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THEORY OF IRREVERSIBLE PROCESSES

I. PARAMETERS OF SMALLNESS

BY

JOSEPH HIGGINS

København 1962
i kommission hos Ejnar Munksgaard

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Synopsis

In part I, the theory of irreversible processes proposed by PRIGOGINE and VAN HOVE is reviewed and the master equation is rederived directly in the phase space without reference to the Fourier space. In part II, the assumptions involved are closely examined with particular emphasis on the justification of the master equation as derived from the Liouville equation. It is demonstrated that the conditions of a parameter of smallness λ associated with the interaction potential energy and large time t compared to a collision time are neither necessary nor sufficient to justify the derivation of the master equation. A necessary, but physically restrictive condition is obtained, and the usefulness of the master equation is discussed.

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Introduction

This is the first of several papers designed to investigate the logical relationship between the Liouville equation and equations describing irreversible processes. While there are many approaches to the development of such equations, they are usually based on philosophical assumptions and no attempt is made to justify analytically these assumptions from the Liouville equation. This, for example, is the case with KRAMERS' equations describing Brownian motion[1] for which the interaction is assumed to have a random character; or the master equation derived by BOGOLUBOV[2], in which it is assumed that the equations describing nature have a Markovian character. Although these assumptions seem physically reasonable, they have not been derived from the Liouville equation. Consequently, the analytical conditions necessary to pass from the reversible properties of the Liouville equation (or the basic equations of motion) to the properties of equations describing irreversible processes are not known.

However, the theory of irreversible processes initiated by VAN HOVE[3], BROUT and PRIGOGINE[4], and further developed by PRIGOGINE and others[5, 6], is distinctive in that it represents an important analytical attempt to develop the equations for irreversible processes directly from the Liouville equation. In this theory, the Fourier space representation of the Liouville equation is studied and a general master equation is developed by assuming (1) a parameter of smallness λ associated with the interaction potential, (2) times t large compared to the average collision time, (3) a large number of particles $N \to \infty$ and infinite volume $\mathcal{V} \to \infty$ but finite concentration N/V, and (4) a weak restriction on the form of the initial density function $\varrho(0)$. Briefly, the Fourier transform of $\varrho(t)$ is expanded in powers of λ, the asymptotic forms of these terms for $\lambda \to 0$, $t \to \infty$, $N \to \infty$, $\mathcal{V} \to \infty$ are determined, and the dominant terms are selected out and summed to produce the master equation. In the first part of this paper (sections 1 and 2), the master equation is rederived directly in the phase space without the use of the Fourier space representation. While this derivation is less cumbersome, it should be emphasized that the logical structure and the assumptions involved are based entirely on the ideas originated by VAN HOVE and PRIGOGINE. The only significant difference in the derivation given here is that, by first summing the

selected terms in λ, a non-Markovian equation is obtained which reduces to the master equation when the limit $t \to \infty$ is taken.

But, in view of the reversible character of the Liouville equation which is not affected by parameters of smallness or large times, it is difficult to understand how the assumptions employed can give rise to the irreversible character of the master equation. In the second part of this paper (section 3), this problem is studied in conjunction with a close analysis of the derivation. Higher order terms in λ and t are examined and a condition is determined to justify the use of the asymptotic forms. The analysis demonstrates that the original assumptions are neither necessary nor sufficient to derive the master equation, while the new conditions appear to severely limit its practical value. However, the apparent discrepancies between the Liouville equation and the master equation are largely resolved and a closer relationship is established between the various theories of irreversible processes.

Part I: Derivation of the Master Equation

Section 1: Liouville Equation

1.1. *General Assumptions*

We shall consider a system of N particles, with momentum p_i and space coordinates x_i, contained in a cubic volume $\mathcal{V}$ whose sides are of length $2L$, subject to the potential $V(\{x_i\})$. The potential is taken as a function of the relative positions and assumed to be pairwise additive:

$$V(\{x_i\}) = \frac{1}{2}\sum_{ij} V_{ij}(x_i - x_j), \tag{1.1.1}$$

from which it follows that the force on any particle is given by

$$\frac{\partial V}{\partial x_i} = \sum_j' \frac{\partial V_{ij}}{\partial x_i} \tag{1.1.2}$$

and

$$\frac{\partial V_{ij}}{\partial x_i} = -\frac{\partial V_{ij}}{\partial x_j}. \tag{1.1.3}$$

Furthermore, we shall assume that the potential and forces vanish at infinity, i. e.,

$$V_{ij}(\pm\infty) = 0 \quad \text{and} \quad \frac{\partial V_{ij}}{\partial x_i}(\pm\infty) = 0. \tag{1.1.4}$$

The Hamiltonian for this system is

$$H = \sum_i' \frac{p_i^2}{2m} + \lambda V(x_i), \tag{1.1.5}$$

where the mass of each particle has been taken equal to m. The parameter λ is introduced primarily as an expansion parameter.

The Liouville equation describes the time dependence of the phase space probability density function*, $\varrho(\{p_i\}, \{x_i\}, t)$, and is given by

$$\frac{\partial \varrho}{\partial t} + \sum_i' \frac{p_i}{m}\frac{\partial \varrho}{\partial x_i} = \lambda \sum_i' \frac{\partial V}{\partial x_i}\frac{\partial \varrho}{\partial p_i} \tag{1.1.6}$$

for the Hamiltonian (1.1.5).

* The words *density function* and *distribution function* are used interchangeably throughout the text, although strictly speaking the quantities referred to are always density functions.

1.2. *Dimensional Changes*

It is convenient to introduce new dimensions as follows:

$$V' = \frac{V}{RT}, \quad p_i' = \frac{p_i}{\sqrt{mRT}}, \quad t' = t\sqrt{\frac{RT}{m}} \tag{1.2.1}$$

where T is the temperature and R is the gas constant. In this case, the equilibrium density function becomes

$$\varrho_{eg} = C \exp\left[-\left(\frac{1}{RT}\right)\left(\sum_i \frac{p_i^2}{2m} + V\right)\right] = C' \exp\left[-\left(\frac{p_i'^2}{2} + V'\right)\right], \tag{1.2.2}$$

where C and C' are normalization constants. The Liouville equation (1.1.6) becomes

$$\frac{\partial \varrho}{\partial t'} + \sum_i p_i' \frac{\partial \varrho}{\partial x_i} = \lambda \sum_i \frac{\partial V'}{\partial x_i} \frac{\partial \varrho}{\partial p_i'}. \tag{1.2.3}$$

Henceforth we shall drop the primes, but consider that all quantities are expressed in these units so that equations (1.2.2) (right side) and (1.2.3) are the appropriate forms.

Finally, it is convenient to use a notation which applies specifically to a one-dimensional real space. Thus, $\mathcal{V}$ is interpreted as a length, and the summations in equation (1.2.3) extend from 1 to N. The results are easily extended to three dimensions, in which case x_i for $i = l \cdot 1,\ l \cdot 2,\ l \cdot 3$ are the three coordinates of the particle l and the summations extend from $i = 1$ to $3N$. Also the potentials $V(x_i - x_j)$ must be interpreted as functions of the three coordinates of each particle i and j. However, specific results derived here for one dimension are easily generalized and the general conclusions are not particularly affected by the dimensionality.

Section 2: Derivation of the Master Equation

2.1. *Equations for the Reduced Density Function*

From the set $[N]$ of N particles we choose a subset S consisting of s particular particles. These particles are labelled $(1, 2, \ldots, s)$ and those in the set $[N-S]$ are labelled $(s+1, \ldots, N)$. We define the S order coordinate-reduced density function by the equation

$$f_s = \mathcal{V}^s \int \varrho \, dx_{s+1} \, dx_{s+2} \ldots dx_N, \tag{2.1.1}$$

which means integration over the entire coordinate space of particles $s+1$ to N. The quantity $\mathcal{V}$ refers to the coordinate space volume (a length in one dimension). The introduction of the factor $\mathcal{V}^s$ in the definition of f_s (2.1.1) is simply a recognition of the volume dependence of the normalization factors of the density func-

tions. In this connection, we are only interested in density functions of physical interest which behave similarly to the equilibrium distribution for the phase space limits. In accord with equation (1.2.2) the equilibrium density function behaves as

$$\varrho_{eq} \to 0 \quad \text{as} \quad p_i \to \pm \infty . \tag{2.1.2}$$

Since the potential energy functions of interest satisfy

we have

$$\left.\begin{aligned} V_{ij}(x_i - x_j \to 0 \quad &\text{as} \quad x_i \to \pm \infty , \\ \varrho_{eq} \to \frac{1}{\mathcal{V}^\circ} \varrho_{eq}^{N-1} \quad &\text{as} \quad x_i \to \pm \infty , \end{aligned}\right\} \tag{2.1.3}$$

where ϱ_{eq}^{N-1} denotes the equilibrium density function for $(N-1)$ particles. And as $\mathcal{V}^\circ \to \infty$, $\varrho_{eq} \to 0$ at the limits.

There are, of course, as many different f_s as there are ways of choosing a particular set $[S]$ from the set $[N]$ (order of particles plays no role). While these different f_s are always functions of a different set of coordinates (at least one particle must be different in each f_s), the f_s may or may not have the same functional form, depending on the symmetry of the problem. Also s can have any value from 0 to N, where $f_0 = f_0(p_1, \ldots, p_N)$ and $f_N = \mathcal{V}^{\circ N} \varrho$.

To obtain the equations for the f_s from the Liouville equation we shall make use of the following facts:

$$\lim_{L \to \infty} \int_{-L}^{+L} \frac{\partial \varrho}{\partial x_i} dx_i = \lim_{L \to \infty} [\varrho(L) - \varrho(-L)] = 0 \tag{2.1.4}$$

because $\varrho(\pm \infty) = 0$*. As $L \to \infty$, $\mathcal{V}^\circ \to \infty$, and to keep the problem meaningful, we must let $N \to \infty$ in such a way that the concentration $C = N/\mathcal{V}^\circ$ remains finite.

In addition, we note that

$$\left.\begin{aligned} \sum_{i=1}^{N} \frac{\partial V}{\partial x_i} \frac{\partial \varrho}{\partial p_i} = \sum_{\substack{ij=1 \\ i \neq j}}^{N} \frac{\partial V_{ij}}{\partial x_i} \frac{\partial \varrho}{\partial p_i} = \sum_{\substack{ij=1 \\ i \neq j}}^{S} \frac{\partial V_{ij}}{\partial x_i} \frac{\partial \varrho}{\partial p_i} \\ + \sum_{i=1}^{S} \sum_{j=s+1}^{N} \frac{\partial V_{ij}}{\partial x_i} \left[\frac{\partial \varrho}{\partial p_i} - \frac{\partial \varrho}{\partial p_j} \right] + \sum_{\substack{ij=s+1 \\ i \neq j}}^{N} \frac{\partial V_{ij}}{\partial x_i} \frac{\partial \varrho}{\partial p_i} , \end{aligned}\right\} \tag{2.1.5}$$

where we have used equations (1.1.2) and (1.1.3).

Integrating the Liouville equation (1.1.3) over the position coordinates of the particles in the set $[N-S]$, and using equations (2.1.1), (2.1.4), and (2.1.5), we obtain

* The same result is obtained if we assume $\varrho(L) = \varrho(-L)$ for $L \to \infty$.

$$\left.\begin{aligned}\frac{\partial f_s}{\partial t}+\sum_{i=1}^{S} p_i\frac{\partial f_s}{dx_i}=\lambda\sum_{\substack{ij=1\\ i\neq j}}^{S}\frac{\partial V_{ij}}{\partial x_i}\frac{\partial f_s}{\partial p_i}+\frac{\lambda}{\mathcal{V}}\sum_{i=1}^{S}\sum_{j=s+1}^{N}\int\frac{\partial V_{ij}}{\partial x_i}\left[\frac{\partial f_{s+1}^{(j)}}{\partial p_i}-\frac{\partial f_{s+1}^{(j)}}{\partial p_j}\right]dx_j\\ +\frac{\lambda}{\mathcal{V}^2}\sum_{\substack{ij=s+1\\ i\neq j}}^{N}\int\frac{\partial V_{ij}}{\partial x_i}\frac{\partial f_{s+2}^{(ij)}}{\partial p_i}\,dx_i\,dx_j\end{aligned}\right\}\tag{2.1.6}$$

for $\mathcal{V}\to\infty$, $N\to\infty$ such that $N/\mathcal{V}=C$, where $f_{s+1}^{(j)}$ is a function of all the $p_i(i=1,\ldots,N)$, the x_i of the particles in the set $[S]$ and in addition x_j for j in the set $[N-S]$; similarly for $f_{s+2}^{(ij)}$. Equation (2.1.6) is valid for $(s=1,\ldots N)$ and is the desired equation for the f_s.

The first three equations are

$$\frac{\partial f_0}{\partial t}=\frac{\lambda}{\mathcal{V}^2}\sum_{\substack{ij=1\\ i\neq j}}^{N}\int\frac{\partial V_{ij}}{\partial x_i}\frac{\partial f_2^{(ij)}}{\partial p_i}\,dx_i\,dx_j,\tag{2.1.7}$$

$$\left.\begin{aligned}\frac{\partial f_1^{(1)}}{\partial t}+p_1\frac{\partial f_1^{(1)}}{\partial x_1}=\frac{\lambda}{\mathcal{V}}\sum_{j=2}^{N}\int\frac{\partial V_{ij}}{dx_i}\left[\frac{\partial}{\partial p_i}-\frac{\partial}{\partial p_j}\right]f_2^{(1\,j)}\,dx_j\\ +\frac{\lambda}{\mathcal{V}^2}\sum_{\substack{ij=2\\ i\neq j}}^{N}\int\frac{\partial V_{ij}}{\partial x_i}\frac{\partial f_3^{(1\,ij)}}{\partial p_i}\,dx_i\,dx_j,\end{aligned}\right\}\tag{2.1.8}$$

$$\left.\begin{aligned}\frac{\partial f_2^{(12)}}{\partial t}+p_1\frac{\partial f_2^{(12)}}{\partial x_1}+p_2\frac{\partial f_2^{(12)}}{\partial x_2}=\lambda\frac{\partial V_{12}}{\partial x_1}\left[\frac{\partial}{\partial p_1}-\frac{\partial}{\partial p_2}\right]f_2^{(12)}\\ +\frac{\lambda}{\mathcal{V}}\sum_{i=1}^{2}\sum_{j=3}^{N}\int\frac{\partial V_{ij}}{\partial x_i}\left[\frac{\partial}{\partial p_i}-\frac{\partial}{\partial p_j}\right]f_3^{(12\,j)}\,dx_j+\frac{\lambda}{\mathcal{V}^2}\sum_{\substack{i,j=3\\ i\neq j}}^{N}\int\frac{\partial V_{ij}}{\partial x_i}\frac{\partial f_4^{(12\,ij)}}{\partial p_i}\,dx_i\,dx_j,\end{aligned}\right\}\tag{2.1.9}$$

where the numbers in the parentheses $f_1^{(1)}$, $f_2^{(12)}$ refer to the particular particles not integrated over. The numbers can always be replaced by k, l as long as the summations exclude them specifically; thus

$$\sum_{i=1}^{2}\sum_{j=3}^{N}\to\sum_{i=k,\,l}\quad\sum_{j=1,\,(j\neq k,\,l)}^{N}.$$

2.2. *Expression in Correlation Functions*

We can always expand an arbitrary distribution function ϱ in terms of the correlation functions as

$$\varrho=\frac{1}{\mathcal{V}^N}\left\{g_0+\sum_i g_1^{(i)}+\sum_P g_2^{(P)}+\sum_i\sum_{\substack{P\\ i\neq P}} g_1^{(i)}\,g_2^{(P)}+\sum_T g_3^{(T)}+\ldots+g_N\right\},\tag{2.2.1}$$

where the g_l are l^{th} order position correlation functions. The indices inside the parenthesis, as $g_2^{(1)}$, $g_2^{(P)}$, refer to the position coordinates of particular particles. The i, P, T represent the particle i, the pairs of particles (h, l), the triplet (μ, ν, w), etc., and the summations are combinations from the set $[N]$. All the g_l may be a function of the momenta of *all* the particles. In particular, g_0 is a function of the momenta only, $g_0 = g_0(p_1, p_2, \ldots, p_N)$. According to their definition as correlation functions, we require that

$$\int_{-\infty}^{+\infty} g_l^{(1,\ldots,l)}\, dx_\mu = 0 \quad \text{for} \quad \mu = 1, \ldots, l. \tag{2.2.2}$$

We now limit our possible initial conditions by requiring that ϱ is a function of the relative coordinates only; i. e.,

$$\varrho = \varrho(\{x_i - x_j\}) \text{ for all } i \text{ and } j. \tag{2.2.3}$$

From the Liouville equation it is easily seen that, if this condition is satisfied at $t = 0$, then it is satisfied at all times. From (2.2.3) it follows that $g_1^{(i)} = 0$ and, hence, equation (2.2.1) reduces to

$$\varrho = \frac{1}{\mathcal{V}^N}\left\{ g_0 + \sum_P g_2^{(P)} + \sum_T g_3^{(T)} + \sum_{\substack{P_1 \\ P_1 \neq P_2}} \sum_{P_2} g_2^{(P_1)}\, g_2^{(P_2)} + \sum_Q g_4^{(Q)} + \ldots + g_N \right\}. \tag{2.2.4}$$

Using the definition of the f_s (2.1.1) and equation (2.2.2), we obtain from (2.2.4) that

$$f_s = \left\{ g_0 + \sum_P g_2^{(P)} + \sum_T g_3^{(T)} + \sum_{\substack{P_1 \\ P_1 \neq P_2}} \sum_{P_2} g_2^{(P_1)}\, g_2^{(P_2)} + \sum_Q g_4^{(Q)} + \ldots + g_s \right\}. \tag{2.2.5}$$

Specifically,

$$\left.\begin{aligned} f_0 &= g_0 \\ f_1 &= g_0 \end{aligned}\right\} \tag{2.2.6}$$

(which is independent of x_i in accord with condition (2.2.3))

$$\begin{aligned} f_2 &= g_0 + g_2^{(ij)} \\ f_3 &= g_0 + g_2^{(ij)} + g_2^{(ik)} + g_2^{(jk)} + g_3^{(ijk)}, \quad \text{etc.} \end{aligned}$$

These equations can be solved for the g_l and yield

$$\left.\begin{aligned} g_0 &= f_0 \\ g_1 &= 0 \\ g_2^{(P)} &= f_2^{(P)} - f_0 \\ g_3^{(T)} &= f_3 - \sum_P f_2^{(P)} + 2 f_0^{(T)} \quad (P \varepsilon T). \end{aligned}\right\} \tag{2.2.7}$$

These equations could have been taken as a definition of the g_l and would yield equation (2.2.2). In fact, the g_l and the f_s form a one-to-one functional transformation of each other; the importance of this particular transformation is shown in section 2.3.

Note that

$$\iint h(x_i - x_j)\, g(x_i - x_j)\, dx_i\, dx_j = \mathcal{V} \int h(x)\, g(x)\, dx, \tag{2.2.8}$$

where h and g are arbitrary functions and the result depends on the limits of integration becoming infinite (i. e., $\mathcal{V} \to \infty$). Then, by substituting equations (2.2.6) into (2.1.6) and applying (2.2.8) as well as the condition (1.1.4), we obtain*

$$\frac{\partial g_0}{\partial t} = \frac{\lambda}{\mathcal{V}^2} \sum_{\substack{ij=1 \\ i \neq j}}^{N} \int \frac{\partial V_{ij}}{\partial x_i} \frac{\partial g_2^{(ij)}}{\partial p_i}\, dx_i\, dx_j \tag{2.2.9}$$

$$\begin{aligned}
&\frac{\partial g_2^{(12)}}{\partial t} + p_1 \frac{\partial g_2}{\partial x_1} + p_2 \frac{\partial g_2}{\partial x_2} = \frac{\partial V_{12}}{\partial x_1} \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2} \right] g_0 + \frac{\partial V_{12}}{\partial x_1} \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2} \right] g_2 \\
&+ \sum_{j=1}^{2} \sum_{i=3}^{N} \int \frac{\partial V_{ij}}{\partial x_i} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right] g_2^{(ij)}\, dx_i - \int \frac{\partial V_{12}}{\partial x_1} \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2} \right] g_2^{(12)}\, dx_1\, dx_2 \\
&+ \sum_{j=1}^{2} \sum_{i=3}^{N} \int \frac{\partial V_{ij}}{\partial x_i} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right] g_3^{(12\,i)}\, dx_i \\
&+ \sum_{i=3}^{N} \sum_{j=3}^{N} \int \frac{\partial V_{ij}}{\partial x_i} \frac{\partial}{\partial p_i} \left[g_3^{(1\,ij)} + g_3^{(2\,ij)} \right] dx_i\, dx_j \\
&+ g_2^{(12)} \sum_{i=3}^{N} \sum_{j=3}^{N} \int \frac{\partial V_{ij}}{\partial x_i} \frac{\partial}{\partial p_i} g_2^{(ij)}\, dx_i\, dx_j \\
&+ \sum_{i=3}^{N} \sum_{j=3}^{N} \int \frac{\partial V_{ij}}{\partial x_i} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right] \left[g_2^{(1\,i)}\, g_2^{(2\,j)} \right] dx_i\, dx_j \\
&+ \sum_{i=3}^{N} \sum_{j=3}^{N} \int \frac{\partial V_{ij}}{\partial x_i} \frac{\partial}{\partial p_i} g_4^{(12\,ij)}\, dx_i\, dx_j
\end{aligned}$$

which are the equations for the g_0 and g_2. The equations for the other g_l are obtained in the same way.

* That the equation for $\partial f_1 / \partial t$ (2.1.8) adds nothing new is easily seen by noting that

$$\begin{aligned}
&\int \frac{\partial V_{ij}(x_i - x_j)}{\partial x_i} \frac{\partial f_3}{\partial p_i} [(x_i - x_j), (x_1 - x_i), (x_1 - x_j)]\, dx_i\, dx_j \\
&= \int \frac{\partial V_{ij}(x)}{\partial x_i} \frac{\partial f_3}{\partial p_i} [x, y - x, y]\, dx\, dy = \mathcal{V} \int \frac{\partial V_{ij}(x)}{\partial x_i} \frac{\partial f_2(x)}{\partial p_i}\, dx
\end{aligned}$$

$$\text{since} \int f_3 [(x_i - x_j), (x_1 - x_i), (x_1 - x_j)]\, dx_1 = \mathcal{V} f_2^{(ij)}$$

2.3. *λ dependence*

We shall now assume that the correlation functions can be expanded in powers of λ-as

$$\left.\begin{aligned} g_0 &= g_0^0 + \lambda g_0^1 + \lambda^2 g_0^2 + \ldots \\ g_l &= \lambda^{l-1}[g_l^0 + \lambda g_l^1 + \lambda^2 g_l^2 + \ldots] \quad \text{for} \quad l \geqslant 2. \end{aligned}\right\} \tag{2.3.1}$$

That is, the l^{th} order correlation function has a λ dependence of no less than λ^{l-1}. Again, it is easy to prove that, if (2.3.1) is valid initially, it is true at all times. This is seen from equations (2.2.9) as well as from the Liouville equation; correlations are created by the operator $\lambda \left\{ \frac{\partial V}{\partial x_i} \frac{\partial}{\partial p_i} \right\}$, and an l^{th} order correlation requires the repeated application of this operator so that g_l can be created only with an order of λ^{l-1}. Consequently, if g_l has initially no λ dependence lower than λ^{l-1}, it will never have any. It is for this reason that we have transformed from the f_s to the g_l. The lowest order λ dependence of the g_l is preserved in time while the f_s will in general contain all powers of λ. It is important to note that equation (2.3.1) also applies to the equilibrium distribution

$$\left.\begin{aligned} \varrho_{\text{eq}} &= C \exp\left[-\sum_i \frac{p_i^2}{2} - \frac{1}{2}\lambda \sum_{\substack{ij \\ i \neq j}} V_{ij}(x_i - x_j) \right] \\ &= C \left[\exp\left(-\sum_i \frac{p_i^2}{2} \right) \right] \left[1 + \frac{\lambda}{2} \sum_{\substack{ij \\ i \neq j}} V_{ij}(x_i - x_j) \right. \\ &\left. + \frac{1}{2}\left(\frac{\lambda}{2}\right)^2 \sum_{P_1} \sum_{P_2} V(P_1)\, V(P_2) + \frac{1}{3!}\left(\frac{\lambda}{2}\right)^3 \sum_{P_1} \sum_{P_2} \sum_{P_3} V(P_1)\, (V(P_2)\, V(P_3) + \ldots \right], \end{aligned}\right\} \tag{2.3.2}$$

where C is a normalization factor and where we can have $P_1 = P_2 = P_3$ etc. From (2.3.2) it is clear that the g_l for the equilibrium distribution satisfy equation (2.3.1). This result is important, as it demonstrates that the equilibrium distribution has not been excluded by our choice of initial conditions.

2.4. *Solution of the Equations for the Correlation Functions*

We shall now solve equations (2.2.9) by iteration to the order λ^2 and for the following initial ($t = 0$) conditions:

$$\left.\begin{aligned} g_0^0(0) &= g_0^0(0) \neq 0 \\ g_0^m(0) &= 0 \quad \text{for} \quad m \geq 1 \\ g_l^m(0) &= 0 \quad \text{for} \quad l \geq 1. \end{aligned}\right\} \tag{2.4.1}$$

While these conditions satisfy the general restrictions (2.3.1) and (2.2.3), they are not preserved in time. They correspond to an initial distribution function $\varrho(t=0)$ which is a function of the momenta $p_1, \ldots p_N$ alone and which is independent of λ.

Inserting equations (2.3.1) into equations (2.2.9) and equating powers of λ, we obtain

$$\frac{\partial g_0^0}{\partial t} = 0 \tag{2.4.2}$$

$$\frac{\partial g_0^1}{\partial t} = 0 \tag{2.4.3}$$

$$\frac{\partial g_0^2}{\partial t} = \frac{1}{\mathscr{V}^2} \sum_{\substack{ij=1 \\ i \neq j}}^{N} \int \frac{\partial V_{ij}}{\partial x_i} \frac{\partial g_2^0(ij)}{\partial p_i} \, dx_i \, dx_j \tag{2.4.4}$$

$$\frac{\partial g_2^0(12,t)}{\partial t} + p_1 \frac{\partial g_0^2(t)}{\partial x_i} + p_2 \frac{\partial g_2^0(t)}{\partial x_2} = \frac{\partial V_{12}}{\partial x_1} \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2} \right] g_0^0(t). \tag{2.4.5}$$

Using the initial conditions (2.4.1), we obtain from (2.4.2)

$$g_0^0(t) = g_0^0(0), \tag{2.4.6}$$

from (2.4.3)

$$g_0^1(t) = 0, \tag{2.4.7}$$

and from (2.4.5)

$$g_2^0(t,12) = \int_0^t \frac{\partial V_{12}}{\partial x_1} (x - pt') \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2} \right] g_0^0(0) \, dt' \, dx, \tag{2.4.8}$$

where $x = x_1 - x_2$ and $p = p_1 - p_2$;

putting (2.4.8) in (2.4.4), we have

$$\frac{\partial g_0^2}{\partial t} = \frac{1}{\mathscr{V}} \sum_{\substack{ij=1 \\ i \neq j}}^{N} \int_x \frac{\partial V_{ij}^{(x)}}{\partial x_i} \int_0^t \frac{\partial}{\partial p_i} \frac{\partial V_{ij}}{\partial x_i} (x - pt') \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right] g_0^0(0) \, dt' \, dx, \tag{2.4.9}$$

where we have also applied equation (2.2.8).

Finally, we can add equations (2.4.2), (2.4.3), and (2.4.9) and write

$$\left.\begin{aligned} \frac{\partial g_0(t)}{\partial t} &= \frac{\partial}{\partial t} [g_0^0 + \lambda g_0^1 + \lambda^2 g_0^2] \\ &= \frac{\lambda^2}{\mathscr{V}} \sum_{\substack{ij=1 \\ i \neq j}}^{N} \int \frac{\partial V_{ij}(x)}{\partial x_i} \frac{\partial}{\partial p_i} \int_0^t \frac{\partial V_{ij}(x - pt')}{\partial x_i} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right] g_0(0) \, dt' \, dx, \end{aligned}\right\} \tag{2.4.10}$$

which is the expression for $g_0(t)$ valid to order λ^2.

2.5. *Extending the Solution*

Equation (2.4.10) is the correct solution to order λ^2 for $\frac{\partial g_0(t)}{\partial t}$. However, it is not Markovian in that it depends on $g_0(0)$. This would appear to be easily rectified. We write equation (2.4.10) as

$$\frac{\partial g_0(t)}{\partial t} = \frac{\lambda^2}{\mathscr{V}} f(t, \bar{p}_\gamma)\, g_0(0), \tag{2.5.1}$$

where

$$f(t, \bar{p}_i, \bar{p}_j) = \sum_{\substack{ij=1 \\ i \neq j}}^{N} \int \frac{\partial V_{ij}(x)}{\partial x_i} \frac{\partial}{\partial p_i} \int_0^t \frac{\partial V_{ij}}{\partial x_i}(x - pt')\, dt'\, dx \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] \tag{2.5.2}$$

is a differential operator in the momenta (denoted by $\bar{p}_\gamma$) as well as a function of t. Integrating equation (2.5.1) with respect to t yields

$$g_0(t) = g_0(0) + \frac{\lambda^2}{\mathscr{V}} F(t, \bar{p}_\nu)\, g_0(0), \tag{2.5.3}$$

where

$$F(t, \bar{p}_\gamma) = \int_0^t f(t', \bar{p}_\gamma)\, dt'. \tag{2.5.4}$$

Solving equation (2.5.3) for $g_0(0)$ yields

$$g_0(0) = \frac{1}{1 + \frac{\lambda^2}{\mathscr{V}} F(t, \bar{p}_\gamma)}\, g_0(t), \tag{2.5.5}$$

which is an operator equation whose meaning is

$$g_0(0) = \left[1 - \frac{\lambda^2}{\mathscr{V}} F(t, \bar{p}_\gamma) + \left(\frac{\lambda^2}{\mathscr{V}} F(t, \bar{p}_\gamma)\right)^2 + \ldots\right] g_0(t), \tag{2.5.6}$$

where the series is that for $1/1+x$. If we now assume that $F^n(t, \bar{p}_\gamma)\, g_0(t)$ is bounded for all t and $\bar{p}$ with an upper bound U_n, and that λ is a parameter of smallness such that

$$1 \gg \frac{\lambda^2}{\mathscr{V}} U_1 \quad \text{and} \quad U_n \gg \frac{\lambda^2}{\mathscr{V}} U_{n+1} \quad \text{for all} \quad n > 1, \tag{2.5.7}$$

then we can set

$$g_0(0) = g_0(t) \quad \text{to order} \quad \lambda^2 \tag{2.5.8}$$

and equation (2.5.1) can be written as

$$\frac{\partial g_0(t)}{\partial t} = \frac{\lambda^2}{\mathscr{V}} f(t, \bar{p}_\gamma)\, g_0(t). \tag{2.5.9}$$

Subject to the condition (2.5.7), equation (2.5.9) is still valid to the order λ^2. The method we have used to obtain equation (2.5.9) is known as the *resolvent method*; it amounts to an elimination of the initial condition in terms of the function and its derivatives, and is in fact the standard procedure for developing a differential equation from its solution. However, to obtain equation (2.5.9), we have made a double approximation: first by cutting off higher powers of λ according to equation (2.4.10), and second according to equation (2.5.8).

These particular approximations are not easily justified and would restrict equation (2.5.8) to cases of little physical interest. However, equation (2.5.9)' can be developed by another procedure for which the approximations seem to be physically reasonable at first sight. This procedure, introduced by PRIGOGINE[6], involves the investigation and summation of all the terms in λ. To do this we examine the value of g_0^4 and in general g_0^{2n} $(n = 2, 3, \ldots)$. The term g_0^4 arises from g_2^3 according to equation (2.2.9). While there are many terms which contribute to g_2^3, we shall only be interested in that which arises from g_0^2. Solving the equations with the initial conditions (2.4.1) we obtain

$$\left.\begin{aligned} g_0^4 = \left[\frac{\lambda^2}{\mathscr{V}}\right]^2 \sum_{\substack{ij=1 \\ i\neq j}}^{N} \int_0^{\bullet t} \int_x^{\bullet} \frac{\partial V_{ij}(x)}{\partial x_i} \frac{\partial}{\partial p_i} \int_0^{\bullet t'} \frac{\partial V_{ij}}{\partial x_i}(x - p\tau) \\ \times \left(\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right) F(t' - \tau)\, d\tau\, dt'\, g_0^0(0), \end{aligned}\right\} \quad (2.5.10)$$

where $F(t)$ is defined by equation (2.5.4). Equation (2.5.10) can be written as

$$g_0^4 = \left[\frac{\lambda^2}{\mathscr{V}}\right]^2 \int_0^{\bullet t} f(t') * \int_0^{\bullet t'} f(t'')\, dt''\, dt'\, g_0^0(0), \quad (2.5.11)$$

where $f(t)$ is defined by equation (2.5.2) and the operation is a type of convolution defined as

$$h(t) * g(t) = \int_0^{\bullet t} h'(\tau)\, g(t - \tau)\, d\tau, \quad (2.5.12)$$

where $h'(t) = \dfrac{dh(t)}{dt}$ is the derivative of $h(t)$, and $h(t)$ and $g(t)$ are arbitrary functions.

Note also that

$$h\ (t) * 1 = \int_0^{\bullet t} h'(\tau)\, d\tau = h(t) - h(0). \quad (2.5.13)$$

It is easily seen from equation (2.2.9) that some terms in g_0^{2n} arise from g_2^{2n-1} which in turn arises from the term $g_0^{2(n-1)}$. Thus the structure of the term g_0^{2n} is apparent from equation (2.5.11), and we obtain

$$\left.\begin{aligned} g_0(t) = \Big[1 + \alpha\int_0^t f(t')\,dt' + \alpha^2\int_0^t f(t') * \int_0^{t'} f(t'')\,dt''\,dt' \\ + \alpha^3\int_0^t f(t') * \int_0^{t'} f(t'') * \int_0^{t''} f(t''')\,dt'''\,dt''\,dt' + \ldots\Big]\, g_0(0), \end{aligned}\right\} \quad (2.5.14)$$

where $\alpha = \dfrac{\lambda^2}{\mathscr{V}^\circ}$.

Differentiating equation (2.5.14) with respect to t we obtain

$$\frac{\partial g_0(t)}{\partial t} = \alpha f(t) * \left[1 + \alpha\int_0^t f(t')\,dt' + \alpha^2\int_0^t f(t') * \int_0^t f(t'')\,dt''\,dt' + \ldots\right] g_0(0) \quad (2.5.15)$$

and, substituting equation (2.5.14) for the series, we have

$$\frac{\partial g_0(t)}{\partial t} = \alpha f(t) * g_0(t) = \alpha\int_0^t f'(\tau)\, g_0(t-\tau)\,d\tau. \quad (2.5.16)$$

Equation (2.5.16) represents a special solution of the general equation given by Zwanzig[7]. Effectively certain terms in the λ expansion of Zwanzig's equation have been disregarded, but equation (2.5.16) retains the same general form. Equation (2.5.16) is still not Markovian, as it depends on the value of g_0 at the time $(t-\tau)$. It is closely related to equation (2.5.1) and can be made Markovian, in a similar manner, by replacing $g_0(t-\tau)$ by $g_0(t)$, in which case one again obtains equation (2.5.9) since $f(0) = 0$. But the necessary conditions to make this replacement are essentially the same as for deriving equation (2.5.9) and restrict the physics to cases of little interest.

However, the problem of making equation (2.5.16) Markovian can be related to an important property of the function $f(t)$ which is derived in the following section.

2.6. *Properties of* $f(t)$

For the function $f(t)$ we can write

$$f(t) = \alpha \sum_{\substack{ij=1 \\ i \neq j}}^{N} \frac{\partial}{\partial p_i}\, \Phi_{ij}(t,p) \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_i}\right], \quad (2.6.1)$$

where

$$\Phi_{ij}(t,p) = \int_x \frac{\partial V_{ij}(x)}{\partial x} \int_0^t \frac{\partial V_{ij}}{\partial x}\,[x - pt']\,dx\,dt'. \quad (2.6.2)$$

Carrying out the time integration of (2.6.2) and for convenience dropping the subscripts, we obtain

$$\Phi(t,p) = -\frac{1}{p}\int_x \frac{\partial V(x)}{\partial x}\,[V(x-pt)-V(x)]\,dx \tag{2.6.3}$$

or

$$\Phi(t,p) = -\frac{1}{p}\int_x \frac{\partial V(x)}{\partial x}\,V(x-pt)\,dx \tag{2.6.4}$$

since the last term in (2.6.3) vanishes when the x integration is carried out.

To investigate (2.6.4) we shall assume a specific form for $\partial V(x)/dx$, namely a force of constant magnitude a over a range $-b<x<b$ and zero elsewhere. This is illustrated in Figure 1 together with $V(x)$. Setting

$$j = pt,$$

the integration over x in equation (2.6.4) is easily carried out for this case and we obtain

$$\Phi(t,p) = +\frac{1}{p}\begin{cases} 0 & \text{for} \quad |j|>2b \\ \frac{1}{2}\frac{j}{|j|}\,a^2\,[2b-|j|^2] & \text{for} \quad b<|j|<2b \\ \frac{1}{2}\;j\;a^2\,[4b-3|j|] & \text{for} \quad 0<|j|<b \end{cases} \tag{2.6.5}$$

a) $$V(|x|) = \begin{cases} ab\,(1-\frac{|x|}{b}) & \text{for} \quad b\geqslant|x|\geqslant 0. \\ 0 & \text{for} \quad |x|>b. \end{cases}$$

b) $$\frac{\partial V(x)}{\partial x} = \begin{cases} -\frac{x}{|x|} & \text{for} \quad b\geqslant|x|\geqslant 0 \\ 0 & \text{for} \quad |x|>b \end{cases}$$

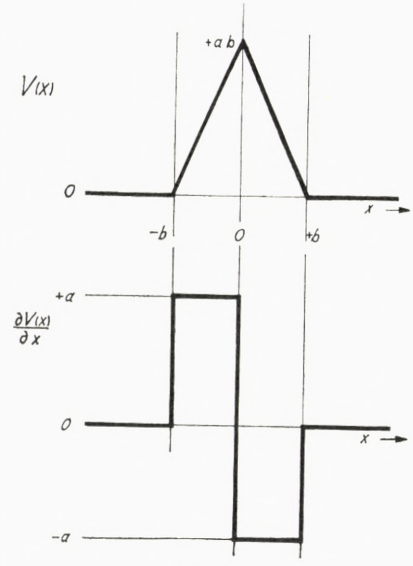

Fig. 1.

From equation (2.6.5) we see that $\Phi(t, p)$ behaves in a manner similar to a Dirac Delta, $\delta(p)$, function as t becomes large, since $\Phi(t, p)$ has a non-zero value only for $p<2b/t$. To demonstrate that $\Phi(t, p)$ is a δ function for large t, we evaluate

$$I = \lim_{t \to \infty} \int_{-\infty}^{+\infty} \Phi(t, p)\, \mathfrak{N}(p)\, dp,$$

where $\mathfrak{N}(p)$ is an arbitrary function. By writing the integral as $\int_0^{\infty} + \int_{-\infty}^{0}$, changing p to $-p$ in the second integral and finally setting $p = j/t$, we obtain

$$I = \lim_{t \to \infty} \int_{j=0}^{\infty} \left\{ \begin{array}{lll} 0 & \text{for} & |j| > 2b \\ \frac{1}{2}\frac{a^2}{j}[2b - j]^2 & \text{for} & b < |j| < 2b \\ \frac{1}{2}a^2[4b - 3j] & \text{for} & 0 < |j| < b \end{array} \right\} \left[\mathfrak{N}\left(\frac{j}{t}\right) + \mathfrak{N}\left(-\frac{j}{t}\right) \right] \mathrm{dj} \qquad (2.6.6)$$

Since j is bounded by $0 < j < 2b$, if we carry through the limit $t \to \infty$, we have $\mathfrak{N}(j/t) \to \mathfrak{N}(0)$ and similarly $\mathfrak{N}\left(-\frac{j}{t}\right) \to \mathfrak{N}(0)$; evaluating the integral over j, we obtain

$$I = 4a^2 b^2 (ln\, 2)\, \mathfrak{N}(0)$$

so that we can write

$$\lim_{t \to \infty} \Phi(t, p) = 4a^2 b^2 (ln\, 2)\, \delta(p). \qquad (2.6.7)$$

The condition that $t \to \infty$ will be studied in detail in a later section, but for the moment we shall follow the arguments given by PRIGOGINE: it is not necessary that $t \to \infty$. If we define the mean collision time t_c in terms of the mean velocity v_M of the particles as

$$t_c = \frac{2b}{v_M}, \qquad (2.6.8)$$

then equation (2.6.7) will be approximately valid for $t \gg t_c$ as long as $\mathfrak{N}(p)$ is essentially constant for $0 < p < p_\beta$, where $p_\beta \ll p_M$.

In other words, $\Phi(t, p)$ becomes independent of t for $t \gg t_c$. We can write

$$\Phi(t, p) \approx \Phi(\infty, p) \quad \text{for} \quad t \geqslant t_\beta \gg t_c$$

and, from equation (2.6.1), it follows that

$$f(t, p) \approx f(\infty, p) \quad \text{for} \quad t \geqslant t_\beta. \qquad (2.6.9)$$

For the problems considered here, t_c will be very small compared to times of interest, so that the condition $t \gg t_c$ presents no difficulty. Finally, for other interesting types of forces, the result will be essentially the same, replacing b by the mean interaction distance and a by the mean value of the force. The only important exception is the $1/r^2$ force which has such a large b that equation (2.6.7) is only valid for t of the order of relaxation times.

2.7. *The Master Equation*

With these properties for $f(t)$, it is now easy to demonstrate that equation (2.5.16) becomes Markovian for $t \geqslant t_\beta$. Integrating (2.5.16) by parts yields

$$\frac{\partial g_0(t)}{\partial t} = \alpha \left\{ f(t)\, g_0(0) - f(0)\, g_0(t) + \int_0^t f(\tau)\, g'(t-\tau)\, d\tau \right\}. \tag{2.7.1}$$

Noting that $f(0) = 0$, splitting the last integral into $\int_0^{t_\beta} + \int_{t_\beta}^t$ and using the property that $f(t) \cong f(\infty)$ for $t \geqslant t_\beta$, yields

$$\left.\begin{aligned} \frac{\partial g_0(t)}{\partial t} = \alpha \Big\{ & f(\infty)\, g_0(0) - \int_0^{t_\beta} f(\tau)\, g_0'(t-\tau)\, d\tau \\ & - f(\infty) \int_{t_\beta}^t g_0'(t-\tau)\, d\tau \Big\} \quad \text{for} \quad t \geqslant t_\beta. \end{aligned}\right\} \tag{2.7.2}$$

An evaluation of the last integral gives

$$\frac{\partial g_0(t)}{\partial t} = \alpha \left\{ f(\infty)\, g_0(t-t) - \int_0^{t_\beta} f(\tau)\, g_0'(t-\tau)\, d\tau \right\} \quad \text{for} \quad t \geqslant t_\beta. \tag{2.7.3}$$

This shows that $g_0'(t)$ is of order α so that both $g_0'(t)$ and $g_0(t)$ do not change very much in a time t_β which is small; hence, we can set $g_0(t-t_\beta) \approx g_0(t)$ and $g_0'(t-\tau) \approx g_0'(t)$. Finally, the last term in equation (2.7.3) is of order α as compared to the first term and can thus be neglected. While an exact condition for these approximations can be easily written down by expanding $g(t-t_\beta)$ in a power series of t_β, a more convenient necessary condition is that

$$\alpha F(t_\beta)\, g_0(t) \ll 1, \tag{2.7.4}$$

where $F(t)$ was previously defined by equation (2.5.4). If this condition holds, we can expect that our approximations are valid and equation (2.7.3) becomes

$$\frac{\partial g_0(t)}{\partial t} = \alpha f(\infty)\, g_0(t). \tag{2.7.5}$$

On replacing $f(\infty)$ by its value we have

$$\frac{\partial g_0(t)}{\partial t} = \frac{\lambda^2}{\mathscr{V}} \sum_{\substack{ij=1 \\ i \neq j}}^{N} \frac{\partial}{\partial p_i} \int_x \frac{\partial V_{ij}(x)}{\partial x} \int_{t'=0}^{\infty} \frac{\partial V_{ij}}{\partial x}(x - pt')\, dx\, dt' \times \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right] g_0(t) \tag{2.7.6}$$

which is identical with the Markovian master equation obtained by Brout, Prigogine, and Van Hove[4], as is demonstrated in Appendix II.

Before comparing the details of this derivation with that given by Prigogine, it is useful to review the application to the problem of Brownian motion.

2.8. *Brownian Motion*

The equation for the Brownian motion of a particle is easily derived from the master equation*. We consider a bath containing N_B particles at equilibrium. Another particle (P) of the same type** is introduced into this bath at $t = 0$ with a given momentum distribution $g_P(p_P, 0)$, and we wish to determine the time dependence of the distribution function g_P.

The momentum distribution for each particle is defined by

$$g_i(p_i, t) = \int_{-\infty}^{+\infty} g_0(\{p\}, t) \prod_{\substack{j=1 \\ j \neq i}}^{N} dp_j, \tag{2.8.1}$$

where $\int g_i(p_i, t)\, dp_i = 1$; that is, the g_i are normalized.

We now require that g_0 can be factorized into particle distribution functions, i. e.,

$$g_0(t) = \prod_{i=1}^{N} g_i(p_i, t). \tag{2.8.2}$$

Again, if (2.8.2) is valid at $t = 0$, it follows from the Liouville equation that it will be true for all t. Since the equilibrium distribution is factorizable, (2.8.2) will apply to Brownian particles if we require that the momentum of the particle P is initially uncorrelated with the momenta of the bath particles.

Since the particles are all of the same type, the interaction potentials $V_{ij}(x_i - x_j)$ will have the same functional form denoted by $V(x_i - x_j)$, and also the masses m_i will be the same. The derivation of the master equation requires that $\mathscr{V} \to \infty$ and hence $N \to \infty$. To make this a physically meaningful situation, we shall require that there exist N_B particles in the bath and n particles P undergoing Brownian motion. Thus,

$$N = N_B + n \tag{2.8.3}$$

as $\mathscr{V} \to \infty$, $N_B \to \infty$ and $n \to \infty$,
such that

$$\frac{N_B}{\mathscr{V}} = C_B \quad \text{and} \quad \frac{n}{\mathscr{V}} = C_P \quad \text{are finite.} \tag{2.8.4}$$

For practical problems we can usually set $n/N_B \simeq 10^{-23}$ (Avogadro's number). The physical interpretation of equations (2.8.4) can be taken either as (1) one system containing $\mathfrak{N} \cdot N_B$ bath particles (where $N_B \approx 10^{23}$) and $\mathfrak{N} \cdot n$ identical Brownian particles ($n \approx 1$), where $\mathfrak{N} \to \infty$ as $\mathscr{V} \to \infty$; or (2) approximately as $\mathfrak{N}$ identical systems, each having a finite volume $\overline{\mathscr{V}}$ and containing N_B bath particles and n Brownian particles, where the number of systems becomes infinite ($\mathfrak{N} \to \infty$) and edge effects of the finite volume $\overline{\mathscr{V}}$ are neglected. Finally, since there are only two types of par-

* The procedure given here is identical to that used by PRIGOGINE (5), (8), (10).

** When the particle is not of the same type the equation is easily derived, but here this example suffices.

ticles, there will be only two different types of particle distribution functions, namely $g_P(p_{P_i}, t)$ for the Brownian particles, where g_P is the same for all these particles but the argument is the p_{P_i} for a particular one and $g_B(p_{B_i}, t)$ for the bath particles, similarly interpreted. Using equations (2.8.2) and (2.6.1), we obtain from the master equation

$$\left.\begin{aligned}\frac{\partial g_1(p_1)\,t}{\partial t} &= \alpha \sum_{\substack{i \\ i \neq j}} \sum_{j=1}^{N} \int_{p_i,\, p_j = -\infty}^{+\infty} \frac{\partial}{\partial p_i} \Phi_{ij}(\infty, p) \\ &\times \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] g_i(p_i, t)\, g_j(p_j, t) \underbrace{dp_i\, dp_j}_{ij \neq 1}\end{aligned}\right\} \tag{2.8.5}$$

when the integration has been carried over all particles but 1, which is taken as some particular particle. The terms in the sum on the right-hand side of (2.8.5) can be broken down and evaluated as follows.

For i and $j \neq 1$, we have

$$\int \frac{\partial}{\partial p_i} \Phi_{ij} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] g_i\, g_j\, dp_i\, dp_j = \int \Phi_{ij}(p_i - p_j) \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_i}\right] g_i\, g_j \Big|_{p_i = -\infty}^{p_i = +\infty} dp_j = 0. \tag{2.8.6}$$

The last equality arises from the definition of (2.6.2) Φ_{ij} and the properties of $V(x)$, from which it follows that $\Phi_{ij} = 0$ for $p_i = \pm\infty$ for all $t \neq 0$ and all p_j except $p_j = \pm\infty$. We make the additional assumption that $g_j(p_j) = 0, \dfrac{\partial g_0}{\partial p_j} = 0$ for $p_j = \pm\infty$, which is necessary for g_i to be normalizable. The remaining terms of (2.8.5) are those for $i = 1$ or $j = 1$. For $j = 1$, we have

$$\int \frac{\partial}{\partial p_i} \Phi_{i1} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_1}\right] g_i\, g_1\, dp_i = 0 \tag{2.8.7}$$

for the same reasons as (2.8.6). Finally, we have the terms for $i = 1$ which yield

$$\left.\begin{aligned}I_{1j} &= \int \frac{\partial}{\partial p_1} \Phi_{1j}(\infty, p) \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_j}\right] g_1\, g_j\, dp_j \\ &= 4\,a^2\, b^2\, ln\, 2 \int \frac{\partial}{\partial p_1} \delta(p_1 - p_j) \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_j}\right] g_1^{(p_1)}\, g_j^{(p_j)}\, dp_j,\end{aligned}\right\} \tag{2.8.8}$$

where we have now used the value of $\Phi_{ij}(\infty, p)$ given by equation (2.6.6). The last term in (2.8.8) has the obvious property that, if g_1 and g_j have the same functional form, then the term is zero. Thus, if particle 1 is a Brownian particle and particle j also, then the integral I_{ij} is zero. Similarly for the bath particles. We may thus write $I_{1j} = 0$ if 1 and j are the same types of particles. Utilizing these results, we have immediately

$$\frac{\partial g_P(p_1, t)}{\partial t} = C_B \beta \int \frac{\partial}{\partial p_1} \delta(p_1 - p_2) \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2} \right] g_P(p_1, t)\, g_B(p_2, t)\, dp_2 \qquad (2.8.9)$$

and

$$\frac{\partial g_B(p_2, t)}{\partial t} = C_P \beta \int \frac{\partial}{\partial p_2} \delta(p_1 - p_2) \left[\frac{\partial}{\partial p_2} - \frac{\partial}{\partial p_1} \right] g_p(p_1, t)\, g_B(p_2, t)\, dp_1, \quad (2.8.10)$$

where $\beta = \lambda^2 4a^2 b^2 ln 2$ and C_B and C_P are the concentrations (equation 2.8.4). The label 1 refers to any one of the Brownian particles and the label 2 to any one of the bath particles.

We now make the additional assumption that the change in the distribution function of the bath particles is negligible in the times we are interested in (i. e., set $C_P = 0$ in 2.8.10) so that we may set

$$g_B(p_2, t) = g_B(p_2, 0) = g_{\mathrm{eq}}(p_2) = exp\left[\tfrac{-p_2^2}{2}\right]. \qquad (2.8.11)$$

Equation (2.8.9) can then be written as

$$\left.\begin{aligned} \frac{\partial g_p(p_1, t)}{\partial t} &= C_B \beta \int \frac{\partial}{\partial p_1} \delta(p_1 - p_2) \\ \times \left[g_{\mathrm{eq}}(p_2) \frac{\partial g_P(p_1, t)}{\partial p_1} - g_P(p_1, t) \frac{\partial g_{eq}(p_2)}{\partial p_2} \right] dp_2. \end{aligned} \right\} \qquad (2.8.12)$$

The integration over p_2 can be carried out to yield

$$\frac{\partial g_P(p_1, t)}{\partial t} = C_B \beta \left\{ \frac{\partial}{\partial p_1} [g_{\mathrm{eq}}(p_1)] \left[\frac{\partial g_P(p_1, t)}{\partial p_1} + p_1 g_P(p_1, t) \right] \right\} \qquad (2.8.13)$$

or

$$\frac{\partial g_P(p_1, t)}{\partial t} = C_B \beta [g_{\mathrm{eq}}(p_1)] \left[\frac{\partial^2 g_P}{\partial p_1^2} + (1 - p_1^2)\, g_P \right], \qquad (2.8.14)$$

which is the equation for the Brownian motion in *one dimension*. From equation (2.8.12) or (2.8.14) it is easily seen that $g_P(p_1, t)$ proceeds from its initial state $g_P(p_1, 0)$ to its final state which must be $g_{\mathrm{eq}}(p_1)$. The details of the approach to the equilibrium distribution are given by equation (2.8.14). The procedure used here gives the various coefficients (as for friction) in terms of the mechanical properties of the particles.

2.9. *Comparison with the Procedure Used by Prigogine*

Aside from the fact that this derivation is carried out directly in the phase space without reference to the Fourier representation, there are several other differences with respect to the derivation given by Prigogine et al.[6] that are worth noting. In this derivation, the selection of higher-order terms in λ, namely g_0^{2n}, was

carried out by comparison with equation (2.5.6) and with the ultimate intention of demonstrating that equation (2.5.9) was actually contained in the complete expansion of $g_0(t)$. In the treatment given by PRIGOGINE, the Fourier transforms of all terms g_0^l are studied with respect to their asymptotic t, λ, N, and V dependence in the limits $t \to \infty$, $\lambda \to 0$ (where ∞ and 0 mean arbitrarily large and arbitrarily small, respectively) such that $\lambda^2 t$ remains finite and $N \to \infty$, $\mathcal{V} \to \infty$ such that $N/\mathcal{V}$ remains finite. Thus, all non-zero terms containing $(\lambda^2 t)^n$ are retained while terms of order $\lambda^2(\lambda^2 t)^n$ are dropped to this order in λ since they are negligible compared to the terms $(\lambda^2 t)^n$. In the next order of approximation all terms $\lambda(\lambda^2 t)^n$ must also be retained. Thus, the asymptotic dependence is taken as a selection rule. The necessity of this selection rule is clear, as we wish to develop an equation valid for small *but fixed* λ and arbitrarily large t so that the quantity $\lambda^2 t$ need not be small compared to $(\lambda^2 t)^2$. That is, λ and t are unrelated and, consequently, $\lambda^2 t$ can and will obtain arbitrarily large values*. Other terms such as $\lambda^3 t^2$ do not exist in the limit either because the Fourier coefficient is zero, or because they vanished as $N \to \infty$ and $V \to \infty$. In principle this is a very powerful procedure, for it contains within itself an immediate proof that the convergence conditions (as presented here) are satisfied.

The asymptotic time analysis is carried out on the Fourier transforms of the terms g_0^l as represented by equation (2.4.9). To indicate briefly the relation of that procedure to the phase space, we note that

$$\left.\begin{aligned} \Phi(t,p) = \int_x \frac{\partial V(x)}{\partial x} \int_0^t \frac{\partial V}{\partial x}(x - pt')\, dt'\, dx \approx \int_x \frac{\partial V(x)}{\partial x} \int_0^t \frac{\partial V}{\partial x}(x - pt')\, dt'\, dx \quad \text{for} \quad |p| > \varepsilon \\ + t \int_x \left[\frac{\partial V(x)}{\partial x}\right]^2 dx \quad \text{for} \quad 0 < |p| < \varepsilon. \end{aligned}\right\} \tag{2.9.1}$$

The Fourier transform of the first integral has poles which lie off the real axis in the complex plane and these are discarded, whereas the second integral has a pole on the real axis and is retained. As pointed out by PRIGOGINE, the poles which lie off the real axis become negligible for $t \gg t_c$. This result is identical to that obtained with the rigorous analysis of $\Phi(t, p)$ (presented in section 2.6) which shows that the first integral in equation (2.9.1) can be effectively neglected for $t \gg t_c$ and, hence, that $\overline{g_0^2}$ behaves asymptotically as $t\delta(p)\overline{g_0(0)}$ (where the bar means the Fourier transform with respect to the x_i). In a similar manner it is shown by PRIGOGINE that $\overline{g_0^{(2n)}}$ behaves as $t^n \delta(p)\overline{g_0(0)}$. When these asymptotic terms are summed and differentiated with respect to t, the Fourier transform of equation (2.7.5) is obtained.

* This is an important point and it is the major distinction between the derivations given by ZWANZIG (7) and by PRIGOGINE. ZWANZIG requires that the quantity λt be small, a nonphysical condition, since λ is related to the size of the interaction potential energy which is time independent, and t necessarily becomes arbitrarily large. By summing all powers of λ/t, PRIGOGINE only requires that λ be small. However, the reader is referred to page 35 for a further discussion of these points.

One may wonder what happened to the convolution aspect of g_0^{2n}. In the asymptotic analysis of these terms in the Fourier space, for example g_0^4, one obtains both a δ and a δ' function. The latter is dropped as being negligible compared to the δ function. If retained it would have led to $g'(t)$ terms which have also been dropped in the treatment given here (see equations 2.7.3 and 2.7.4). It is worth mentioning that the result obtained by the resolvent method (eq. 2.5.6) is also used as a guide to enhance the proper selection and analysis of the terms g_0^l in the treatment given by PRIGOGINE.

Part II: Analysis of the Master Equation

Section 3: Analysis of the Master Equation

3.1. *Discussion of the Master Equation*

While we shall shortly investigate the approximations involved, it is important to realize the generality of the master equation (2.6.8) if the presentation is correct. The $\{x_i\}$ dependence of the initial distribution function $\varrho(0)$ is limited by the conditions (2.2.3) and (2.3.1), but the momentum distribution $g_0(\{p_i\})$ is not restricted and can have any normalizable form. The master equation expresses the time dependence of $g_0(t)$ and is valid for λ small and $t \gg t_c$, as well as N and $\mathcal{V}$ becoming infinite such that concentrations remain finite. While not all physical systems will have a small λ, for purposes of discussion we shall allow λ to be made arbitrarily small, but not zero. The quantities λ and t are not related so that the master equation is valid no matter how large t becomes. Also we can take $g_0(t)$ as an approximation to $\varrho(t)$ in accord with equation (2.2.4), since all higher correlation functions (g_2, $g_3 \ldots$) enter to higher orders in λ and can presumably be ignored for small λ*. In effect, the master equation is another form of the Liouville equation valid when the stated conditions are satisfied. It is easily demonstrated that the entropy production (for $S(t) = \int g_0 \ln g_0 \Pi_i dp_i$, where $g_0(t)$ is the solution of the master equation) is positive definite ($\partial S/\partial t > 0$). Furthermore, starting from any initial state $g_0(0)$, the distribution function will eventually approach a time independent state (as $t \to \infty$).

The nature of the solution is particularly easy to realize when the momentum distribution function is initially factorized (equation 2.8.2), in which case equation (2.8.5) can be applied. Starting from any initial set of $g_i(p_i, 0)$, after a short time ($t \gg t_c$), the only contributions to changing the functional forms $g_i(p_i, t)$ occur when $p_i = p_j$ and the time evolution proceeds until $g_i(p) = g_j(p)$ (that is, the functional forms become identical). At this point (which is $t = \infty$), the system is stationary, and all the g_i are functionally identical. Note that, in general, $g_i(p_i, 0) \neq g_i(p_i, \infty)$. The master equation does *not* possess an oscillatory solution.

* This approximate relationship between $\varrho(t)$ and $g_0(t)$ is not an explicit part of the theory as presented by PRIGOGINE, but it seems to be the source of some confusion in the literature as well as an interesting feature to investigate.

3.2. *Difficulties with the Master Equation*

However, we must recall the reversible properties of the Liouville equation, particularly the entropy production which is always zero and the existence of the Poincaré time at which the system returns to its original state. Since these properties do not depend on the size of λ, it is difficult to understand how the solution of the master equation, which is an approximation to the solution of the Liouville equation, can exhibit irreversible properties. As the Poincaré time depends on the number of particles N, this difficulty can be resolved by assuming that the Poincaré time becomes infinite for an infinite number of particles and hence can be forgotten, although the use of the master equation to describe real systems with a finite number of particles is implicitly limited to times much less than the Poincaré time*. The difference in the entropy production of the two equations is not explained.

There is still another difficulty. If all the particle density functions $g_i(p_i)$ have identical functional forms, *regardless* of what that form is (i. e., it need not be the equilibrium form), the momentum density function g_0 will not change in time according to the master equation (see eqs. 2.8.6, 2.8.8). Or, in the study of Brownian motion (section 2.8), if the density function of the bath particles g_B had *any* functional form, the Brownian particle would have approached this form as $t \to \infty$. This property of the master equation is in complete contradiction to the Liouville equation which states that, in general, such functions must change in time (except for the equilibrium density functions). This property of the Liouville equation does neither depend on the size of λ nor on whether the volume is finite or infinite. In view of these differences, we must conclude that the solution of the master equation is not an approximation to the solution of the Liouville equation $\varrho(t)$ nor to the corresponding momentum density function $g_0(t)$. Consequently, the derivation of the master equation starting from the Liouville equation cannot be justified with only the assumptions employed thus far.

3.3. *Resolution of the Inconsistencies – g_0 as an approximation to ϱ.*

The difference in entropy production between the Liouville equation and the master equation presents a problem only if g_0 is assumed to be equal to ϱ to the order λ. This possibility appears from equations (2.2.4) and (2.3.1) which state that

$$\varrho = \left[g_0^0 + \lambda \sum_P g_2^0 + \lambda^2 \sum_P g_2^1 \right] + \lambda^2 \left[g_0^0 + \lambda \sum_P g_2^2 + \lambda \sum_T g_3^0 \right] + \ldots \tag{3.3.1}$$

Equation (3.3.1) is written so as to demonstrate that each term of higher order correlation functions, g_2^l, g_3^m, etc., can be compared to g_0^n and is of higher order in λ. If in *each* bracket the higher order terms can be neglected with respect to the first term for small λ, then ϱ can be replaced by g_0. It is important to note that the

* This explanation was given by PRIGOGINE (4).

entire position dependence of ϱ is contained in the $g_l\,(l \geq 1)$, while g_0 expresses only a part of the momentum dependence.

To study this problem, we may start by examining the term g_2^0 which is given by equation (2.4.8) and can be written as

$$g_2^0(i, j, t) = -\frac{1}{p}\,[V(x - pt) - V(x)]\left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] g_0^0(0) \tag{3.3.2}$$

after the time integration has been carried out. This term must be compared to $g_0^0(t) = g_0^0(0)$. For almost all density functions $g_0^0(0)$ of interest, the term g_2^0 will become arbitrarily large relative to g_0^0 as the p_i and p_j approach infinity. Specific examples are $g_0^0 = \prod_i g_i(p_i)$, where $g_i(p_i) = \delta(p_i - p_i')$ or $g_i(p_i) = \exp(-p_i^4)$. In the neighbourhood of $p = 0$, equation (3.3.2) reduces to

$$g_2^0(i, j, t) = +t\frac{\partial V(x)}{\partial x}\left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] g_0^0(0) \tag{3.3.3}$$

so that g_2^0 will become arbitrarily large as $t \to \infty$, even for $p = 0$. Finally, if $V(x)$ has an infinity as is the case for many potentials of physical interest, then g_2^0 will again become arbitrarily large when the arguments in (3.3.2) lie in the neighbourhood of these infinities. For any one of these reasons, it is clear that no matter how small λ is made, the term λg_2^0 will dominate the term g_0^0 for some values of $\{p_i\}$, $\{x_i\}$, and t so that it cannot be neglected. The same reasoning applies to each of the brackets of (3.3.1).

The importance of these higher-order correlation functions in regard to the entropy production is easily realized. If the expansion of ϱ given by (3.3.1) is inserted in the definition of the entropy, $S = \int \varrho \ln \varrho \prod_i dp_i\,dx_i$, and the entropy is then expanded in powers of λ, it is easy to demonstrate that $\partial S/\partial t = 0$ for all t and for each power of λ by using the values of the g_l derived from equations (2.2.9) in section 2.4.

We can conclude that $g_0(t)$ is not an approximation to $\varrho(t)$, regardless of how small λ may be. Consequently, there is no inconsistency in the different entropy productions associated with the Liouville equation and the master equation.

3.4. *The Master Equation as an Equation for* g_0

While $g_0(t)$ cannot be taken as an approximation to $\varrho(t)$, it is still possible that the g_0, which satisfies the master equation, is a valid approximation to the g_0 which arises from the Liouville equation (1.1.6). However, we must still resolve the inconsistency which arises from the fact that stationary solutions g_0 of the master equation are not stationary solutions of the Liouville equation. Again we shall look at the higher-order terms in λ. We begin with the term g_0^2 which has an order λ^3. This term arises from g_2^1 and, in the development of g_2^1, we consider only the first term on the

right in equation (2.2.9). All other terms in this equation are of different powers in the concentrations, as indicated by the summation signs. Solving this reduced equation for g_2^1, and inserting the result in equation (2.2.9), gives finally

$$\left.\begin{aligned}\frac{\partial g_0^3(t)}{\partial t} = \frac{\lambda^3}{\mathscr{V}} \sum_{ij}{}' \frac{\partial}{\partial p_i} \int_{x=-\infty}^{+\infty} \frac{\partial V(x)}{\partial x} \int_0^t E(-p\tau) \frac{\partial V(x)}{\partial x} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] \\ \int_0^{t-\tau} \frac{\partial V}{\partial x}(x - pt')\, dt'\, d\tau\, dx \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] g_0^0(t).\end{aligned}\right\} \tag{3.4.1}$$

The exact analysis of this term is carried out in Appendix II, and it is shown that equation (3.4.1) can be reduced to

$$\frac{\partial g_0^3(t)}{\partial t} = \frac{-2\lambda^3}{\mathscr{V}} \sum_{ij}{}' \frac{\partial}{\partial p_i} \left\{\frac{t}{p^2} I_{21}(j) + \frac{1}{p^3} I_{22}(j)\right\} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] g_0^0(0), \tag{3.4.2}$$

where $j = pt$ is confined to $|j| < 2b$. The character of $g_0^3(t)$ is already apparent from this equation which shows that $g_0^3(t)$ depends on $\lambda^3 t^2/p^2 + \lambda^3 t/p^3$ and has poles for $p = 0$ and $t = \infty$. Since the operators outside the brackets $\{\ \}$ are identical with those for the term in $g_0^2(t)$ which depends on $\lambda^2 t/p$ (see eqs. 2.6.1 and 2.6.5), these terms can be compared directly. As the poles for g_0^3 are of higher order than for $g_0^2(t)$ we cannot expect that the higher-order terms can be neglected with respect to the lower-order terms, however small λ is made. But such analysis, while indicative of much that follows, is not rigorous. To determine the exact value of $\frac{\partial g_0^3}{\partial t}(t)$ for $t \to \infty$, we proceed as in section 2.6 by considering the integration over p_i. The complete evaluation of equation (3.4.2) for the constant force is carried out in Appendix II and yields

$$\frac{\partial g_0^3(t)}{\partial t} = -\lambda^3 \frac{4}{3} a^3 b^3 (1 - ln\, 2) \sum_{ij}{}' \frac{\partial}{\partial p_i} \delta(p_i - p_j) \frac{\partial^2}{\partial p_j^2} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] g_0^0(0). \tag{3.4.3}$$

This equation shows that the asymptotic time dependence of $g_0^3(t)$ is $\lambda^3 t$ and, as pointed out by PRIGOGINE, can be neglected for small λ in comparison to $g_0^2(t)$ whose dependence is $\lambda^2 t$. However, a comparison of these terms on the basis of the time and λ dependence alone is not meaningful, since the momentum operator on the right of (3.4.3) is not identical with that which occurs in $g_0^2(t)$ (eqs. 2.6.1 and 2.6.7). Thus, if we again assume that $g_0(0)$ is factorized into $\prod_i g_i(p_i)$, then even if all the $g_i(p_i)$ have identical functional forms, $\partial g_0^3/\partial t$ will not in general* be zero, whereas we have

* There may well be particular functional forms which are exceptions to this statement, but, arbitrarily chosen, $g_i(p_i)$ (identical for all i) will *not* make $\partial g_0^3/\partial t = 0$. This is easily proved by picking particular forms for $g_i(p_i)$ and inserting them into equation (3.3.4).

already shown that $\partial g_0^2/\partial t = 0$ under this condition. This result affords the resolution of the difficulty discussed in the previous section, for the special factorized form is no longer a stationary solution of the extended master equation (i. e., the λ^3 term included). At the same time it demonstrates that the λ^3 term cannot in general be neglected relative to the λ^2 term, no matter how small λ is taken.

However we now have another difficulty. Equation (3.4.3) has done its job so well that even if we take all g_i identical and equal to the equilibrium form, i. e., $g_i(p_i) = g_{\mathrm{eq}}(p_i) = C \exp\left(-\frac{p^2}{2}\right)$, we find that $\partial g_0^3/\partial t \neq 0$. This is at first rather difficult to understand since the equilibrium distribution is a time independent solution of the Liouville equation and g_{eq} is the correct form of the reduced equilibrium density function. Furthermore, of the terms which we have neglected, none can affect this result since they all occur to different powers of λ or C (concentration). However, the equilibrium distribution is given by equation (2.3.2) and is a function of the potential energy as well as the p_i. While this does not affect the momentum density functions g_{eq}, it does affect the initial conditions. The initial conditions thus far employed are incompatible with the fact that, at $t = 0$, the distribution function was the equilibrium distribution. Comparison with equation (2.3.2) shows that we must take

$$\left.\begin{aligned} g_0^0(0) &= g_0^0(0) \\ g_0^\nu &= 0 \quad \text{for} \quad \nu > 0 \\ g_1^\nu &= 0 \quad \text{for all} \quad \nu \\ g_2^0(0) &= -\, g_0^0(0)\, V(x) \\ g_2^1(0) &= g_0^0(0)\, V^2(x). \end{aligned}\right\} \tag{3.4.4}$$

For these initial conditions we obtain (see section 5.3)

$$\left.\begin{aligned} \frac{\partial g_0^3(t)}{\partial t} = \frac{\lambda^3}{\mathcal{V}} \frac{8 a^3 b^3}{3} \sum_{ij} \frac{\partial}{\partial p_i} \Bigg\{ & -\ln 2\, \delta(p_i - p_j) \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] \\ & + (1 - \ln 2)\, \delta(p_i - p_j) \frac{\partial}{\partial p_j} - \frac{(1 - \ln 2)}{2} \delta(p_i - p_j) \frac{\partial^2}{\partial p^2} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] \Bigg\} g_0^0(0). \end{aligned}\right\} \tag{3.4.5}$$

If we now assume that $g_0^0 = \prod_i g_{\mathrm{eq}}(p_i)$, equation (3.4.5) gives

$$\frac{\partial g_0^3}{\partial t} = 0,$$

showing that the equilibrium density function is time independent. But equation (3.4.5) still retains the property that $\frac{\partial g_0^3}{\partial t}(t) \neq 0$ for arbitrary distributions $g_i(p_i)$, even if the functional forms are identical for all i. We shall consider the effects of

these higher-order terms in λ still further in section 3.6, but first it is important to investigate some of the other approximations involved in the derivation of the master equation.

3.5. *The Value of the Collision Time*

In the derivation of the master equation, it was necessary to assume the existence of a time t_β sufficiently large so that for all $t > t_\beta$ we could set $f(t) \approx f(\infty)$ (eq. 2.6.9). But we also had to assume that t_β was sufficiently small so that $g_0(t - t_\beta) \approx g_0(t)$ (eq. 2.7.4). It is necessary to investigate the requirements for which both these conditions can be satisfied simultaneously. To determine the largeness of t_β, we retain the next non-zero term which arises from the Taylor expansion of $[\mathfrak{R}(j/t) + \mathfrak{R}(-j/t)]$ in equation (2.6.6). In the place of equation (2.7.5) we obtain

$$\left.\begin{aligned} \frac{\partial g_0(t)}{\partial t} = \frac{1}{\mathscr{V}} \sum_{ij}{}' \frac{\partial}{\partial p_i} \Bigg\{ & 4\, a^2 b^2 \ln 2\, \delta(p) \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] \\ & + \frac{a^2 b^4}{2\, t^2} \delta(p) \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] \frac{\partial^2}{\partial p_j^2} - \frac{a^2 b^4}{t^2} \delta(p) \frac{\partial}{\partial p_j} \Bigg\} g_0(0), \end{aligned}\right\} \quad (3.5.1)$$

where the third term arises from the use of the new initial conditions discussed in section 3.4 (eqs. 3.4.1). We must choose t_β sufficiently large so that the terms in $1/t^2$ can be neglected with respect to the first term. Several features of the $1/t^2$ terms should be noted. First, while they occur to higher order in b (the range of the force) than the first term, they have the same a dependence (namely a^2) as the first term. Thus, it is necessary to assume that b^2/t^2 is small even to expect that these terms can be neglected. Secondly, the $1/t^2$ terms have the same property as the λ^3 terms; they do *not* vanish if $g_0(\{p_i\})$ is a factorized function with all factors having the same functional form, i. e., $g_0(p_i) = \prod_i g_i(p_i)$ with $g_i(p_i) = g_j(p_i)$, while the first term does vanish. In this case, $1/t^2$ terms can never be neglected except for $t_\beta = \infty$ (or $b = 0$ which is not allowed). But it should be noted that all terms vanish for g_0 equal to the equilibrium distribution.

To examine the conditions in t_β in further detail, we shall assume two types of particles, labelled α and β, having concentrations C_α and C_β. Furthermore, we shall assume that initially the density function $g(0)$ is factorized and that the two types of particles have the density functions

$$\left.\begin{aligned} g_\alpha(p_\alpha, t) &= A_\alpha \quad \exp \left[-\frac{p_\alpha^2}{2\, \sigma_\alpha}\right] \\ g_\beta(p_\beta, t) &= A_\beta \quad \exp \quad -\frac{p_\beta^2}{2\, \sigma_\beta}, \end{aligned}\right\} \quad (3.5.2)$$

where A_α and A_β are normalization constants and $\sigma_\alpha(t)$ and $\sigma_\beta(t)$ are parameters corresponding to the mean square deviation. For $\sigma_\alpha,\ \sigma_\beta = 1$, the density functions become the equilibrium density functions, while for $\sigma_\alpha,\ \sigma_\beta = 0$ they correspond to a delta function. The equations for $g_\alpha(p_\alpha, t)$ and $g_\beta(p_\beta, t)$ are developed in the same manner as for the case of Brownian motion (section 2.8) by integrating over all particles but the one of interest. Thus equation (3.5.1) yields

$$\begin{aligned}\frac{\partial g_\alpha(p_\alpha, t)}{\partial t} = \frac{\partial}{\partial p_\alpha}\Bigg\{ & 4\,a^2 b^2 \ln 2\, C_\beta \left[\frac{\partial g_\alpha(p_\alpha, t)}{\partial p_\alpha} g_\beta(p_\alpha, t) - g_\alpha(p_1, t)\frac{\partial g_\beta(p_\alpha, t)}{\partial p_\alpha}\right] \\ & + \frac{a^2 b^4}{2 t^2}\left[C_\beta \frac{\partial g_\alpha(p_\alpha, t)}{\partial p_\alpha}\frac{\partial^2 g_\beta(p_\alpha, t)}{\partial p_\alpha^2} - C_\beta \frac{\partial^3 g_\beta(p_\alpha, t)}{\partial p_\alpha^3} g_\alpha(p_\alpha, t)\right. \\ & \left. + C_\alpha \frac{\partial g_\alpha(p_\alpha, t)}{\partial p_\alpha}\frac{\partial^2 g_\alpha(p_\alpha, t)}{\partial p_\alpha^2} - C_\alpha \frac{\partial^3 g_\alpha(p_\alpha, t)}{\partial p_\alpha^3} g_\beta(p_\alpha, t)\right] \\ & + \frac{a^2 b^4}{t^2}\left[C_\beta \frac{\partial g_\beta(p_\alpha, t)}{\partial p_\alpha} g_\alpha(p_\alpha, t) + C_\alpha \frac{\partial g_\alpha(p_\alpha, t)}{\partial p_\alpha} g_\alpha(p_\alpha, t)\right]\Bigg\}\end{aligned} \tag{3.5.3}$$

with a similar equation for $\partial g_\beta(p_\beta, t)/\partial t$ obtained from (3.5.3) by interchanging α and β. By inserting equations (3.5.2) into (3.5.3), the condition for neglecting the $1/t^2$ terms relative to the first term is readily obtained. For the $\partial g_\alpha/\partial t$ equation, we must require

$$\frac{b^2}{t_\beta^2}\left|\left\{C_\alpha\left(1-\frac{1}{\sigma_\alpha}\right) + C_\beta\left[\frac{1}{2}\frac{p_\alpha^2}{\sigma_\beta}\left(\frac{1}{\sigma_\beta}-\frac{1}{\sigma_\alpha}\right)+\frac{1}{2}\left(\frac{1}{\sigma_\alpha}-\frac{3}{\sigma_\beta}+2\right)\right]\right\}\right| \ll 4\ln 2\, C_\beta\left(1-\frac{\sigma_\beta}{\sigma_\alpha}\right) \tag{3.5.4}$$

and for the $\partial g_\beta/\partial t$ equation the condition is the same as (3.5.4), but with α and β interchanged.

For the condition on the smallness of t_β, when $g_0(0)$ is factorized, we note that equation (2.7.3) reduces to two equations

$$\begin{aligned}\frac{\partial g_\alpha(p_\alpha, t)}{\partial t} = 4\,a^2 b^2 \ln 2\, C_\beta \frac{\partial}{\partial p_\alpha}\Bigg\{ & \frac{\partial g_\alpha(p_\alpha, t-t_\beta)}{\partial p_\alpha} g_\beta(p_\alpha, t-t_\beta) \\ & - g_\alpha(p_\alpha, t-t_\beta)\frac{\partial g_\beta(p_\alpha, t-t_\beta)}{\partial p_\alpha}\Bigg\}\end{aligned} \tag{3.5.5}$$

and

$$\frac{\partial g_\beta(p_\beta, t)}{\partial t} = \text{same as above but } \alpha \rightleftarrows \beta,$$

where we have neglected the integral term occurring in (2.7.3). The master equation is obtained by setting $t_\beta = 0$ in equations (3.5.5), and the conditions for doing this may be taken as

$$t_\beta \frac{\partial g_\alpha(t)}{\partial t} \ll g_\alpha(t) \quad t_\beta \frac{\partial g_\beta(t)}{\partial t} \ll g_\beta(t) \tag{3.5.6}$$

and correspond to the condition (2.7.4). To examine these conditions more fully, we shall use the functional forms given by (3.5.2) and determine $\partial g_\alpha(t)/\partial t$ from the master equation (i. e., 3.5.5. with $t_\beta = 0$). In that case, the conditions (3.5.6) become

$$\left| 4\, a^2 b^2 \ln 2\, t_\beta C_\beta g_\beta^{(p_\alpha)} \left[1 + p_\alpha^2 \left(\frac{1}{\sigma_\beta} - \frac{1}{\sigma_\alpha} \right) \right] \right| \ll 1 \tag{3.5.7}$$

and the same equation with $\alpha \rightleftarrows \beta$, except that p_α is not changed.

The conditions (3.5.4) and (3.5.7) in the values of t_β are not necessarily compatible, regardless of how small (but not zero) the quantities a or b are chosen. Thus, if $\sigma_\beta = \sigma_\alpha \neq 1$, equation (3.5.4) can only be satisfied for $t_\beta = \infty$, while equation (3.5.7) requires $t_\beta = 0$, demonstrating that the master equation is not correct. This case is not surprising in view of our previous discussions, but it is now clear that σ_β and σ_α must be sufficiently different so that there will exist a t_β which satisfies both conditions. As another example, we can consider the case related to Brownian motion by taking $\sigma_\beta = 1$. In this case, the conditions (3.5.4) and (3.5.7) reduce to

$$\frac{b^2}{t_\beta^2} \left| \frac{C_\alpha}{C_\beta} + \frac{1}{2}(p_\alpha^2 - 1) \right| \ll 4 \ln 2 \quad \text{for} \quad \frac{\partial g_\alpha}{\partial t} \tag{3.5.8}$$

$$\frac{1}{2} \frac{b^2}{t_\beta^2} \left| \frac{p_\beta^2}{\sigma_\alpha^2} - \frac{3}{\sigma_\alpha} \right| \ll 4 \ln 2 \quad \text{for} \quad \frac{\partial g_\beta}{\partial t} \tag{3.5.9}$$

and

$$4\, a^2 b^2 (\ln 2)\, t_\beta C_\beta g_\beta^{(p_\alpha)} \left| 1 + p^2 \left(1 - \frac{1}{\sigma_\alpha} \right) \right| \ll 1 \tag{3.5.10}$$

$$4\, a^2 b^2 (\ln 2)\, t_\beta C_\beta g_\beta^{(p_\alpha)} \left| 1 + p^2 \left(\frac{1}{\sigma_\alpha} - 1 \right) \right| \ll 1, \tag{3.5.11}$$

where the first condition serves for neglecting the $1/t^2$ terms in the equation for $\partial g_\alpha(p_\alpha, t)/\partial t$, while the second applies to the equation for $g_\beta(p_\alpha, t)/\partial t$ and can be ignored if we wish to consider only the motion of the Brownian particle (i. e., g_α). The last two conditions apply to both equations. In any case, there are again no compatible values of t_β for $\sigma_\alpha = 0$; i. e., when the Brownian particle has initially a $\delta(p_\alpha)$ density function. Thus, we must assume that σ_α is sufficiently different from zero to satisfy the first, third, and fourth conditions. The second condition further restricts the value of σ_α, but is concerned with the equation for $g_\beta(p_\beta)$ describing the motion of the bath particles.

Furthermore, it should be recognized that the values of t_β which satisfy the conditions (3.5.7) also depend on the momentum (p_α or p_β). In general, it is necessary to restrict the range of momenta p_α for which the master equation can be considered correct. Thus, for large values of p_α, it is necessary to choose a large value of t_β to satisfy the condition (3.5.8); in fact $t_\beta \to \infty$ as $p_\alpha \to \infty$. However, this value of t_β *will* be compatible with equation (3.5.10) because of the presence of the factor $g_\beta(p_\alpha)$ in (3.5.10). While it is clear that we must choose a different value of t_β for each p_α, this presents no major problems, except to restrict the range of momenta for which the master equation is valid at a given time t. As t becomes larger, t_β for particular p_α can be made larger and we can neglect the terms in $1/t^2$ for a wider range of momenta.

Finally, we must realize that the values of σ used in the conditions (3.5.3) and (3.5.7) are time dependent. Thus, in the case of Brownian motion where, at $t = 0$, we take $\sigma_\beta(0) = 1$ and $\sigma_\alpha(0) \neq 1$, it will be possible to satisfy the conditions for some region of momentum if a and b are small. As was already pointed out in section 3.2, the master equation (eq. 3.5.1 *without* the $1/t^2$ terms) will drive the system to a state where $\sigma_\beta = \sigma_\alpha \neq 1$. As the system approaches this state the terms in $1/t^2$ will become increasingly important and finally dominate the other terms, as indicated by the fact that the conditions will no longer be satisfied. This result depends on the fact that $\sigma_\alpha \to \sigma_\beta$ exponentially in time, while we can only neglect the other terms to an order $1/t^2$.

3.6. *Effect of Higher Order Terms in* λ

In the previous section, we have concerned ourselves with an analysis of the condition necessary to reduce the non-Markovian equation (2.5.16) to the Markovian master equation (2.7.5). These equations only involved certain terms of order $(\lambda^2)^n$ and the reduction to the master equation primarily required conditions which allow these terms to be replaced by their asymptotic forms. In this section we shall examine the effect of higher-order terms in λ, such as $(\lambda^3)^n$, using the asymptotic forms of these terms without regard to the conditions necessary to justify these forms. In place of the master equation, we then obtain

$$\frac{\partial g_0(\{p_i\}, t)}{\partial t} = \{\lambda^2 [2.7.6] + \lambda^3 [3.4.6]\} g_0(\{p_i\}, t), \tag{3.6.1}$$

where the numbers in brackets refer to the operators given by those equations. The λ^2 terms are just those of the master equation. The only difference between the λ^3 term here and that given by equation (3.4.6) is that it now operates on $g_0(t)$ instead of $g_0(0)$. This replacement can be justified by examining and summing special terms of all orders in $(\lambda^3)^n$ and $(\lambda^2)^m(\lambda^3)^l$ in the same manner as for the derivation of the master equation given in sections 2.5 to 2.7.

As shown by equation (3.4.6), the λ^3 operator can be broken into two parts. One part (the first term of 3.4.6) has exactly the same form as the master equation and can always be ignored if λ is small (i. e. $\lambda^3 \ll \lambda^2$); but even if λ is not small, this term will not alter the form of the master equation, except for the change of the numerical coefficient from $(4\lambda^2 a^2 b^2 ln\, 2)$ to $\left(4\lambda^2 a^2 b^2 ln\, 2\left[1-\frac{2}{3}\lambda ab\right]\right)$. We shall ignore this term in the following. The other part of the λ^3 operator (the second and third terms of eq. 3.4.6) is identical with the terms in $1/t^2$ in equation (3.5.1); in fact it is only necessary to let the quantity in equation (3.5.1) go to

$$\frac{a^2 b^4}{t^2} \to a^3 b^3 [(ln\, 2) - 1] \tag{3.6.2}$$

to obtain equation (3.6.1). As in section 3.5, we can assume that $g_0(0)$ is factorized and there exist only two types of particles, α and β. Equation (3.6.1) reduces to two simultaneous equations identical with the equation (3.5.3) when the substitution (3.6.2) is made. If we further assume that the density functions are represented by equation (3.5.2), then the conditions for neglecting the λ^3 terms become identical with the conditions (3.5.4) so long as we set

$$\frac{b^2}{t^2} \to ab\,[1 - ln\, 2]. \tag{3.6.3}$$

The analysis of these conditions is essentially identical to that previously given, except that the λ^3 terms are not directly affected by the size of t. For any value of ab we must limit the momentum space and the nature of the density functions in order to neglect the terms in λ^3. Finally, we must again realize that σ_α and σ_β are time dependent. The equation of motion for the density functions (eqs. 3.5.3 with 3.6.2) can be schematically written as

$$\left.\begin{aligned} \frac{\partial g_\alpha(p_\alpha, t)}{\partial t} &= \lambda^2 C_\beta(\sigma_\alpha = \sigma_\beta) + \lambda^3 C_\alpha(\sigma_\alpha = 1) \\ \frac{\partial g_\beta(p_\beta, t)}{\partial t} &= \lambda^2 C_\alpha(\sigma_\alpha = \sigma_\beta) + \lambda^3 C_\beta(\sigma_\beta = 1), \end{aligned}\right\} \tag{3.6.4}$$

where the equalities in parenthesis indicate the conditions under which the coefficients *are zero*. Thus, if we consider Brownian motion where initially $0 < \sigma_\alpha(0) \ll 1$ and $\sigma_\beta(0) = 1$, we can neglect the λ^3 terms for some range of momenta (λ is assumed small). But the effect of the λ^2 terms is to make $\sigma_\alpha = \sigma_\beta \neq 1$. As this state is approached, the λ^3 terms will dominate the motion. It is also clear that the λ^3 terms become important more rapidly for $\partial g_\beta/\partial t$ since they enter to an order C_β in that equation.

3.7. *Discussion of the Analysis*

The analysis given in this and the preceding section can be considered as a first-order analysis of the conditions necessary for the master equation to be correct. The presence of the λ^3 terms will affect the conditions necessary for the neglect or retention of the $1/t^2$ terms as well as the conditions for making the equation Markovian. Basically, it is also necessary to determine the condition for neglecting other terms which arose in the original expansion of the Liouville equation (2.2.9). In any case, the conditions we have determined already place the master equation in its proper perspective.

As in the case of Brownian motion, by imposing limitations on the momentum space, the time coordinate, and the nature of the initial distribution function, the motion of the system will be determined by the master equation (λ^2 terms). This motion is such that the system will approach a state (not the equilibrium state) where the master equation will be satisfied and where the λ^2/t^2 and λ^3 terms will become important in determining the motion of the system. When these terms are included we can expect that the system will approach a state (again, not the equilibrium state) which satisfies the collection of λ^2, λ^2/t^2 and λ^3 terms and will require the retention of still higher order terms (λ^2/t^4 and λ^4). Furthermore, the equations (with λ^2/t^2 and λ^3 terms retained) are such that the system need not approach the new stationary states in a monotonic manner, but rather can undergo damped oscillations. When all orders of λ and t are retained, the system need no longer approach a stationary solution; instead, it will obtain an oscillatory solution. This effect will be further studied in a later paper for it relates to the Poincaré time and the entropy production.

However, there is one exception to the preceding discussion, which arises in the case of Brownian motion. If we assume that the concentration of the Brownian particles α is zero, then the bath particles β will remain at equilibrium, as shown by equation (3.6.4). While it is still necessary to impose limitations on the momentum-time space, the master equation will be correct within these limits and describe the motion of the Brownian particle to the final equilibrium state. The limitation on the momentum space involves p^2 and can be expressed as a condition on the energy, namely as $E_\alpha \ll kT$, where E_α is the energy of the particle. As was pointed out in section 3.6, even when λ is not small, the master equation (with only a change in numerical coefficients) may still be satisfied, although the momentum space will be more severely restricted. Still, it should be noted that any changes in the interaction potential or the Hamiltonian will affect the nature of these conditions, so that the particular form of the master equation may not be justified in regions of physical interest and some other form wuold have to be developed.

In view of these results, the similarity under certain conditions of the Brownian motion equation given here to equations derived by other techniques is not surprising. Thus, the stochastic derivation given by KRAMERS[1] assumes that the Brownian particle is affected by random forces in the bath which is not itself affected by the particle; and the final equation is intuitively subjected to the condition that $E_\alpha \ll kT$. The

derivation of a Brownian motion equation given by ROSENBLUTH[9] is similar to the derivation given here. Starting from the Liouville equation an expansion is made in correlation functions and λ; only the first iteration is carried out (in fact, only the $\lambda^2 t$ term is retained). The Brownian motion equation is then obtained by assuming that the bath particles are at equilibrium and are not disturbed, as well as that $t \to \infty$. This procedure is more direct and avoids the summation of all powers of $(\lambda^2 t)^n$ and the intermediate formulation of the master equation. A condition is imposed on the energy by requiring that the expansion be valid for average values; such a condition must be considered to be intuitive since it was not and cannot be used to analytically justify the application of the resulting equations. The resulting equation is identical with that obtained by use of the master equation. Finally, we may realize that the condition imposed by ZWANZIG in his derivation of the master equation, namely, that the quantity λt be small (see footnote p. 25), is actually required to justify the master equation. For the analysis presented here shows that the master equation is not valid after a time related to λ and the specific form of the initial density function.

The usefulness of the master equation is probably best discussed in terms of states of the density functions. Starting from some state for which the conditions are satisfied, the master equation will approximately describe the evolution of the system to some new state in which the conditions are no longer satisfied. If it happens that the two states are of physical interest, then the equation is useful. This is the case for a Brownian motion even when the ratio of particles is finite ($\approx 10^{23}$). The conditions (3.5.4) can be satisfied for initial states of physical interest and the evolution will be approximately described by the master equation until the state for $\sigma_\alpha = \sigma_\beta \neq 1$ is reached. This final state will be very near the equilibrium state, and the equation will be of physical importance. However, for other initial states which are not so closely related to the equilibrium state, the conditions will be more difficult to satisfy for problems of physical interest. It is worth noting that some form of time-coarse-graining in place of time limits ($t \to \infty$) may considerably reduce the stringency of the conditions while still yielding essentially the same equations; this will be discussed further in a later paper.

Section 4

Conclusions and Summary

The theory of irreversible processes developed by PRIGOGINE and others applies to infinite systems ($\mathcal{V} \to \infty$, $N \to \infty$) and is based on the assumption of a parameter of smallness associated with the interaction potential and the condition that t is large. It is further assumed that the initial density function $\varrho(\{p_i\}, \{x_i\}, 0)$ has a λ dependence similar to that of the equilibrium density function. The coordinate space Fourier transform of the solution of the Liouville equation $\varrho(\{p_i\}, \{x_i\}, t)$ is expanded in powers of λ, and the asymptotic time dependence of each term is studied. All terms having a dominant t dependence are selected out of the complete array. Thus, all powers of $(\lambda^2 t)^n$ are retained while terms such as $\lambda^3 t^2$ do not arise in the asymptotic

expansion. The asymptotic forms are then summed and lead immediately to the master equation which describes an irreversible process, since its solution implies a positive entropy production. In order to justify the use of the asymptotic forms, it is necessary to require that $t \gg t_c$, the collision time, which is assumed to be small in many cases of interest. Based on this derivation, the master equation would appear to be a representation of the Liouville equation, valid when λ is small, t is large, and the other weak restrictions are satisfied.

In part I of this paper (sections 1 and 2) we have rederived the master equation directly in the phase space, using only the conditions discussed above. It was demonstrated that the Fourier transform of the master equation obtained here is identical to that derived by PRIGOGINE. The only variation in the derivation given here was that the terms in $(\lambda^2 t)^n$ were summed before taking the limit of t large; this resulted in a *non*-Markovian equation closely related to the operational development of the master equation given by ZWANZIG. When the condition $t \gg t_c$ was imposed, this non-Markovian equation reduced to the Markovian master equation.

In view of the apparent generality of the master equation and its close relation to the Liouville equation, the differences in the properties of their solutions appear as inconsistencies. For example, the master equation basically describes the evolution of the momentum density function, $g_0(\{p_i\}, t)$, which would seem to be an approximation of the complete density function $\varrho(\{p_i\}, \{x_i\}, t)$ to the order λ; as such it is difficult to understand the difference in entropy production of the two equations. As another example, the master equation possesses stationary solutions which are not stationary solutions of the Liouville equation. In part II (section 3), a detailed analysis of the master equation is given in order to resolve these inconsistencies. The analysis demonstrates that the assumptions used in the derivation of the master equation are by no means sufficient to justify the neglect of higher-order terms in λ (such as $\lambda^3 t$) neither for the expansion of $\varrho(t)$ nor g_0, no matter how small λ is taken (but not zero). When these higher-order terms are retained the inconsistencies are removed.

The fundamental analytical error in the derivation of the master equation lies in the use of the asymptotic time dependence as the basis for selecting the dominant terms in λ. Every term in λ is a function of both t and $\{p_i\}$. This momentum dependence can be expressed as a differential momentum operator acting on the initial momentum density function $g_0(0, p_i)$ and such that higher terms in λ have higher order differential operators. While a particular term in λ may appear dominant for λ small and t large, the momentum dependence may make this term negligible, and some higher order term dominant. Furthermore, the lower order terms in λ always cause the density function $g_0(t, \{p_i\})$ to change such that the higher λ terms become dominant. Consequently, the selection rule based on λ, t dependence is not satisfactory and the momentum dependence of all terms must also be analyzed.

The preceding results do not directly affect the use of asymptotic forms for t large. The time dependence of any term in λ^n can be expanded about $t = \infty$ and pro-

duces terms in powers of l/t^2 which are associated with powers of the range b of the force. Again these terms also depend on the momentum $\{p_i\}$, and cannot in general be neglected, no matter how small b is made (but not zero) or how large t is made (but not infinite). This result shows that the Liouville equation cannot be reduced to a Markovian master equation for b small and t large without some additional conditions on the momentum density function. We may summarize these results as follows:

Even if the volume $\mathcal{V}$ and the number of particles N are infinite, it is not possible to expand the density function $\varrho(\{p_i\}, \{x_i\}, t)$ which satisfies the Liouville equation, or the associated reduced density functions such as $g_0(\{p_i\}, t)$ or $g_1(p_i, t)$, in powers of a parameter of smallness, be it the magnitude of the force or the range of the force or the concentration, such that higher-order terms in the parameter can be neglected in describing the evolution of any of the density functions for all values of time, momentum (and/or position) or all initial states of the density function.

This conclusion represents a generalisation of a well-known theorem due to POINCARÉ. However, it does not exclude the possibility of establishing equations, such as the master equations, which can correctly describe the evolution when conditions are imposed on the range of time, the momentum space, and the initial state of the system. In this regard, a necessary condition for the master equation to hold was established and studied with particular emphasis on the problem of Brownian motion. It was shown that the condition can be satisfied by reasonable physical limitations on the range of momentum and initial distribution and that the master equation can be expected to describe the motion of the Brownian particle density function until it is *almost* at equilibrium. The condition also shows that even if λ is not small, the evolution of the density function may still be described by the master equation (with a change in numerical coefficients), although it will be necessary to impose stronger limits on the momentum space. That is, the condition that λ is small is neither necessary nor sufficient to justify the master equation. This result explains the close similarity of Brownian motion equations under certain conditions although these equations are obtained by widely different approaches such as the stochastic assumptions used by KRAMERS.

However, it must be realized that the condition developed here is only necessary; it may not be sufficient even for the case considered here. Furthermore, any change in the interaction potential or the Hamiltonian will affect the nature of the condition. Thus, the extension of the master equation to more complex systems by the use of action and angle variables[8), (10)] will yield very different conditions. Whether these conditions can be satisfied for cases of physical interest remains to be seen.

While the study carried out here has emphasized the one-dimensional case, the extension of the derivation of the master equation (section 2) to three dimensions

is trivial. The extension of the analysis (section 3) to three dimensions is more difficult as the integrals involved become complicated, and have not yet been evaluated. However, there is no indication, neither in the method nor in the results, that the general conclusions would be affected by the dimensionality.

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Section 5: Appendices

5.1. *Appendix I: Solution of the equation*

Equations of the type (2.4.4) are most easily solved by the use of a displacement operator

$$E(pt) = e^{pt\frac{\partial}{\partial x}} \tag{5.1.1}$$

which has the property

$$E(pt)\, f(x, p, t) = f[x + pt, p, t] \tag{5.1.2}$$

as well as the commutation properties

$$E(pt)\frac{\partial}{\partial t} f(x, p, t) = \left[\frac{\partial}{\partial t} E(pt) - p\frac{\partial}{\partial x} E(pt)\right] f(x, p, t) \tag{5.1.3}$$

$$E(pt)\frac{\partial}{\partial p} f(x, p, t) = \left[\frac{\partial}{\partial p} E(pt) - t\frac{\partial}{\partial x} E(pt)\right] f(x, p, t) \tag{5.1.4}$$

$$E(pt)\, g(p, t)\frac{\partial f}{\partial x}(x, p, t) = g(p, t)\frac{\partial}{\partial x} E(pt)\, f(x, p, t), \tag{5.1.5}$$

and

$$E(pt_1)\, E(pt_2) = E[p(t_1 + t_2)] \tag{5.1.6}$$

$$E(pt)\, g(x, p, t)\, h(x, p, t) = [E(pt)\, g(x, p, t)]\, [E(pt)\, h(x, p, t)]. \tag{5.1.7}$$

To solve the equation

$$\frac{\partial g^{(x, p, t)}}{\partial t} + p\frac{\partial g^{(x, p, t)}}{\partial x} = h(x, p, t) \tag{5.1.8}$$

we operate with $E(pt)$ and, after using the commutation properties (eq. 5.1.3), obtain

$$\frac{\partial}{\partial t} E(pt)\, g(x, p, t) = E(pt)\, h(x, p, t). \tag{5.1.9}$$

Integrating with respect to t, and noting that $E(0) = 1$, we have

$$E(pt)\, g(x, p, t) - g(x, p, 0) = \int_0^t E(pt')\, h(x, p, t')\, dt'. \tag{5.1.10}$$

Applying the inverse operator $E(-pt)$ yields

$$g(x, p, t) = E(-pt)\, g(x, p, 0) + E(-pt) \int_0^t E(pt')\, h(x, p, t')\, dt' \qquad (5.1.11)$$

which can be written as

$$g(x, p, t) = g(x - pt, p, 0) + \int_0^t E[p(t - t')]\, h(x, p, t')\, dt'. \qquad (5.1.12)$$

Finally, we may set $\tau = t - t'$ and obtain

$$g(x, p, t) = g(x - pt, p, 0) + \int_0^t h(x - p\tau, p, t - \tau)\, d\tau.$$

5.2. *Appendix II: Evaluation of Higher-Order Terms in* λ

1) In accord with equations (2.2.9) and (2.4.1) we obtain

$$\left.\begin{aligned} \frac{\partial g_0^3}{\partial t} = \frac{1}{\mathscr{V}} \sum_{\substack{(2) \\ 2 \neq 1}} \frac{\partial}{\partial p_1} \int_x \frac{\partial V(x)}{\partial x} \int_0^t E(-p\tau) \frac{\partial V(x)}{\partial x} \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2}\right] \\ \cdot \int_0^{t-\tau} \frac{\partial V}{\partial x}(x - pt')\, dt'\, d\tau\, dx \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2}\right] g_1(p_1)\, g_2(p_2), \end{aligned}\right\} \qquad (5.2.1)$$

where $p = (p_1 - p_2)$ and the operator, $E(-p\tau)$, acts on everything to the right. Since this operator does not commute with the differential operator $[\partial/\partial p_1 - \partial/\partial p_2]$, it is easiest to carry through the latter operator and then apply $E(-p\tau)$. This yields

$$\frac{\partial g_0^3}{\partial t} = \frac{1}{\mathscr{V}} \sum_{\substack{(2) \\ 2 \neq 1}} \frac{\partial}{\partial p_1} [I_1(t, p)\, \Phi_1(t, p_1, p_2) - 2\, I_2(t, p)\, \Phi_2(t, p_1, p_2)], \qquad (5.2.2)$$

where

$$\left.\begin{aligned} \Phi_1(t, p_1, p_2) &= \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2}\right]^2 g_1(p_1)\, g_2(p_2) \\ \Phi_2(t, p_1, p_2) &= \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2}\right] g_1(p_1)\, g_2(p_2) \end{aligned}\right\} \qquad (5.2.3)$$

and

$$\left.\begin{aligned} I_1 &= \int_{x=-\infty}^{+\infty} \frac{\partial V(x)}{\partial x} \int_0^t \frac{\partial V}{\partial x}(x - p\tau) \int_0^{t-\tau} \frac{\partial V}{\partial x}[x - p(t' + \tau)]\, dt'\, d\tau\, dx \\ I_2 &= \int_{x=-\infty}^{+\infty} \frac{\partial V(x)}{\partial x} \int_0^t \frac{\partial V}{\partial x}(x - p\tau) \int_0^{t-\tau} t' \frac{\partial^2 V}{\partial x^2}[x - p(t' + \tau)]\, dt'\, d\tau\, dx. \end{aligned}\right\} \qquad (5.2.4)$$

2) It is easily seen that the first integral (I_1) is zero. Note, first, that for an arbitrary function $F(t', \tau)$

$$\int_0^t \int_0^{t-\tau} F(t', \tau)\, dt'\, d\tau = \int_0^t \int_0^{t-t'} F(t', \tau)\, dt'\, d\tau, \tag{5.2.5}$$

since the area covered is the same and the two integrals differ only in the way it is covered. In the integral I_1, change the integration variable x to $x' = x - p(t' + \tau)$ and we have

$$\left.\begin{aligned} I_1 &= \int_0^t \int_0^{t-\tau} \int_{x'=-\infty}^{+\infty} \frac{\partial V}{\partial x}[x' + p(t' + \tau)] \frac{\partial V}{\partial x}[x' + pt'] \frac{\partial V(x)}{\partial x}\, dx'\, dt'\, d\tau \\ &= \int_{x=-\infty}^{+\infty} \int_0^t \int_0^{t-\tau} \frac{\partial V(x)}{\partial x} \frac{\partial V}{\partial x}(x + p\tau) \frac{\partial V}{\partial x}[x + p(t' + \tau)]\, dt' d\tau\, dx, \end{aligned}\right\} \tag{5.2.6}$$

where the last integral has been obtained by applying equation (5.2.5), then interchanging the labels t' and τ and setting $x' = x$ because these are all dummy variables of integration. Adding equations (5.2.6) and (5.2.4) gives

$$\left.\begin{aligned} I_1 = \frac{1}{2} \int_{x=-\infty}^{+\infty} \int_0^t \int_0^{t-\tau} \frac{\partial V(x)}{\partial x} \Big\{ &\frac{\partial V}{\partial x}(x - p\tau) \frac{\partial V}{\partial x}[x - p(t' + \tau)] \\ &+ \frac{\partial V}{\partial x}(x + p\tau) \frac{\partial V}{\partial x}[x + p(t' + \tau)] \Big\}\, dt'\, d\tau\, dx. \end{aligned}\right\} \tag{5.2.7}$$

Note that $\partial V(x)/\partial x$ is an odd function, i. e., $\partial V(-x)/\partial x = -\partial V(x)/\partial x$; then it is immediately seen that the integral in (5.2.7) is an odd function of x and, hence,

$$I_1 = 0. \tag{5.2.8}$$

3) For the integral I_2, we first make an integration by parts for the variable t' and obtain

$$I_2 = -\frac{1}{p} \int_x \frac{\partial V(x)}{\partial x} \frac{\partial V}{\partial x}(x - pt) \int_0^t \frac{\partial V}{\partial x}(x - p\tau)\, (t - \tau)\, d\tau\, dx + \frac{1}{p} I_1(pt) \tag{5.2.9}$$

and $I_1 = 0$ according to (5.2.8). Define

$$\bar{V}(x) = \int_{-\infty}^{x} V(x')\, dx' - \alpha, \tag{5.2.10}$$

where α is a constant chosen so as to make $\bar{V}(x)$ an odd function if $V(x)$ is an even function. Subsequently, an integration by parts over τ gives

$$\left.\begin{aligned} I_2 &= \frac{t}{p^2}\int_x^{\bullet} \frac{\partial V(x)}{\partial x}\, V(x)\, \frac{\partial V}{\partial x}(x-pt)\, dx \\ &- \frac{1}{p^3}\int_x^{\bullet} \frac{\partial V(x)}{\partial x}\, \frac{\partial V}{\partial x}(x-pt)\, [\bar{V}(x-pt)-\bar{V}(x)]\, dx. \end{aligned}\right\} \quad (5.2.11)$$

The inclusion of α in the definition of $\bar{V}$ (5.2.10) is allowed by (5.2.11) because of the difference which occurs. If the two terms of the second integral in (5.2.11) are separated and the variable of integration changed to $x' = x - pt$ in the first of these terms, we obtain

$$I_2 = +\frac{t}{p^2} I_{21} + \frac{1}{p^3} I_{22}, \quad (5.2.12)$$

where

$$I_{21} = -\int_x^{\bullet} \frac{\partial V(x)}{\partial x}\, V(x) \frac{\partial V}{\partial x}(x-j)\, dx, \quad (5.2.13)$$

$$I_{22} = -\int_x^{\bullet} \frac{\partial V(x)}{\partial x}\, \bar{V}(x) \left[\frac{\partial V}{\partial x}(x+j) - \frac{\partial V}{\partial x}(x-j)\right] dx, \quad (5.2.14)$$

and

$$j = pt. \quad (5.2.15)$$

4) Even and Odd Character.

Changing x to $x' = -x$ in equation (5.2.13), using the even and odd properties of $V(x)$ and $\partial V/\partial x$, and noting that $\int_{-\infty}^{+\infty} = -\int_{+\infty}^{-\infty}$, we obtain I_{21} as above, but with $x-j$ replaced by $x+j$. Adding this to I_{21} in (5.2.13), we can write

$$I_{21}(j) = -\frac{1}{2}\int_x^{\bullet} \frac{\partial V(x)}{\partial x}\, V(x) \left[\frac{\partial V}{\partial x}(x-j) + \frac{\partial V}{\partial x}(x+j)\right] dx, \quad (5.2.16)$$

which is easily seen to be an even function of j; i. e.

$$I_{21}(-j) = I_{21}(j), \quad (5.2.17)$$

while, from (5.2.14), we have that I_{22} is an odd function of j:

$$I_{22}(-j) = -I_{22}(j). \quad (5.2.18)$$

5) The exact evaluation of I_{21} and I_{22} for a constant force over a range $-b$ to b is not difficult. We have

$$\left.\begin{aligned}
\frac{\partial V(x)}{\partial x} &= \begin{cases} \dfrac{-x}{|x|}\,a & 0 \leqslant |x| \leqslant b \\ 0 & b < |x| \end{cases} \\
V(x) &= \begin{cases} a(b-|x|) & 0 \leqslant |x| \leqslant b \\ 0 & b < |x| \end{cases} \\
\bar{V}(x) &= \begin{cases} \dfrac{x}{|x|}\dfrac{ab^2}{2} & b < |x| \\ \dfrac{a}{2}x\,[2b-|x|] & 0 \leqslant |x| \leqslant b \end{cases}
\end{aligned}\right\} \qquad (5.2.19)$$

where α has been chosen to be $\alpha = ab^2/2$ according to the definition (5.2.10). The integrations for I_{21} and I_{22} are easily carried out and one obtains

$$\left.\begin{aligned}
I_{21}(j) &= \begin{cases} +\dfrac{a^3}{2}(2b-|j|)^2 & b \leqslant |j| \leqslant 2b \\ +\dfrac{a^3}{2}\{2b^2-[2b-|j|]^2\} & 0 \leqslant |j| \leqslant b \\ 0 & 2b \leqslant |j| \end{cases} \\
I_{22}(j) &= \begin{cases} +\dfrac{a^3 j}{3}[3b^2-6b|j|+j^2] & 0 \leqslant |j| \leqslant b \\ +\dfrac{a^3 j}{3|j|}[2b-|j|]\,[b^2-4b|j|+j^2] & b \leqslant |j| \leqslant 2b \\ 0 & 2b \leqslant |j|\,. \end{cases}
\end{aligned}\right\} \qquad (5.2.20)$$

These functions are illustrated in figure 2.

6) To determine the meaning of I_2, we may consider reducing g_0^3 by integration over all p_i for $i \neq 1$. This requires the evaluation of the integral

$$I = \int_{p_2=-\infty}^{+\infty} I_2(p, t)\,\Phi_2(t, p_1, p_2)\,dp_2. \qquad (5.2.21)$$

The integration over p_2 is easily transferred to an integration over p, by

$$p = (p_1 - p_2) \qquad (5.2.22)$$

to give

$$I = \int_{p=-\infty}^{+\infty} I_2(p, t)\,\Phi_2(t, p_1, p)\,dp. \qquad (5.2.23)$$

Finally, we can transform to

$$j = pt \qquad (5.2.24)$$

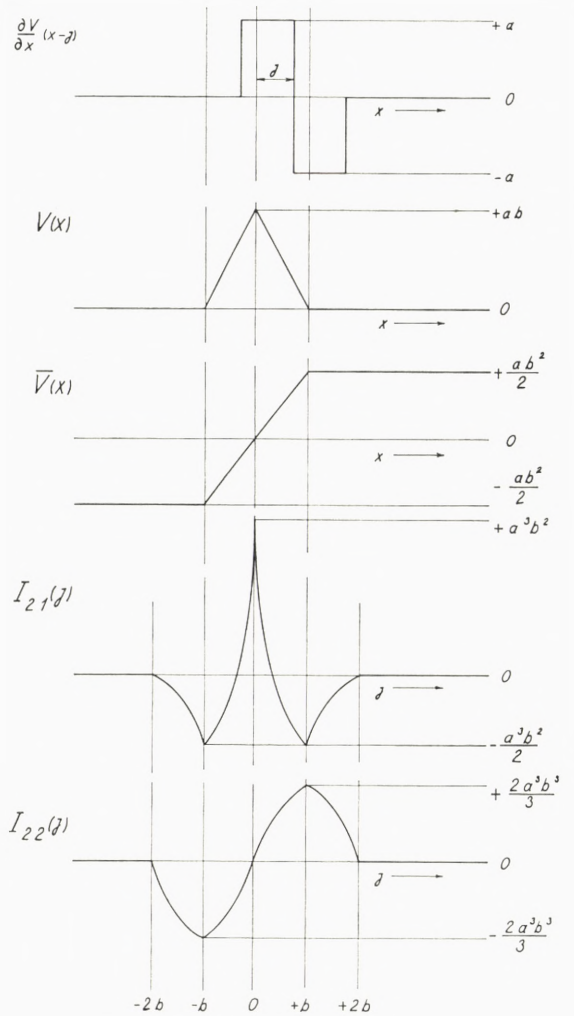

Figure 2: Illustration of the functions described by equations 5.2.19 and 5.2.20.

and have

$$I = \frac{1}{t} \int_{j=-\infty}^{+\infty} I_2\left(\frac{j}{t}, t\right) \Phi_2\left(t, p_1, \frac{j}{t}\right) dj. \tag{5.2.25}$$

Using the equation for I_2 (5.2.12), equation (5.2.24) becomes

$$I = t^2 \int_{-2b}^{+2b} \left[\frac{j I_{21}(j) + I_{22}(j)}{j^3}\right] \Phi_2\left(t, p_1, \frac{j}{t}\right) dj, \tag{5.2.26}$$

where we have noted that I_{21} and I_{22} are zero for $|j| > 2b$. The integral can now be broken into $\int_0^{2b} + \int_{-2b}^{0}$. Transforming $j \to -j$ in the second integral and using the even and odd properties of I_{21} and I_{22}, we obtain

$$I = t^2 \int_0^{2b} \left[\frac{j I_{21}(j) + I_{22}(j)}{j^3}\right] \left[\Phi_2\left(t, p_1, \frac{j}{t}\right) + \Phi_2\left(t, p_1, -\frac{j}{t}\right)\right] dj. \tag{5.2.27}$$

Finally, $\Phi_2\left(t, p_1, \frac{j}{t}\right)$ and $\Phi_2\left(t, p_1, -\frac{j}{t}\right)$ are expanded in a power series of j/t to yield

$$\left.\begin{aligned} I = t^2 \int_0^{2b} &\left[\frac{j I_{21}(j) + I_{22}(j)}{j^3}\right] \\ \cdot &\left[2\Phi_2(t, p_1, 0) + \left(\frac{j}{t}\right)^2 \Phi_2''(t, p_1, 0) + \frac{1}{2\cdot 3}\left(\frac{j}{t}\right)^4 \Phi_2^{\mathrm{IV}}(t, p_1, 0)\right] dj, \end{aligned}\right\} \tag{5.2.28}$$

where the primes (') on the Φ_2 denote derivatives with respect to p; i. e., $\Phi_2'' = (\partial^2/\partial p^2)\, \Phi_2(t, p_1, p)$. Using the values of I_{21} and I_{22} given by (5.2.20) it is easy to carry out the integrations in (5.2.28) and show that

$$\int_0^{2b} \left[\frac{j I_{21}(j) + I_{22}(j)}{j^3}\right] dj = 0, \tag{5.2.29}$$

while

$$\int_0^{2b} \left[\frac{j I_{21}(j) + I_{22}(j)}{j}\right] dj = \frac{2a^3 b^3}{3}(1 - ln\, 2). \tag{5.2.30}$$

For all other terms in the series of (5.2.28) (namely $\Phi_2^{(2n)}$), the integral over j is finite (there are no poles in the integrand for these terms) while the t dependence is of order $(1/t_2)^{n-1}$; and as t becomes large such that $2b/t \ll 1$, all other terms can be neglected so long as we make the reasonable assumption that $\Phi_2^{(2n)}(t, p_1, 0)$ remains bounded for all t and p_1.

Hence we have

$$I = \frac{2a^3 b^3}{3}(1 - ln\, 2)\, \Phi_2''(t, p_1, 0). \tag{5.2.31}$$

From the definition of Φ_2 we can therefore write

$$I_2 = \frac{2a^2 b^3}{3}(1 - ln\, 2)\, \delta(p_1 - p_2) \frac{\partial^2}{\partial p_2^2} \tag{5.2.32}$$

and thus

$$\left.\begin{aligned}\frac{\partial g_0^3}{\partial t} = &-\frac{\lambda^3 4 a^3 b^3}{3}(1-ln\,2)\sum\frac{\partial}{\partial p_i}\delta(p_i-p_j)\\ &\frac{\partial^2}{\partial p_j^2}\left[\frac{\partial}{\partial p_i}-\frac{\partial}{\partial p_j}\right]g_i(p_i)\,g_j(p_j).\end{aligned}\right\} \quad (5.2.33)$$

5.3. *Appendix III: Effects of Equilibrium Type Initial Conditions*

1) In this section, we calculate the equations for g_0 for a set of initial conditions in which the higher-order correlation functions g_l have a position dependence identical with the equilibrium distribution. Comparison with the expansion of the equilibrium distribution (eq. 2.3.2) shows that we must take

$$g_0^0(0) = g_0^0(0) \quad (5.3.1)$$

$$g_0^\nu = 0 \quad \text{for} \quad \nu > 0$$

$$g_1^\nu = 0 \quad \text{all} \quad \nu$$

$$g_2^0(0) = -g_0^0(0)\,V(x) \quad (5.3.2)$$

$$g_2^1 = g_0^0(0)\,V^2(x), \quad \text{etc.,} \quad (5.3.3)$$

$$\text{for all higher orders } g_2 \text{ and } g_1. \quad (5.3.4)$$

In section 5.3 we have developed the terms which arise from the initial conditions (5.3.1) and it is only necessary to add to those terms the one arising from the non-zero initial conditions (5.3.2), (5.3.3), and (5.3.4). To simplify the notation we shall let brackets [ ] represent all the terms previously calculated, where the number inside the brackets indicates the particular equation giving the value of these terms. Furthermore, we shall immediately replace $g_0^0(0)$ by $g_0(t)$ which is justified by selecting and summing various terms in higher powers of λ in the same manner as developed in sections 2.5 to 2.7.

2) Using equation (2.2.9) we obtain

$$g_2^0 = -V(x-pt)\,g_0^0(t) + [2.4.8] \quad (5.3.5)$$

which gives rise to

$$\frac{\partial g_0(t)}{\partial t} = -\frac{\lambda^2}{\mathscr{V}}\sum_{ij}\frac{\partial}{\partial p_i}\int_0\frac{\partial V(x)}{\partial x}\,V(x-pt')\,dt'\,dx\,g_0(t) + [2.4.10] \quad \text{to order} \quad (\lambda^2)^n.$$

In the limit of $t \to \infty$, this term vanishes so that we are again left with our previous result (eq. 2.4.10).

3) However, if we now calculate the contribution to $\partial g_0^3/dt$, we obtain

$$\left.\begin{aligned}\frac{\partial g_0^3}{\partial t} = \sum_{\substack{ij\\ i\neq j}} \frac{1}{\mathscr{V}} \Bigg\{ \frac{\partial}{\partial p_i} \int_x^{\bullet} \frac{\partial V(x)}{\partial x} \int_0^t V^2(x-pt')\, dt'\, dx \\ - \frac{\partial}{\partial p_i} \int_x^{\bullet} \frac{\partial V(x)}{\partial x} \int_0^t E(-p\tau) \frac{\partial V(x)}{\partial x} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] V[x-p(t-\tau)]\, d\tau\, dx \Bigg\} g_0 \\ + [5.2.33]\, g_0 .\end{aligned}\right\} \tag{5.3.7}$$

Here again the first term in the $\{\ \}$ vanishes for $t \to \infty$, and it is the second term which is of interest.

Carrying through the operator $[\partial/\partial p_i - \partial/\partial p_j]$, equation (5.3.7) becomes

$$\frac{\partial g_3^0}{\partial t} = \sum_{ij} \frac{1}{\mathscr{V}} \left\{ \frac{\partial}{\partial p_i} (-) I_{31} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] g_0 + 2 \frac{\partial}{\partial p_j} I_{32}\, g_0 \right\} + [5.2.33], \tag{5.3.8}$$

where

$$I_{31} = \int_x^{\bullet} \frac{\partial V(x)}{\partial x} \int_0^t \frac{\partial V}{\partial x}(x-p\tau)\, V(x-p\tau)\, d\tau\, dx \tag{5.3.9}$$

and

$$I_{32} = \int_x^{\bullet} \frac{\partial V(x)}{\partial x} \int_0^t \frac{\partial V}{\partial x}(x-p\tau)\, [t-\tau] \frac{\partial V}{\partial x}(x-pt)\, d\tau\, dx . \tag{5.3.10}$$

4) A comparison of I_{32} with I_2 (eq. 5.2.9), Appendix II, shows

$$I_{32} = -pI_2 = -\frac{t}{p} I_{21} - \frac{1}{p^2} I_{22} \tag{5.3.11}$$

from equation (5.2.12). Proceeding as in section 5.2, we find that

$$\lim_{t\to\infty} \int_{-\infty}^{+\infty} I_{32}(p_1, t)\, \Phi(t, p_1, p)\, dp = -\frac{4a^3b^3}{3} (1 - ln\, 2)\, \Phi'(t, p_1, 0) \tag{5.3.12}$$

so that we can write

$$I_{32} = +\frac{4a^3b^3}{3} (1 - ln\, 2)\, \delta(p_1 - p_2) \frac{\partial}{\partial p} . \tag{5.3.13}$$

5) The integral I_{31} is easily reduced to

$$I_{31} = \frac{1}{4p} \int V_{(x)}^2 \left[\frac{\partial V}{\partial x}(x-j) - \frac{\partial V}{\partial x}(x+j)\right] dx \tag{5.3.14}$$

and integration over x gives

$$I_{31} - \frac{1}{2p}(-)\begin{cases} 0 & \text{for} \quad 2b \leqslant |j| \\ \frac{a^3}{3}\frac{j}{|j|}[2b - |j|]^3 & b \leqslant |j| \leqslant 2b \\ \frac{a^3}{3} j [6b(b - |j|) + j^2] & 0 \leqslant |j| \leqslant b. \end{cases} \tag{5.3.15}$$

Finally,

$$\lim_{t \to \infty} \int_{+\infty}^{-\infty} I_{31}(p, t)\, \Phi(p)\, dp = \frac{8 a^3 b^3}{3} ln\, 2\, \Phi(0) \tag{5.3.16}$$

so we can write

$$I_{31} = \frac{8 a^3 b^3}{3} ln\, 2\, \delta(p_1 - p_2). \tag{5.3.17}$$

6) Equation (5.3.8) can then be written as

$$\begin{aligned} \frac{\partial g_0^3}{\partial t} = \frac{1}{\mathscr{V}} \sum_{ij}' \frac{\partial}{\partial p_i} \Bigg\{ & -\frac{8 a^3 b^3}{3} ln\, 2\, \delta(p_1 - p_2) \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2}\right] \\ & + \frac{8 a^3 b^3}{3} (1 - ln\, 2)\, \delta(p_1 - p_2) \frac{\partial}{\partial p_2} \\ & - \frac{4 a^3 b^3}{3} (1 - ln\, 2)\, \delta(p_1 - p_2) \frac{\partial^2}{\partial p_2^2} \left[\frac{\partial}{\partial p_1} - \frac{\partial}{\partial p_2}\right] \Bigg\} g_0^0. \end{aligned} \tag{5.3.18}$$

If we further assume that g_0^0 is factorized, i. e.,

$$g_0^0 = \prod_i {}^{(i)}g(p_i) \tag{5.3.19}$$

such that

$$\int {}^{(i)}g(p_i)\, dp_i = 1, \tag{5.3.20}$$

we obtain

$$\begin{aligned} \frac{\partial\, {}^{(i)}g^3}{\partial t} = \frac{1}{\mathscr{V}} \sum_{ij}' \frac{\partial}{\partial p_i} \Bigg\{ & -\frac{8 a^3 b^3}{3} ln\, 2 \int \delta(p_i - p_j) \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] {}^{(i)}g^0\, {}^{(j)}g^0\, dp_j \\ & + \frac{8 a^3 b^3}{3} (1 - ln\, 2) \int \delta(p_i - p_j) \frac{\partial}{\partial p_j}\, {}^{(i)}g^0\, {}^{(j)}g^0\, dp_j \\ & - \frac{4 a^3 b^3}{3} (1 - ln\, 2) \int \delta(p_i - p_j) \frac{\partial^2}{\partial p_j^2} \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j}\right] {}^{(i)}g^0\, {}^{(j)}g^0\, dp_j \Bigg\}. \end{aligned} \tag{5.3.21}$$

Finally, if we assume that *all* particles were at equilibrium initially, we have

$${}^{(i)}g^0(p_i) = C \exp\left[-\frac{p_i^2}{2}\right] = {}^{(i)}g_{\text{eq}} \quad \text{for all} \quad i. \tag{5.3.22}$$

Inserting this in equation (5.3.21), we find that the first term on the right is zero while the second and third terms give

$$\frac{\partial g^3}{\partial t} = \frac{N}{\mathscr{V}^\circ}\frac{\partial}{\partial p_i}\left\{\frac{8\,a^3b^3}{3}(1-ln\,2)\,[-p_1]-\frac{4\,a^3b^3}{3}(1-ln\,2)\,[-2\,p_1]\right\}{}^{(i)}g_{\mathrm{eq}}\,{}^{(j)}g_{\mathrm{eq}} = 0\,. \qquad (5.3.23)$$

5.4. *Appendix IV: Identity of the Master equations*

1) In this section a proof is given to demonstrate that the master equation obtained by PRIGOGINE and the master equation (2.7.6) presented here are in fact identical. For a problem in one dimension, the master equation is given by PRIGOGINE as

$$\frac{\partial g^0}{\partial t} = \lambda^2 \sum_{ij}{}' \int dk\,|\,V_k\,|^2 k\left(\frac{\partial}{\partial p_i}-\frac{\partial}{\partial p_j}\right)\delta_-\,[k(p_i-p_j)]\,k\left(\frac{\partial}{\partial p_i}-\frac{\partial}{\partial p_j}\right)g_0\,(p,\,t), \qquad (5.4.1)$$

where

$$V_k = \lim_{\mathscr{V}^\circ\to\infty}\frac{1}{\mathscr{V}^{\circ 1/2}}\int e^{-ikx}\,V(x)\,dx \qquad (5.4.2)$$

and $\mathscr{V}^\circ$ is the volume.

From the definition of V_k, we readily obtain

$$\frac{1}{\mathscr{V}^{\circ 1/2}}\int e^{-ikx}\frac{\partial V(x)}{\partial x}\,dx = +\frac{ik}{\mathscr{V}^{\circ 1/2}}\int e^{-ikx}\,V(x)\,dx = \frac{ik}{\mathscr{V}^{\circ 1/2}}\,V_k \qquad (5.4.3)$$

and, hence,

$$k^2\,|\,V_k\,|^2 = \frac{1}{\mathscr{V}^\circ}\int e^{-ikx}\frac{\partial V(x)}{\partial x}\,dx\int e^{+ikx'}\frac{\partial V(x')}{\partial x'}\,dx'. \qquad (5.4.4)$$

From its definition we may set

$$\delta_-\,[k(p_i-p_j)] = \int_0^\infty e^{+\,ik\,(p_i-p_j)\,t'}\,dt'. \qquad (5.4.5)$$

Inserting equations (5.4.4) and (5.4.5) in (5.4.1), we obtain

$$\left.\begin{aligned}\frac{\partial g_0\,[\{p_i\},\,t]}{\partial t} = \frac{\lambda^2}{\mathscr{V}^\circ}\sum_{i<j}{}'\left(\frac{\partial}{\partial p_i}-\frac{\partial}{\partial p_j}\right)\int_{t=0}^{\infty}\int_{x'}\int_{x}\int_{k=-\infty}^{+\infty}dk\,e^{-ik\,(x-x'-pt')}\\ \cdot\frac{\partial V(x)}{\partial x}\,\frac{\partial V(x')}{\partial x'}\,dx\,dx'\,dt'\left(\frac{\partial}{\partial p_i}-\frac{\partial}{\partial p_j}\right)g_0(\{p_i\},\,t).\end{aligned}\right\} \qquad (5.4.6)$$

This equation is found in reference (11) as equation (1.14), page 557. As shown by PRIGOGINE (5), the $\pi\delta(kp)$ which occurs there should be corrected to read $\delta_-(kp)$.

Performing the integration over k gives

$$\left.\begin{aligned}\frac{\partial g_0}{\partial t} &= \frac{\lambda^2}{\mathscr{V}} \sum_{ij=1}^{N}{}' \frac{\partial}{\partial p_i} \int_x \int_{x'} \int_{t=0}^{\infty} \delta(x - x' - pt) \\ &\cdot \frac{\partial V(x)}{\partial x} \frac{\partial V(x')}{\partial x} \, dx \, dx' \, dt' \left(\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right) g_0(\{p_i\}, t),\end{aligned}\right\} \tag{5.4.7}$$

where we have noted that

$$\left.\begin{aligned}\sum_{i<j}{}' \left(\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right) \left(\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right) &= 1/2 \sum_{ij=1}^{N}{}' \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right] \left[\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right] \\ &= 1/2 \left[\sum_{ij=1}^{N}{}' \frac{\partial}{\partial p_i} \left(\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right) - \sum_{ij=1}^{N}{}' \frac{\partial}{\partial p_j} \left(\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right) \right] \\ &= \sum_{ij=1}^{N}{}' \frac{\partial}{\partial p_i} \left(\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right).\end{aligned}\right\} \tag{5.4.8}$$

Finally, integrating equation (5.4.7) over x' yields

$$\frac{\partial g_0}{\partial t} = \frac{\lambda^2}{\mathscr{V}} \sum_{ij=1}^{N}{}' \frac{\partial}{\partial p_i} \int_x \int_{t=0}^{\infty} \frac{\partial V(x)}{\partial x} \frac{\partial V}{\partial x}(x - pt') \, dx \, dt' \cdot \left(\frac{\partial}{\partial p_i} - \frac{\partial}{\partial p_j} \right) g_0(\{p_i\}, t) \tag{5.4.9}$$

which is identical with equation (2.7.6).

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TWO-QUASI-PARTICLE STATES IN EVEN-MASS NUCLEI WITH DEFORMED EQUILIBRIUM SHAPE

BY

C. J. GALLAGHER, JR., AND V. G. SOLOVIEV

København 1962
i kommission hos Ejnar Munksgaard

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Synopsis

The energy levels in even-even nuclei and the beta transition rates between even-even and odd-odd nuclei in the $150 < A < 190$ region are analyzed. The excitations in these nuclei are describable as rotational states based upon intrinsic states. With the exception of systematically occurring excited $2+$ states in even-even nuclei, it is shown that the intrinsic states are describable as two-particle excitations, if the Nilsson wave functions are used to characterize the single-particle states. The level energies and beta transition rates are compared with theoretical values which take into account the effect of pairing correlations. The pairing correlations are evaluated with inclusion of "blocking" as described in a previous paper by one of the authors (Mat. Fys. Skr. Dan. Vid. Selsk. **1**, 11 (1961)).

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I. INTRODUCTION

Within the last few years significant theoretical clarification of the coupling schemes applying to the low lying states of nuclei has taken place[1,2,3,4].

In the mass region $150 < A < 190$, where the strong coupling model of BOHR and MOTTELSON is a useful description of the nuclear system[4], an extensive classification of the properties of intrinsic nuclear states has been made possible through the introduction by NILSSON of single-particle states calculated for a deformed potential well[5]. In the compilation of MOTTELSON and NILSSON it has been clearly demonstrated that many of the properties of the intrinsic levels of odd-mass nuclei in this region can be described by these wave functions[6]. The ground states of odd-odd nuclei in this region are now known to be simple proton-neutron systems in which the last odd proton and odd neutron are usually the Nilsson states appropriate for the Z and N in question, coupled in such a way that the particle intrinsic spins couple parallel[7]*. Finally, on the basis of an analysis of beta decay rates from deformed odd-odd nuclei using simple two-particle Nilsson wave functions and single-particle operators, it has been pointed out that there exist some experimental data which indicate that the excited levels of deformed even-even nuclei may also be describable simply as two-particle Nilsson proton or neutron states strongly coupled to the deformed core[8].

We can summarize these results for deformed odd-odd and odd-mass nuclei by the statement that the experimental data indicate that, at least at low excitation energies, unpaired particles in these nuclei, while being strongly coupled to the deformed core, apparently interact only weakly, if at all, with each other. The extent to which this is also true in the excited states of even-even nuclei has until now not been determined.

A salient feature of the excitation spectra of all deformed even-even nuclei observed to date, and one which has not been explained by the above-mentioned

* In some cases, the experimental data indicate that configurations other than the last odd-proton odd-neutron state are the lowest. The extent to which this competition between different configurations occurs is not known experimentally at present. However, even where the observed proton-neutron configurations differ from those expected, the lowest lying state is that in which the intrinsic particle spins are coupled parallel.

models, is that an energy gap of approximately 1 Mev is observed between the ground and first-excited intrinsic states. BOHR, MOTTELSON, and PINES pointed out that this gap might arise, in analogy to the energy gap in super-conductors, from correlations between coupled particle pairs in the core[9]. Detailed mathematical studies of this problem show that a general feature of the excitation spectra of even-even nuclei based on pairing correlation calculations is the occurrence of an energy gap, the exact energy of this gap depending on the more detailed assumptions within the theory[10,11]. We will discuss some of these studies in more detail in Section II. However, in a nuclear model including pairing correlations developed by one of us (VGS), which should be valid for deformed nuclei, certain mathematical difficulties inherent in earlier approaches are avoided. The independence of the quasi-particle excitations in both the odd- and even-mass nuclei, an effect which we noted as an empirical fact above, is also contained quite naturally in this model[12]. In addition, the energy spectra and beta decay transition rates in these nuclei can be calculated on the basis of the model. These features will also be discussed in more detail in Section II.

The level spectra of deformed even-even nuclei are particularly good cases for testing this model, because all the parameters necessary for the calculation of even-even spectra can be adjusted using the experimental data on the levels of odd-mass nuclei and pairing energies from experimental mass tables. Unfortunately, from the point of view of making such a test, the amount of experimental data available on the intrinsic levels of deformed even-even nuclei is at present small. Furthermore, although some evidence has been presented suggesting the presence of two-particle excitations in even-even nuclei[8], a detailed analysis of the existing data which demonstrates that the body of experimental data supports such an interpretation has not yet been presented.

The present paper has therefore been prepared with a twofold purpose in mind. It is an attempt, first of all, to analyze the existing experimental data on the intrinsic levels of deformed even-even nuclei in the $150 < A < 190$ mass region in order to determine whether they can be explained as simple two-particle-like excitations, and secondly, to compare the observed spectra with those calculated on the basis of a specific nuclear model including pairing correlations, with the hope that the comparison will provide a means of determining the degree of validity of the model and hence serve to guide further developments.

In carrying out this comparison, we have borne in mind that many data exist on excitations in even-even nuclei, which, because of their measured transition probabilities and energies, have come to be interpreted as being collective in nature. These excitations, for which no provision has been made in the present model, have been widely discussed in the literature and have been interpreted qualitatively as collective nuclear vibrations[13,14], and much progress has been made in accounting for them in a quantitative way[15]. By defining the intrinsic excitations in the nuclei where these excitations occur we hope that a clearer definition of the collective states will emerge, especially with respect to intrinsic excitations of the same spin and parity.

In Section II the general features of the model are discussed. Section III contains the presentation of the experimental data and their analyses. In Section IV we discuss the data and present the conclusions that we believe can be drawn on the basis of the analysis.

II. THEORETICAL

A. General Features of Pairing Correlations Applied to Deformed Nuclei

Investigations of nucleon pairing correlations in heavy nuclei provide an explanation of those nuclear properties which could not be accounted for within the framework of the independent-particle model, particularly the moments of inertia of deformed nuclei and the gap in the excited spectra of even-even nuclei[10,11,16,17]. These investigations have shown that the residual short-range forces between nucleons are attractive, and the ground state of any nucleus is the superfluid state, that is, the state in which the amplitude of the last few pairs is spread over several levels. This state is energetically more favourable than that with successively filled levels of the average field in the independent-particle model.

In the present paper, we attempt to compare some of the observed properties of strongly deformed even-mass nuclei with the results calculated on the basis of a model which applies pairing correlations to nuclei with a deformed core.

This model, in addition to including the average field of the independent-particle model, also includes the short range part of nucleon-nucleon interactions which lead to pairing correlations. These residual interactions between nucleons are described by the Bardeen-type Hamiltonian. The main equations of the problem have been found with the aid of the variational principle and are given in ref. 18.

Basically, the present model is a model of independent quasi-particles. However, in addition, we take into account in a systematic way the influence of unpaired particles on the superfluid properties of the system, i. e., the blocking effect which is important in the case of deformed nuclei.

B. Comparison with Earlier Results

The most important differences between the basic assumptions of the present model and those of previous investigations of the effect of pairing correlations[10,11] are:

a) it takes into account the influence of quasi-particles on the superfluid properties of the nucleus, i. e., the blocking effect, and therefore differences exist between the properties of the ground and excited states in the different models;

b) in it the number of particles is on the average equal to the true number of particles in the nucleus for both the ground and excited states.

The concept of independent quasi-particles inherent in the present model seems to find some justification in experimental data. Thus, the clear correspondence between the levels predicted by the Nilsson diagram and the observed level spectra in odd-A nuclei in the region of deformed nuclei seems to indicate that the Nilsson states are good representations of independent quasi-particles. The two-Nilsson-particle interpretation of the energy levels of deformed even-mass nuclei, which has been used by one of us (CJG) to analyze the beta-decay rates of deformed odd-odd nuclei and the levels of deformed even-even nuclei, is also essentially an independent quasi-particle model.

It should be noted at this point that the ideas discussed here for the $150 < A < 190$ mass region should be equally valid in other mass regions in which the nuclear core is deformed.

C. Calculations

In the present paper, we present the results of calculations of the spectra of two-quasi-particle states in even-even nuclei and corrections to beta-decay transition rates arising from nuclear superfluidity.

The main assumptions underlying the detailed calculation of the spectra of two-quasi-particle levels in even-even nuclei and the magnitudes of beta decay log ft's discussed below are formulated in order to exclude as much as possible the ambiguity and inaccuracy associated with the poor knowledge of the levels and wave functions of the average field. Thus, instead of attempting to calculate the even-even spectra and log ft's directly from the wave functions and energies as given by Nilsson, the Nilsson potential was first adjusted to give the best possible fit with the observed odd-A level spectra and experimental pairing energies, and then the calculations were carried out using the adjusted values.

1. *Energy Levels of Deformed Even-Even Nuclei*

We have investigated the properties of the strongly deformed nuclei in the region $150 < A < 190$. The nuclei under consideration were divided into three groups: the first group with $156 \leqslant A \leqslant 174$ ($64 \leqslant Z \leqslant 70$; $92 \leqslant N \leqslant 104$), the second group with $174 < A \leqslant 186$ ($70 < Z \leqslant 74$; $104 < N \leqslant 112$). The nuclei with $A = 152$ and 154, and the levels in the even-even osmium isotopes and W^{184} and W^{186} make up the third group. At the mass numbers where these nuclei occur the deformations are changing rapidly; hence, although they should probably be considered as strongly deformed nuclei, a reasonably correct calculation would require detailed consideration of each nucleus separately. Because such detailed calculations are not in the spirit of the present paper, no calculations have been made for these nuclei.

For the first two groups one set of the single-particle levels of the average field and one pairing interaction constant for both the proton and neutron systems were

TABLE I 1. *Single-particle energy levels.*

Neutron system				Proton system			
N	Assigned orbital	Energy ($\hbar\mathring{w}_0$) I	II	Z	Assigned orbital	Energy ($\hbar\mathring{w}_0$) I	II
93	$3/2-[521\uparrow]$	0	0	63	$5/2+[413\downarrow]$	0	0
95	$5/2+[642\uparrow]$	0.04	0.04	65	$3/2+[411\uparrow]$	0.04	0.04
97	$5/2-[523\downarrow]$	0.07	0.07	67	$7/2-[523\uparrow]$	0.12	0.12
99	$7/2+[633\uparrow]$	0.22	0.22	69	$1/2+[411\downarrow]$	0.20	0.20
101	$1/2-[521\downarrow]$	0.24	0.24	71	$9/2-[514\uparrow]$	0.42	0.30
103	$5/2-[512\uparrow]$	0.29	0.29	73	$7/2+[404\downarrow]$	0.31	0.31
105	$7/2-[514\downarrow]$	0.41	0.33	75	$5/2+[402\uparrow]$	0.36	0.43
107	$9/2+[624\uparrow]$	0.48	0.41	77	$1/2+[400\uparrow]$	0.52	0.52
109	$1/2-[510\uparrow]$	–	0.48				
111	$3/2-[512\downarrow]$	–	0.55				
113	$7/2-[503\uparrow]$	–	0.59				

However, it should be noted that inherent in the present approach is the possibility of investigating the change of the average field in passing from one nucleus to another, as well as investigating the importance of other factors which were not taken into account in the present calculation, above all the interactions of quasiparticles.

The calculations of the basic superfluid properties of the ground and two-quasi-particle excited states were carried out on an electronic computer, using the values of the pairing interactions G_N and G_Z and the schemes of single-particle levels given in Table II 1. The absolute values of the excitation energies of the two-quasiparticle states are calculated on the average with an accuracy of $\approx 10\,\%$, but sometimes are probably not more accurate than $20\,\%$. The calculated energy spectra for the individual even-even nuclei are written down in Section III in the second table for each mass number.

2. *Beta Decay*

a) *Selection Rules for Beta Decay.* Selection rules for single-particle transitions in even-mass nuclei based on ALAGA's selection rules for odd-mass nuclei have been given in ref. 8. The main difference between the even- and odd-mass systems was therein shown to be the possibility of A-forbiddenness in even-mass nuclei. An additional classification of beta transitions within the framework of the present model was formulated in ref. 19, where its importance from the point of view of the properties of the nuclear superfluid is discussed. This classification is based on the change in the number of quasiparticles during a beta transition, viz., all beta transitions were divided into three groups:

chosen, which gave the best agreement with the single-particle spectra of the odd nuclei and the pairing energies. In Table II 1 are indicated the relative energies of some of the most important levels for the first and second groups of nuclei. Note that the behaviour of some levels of the first group is different from that of the corresponding levels of the second group, which is not unreasonable because of the different deformations necessary to reproduce the observed odd-A spectra.

In this calculation, in order to correct for the observed variation of pairing energies from nucleus to nucleus, a rather rough averaging has been made. After the parameters of the Nilsson potential had been adjusted to give the best fit, we obtained for the whole region $156 \leqslant A \leqslant 188$ the following values of the pairing interaction constant:

$$G_N = 26/A \text{ MeV}; \quad G_Z = 28/A \text{ MeV}. \tag{1}$$

The calculations, when carried out using the accepted scheme of the average field single-particle levels and by the chosen values of G, lead, as shown in ref. 18, to a fairly acceptable description of the behaviour of the single-particle levels of the odd-A nuclei.

An exception is the change in the sequence of the $7/2+[404\downarrow]$ and $9/2-[514\uparrow]$ proton levels, and the change in the spin of the ground state of the odd-N nuclei when $N = 95$. When $N = 95$ the scheme used fails to give correct values for the spin of the ground state of some odd nuclei. Therefore, for the case with $N = 91$, we substituted the level $11/2-[505\uparrow]$ in place of the level $5/2-[503\downarrow]$ which, with the other two levels, drops down a place. We expect this will only affect the neutron levels in *Gd*.

We point out here that, for the given system of levels of the average field and for the G_N and G_Z of fixed magnitude, the calculations based on the present model are entirely unambiguous. That is, because only one configuration of the single-particle levels is used for calculating the properties of a group of nuclei, the results of the calculation cannot be interpreted as a "fitting" of the calculated spectra to the corresponding experimental data. Furthermore, no new parameters have been introduced for the calculation of the properties of the even-even nuclei. Therefore, a comparison of the calculated properties of even-even nuclei with the experimental data is very important from the point of view of verifying whether the present model gives a valid approximation to the effective forces in these nuclei.

A calculation using only two sets of the average field levels and only two values of G for a large group of nuclei is a rather rough approximation, as the behaviour of the average field levels, the equilibrium deformations, and the pairing energies change noticeably. This approximation is made first of all to exclude any arbitrariness in calculating the spectra of even-even nuclei, and secondly to allow comparison of the log ft's in even-A nuclei to those in odd-A nuclei. A third, more practical, reason for so few adjustments is that, although there are relatively few single-particle levels in odd-A nuclei, relatively little is known about them, and the available experimental data did not indicate the necessity of forming more than two groups.

$$\begin{array}{lll} \text{I.} & R(G=0)=1 & 0<R(G\neq 0)<1 \\ \text{II.} & R(G=0)=0 & 0<R(G\neq 0)<1 \\ \text{III.} & R(G=0)=0 & R(G\neq 0)=0. \end{array}$$

The first and second groups contain those beta decays in which only one quasi-particle in the proton (neutron) systems disappears or appears and the configuration of the remaining particles is left unaltered. These are essentially the cases considered in ref. 8. In the third group, which is totally forbidden on the basis of the present model and denoted in the classification of beta transitions by F, are included

a) transitions in which, besides the change in the number of quasi-particles by one, the configuration of other quasi-particles changes (the "non-overlap" forbiddenness of ref. 8);

b) transitions in which the number of quasi-particles of the proton (neutron) system changes by more than one.

Transitions of this latter group imply quasi-particle interactions which are not included in the present independent quasi-particle model and are therefore a powerful means of testing the validity of this important assumption of the model.

b) *Corrections to Beta Decay Transition Rates Arising from Nuclear Superfluidity.* As has been mentioned previously, the effect of the pairing correlation is to spread the amplitude of the last few pairs over a number of states. This distribution will differ if the proton or neutron core in question contains an even or odd number of particles. Thus, for example, a beta transition which changes an odd-neutron core plus an odd-proton core into an even-neutron core plus an even-proton core will involve considerable rearrangement of the many-body system. The effects of these changes on the single-particle transition rate can be calculated on the basis of the present model. As is shown in ref. 20, the superfluid corrections $R = R_Z R_N$ to the beta transition probabilities can be important. (In the present discussion, the notation of ref. 20 is used). Values of $\log (ft)_c$ for even-even nuclei were calculated using experimental data and superfluid corrections determined for the same single-particle beta transitions in odd-A nuclei. The matrix elements were determined from the odd-particle transitions indicated, and the values of the $\log (ft)_c$ listed for the even-mass nuclei were calculated assuming these matrix elements and the superfluid corrections calculated on the basis of the model. The comparison of the beta transition probabilities is valid only when the transition is a non-A-forbidden transition of group I or II, in which ΔI is the same in the odd- and even-mass nucleus. We have also calculated $\log [(ft)_e R_\eta]$ which is designed to improve the relative agreement of transitions in even-mass nuclei by correcting the experimental $\log (ft)_e$ for the superfluid (R) and statistical (η) factors.

3. *Other Physical Properties*

Within the framework of the present model it is also possible to consider gamma-ray transitions, magnetic moments, and moments of inertia. Superfluid corrections to gamma-ray transition probabilities are complicated, and together with the fluctuations in gamma-ray transition rates arising from small variations of the nuclear wave functions their role is not at present clear. To the extent that two quasi-particle states are approximated by two Nilsson particles the Nilsson wave functions should be useful for calculating their magnetic moments. Expressions for the magnetic moments of deformed odd-odd nuclei have been given previously[6,7,21] and satisfactory agreement between the observed and calculated moments has been found. The calculation of moments of inertia for the ground states of even-even nuclei has been the subject of several recent papers, and the extension of these calculations to two-quasi-particle excitations in even-even nuclei promises to be a formidable task. In the present paper we shall not attempt a further discussion of these topics.

Several features, especially quasi-particle interactions and other residual interactions, cannot be investigated within the framework of the present model without the addition of perturbation terms in the Hamiltonian. For example, the spin-dependent forces which might be expected to remove the degeneracy of the $\Omega_1 \pm \Omega_2$ doublets in the excited states of even-even nuclei, in analogy to the spin splitting observed in odd-odd nuclei, are not included. At present, however, the role of these interactions is not clear, and we hope that the present investigation will help to clarify it.

As was mentioned in the Introduction, no provision for collective vibrations has been made in the present model. However, the important role of such excitations is experimentally established, and in cases where definite disagreement between calculated and observed energies occurs for states with $K\pi = 0\pm$, and $K\pi = 2+$ we have tended to assign the states as collective in the interpretation. In these cases, we have in general also included the most probable alternative two-quasi-particle interpretation of the states.

III. INTERPRETATION OF THE OBSERVED LEVEL SPECTRA

A. Summary of Parameters Used in Discussing the Spectra of Non-Spherical Even-Mass Nuclei

The analysis of even-even spectra attempted in the present paper is based primarily on the idea that the energy levels of deformed nuclei can be divided into rotational and intrinsic states, because the introduction of pairing correlations into the discussion of the intrinsic structure does not change this description. We will therefore follow rather closely the format used by Mottelson and Nilsson in their extensive analysis of the levels in deformed odd-mass nuclei. Thus, before beginning a discussion of the analysis, we shall briefly review some of the relevant parameters.

1. *Coupling Scheme*

A vector representation of the strong coupling scheme of BOHR and MOTTELSON is shown in Fig. 1. The nomenclature is discussed in the caption. For the case in which $K = \Omega = \Lambda + \Sigma$ for the intrinsic state (the asymptotic limit approximation), the doubly degenerate states of the two-particle system can be represented as states in which the intrinsic spins are aligned parallel or antiparallel. For these states we adopt

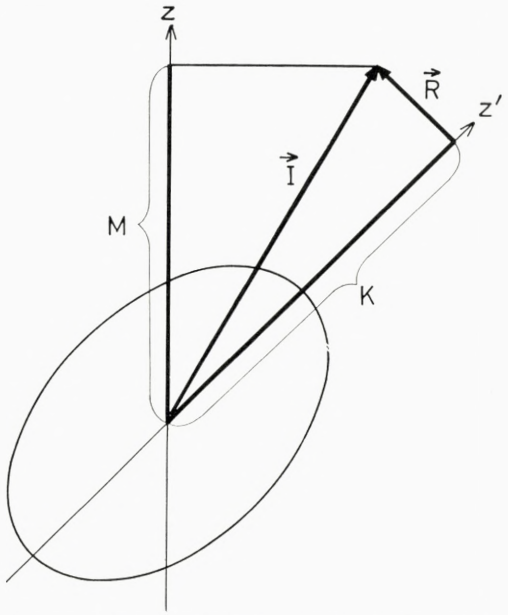

Fig. 1. *Angular momentum coupling scheme for deformed nuclei.* The total angular momentum, I, has the component M along the fixed z-axis and the component K along the nuclear symmetry axis, z'. The collective rotational angular momentum, R, is perpendicular to the nuclear symmetry axis; thus, K is entirely a property of the intrinsic motion.

the shorthand notation $\Sigma = 1$ and $\Sigma = 0$, respectively. In odd-odd nuclei the $\Sigma = 1$ states are lower in energy. At this time no clear-cut exception to this rule is known, and hence it has been used as a guide in assigning odd-odd configurations when the experimental data do not permit a definite assignment.

2. *Rotational Bands*

The energy of a rotational state of spin I in an even-mass nucleus is given by the relationship

$$E_I = E_0 + \frac{\hbar^2}{2\Im} I(I+1),$$

where E_0 is the zero point energy.

The level sequence for levels with $K \neq 0$ is $I, I+1, I+2$, etc. For $K = 0$ three cases occur. $K = 0+$ levels with paired particle configurations have a level sequence $0+$, $2+$, $4+$, etc. Experimentally, $K\pi = 0-$ bands have been found in elements with $A > 220$, which have a spin sequence 1, 3, 5 etc., with no even-spin bands observed as yet[22]. Two-quasi-particle levels with $K = 0$ have rotational bands with both odd and even spin states, but the odd and even bands may be displaced depending on the properties of the intrinsic configuration[8, 23, 24, 25].

The moment of inertia $\Im$ appearing in the expression for the energy has been considered elsewhere in detail for the ground-state rotational band[16, 17], but moments of inertia of two-quasi-particle states have not as yet been calculated, and we will therefore not attempt a discussion of them.

Associated with the rotational bands are selection and intensity rules which depend on the quantum number K discussed in the caption of Fig. 1. These rules have been given previously[26]. In particular, however, transitions of order λ between states in which

$$\lambda < | K_f - K_i |$$

are formally K-forbidden, although they may be allowed by selection rules which depend only on the spin change ΔI and parity change. In addition, as a result of the K quantum number, intensity rules between states of rotational bands occur. For allowed beta decays from an initial state characterized by $I_i \pi_i K_i$ to final states of a rotational band characterized by $I_f \pi_f K_f$, $I_f' \pi_f K_f$, we have the expression

$$\frac{ft\,(I_i \to I_f)}{ft\,(I_i \to I_f')} = \frac{\langle I_i L K_i K_f - K_i \mid I_f' K_f \rangle^2}{\langle I_i L K_i K_f - K_i \mid I_f K_f \rangle^2}.$$

Similar K selection and intensity rules are predicted for gamma-ray transitions, and their validity should depend on the extent to which the gamma-ray transitions are not hindered by other intrinsic selection rules and to which the K quantum number is valid.

3. *Selection Rules Associated with the Intrinsic Structure*

Mottelson and Nilsson have discussed the operative selection rules for transitions between states described by the Nilsson wave functions, assuming single-particle transition operators. Alaga has calculated these selection rules when the Nilsson wave functions can be described by the asymptotic limit quantum numbers $(Nnz\Lambda\Sigma)$[27]. These selection rules for beta decay are reproduced in Table III 1. The Nilsson diagrams for the regions $50 \leqslant Z \leqslant 82$ and $82 \leqslant N \leqslant 126$ are reproduced in Fig. 2 and Fig. 3. As has been discussed previously, for two-quasi-particle states connected by single-particle operators, these selection rules apply exactly if the particles in the final and initial states have the same relative coupling and only one

TABLE III 1. *Selection rules for beta transitions in terms of the asymptotic quantum numbers N, n_z, and Λ.*

Transition	ΔK	Operator	$\Delta\Lambda$	Δn_z	ΔN
Allowed (a)	0	1	0	0	0
		σ_z	0	0	0
	1	σ_+	0	0	0
First forbidden (1)	0	z	0	1 −1	1 −1
		$\sigma_z z$, $\sigma_z \nabla_z$	0	1 −1	1 −1
		$\sigma_+(x-iy)$, $\sigma_+ \nabla_-$	−1	0	±1
		$\sigma_-(x+iy)$, $\sigma_- \nabla_+$	1	0	±1
	1	$(x+iy)$	1	0	±1
		$\sigma_+ z$, $\sigma_+ \nabla_z$	0	1 −1	1 −1
		$\sigma_z(x+iy)$, $\sigma_z \nabla_+$	1	0	±1
First forbidden with α-type shape (1*)	0	$\sigma_z z$	0	1 −1	1 −1
		$\sigma_+(x-iy)$	−1	0	±1
		$\sigma_-(x+iy)$	1	0	±1
	1	$\sigma_+ z$	0	1 −1	1 −1
		$\sigma_z(x+iy)$	1	0	±1
	2	$\sigma_+(x+iy)$	1	0	±1

These selection rules were first given by G. ALAGA (ref. 27).

The entries of the table are ordered according to multipolarity and change in angular momentum component ΔK between initial and final states. Column three then contains the corresponding multipole operator. The selection rules in terms of Λ, the component of orbital angular momentum along the nuclear symmetry axis z', N, the total number of nodes in the harmonic oscillator wave function, and n_z, the number of nodal planes perpendicular to the z'-axis are given in columns four, six, and five, respectively.

particle changes in the transition. A second case exists when the relative coupling of the particles is different in the final and initial states. Here, although only one particle changes, and although the matrix elements for the single-particle transition may be non-vanishing, the transition is Λ-forbidden. These transitions are included in groups I and II of Section II. Two-particle transitions are completely forbidden in this scheme. These are considered in group III a of Section II.

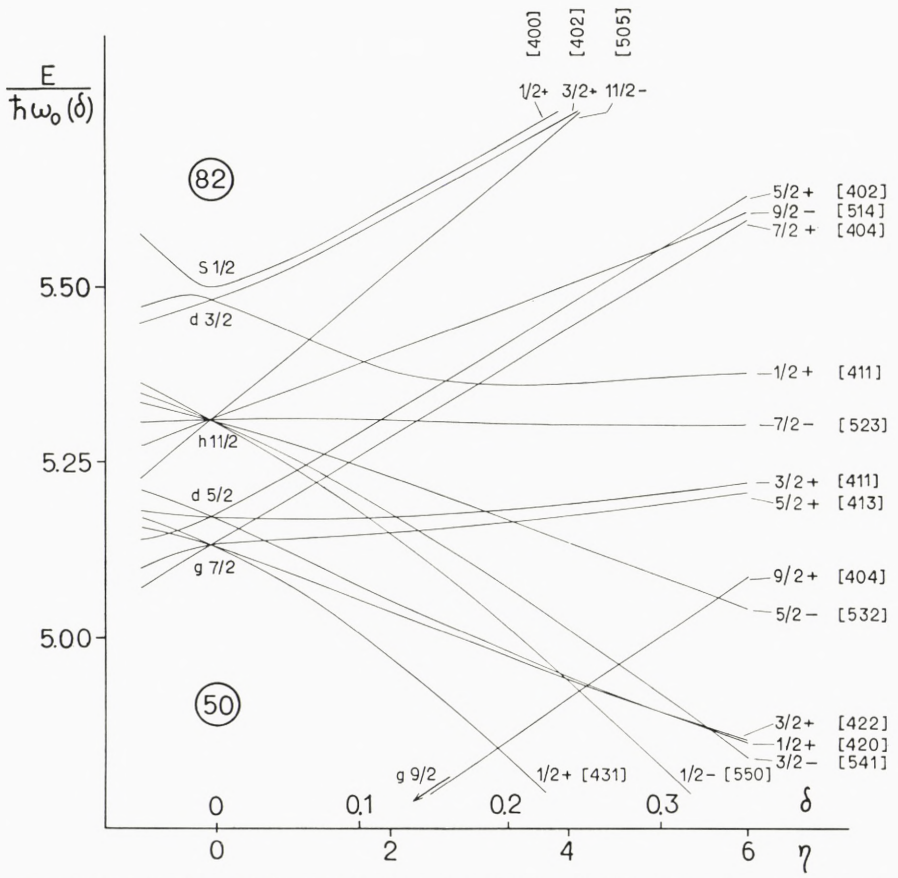

Fig. 2. *Single-particle levels for odd-Z nuclei in the region* $50 < Z < 82$. This figure is a reproduction of fig. 3 in ref. 6, where the parameters which characterize the levels are discussed. Levels used in the present work have been adjusted slightly from the values quoted in ref. 6. (See text and Table II 1).

In discussing the beta transitions we will use the following notations:

a = allowed beta transitions, i. e. $\Delta I = 0$, or 1 (no);
1 = first forbidden beta transitions with $\Delta I = 0$, or 1 (yes);
1* = alpha type first order beta transition, i. e. $\Delta I = 2$ (yes);
u = the transition does not violate the asymptotic selection rules of Table III 1 (i. e. unhindered);
h = the transition violates the selection rules of Table III 1;
Λ = the transition is Λ-forbidden;
K = the transition is K-forbidden. K-forbiddenness is essentially the same as Λ-forbiddenness, but we use K-forbiddenness exclusively for transitions to excited rotational states. (Thus in our notation a transition can be both K- and Λ-forbidden);
F = transitions included in group III of Section II.

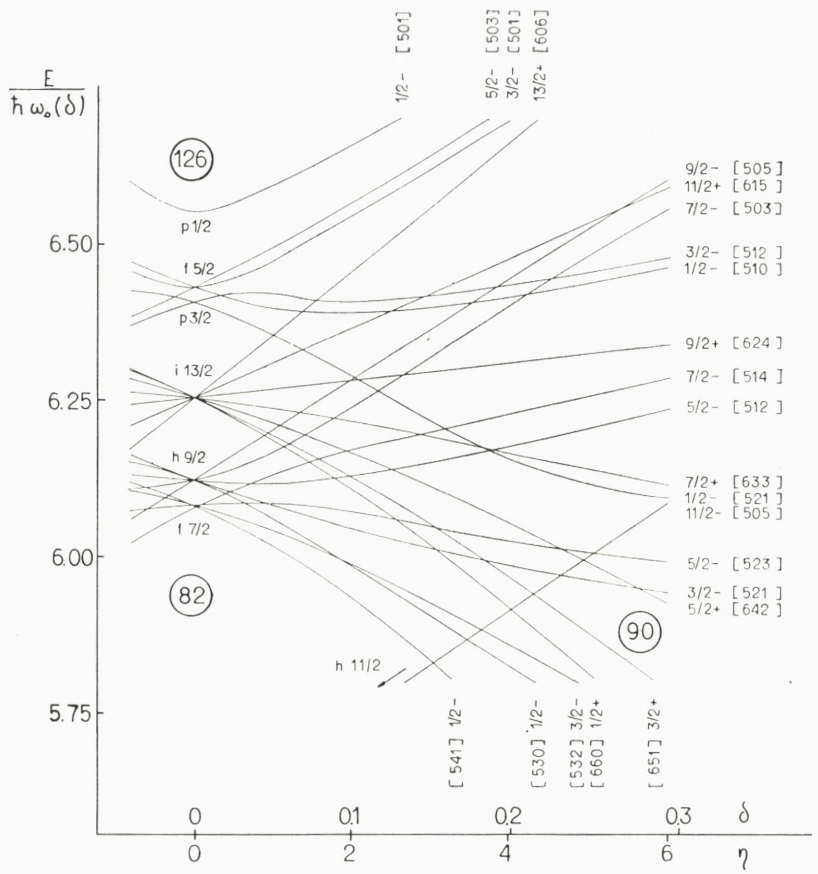

Fig. 3. *Single-particle levels for odd-N nuclei in the region* $82 < N < 126$.. This figure is a reproduction of fig. 4 in ref. 6, where the parameters which characterize the levels are discussed. Levels used in the present work have been adjusted slightly from the values quoted in ref. 6. (See text and Table II 1).

4. *Presentation of Experimental Data*

In the presentation of experimental data we shall discuss separately the level schemes for each mass number. References to the original experimental work are given in the captions to the figures. In general, only experimental references appearing after the 1958 edition of the Table of Isotopes[28] are specifically mentioned. The abbreviations employed are:

half-lives are given in y years, d days, h hours, m minutes, s seconds;
decay energies are indicated where known;
beta decay log ft's are given for each beta group and are indicated by underlining;
excitation energies are given in keV.
The *spin I*, and *parity* π are written at the right side of each level in the order $I\pi$.

To the right of each of the more complex level schemes, the theoretical analysis of the experimental data is given in 3 columns.

The first column gives the assigned K quantum number of the state in addition to the spin I and parity π, in the order $I\pi K$.

In the second column, the type of state is indicated, where the following abbreviations are used:

g = the ground or vacuum state;
c = a state of collective character (see Sec. II. C. 3);
nn = a neutron two-quasi-particle state;
pp = a proton two-quasi-particle state;
i = an intrinsic excitation for which a number of interpretations are possible.

In the third column, the specific configuration for intrinsic states is given in square brackets, viz. ($[Nn_z\Lambda\Sigma \pm N'n'_z\Lambda'\Sigma']$), where the nomenclature is that of the asymptotic limit configurations of the Nilsson wave functions. The intrinsic spin Σ aligned in the direction of the orbital angular momentum directed along the symmetry axis, Λ, is designated $\uparrow$; when it is aligned antiparallel to Λ it is designated $\downarrow$. For odd-odd nuclei the proton state is always listed first; in even-even nuclei the ordering is arbitrary.

In classifying the experimental data shown in the figures we have followed the practice, introduced by MOTTELSON and NILSSON, of assigning the following somewhat arbitrary grades to the data:

A: Sufficient evidence available to establish the existence of the level and also to indicate quite strongly the spin and parity.
B: Position of the level well-established, but the available data does not uniquely determine the spin and parity.
C: Position of the level based largely on conjecture guided by established systematics or an energy fit with otherwise unassigned gamma rays.

In cases where the complexity of the full level scheme obscures the band structure, we have drawn a separate figure to illustrate the classification of the observed levels into rotational bands.

For simple decay schemes, and for the parent odd-odd nuclei, the format described above has been modified in an obvious way.

5. *Interpretation of Experimental Spectra*

The analysis of data shown in the figures is amplified in Tables III a and b for each mass number. In Table III a, an analysis of the experimental data is made which shows the possible configurations which can be assigned to the level (if more than one exists) and also indicates the classification of the beta transition which populates the state. The calculated energies for the configurations are also listed, as are the observed energies. In cases where the odd-odd configuration assignment is uncertain, multiple assignments for the odd-odd nucleus are listed.

Table III b contains for the specified even-even nucleus the calculated level spectrum. The various configurations are listed in these tables, using the shorthand notation K, $K+1$, etc. In every case, K refers to the last filled orbital, $K-1$, the last filled orbital but one, $K+1$, the first empty orbital, etc. Because the Nilsson levels are in general filled successively, the Nilsson states corresponding to the various indices change regularly. However, as a convenience, the meanings for the index designations for each mass number are indicated at the foot of the corresponding Table III b. The calculated energies are those of the degenerate doublet. The two states of each doublet are listed in the order $\Sigma = 0$, $\Sigma = 1$. In the right-hand columns of Table III b under class are classified all the possible beta transitions from the odd-odd configuration given at the head of the column to the corresponding even-even levels, although in many cases energy considerations preclude the transitions. In several cases, more than one odd-odd configuration is listed, indicating uncertainty in the odd-odd assignments. In the right-hand columns under log ft are given the experimental log ft values observed. In addition we sometimes include log ft values in parentheses. These latter are average values for the same single-particle transition observed in odd-mass nuclei.

B. Level Schemes

A = 152.

The 3− ground state and magnetic moment of 2.0 nm of Eu^{152} support the assignment of the configuration $411\uparrow + 521\uparrow$ to the state. The configuration of the 0− isomeric state is uncertain as three lowlying 0− configurations are possible. The state is most easily assigned as the $\Sigma = 0$ doublet state of the ground-state configuration, but the reported upper limit on the intensity of the allowed $M3$ transition between the isomers casts doubt on this assignment. The best overall fit to the data is achieved if the 0− isomer has the configuration $532\uparrow - 642\uparrow$ (see Table III 2).

The energies of the intrinsic states in Sm^{152} and Gd^{152} have not been calculated (see Section II).

Electron capture decay of 3− Eu^{152} populates a 1531 keV 2− level with a log ft = 9.0 for the transition. No low lying $K\pi = 2-$ states are expected in the spectrum and the large log ft for this $\Delta I = 1$, no, transition could be explained if the state is a rotational state of a $K = 0-$ or 1− band, whence the transition is K-forbidden. This interpretation is further supported by the 1− state at 1511 keV populated by the decay of the 0− isomer. The apparent absence of a 0− state suggests $K\pi = 1-$ as the most probable assignment. The similarity of the decay properties of the 1531 − keV 2− state to the 2− state at 1399 keV in Gd^{154} observed in the decay of Eu^{154} (which has the same ground state as Eu^{152}) suggests that the state is a neutron state. If this is the case, the most probable assignment is $521\uparrow - 642\uparrow$. In Table III 2, the other possible assignment for $K\pi = 1-$ is also listed.

The 3+ level at 1235 keV probably is the first rotational state based on a

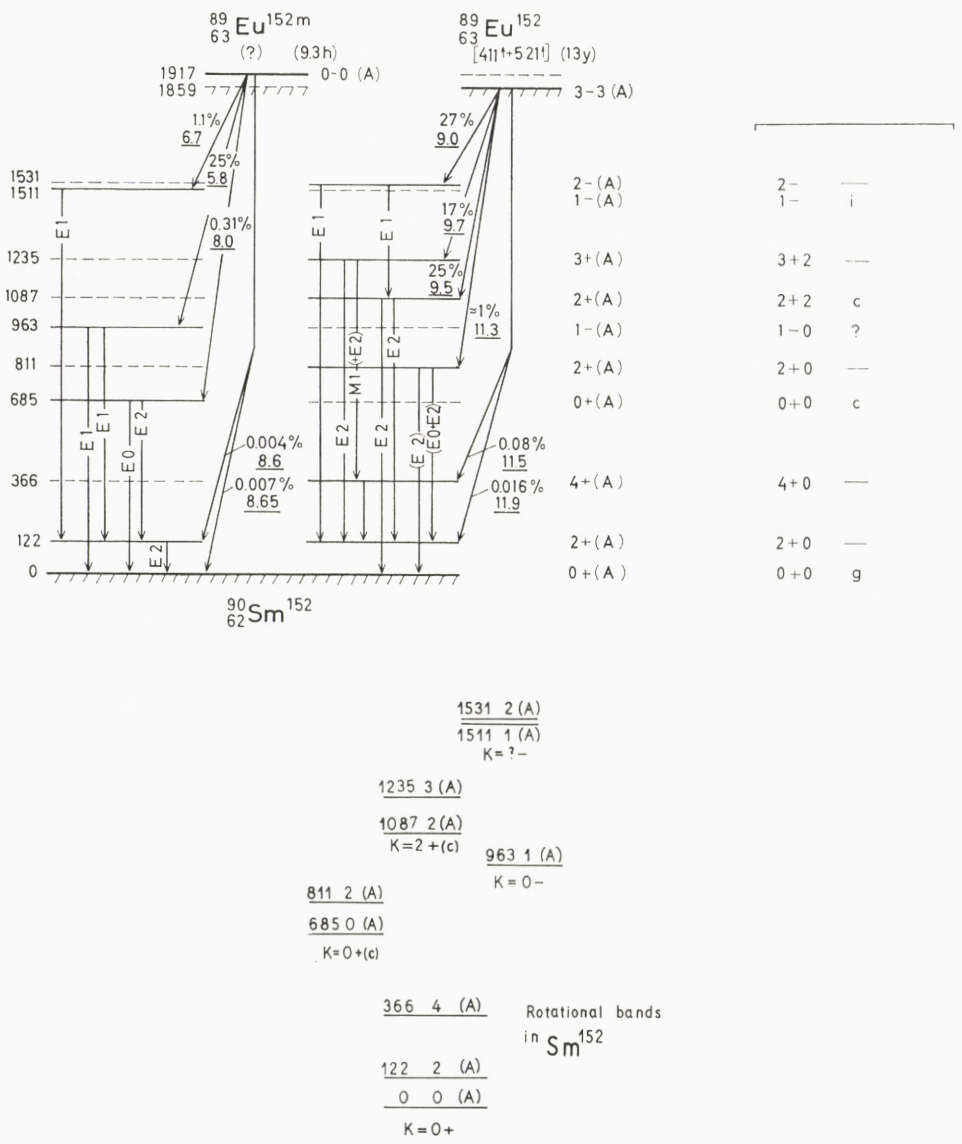

Fig. 4. A = 152.

The spin 0 of the 9.3 h Eu^{152} has been deduced from the upper limit on the magnetic moment of Eu^{152} of $\leqslant 0.004$ nm, reported by V. W. Cohen, J. Schwartz, and R. Novick, Phys. Rev. Letters **2**, 305 (1959). The spin 3 of the 13 *y* Eu^{152} has been deduced from paramagnetic resonance measurements (see SHS). The negative parity assignment to both isomers is as reported by L. Grodzins and A. W. Sunyar, Phys. Rev. Letters **2**, 307 (1959). The energy difference, 50 ± 15 keV, between the Eu isomers has been established by D. Alburger, S. Ofer, and M. Goldhaber, Phys. Rev. **112**, 1998 (1958) who also report a limit on the intensity of the transition between the isomers. A comprehensive review of the experimental data which establish the decay schemes of the 9.3 *h* and 13 *y* Eu^{152} isomers is to be found in the Nuclear Data Sheets (hereinafter called NDS). Additional data on the 9.3 *h* Eu^{152} decay scheme is in I. Marklund, O. Nathan, and O. B. Nielsen, Nuclear Phys. **15**, 199 (1960). Evidence for direct population of the 811 keV 2+ level by 9.3 *h* Eu^{152} has recently been obtained (G. Ewan, priv. comm., 1960; O. Nathan and O. B. Nielsen, priv. comm., 1961).

Eu^{152} (0 – 0) – 1 a, b, c
(3 – 3) – 2

TABLE III 2.

$^{90}_{62}Sm^{152}$

Experimental		Theoretical		1 a†		1 b†		1 c†		2†	
$I\pi$	E	Final configuration	$I\pi K$	Class	log ft	Class	log ft	Class	log ft	Class	log ft
2 –	1.531	No	2 – 2	..	..	..	..	..	..	..	9.0
		642 ↑ – 521 ↑ n	2 – 1	..	..	..	..	..	..	$aK(ah)$	
		651 ↑ – 521 ↑ n	2 – 0	..	..	..	..	..	..	$aK(ah)$	
		532 ↑ – 411 ↑ p	2 – 1	..	..	..	..	..	..	$aK(ah)$	
		413 ↓ – 532 ↑ p	2 – 0	..	..	..	..	..	..	aF	..
1 –	1.511	642 ↑ – 521 ↑ n	1 – 1	ah	6.7	aF	6.7	ah	6.7	..	..
		651 ↑ – 521 ↑ n	1 – 0	ah	..	aF	..	aF	..	..	..
		532 ↑ – 411 ↑ p	1 – 1	ah	..	aF	..	ah	..	..	..
		413 ↓ – 532 ↑ p	1 – 0	aF	..	ah	..	ah	..	..	..
2 +	1.087	No	2 + 2	..	..	..	..	..	..	..	9.5
		(collective)	2 + 2	..	..	..	..	..	..	1 ?	..
1 –	.963	642 ↑ – 523 ↓ n	1 – 0	aF	5.8	ah	5.8	ah	5.8	..	..
		651 ↑ – 521 ↑ n	1 – 0	ah	..	aF	..	aF	..	..	..
		413 ↓ – 532 ↑ p	1 – 0	aF	..	ah	..	ah	..	..	..
		(collective)	1 – 0	..	..	..	..	..	..	..	..
2 +	.811	(collective)	2 + 0	..	..	..	..	..	..	1 ?	11.3
4 +	.366	ground	4 + 0	..	..	..	..	..	..	$1K(1u)$	11.5
2 +	.122	ground	2 + 0	$1^*h(1u)$	8.6	$1^*h(1u)$	8.6	$1^*h(1u)$	8.6	$1K(1u)$	11.9
0 +	0	ground	0 + 0	–	8.7	–	8.7	–	8.7	..	..

† 1 a) 411 ↑ – 521 ↑ 1 b) 413 ↓ – 523 ↓ 1 c) 532 ↑ – 642 ↑ 2) 411 ↑ + 521 ↑

$K = 2+$ state at 1087 keV. No low lying 2+ states are expected in the intrinsic spectrum, suggesting the state is collective. The assignment of the 2+ state at 811 keV as a rotational state based on a 0+ level at 685 keV is established by the mixed $E0 + E2$ transition to the 2+ state of the ground rotational band. The 0+ state is probably best described as a collective state.

The 963 keV 1– state is assigned as a $K\pi = 0-$ state on the basis of its gamma-ray branching to the ground-state band. Two intrinsic excitations with $K\pi = 0-$ are expected, but a rough estimate of the excitation energies of these levels gives a considerably higher energy than that observed.

A = 154.

The magnetic moment of 2.1 nm and spin 3 of the Eu^{154} ground state are consistent with the assignment of the configuration 411 ↑ + 521 ↑[21]. The similarity of both magnetic moment and decay scheme of Eu^{124} to that of 3 – Eu^{152} is additional evidence for the assignment of the same ground state to both.

In Gd^{154}, with 90 neutrons, the same problem exists in calculating the neutron spectrum as in Sm^{152} (see Section II).

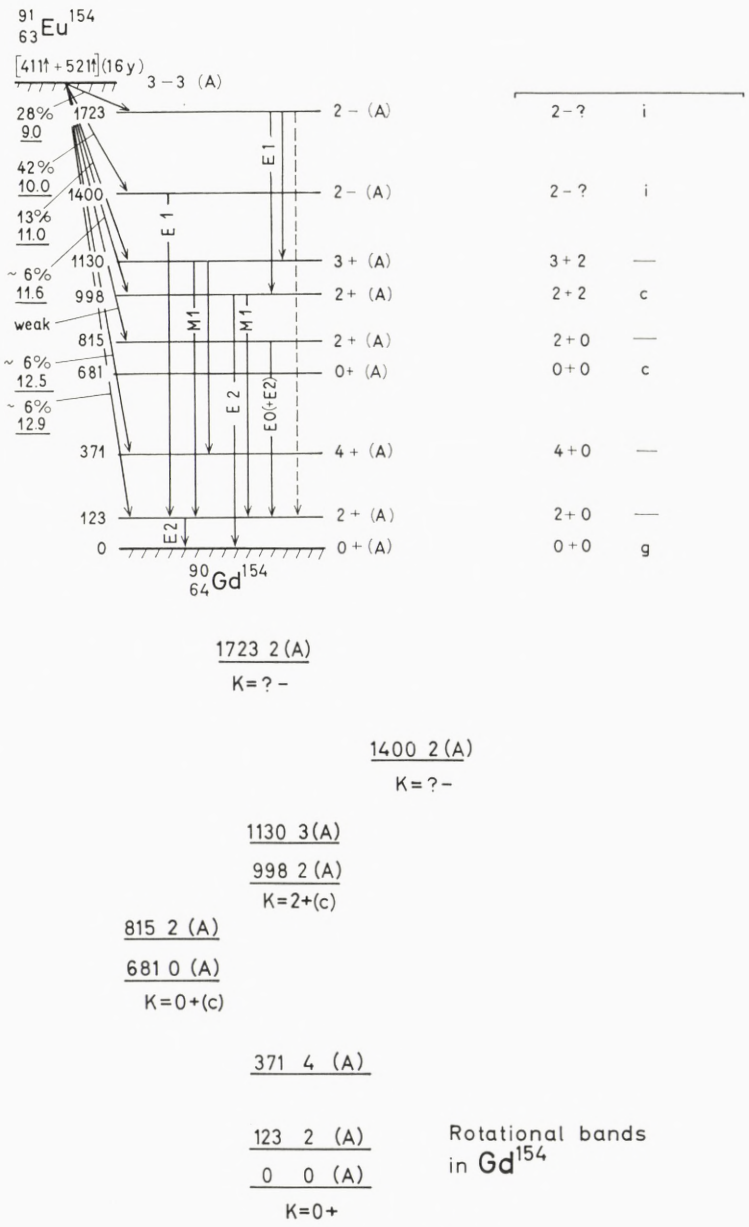

Fig. 5. A = 154.

The spin 3 and magnetic moment of 2.1 nm of Eu^{154} have been deduced from paramagnetic resonance measurements (see SHS). The basic decay scheme of 16 *y* Eu^{154} was established by J. O. Juliano and F. S. Stephens, Phys. Rev. **108**, 341 (1957); more detailed references to other experimental work are to be found in the NDS. The 815 keV 2+ level has been observed in Eu^{154} decay (unpublished results quoted in O. Nathan and S. Hultberg, Phys. Rev. **10**, 118 (1959)), but the assignment of the 681 keV 0+ and 815 keV levels is based on preliminary results on the decay scheme of Tb^{154} (B. Harmatz, T. H. Handley, and J. W. Mihelich, Phys. Rev. **123**, 1758 (1961) hereinafter referred to as HHM 61; M. Jørgensen, O. Nathan, and O. B. Nielsen, priv. comm. (1960). The 2− assignment of the 1400 and 1723 keV levels has been established by P. Derbrunner and W. Kündig, Helv. Phys. Acta **33**, 395 (1960), and R. Stiening and M. Deutsch, Phys. Rev. **121**, 1484 (1961).

Eu^{154} (3 – 3) –1 TABLE III 3. $^{90}_{64}Gd^{154}$

Experimental		Theoretical			1†	
I π	E	Final configuration	I πK	E	Class	log ft
2 –	1.723	411 ↑ – 523 ↑ p	2 – 2	2.0	$\alpha A(2)$	9.0
		651 ↑ – 521 ↑ n	2 – 0	..	$\alpha K(ah)$	..
		642 ↑ – 521 ↑ n	2 – 1	..	$\alpha K(ah)$	..
		532 ↑ – 411 ↑ p	2 – 1	1.7	$\alpha K(ah)$	..
		532 ↑ – 413 ↓ p	2 – 0	1.9	αF	..
		413 ↓ – 523 ↑ p	2 – 1	1.9	αF	..
2 –	1.400	same as 1.723	..	..	..	10.0
2 +	.998	413 ↓ – 411 ↓ p	2 + 2	2.4	$1A(1h)$	11.6
		(collective)	2 + 2	..	1 ?	..
2 +	.815	(collective)	2 + 0	..	1 ?	large
4 +	.371	ground	4 + 0	..	$1K(1u)$	12.5
2 +	.123	ground	2 + 0	..	$1K(1u)$	12.9

† 1) 411 ↑ + 521 ↑

The interpretation of the levels in Gd^{154} at 1400, 1130, 998, 815, and 681 keV seems identical to that of the 1531, 1235, 1087, 811, and 685 keV levels in Sm^{152}. The decay of the 2 – level at 1723 keV to the $K\pi = 2+$ states at 998 and 1130 keV suggests $K\pi = 1-$ or $2-$ for the state. The only $K\pi = 2-$ state is expected at somewhat higher energy. The log $ft = 9.0$ for the beta transition to this state indicates a retarded transition, but this does not help appreciably in classifying the level, because it is predicted that transitions to all low lying negative parity states are retarded.

A = 156.

The assignment of the 3– configuration 411 ↑ + 521 ↑ to Tb^{156} seems reasonable on the basis of the decay scheme. The 4– level at 2042 keV seems better described as the intrinsic state 521 ↑ + 642 ↑ (n) than the state 532 ↑ + 411 ↑ (p) because of the somewhat lower energy predicted for the neutron state, although the log ft's for the transitions 411 ↑ (p) → 642 ↑ (n) and 532 ↑ (p) → 642 ↑ (n) are of the same order of magnitude. Only one intrinsic 3 – state is available in the low energy spectrum, 651 ↑ + 521 ↑ (n), and the observed log ft for the single-particle transition 411 ↑ (p) → 651 ↑ (n) is 7.0, consistent with the log ft for the $Tb^{156} \rightarrow Gd^{156}$ transition. However, the 3 – state appears at somewhat lower energy than that calculated for the configuration listed. No 5 + intrinsic states are expected, so the 1620 keV state seems best assigned as a rotational state. The 4 + state at 1507 keV is quite naturally assigned as the $\Sigma = 0$ member of the K, $K+1$ proton state 413 ↓ + 411 ↑. The 1154 and 1246 keV states are well described as a $K\pi = 2+$ rotational band, probably collective in nature, as no low lying 2 + states are expected in the spectrum.

The Eu^{156} ground state seems fairly well described by the 1 – configuration 413 ↓ – 521 ↑. The transition to the Gd^{156} ground state is somewhat more strongly

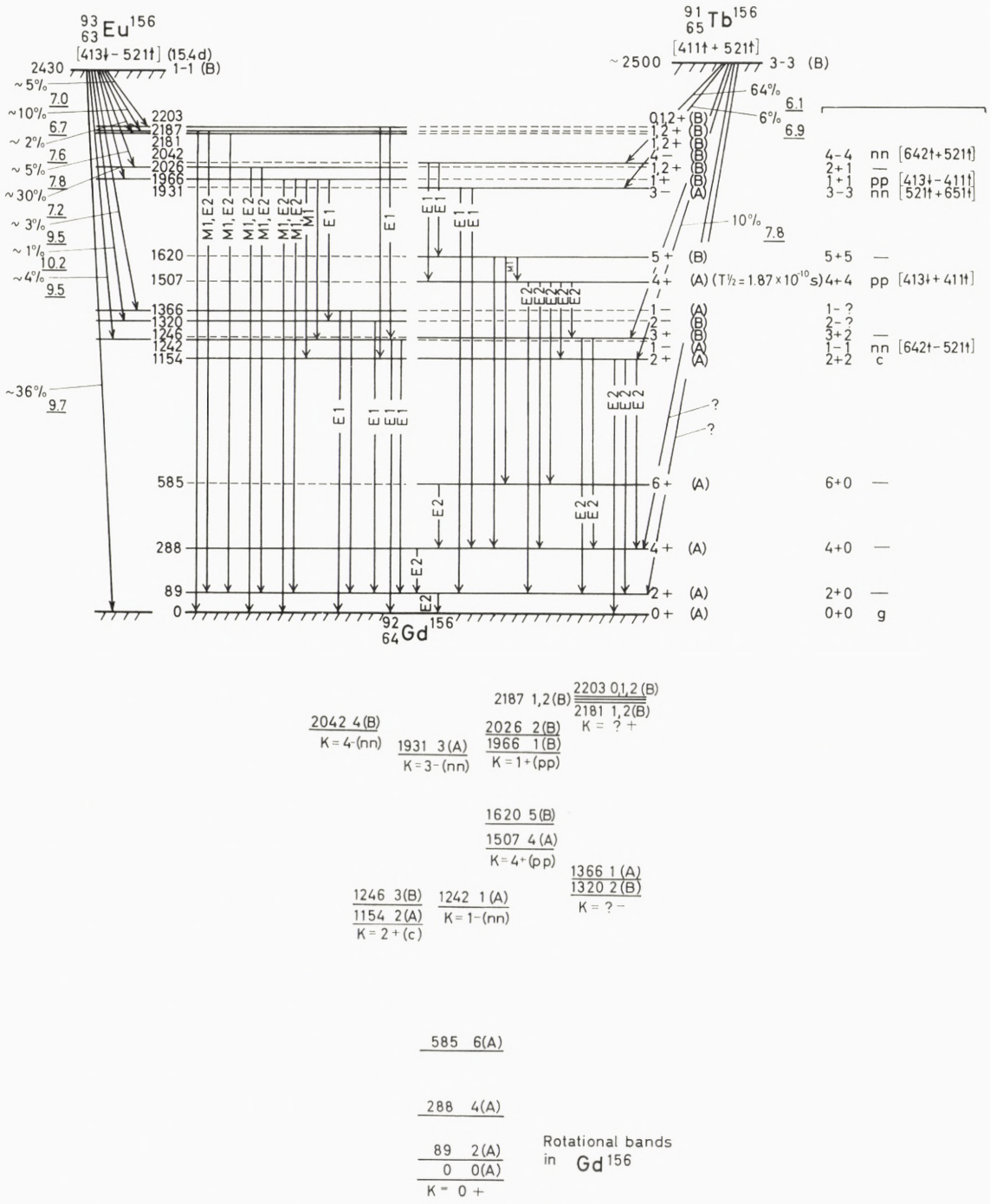

Fig. 6. A = 156.

The decay scheme of Eu^{156} has been proposed by G. Ewan, J. S. Geiger, and R. L. Graham (to be published); many features of this decay scheme are supported by the gamma-ray measurements of J. E. Cline and R. L. Heath, Nuclear Phys. **22**, 598 (1961). The Tb^{156} decay scheme is as reported by P. G. Hansen, O. B. Nielsen, and R. K. Sheline, Nuclear Phys. **12**, 389 (1959); S. Ofer, Phys. Rev. **115**, 412 (1959). The lifetime of the 1507 keV level has been reported by R. E. Bell and M. H. Jørgensen, Nuclear Phys. **12**, 413 (1959). References to earlier measurements are quoted in the references above, and in SHS and the NDS.

Eu^{156} (1 – 1) – 1
Tb^{156} (3 – 3) – 2

TABLE III 4 a.

$^{92}_{64}Gd^{156}$

Experimental		Theoretical			1†		2†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft	Class	log ft
0,1,2+	2.203	–	..	..	1?	7.0	..	..
1,2+	2.187	–	..	..	1?	6.7	..	..
1,2+	2.181	–	..	..	1?	7.6	..	..
4–	2.042	642 ↑ + 521 ↑ n	4 – 4	1.5	..	..	ah	6.1
		532 ↑ + 411 ↑ p	4 – 4	1.7	..	..	ah	..
1,2+	2.026	rot. state 1.966	2 + 1	..	..	7.8	..	..
1+	1.966	413 ↓ – 411 ↑ p	1 + 1	1.4	1u	7.2	..	..
		523 ↓ – 521 ↑ n	1 + 1	1.7	1u	..	..	..
3–	1.931	521 ↑ + 651 ↑ n	3 – 3	2.0	..	..	ah	6.9
4+	1.507	413 ↓ + 411 ↑ p	4 + 4	1.4	..	..	1h	8.0
		523 ↓ + 521 ↑ n	4 + 4	1.7	..	..	1h	..
1–	1.366	521 ↑ – 651 ↑ n	1 – 0	..	ah	9.5	..	..
		642 ↑ – 521 ↑ n	1 – 1	1.5	ah	..	..	..
		532 ↑ – 411 ↑ p	1 – 1	1.7	aF	..	..	..
2–	1.320	521 ↑ – 651 ↑ n	2 – 0	..	..	10.2	..	..
		642 ↑ – 521 ↑ n	2 – 1	..	..	..	..	..
		532 ↑ – 411 ↑ p	2 – 1	..	..	..	..	..
1–	1.242	same as 1.366	..	..	..	9.5	..	..
2+	1.154	(collective)	2 + 2	..	1?	–	1?	7.8
4+	.288	ground	4 + 0	..	..	..	1K(1u)	large
2+	.089	ground	2 + 0	..	1h	large	1K(1u)	large
0+	0	ground	0 + 0	..	1h	9.7	..	..

† 1) 413 ↓ – 521 ↑ 2) 411 ↑ + 521 ↑

retarded (log ft = 9.5) than the single-particle rate observed in Eu^{155} decay, where a log ft = 8.7 is observed for the transition. It should be noted that the 0+ assignment proposed for Eu^{156} by G. EWAN et al. (ref. 29) can also explain many features of the decay scheme if the 0+ configuration 413 ↓ – 642 ↑ is assumed. A choice between these two assignments does not seem possible on the basis of the present data.

The levels populated by Eu^{156} cannot be interpreted unambiguously. Low lying $\Sigma = 0$ negative parity states are expected on the basis of the $\Sigma = 1$ 3– and 4– states observed in Tb^{156} decay, but the data can be interpreted in a number of ways. The observed log ft's for transitions to the 1966 keV and 2187 keV levels suggest that these levels have the configurations 411 ↑ – 413 ↓ (p) and 521 ↑ – 523 ↓ (n), although which is which is not clear. The experimental assignment of the other levels is at present uncertain.

A = 160.

The $K\pi = 3-$ assignment and magnetic moment of 1.6 ± 0.25 of Tb^{160} are in agreement with the assignment of the configuration 411 ↑ + 521 ↑ to Tb^{160} (ref. 30).

$^{92}_{64}Gd^{156}$

TABLE III 4 b.

State	$K\pi$	Energy (MeV)		$^{91}_{65}Tb^{156}$ $p = K+1$; $n = K$	$3-$	$^{93}_{63}Eu^{156}$ $p = K$;	$1-$
		Calc.	Exper.	Class	log ft	Class	log ft
neutron levels							
$K, K+1$	$1-$	1.5	..	..	..	ah	9.5 (7.5)
	$4-$	..	2.042	ah	6.1	..	..
K, K ..... } $K+1, K+1$ ..... }	$0+$	1.6	..	..	..	$1h$	..
$K, K+2$	$4+$	1.7	1.507	$1h$	large	..	..
	$1+$		1.966	$1^*A(1^*h)$	..	$1u$	7.2
$K+1, K+2$	$5-$	1.9	..	..	..	..	..
	$0-$	..	..	..	..	aF	..
$K, K+3$	$4-$	2.0	..	$aA(3)$	..	..	..
	$7-$		..	..	..	..	..
$K-1, K+1$	$1+$	2.0	..	1^*F	..	$1F$	..
	$4+$	..	..	$1F$	..	..	..
$K-1, K$	$0-$	2.0	..	..	..	ah	..
	$3-$	..	1.931	ah	6.9	..	..
$K+1, K+3$	$3-$	2.1	..	aF	..	..	..
	$8-$	..	..	..	..	..	..
$K-1, K+2$	$4-$	2.1	..	aF	..	..	..
	$1-$	..	..	..	..	aF	..
$K-2, K$	$1-$	2.3	..	..	..	ah	..
	$2-$	..	..	ah	..	$aA(ah)$	..
$K-2 = 660\uparrow$ $K-1 = 651\uparrow$ $K = 521\uparrow$ $K+1 = 642\uparrow$ $K+2 = 523\downarrow$ $K+3 = 505\uparrow$							
proton levels							
$K, K+1$	$4+$	1.4	1.507	$1h$	large (8.5)	..	..
	$1+$		1.966	$1^*A(1^*h)$	..	$1u$	7.2
K, K ..... } $K+1, K+1$ ..... }	$0+$	1.6	..	..	..	$1h$	..
$K-1, K+1$	$1-$	1.7	..	..	..	aF	..
	$4-$	..	2.042	ah	6.1	..	..
$K-1, K$	$5-$	1.9	..	..	..	..	..
	$0-$	..	..	..	..	ah	..
$K, K+2$	$6-$	1.9	..	..	..	..	..
	$1-$	..	..	..	..	a(2)	..
$K+1, K+2$	$2-$	2.0	..	$aA(2)$	..	aF	..
	$5-$	..	..	..	..	..	..
$K-1, K+2$	$1+$	2.0	..	1^*F	..	$1F$	..
	$6+$	..	..	..	..	..	..
$K, K+3$	$2+$	2.4	..	$1F$	..	$1u$	(6.2)
	$3+$		..	..	..	$1^*A(1u)$	..
$K+1, K+3$	$2+$	2.5	..	$1u$	..	$1F$	..
	$1+$	..	..	$1^*A(1u)$	..	$1F$	..
$K-1 = 532\uparrow$ $K = 413\downarrow$ $K+1 = 411\uparrow$ $K+2 = 523\uparrow$ $K+3 = 411\downarrow$							

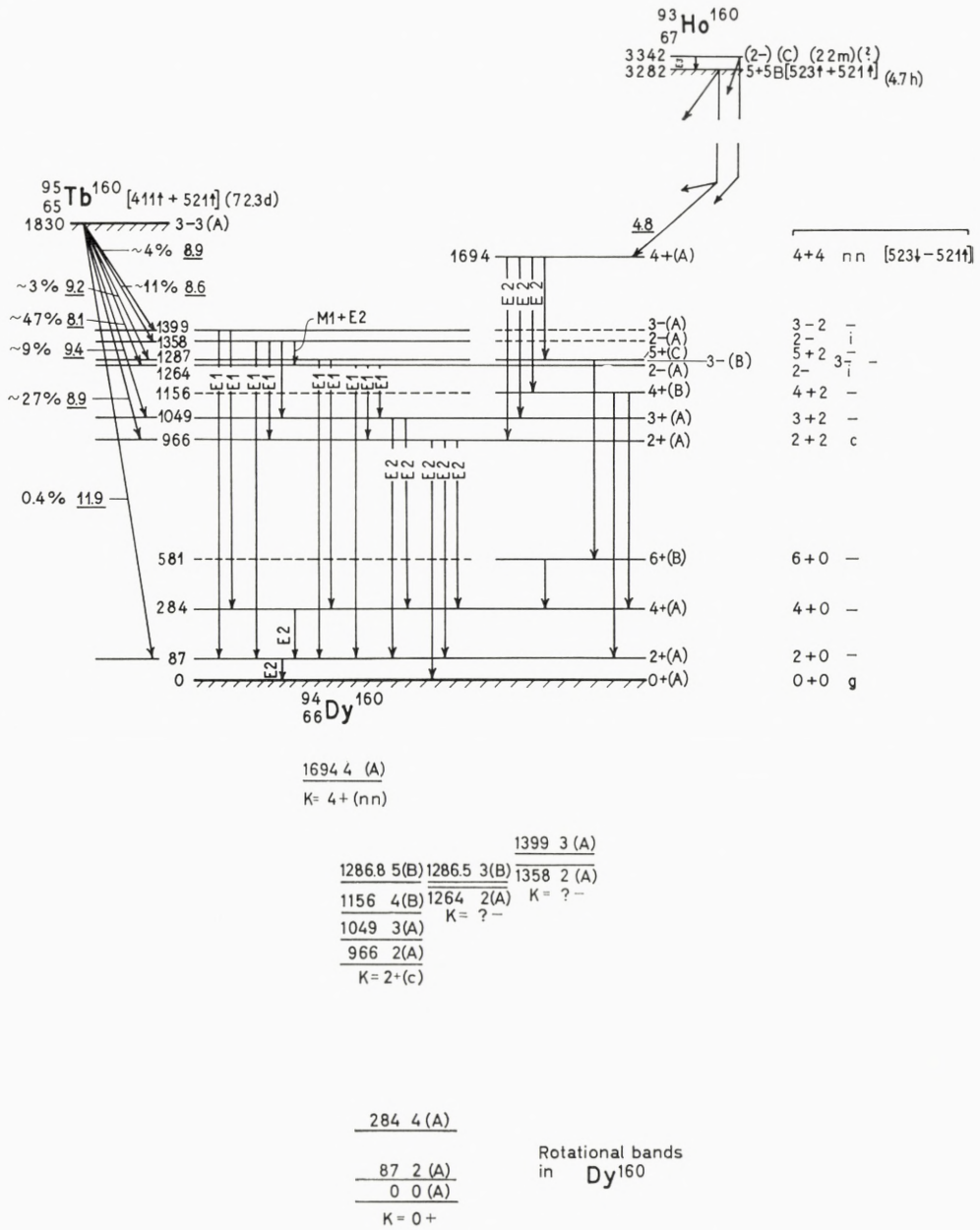

Fig. 7. A = 160.

The decay scheme of Tb^{160} has been extensively studied. The newest experimental data and reviews of previous work are reported by C. E. Johnson, J. F. Schooley, and D. A. Shirley, Phys. Rev. **120**, 2108 (1960); G. T. Ewan, R. L. Graham, and J. S. Geiger, Nuclear Phys. **22**, 610 (1961). (See also N. A. Voinova, B. S. Dzhelepov, N. N. Zhukovskii, and Yu. V. Khol'nov, Izvest. Akad. Nauk SSSR, Ser Fiz. **24**, 852 (1960); A. V. Kogan, V. D. Kul'kov, L. P. Nikitin, N. M. Reinov, I. A. Sokolov, and M. F. Stelmakh, Programma i Tezisy Dokladov 11 Ežegdnogo Soveščanija po Jadernoj Spektroskopii v Rige, Akad. Nauk SSSR, p. 89).

Studies of the Ho^{160} decay scheme have been made. (See the NDS; also K. S. Toth and J. O. Rasmussen, Phys. Rev. **115**, 150 (1959); B. S. Dzhelepov, I. Zvol'skii, M. K. Nikitin, and V. A. Sergienko, Izvest. Akad. Nauk SSSR, **25**, 1246 (1961); E. P. Grigoriev, B. S. Dzhelepov, V. Zvol'ska, and A. V. Zolotavin, Programma i Tezisy Dokladov 11 Ežegdnogo Soveščanija po Jadernoj Spektroskopii v Rige, Akad. Nauk SSSR, p. 55. These results all indicate the very great complexity of the decay scheme. However, the 4+ level at 1694 keV is populated by an allowed, unhindered β+ group (E. P. Grigoriev, B. S. Dzhelepov, and A. V. Zolotavin, Izvest. Akad. Nauk, SSSR, Ser. Fiz. **22**, 821 (1958), for which reason we include it in the Dy^{160} level scheme.

Note that the 1694 keV level configuration should be $523\downarrow + 521\uparrow$.

Tb^{160} $(3-3)-1$
Ho^{160} $(5+5)-2$

TABLE III 5 a.

$^{94}_{66}Dy^{160}$

Experimental		Theoretical			1†		2†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft	Class	log ft
4+	1.694	$523\downarrow+521\uparrow n$	4+4	1.6	..	..	au	≈ 4.8
3−	1.399	rot. state 1.358	3−?	..	−	8.9	..	..
2−	1.358	$521\uparrow-642\uparrow n$	2−1	1.5	$aK(ah)$	8.6	..	..
		$411\uparrow-523\uparrow p$	2−2	1.4	$aA(ah)$	..	..	..
3−	1.287	rot. state 1.264	..	..	−	9.2	..	..
2−	1.264	same as 1.358	..	..	..	8.1	..	..
3+	1.049	rot. state .966	3+2	−	−	9.4	..	..
2+	.966	$411\uparrow+411\downarrow p=411\downarrow p$	2+2	2.0	$1u$	8.9	..	..
		(collective)	2+2	..	1?	..	..	..
2+	.087	ground	2+0	−	$1K(1u)$	11.9	..	..

† 1) $411\uparrow+521\uparrow$ 2) $523\uparrow+521\uparrow$

Two rotational bands of negative parity are observed in Dy^{160} although the K quantum numbers of the bands are not clear. Possible assignments of the bands are indicated in Table III 5 a. It is interesting to note that all transitions are strongly forbidden, as observed, and that states to which faster transitions could occur all appear to have somewhat higher energy than the decay energy of Tb^{160}. The 966 and 1049 keV levels are well established as members of a $K\pi = 2+$ band, and their low energy relative to the calculated 2+ state energies supports their assignment as collective states.

The similarity of the (3−) Eu^{152}, Eu^{154}, and Tb^{160} decay schemes should be noted. In all these isotopes the ground-state configuration is identical, all have relatively little decay energy, and all decay by highly retarded (probably K-forbidden) transitions to apparently the same levels in the daughter nuclei. It would be interesting, if this analogy were pursued further experimentally, to see whether the decays of Eu^{152} and Eu^{154} also populate 3− levels above the 1531 keV and 1400 and 1723 keV levels, respectively.

Much additional information on the levels of Dy^{160} will be provided by further studies of Ho^{160} decay, as preliminary measurements have indicated an extremely complex spectrum. We have included a level at 1694 keV in the illustrated decay scheme, which, on the basis of the $E2$ transitions from it to the 2+, 3+, and 4+ levels at 966, 1049, and 1156 keV is 4+. The log ft = 4.8 from the 4.7 h Ho^{160} to this level is clearly associated with the $523\uparrow$ (p)→$523\downarrow$ (n) transition, establishing the 4+ level as the $523\downarrow+521\uparrow$ neutron configuration and the Ho^{160} isomer as the 5+ configuration $523\uparrow+521\uparrow$.

A = 162.

The log ft = 4.6 observed in the decays of both members of the Ho^{162} isomeric pair clearly establishes that the decays involve the transition $523\uparrow$ (p)→$523\downarrow$ (n).

$^{94}_{66}Dy^{160}$

TABLE III 5 b.

State	$K\pi$	Energy (MeV)		$^{95}_{65}Tb^{160}$ $p = K$	$3-$ $n = K$	$^{93}_{67}Ho^{160}$ $p = K+1$	$5+$ $n = K$
		Calc.	Exper.	Class	log ft	Class	log ft
neutron levels							
$K, K+1$	$1-$	1.5	..	..	..	..	..
	$4-$	..	..	ah	..	$1h$	..
$K, K+2$	$4+$	1.6	1.694	$1h$	..	au	4.8 (5.0)
	$1+$	..	..	$1^*A(1^*h)$	..	..	..
K, K / $K+1, K+1$	$0+$	1.6	..	..	..	..	..
$K-1, K+1$	$1+$	1.7	..	1^*F	..	..	..
	$4+$	..	..	$1F$	..	aF	..
$K+1, K+2$	$5-$	1.7	..	..	..	$1F$	..
	$0-$	..	..	..	..	..	..
$K-1, K+2$	$4-$	1.8	..	aF	..	$1F$	..
	$1-$	..	..	..	..	..	..
$K-1, K$	$0-$	1.8	..	..	..	..	..
	$3-$	..	..	ah	..	1^*h	..
$K, K+3$	$2-$	2.6	..	$aA(ah)$	..	..	..
	$5-$	..	..	..	..	$1u$	(6.1)
$K+1, K+3$	$1+$	2.7	..	1^*F	..	..	..
	$6+$	..	..	..	..	aF	..

$K-1 = 651\uparrow \quad K = 521\uparrow \quad K+1 = 642\uparrow \quad K+2 = 523\downarrow \quad K+3 = 633\uparrow$

proton levels							
$K, K+1$	$2-$	1.4	..	$aA(2)$	..	..	..
	$5-$	..	..	..	..	$1u$	..
$K-1, K+1$	$6-$	1.7	..	..	..	$1h$	(8)
	$1-$	..	..	..	..	..	..
K, K / $K+1, K+1$	$0+$	1.8	..	..	..	..	..
$K, K+2$	$2+$	2.0	..	$1u$	(6.3)	..	..
	$1+$	..	..	$1^*A(1u)$	..	..	..
$K-2, K+1$	$1+$	2.0	..	1^*F	..	..	..
	$6+$	..	..	..	..	ah	..
$K-1, K$	$4+$	2.1	..	$1h$	..	aF	..
	$1+$	..	..	$1^*A(1h)$	..	..	..
$K-1, K+2$	$2+$	2.2	..	$1F$	..	..	..
	$3+$	..	..	$1F$	..	..	..
$K+1, K+2$	$4-$	2.2	..	aF	..	$1u$	(7.0)
	$3-$	..	..	aF	..	$1^*A(1u)$	..
$K+1, K+3$	$7-$	2.9	..	..	..	1^*h	..
	$0-$	..	..		..	..	..

$K-2 = 532\uparrow \quad K-1 = 413\downarrow \quad K = 411\uparrow \quad K+1 = 523\uparrow \quad K+2 = 411\downarrow \quad K+3 = 404\downarrow$

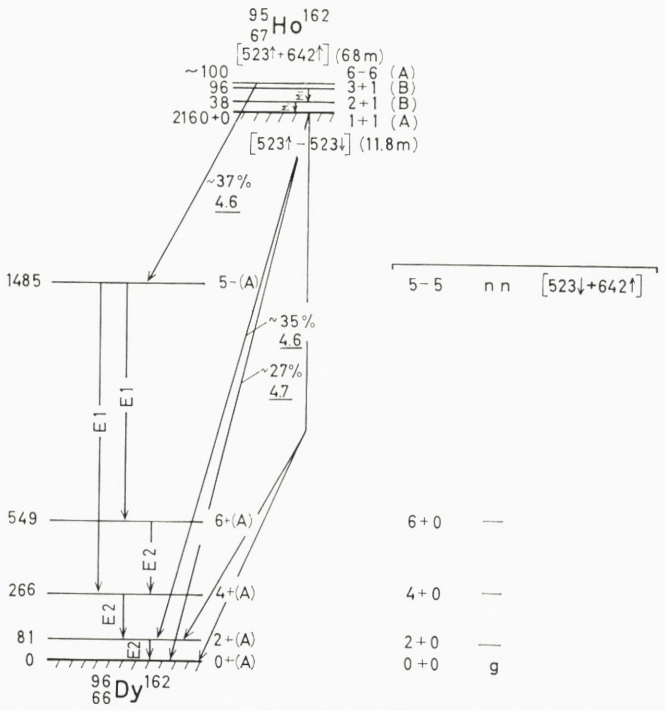

Fig. 8. A = 162.
The isomers of Ho^{162} and the decay schemes have recently been established by M. JØRGENSEN, O. B. NIELSEN, and O. SKILBREID, Nuclear Phys. **24**, 443 (1961). The configuration assignments were originally proposed by these authors.

Ho^{162} $(6-6)-1$
$(1+1)-2$

TABLE III. 6 a. $^{96}_{66}Dy^{162}$

Experimental		Theoretical			1†		2†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft	Class	log ft
5−	1.485	$523\downarrow+642\uparrow$	5−5	1.3	*au*	4.6	..	..
2+	.081	ground	2+0	–	..	..	*au*	≈ 4.6
0+	0	ground	0+0	–	..	..	*au*	≈ 4.7

† 1) $523\uparrow+642\uparrow$ 2) $523\uparrow-523\downarrow$

A 6− assignment for the upper isomer is definite from its allowed decay to the 5− level in Dy^{162} at 1485 keV, which in turn is clearly established from its decay properties. The 6− Ho^{162} configuration can therefore only be $523\downarrow+642\uparrow$, and the 5− state the neutron state $523\downarrow+642\uparrow$. The allowed decay to the Dy^{162} ground state clearly establishes the 11.8 min isomer as the 1+ state $523\uparrow-523\downarrow$. These assignments have previously been made by M. JØRGENSEN, O. B. NIELSEN, and O. SKILBREID[31].

$^{96}_{66}Dy^{162}$

TABLE III 6b.

State	$K\pi$	Energy (MeV)		$^{95}_{67}Ho^{162}$ $p = K+1$;	$1+$ $n = K+1$	$^{95}_{67}Ho^{162}$ $p = K+1$;	$6-$ $n = K$
		Calc.	Exper.	Class	log ft	Class	log ft
neutron levels							
$K, K+1$	$5-$	1.3	1.485	..	..	au	4.6 (5.2)
	$0-$	..	..	$1u$	..	..	..
K, K ..... } $K+1, K+1$ ..... }	$0+$	1.4	..	au	..	..	..
$K-1, K+1$	$4+$	1.6	..	..	..	1^*F	..
	$1+$	..	..	$a(2)$	..	..	..
$K-1, K$	$1-$	1.8	..	$1F$	..	..	..
	$4-$	..	..	..	..	..	..
$K-2, K+1$	$4-$	1.9	..	..	..	..	..
	$1-$	..	..	1^*h	..	..	..
$K-2, K$	$1+$	2.1	..	aF	..	..	..
	$4+$	..	..	..	..	1^*h	..
$K, K+2$	$1+$	2.2	..	aF	..	..	..
	$6+$	..	..	..	..	$1u$	..
$K+1, K+2$	$6-$	2.2	..	..	..	aF	..
	$1-$	..	..	$1u$	..	..	..
$K, K+3$	$3-$	2.3	..	1^*F	..	..	..
	$2-$	..	..	$1F$	..	..	..

$K-2 = 651\uparrow$, $K-1 = 521\uparrow$, $K = 642\uparrow$, $K+1 = 523\downarrow$, $K+2 = 633\uparrow$, $K+3 = 521\downarrow$

proton levels							
$K, K+1$	$2-$	1.4	..	$1h$	..	..	..
	$5-$	..	..	..	..	ah	..
$K-1, K+1$	$6-$	1.7	..	..	..	ah	..
	$1-$	..	..	$1u$	..	..	..
K, K ..... } $K+1, K+1$ ..... }	$0+$	1.8	..	au	..	..	..
$K, K+2$	$2+$	2.0	..	aF	..	..	..
	$1+$	..	..	aF	..	..	..
$K-2, K+1$	$1+$	2.0	..	ah	..	..	..
	$6+$	..	..	..	..	$1u$	..
$K-1, K$	$4+$	2.1	..	..	..	..	..
	$1+$	..	..	aF	..	..	..
$K-1, K+2$	$2+$	2.2	..	aF	..	..	..
	$3+$	..	..	..	..	..	..
$K+1, K+2$	$4-$	2.2	..	..	..	..	..
	$3-$	..	..	1^*h	..	..	..
$K+1, K+3$	$7-$	2.9	..	..	..	ah	..
	$0-$	..	..	$1u$	..	..	..

$K-2 = 532\uparrow$ $K-1 = 413\downarrow$ $K = 411\uparrow$, $K+1 = 523\uparrow$, $K+2 = 411\downarrow$, $K+3 = 404\downarrow$

A = 164.

The Ho^{164} isomers are identical to the Ho^{162} isomers, except the lower decay energy rules out the beta decay from the 6− isomer to the 5− state in Dy^{164}. The assignments have previously been proposed by M. JØRGENSEN, O. B. NIELSEN, and O. SKILBREID[32]. The allowed, unhindered decay of Tm^{164} to Er^{164} seems clearly to establish the 2 m Tm^{164} isomer as having the 1+ configuration 523 ↑ − 523 ↓.

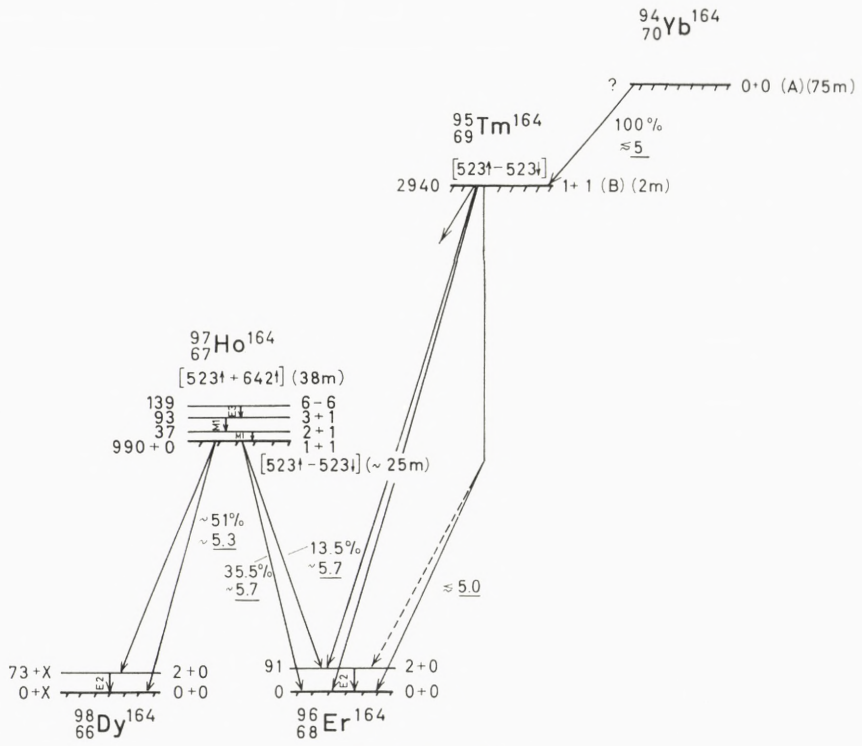

Fig. 9. A = 164.

The presence of two isomers of Ho^{164} has been established by M. JØRGENSEN, O. B. NIELSEN, and O. SKILBREID (priv. comm., Feb. 1961), who assigned the decay scheme of Ho^{164} as reported by H. N. BROWN and R. A. BECKER, Phys. Rev. **96**, 1372 (1954) to arise from the decay of the 1+ isomer. The configuration assignments were originally proposed by M. JØRGENSEN et al.

The data on the $Yb^{164} \rightarrow Tm^{164} \rightarrow Er^{164}$ decay chain are as reported by A. ABDURAZAKOV, K. GROMOV, B. DALKHSUREN, B. DZHELEPOV, I. LEVENBERG, A. MURIN, YU. NORSEYEV, V. POKROVSKY, V. CHUMIN, and I. YUTLANDOV, Nuclear Phys. **21**, 164 (1960).

A = 166.

The levels in Ho^{166} populated by Dy^{166} decay seem well described by rotational states based on a $K = 0-$ state. The band manifests a displacement of the odd-spin levels with respect to those with even spin. An intrinsic 1+ level at 428 keV is populated with a $\log ft = 4.8$, clearly identifying the level as the configuration 523 ↑ − 523 ↓. Of the levels reported from Ho^{165} (n, γ), Ho^{166} reactions, the 3+ level at 194 keV

$Ho^{164}(1+1)-1$
$Tm^{164}(1+1)-2$

TABLE III 7.

$^{98}_{66}Dy^{164}$ $^{96}_{68}Er^{164}$

Experimental		Theoretical			1†		2†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft	Class	log ft
2+	.091	ground (Er^{164})	2+0	–	*au*	≈5.4	..	..
0+	0	ground (Er^{164})	0+0	–	*au*	≈5.7	*au*	≲5.0
2+	.073	ground (Dy^{164})	2+0	–	*au*	≈5.3	..	..
0+	0	ground (Dy^{164})	0+0	–	*au*	≈5.3	..	..

† 1) 523↑−523↓ 2) 523↑−523↓

is assigned the configuration 523↑−521↓, and the 4− level seems well described as a rotational state of the 0− band. The $K\pi = 7-$, $\Sigma = 1$, member of the Ho^{166} ground state doublet (the long lived Ho^{166}) is essentially degenerate with the $\Sigma = 0$ state, the 7− state having an energy 9 ± 33 keV lower than the 0− state.

The levels observed in Ho^{166} are all formed by coupling the 523↑ proton to different neutron configurations. The neutron level ordering is identical to that observed in Er^{167}.

The beta decay of 27 h Ho^{166} populates a 1− level at 1826 keV with a log ft = 5.2, which establishes the level configuration as 523↓−633↑(n) (ref. 33). The long lived Ho^{166} decays entirely to a 6− state at 1785 keV with a log $ft \leqslant 6.7$. Although the decay rate is somewhat retarded for an *au* transition, we assign the 6− state as the $\Sigma = 0$ state of the 633↑+523↓(n) configuration (ref. 34), as no other 6− state is expected at such a low energy. The doublet spacing in the even-even nucleus is 40 keV. This difference is considerably smaller than the spacing observed in other nuclei, although experimentally this is the best established case.

The 1− state at 1663 keV populated by the 27 h Ho^{166} can be interpreted as the intrinsic $K\pi = 0-$ state 404↓−523↑(p) (the 1− state lying lower than the 0−), but it occurs at a somewhat lower energy than that calculated for the level. The 1460 keV 0+ state is quite naturally interpreted as the $K, K; K+1, K+1$ proton pair excitation.

The decay of the 6− level at 1785 keV populates 7+, 6+, and 5+ states of a $K\pi = 2+$ band. The 4+, 3+ and 2+ levels of this band are then excited by cascade transitions. These latter three levels are well established by the decay of Tm^{166}, in which these levels are strongly excited by cascade transitions. The 7 h Tm^{166} has a measured spin of 2, and two configurations can be assigned this spin, the $2- \Sigma = 0$ configuration 411↓−523↓, and the $2+ \Sigma = 1$ configuration 411↓−642↑. A measurement of the magnetic moment should be decisive in establishing the correct assignment†.

The decay scheme of Tm^{166} is complex, and because of the uncertainty in most of the experimental assignments we do not attempt a more detailed analysis of the level scheme.

† See caption of Fig. 10.

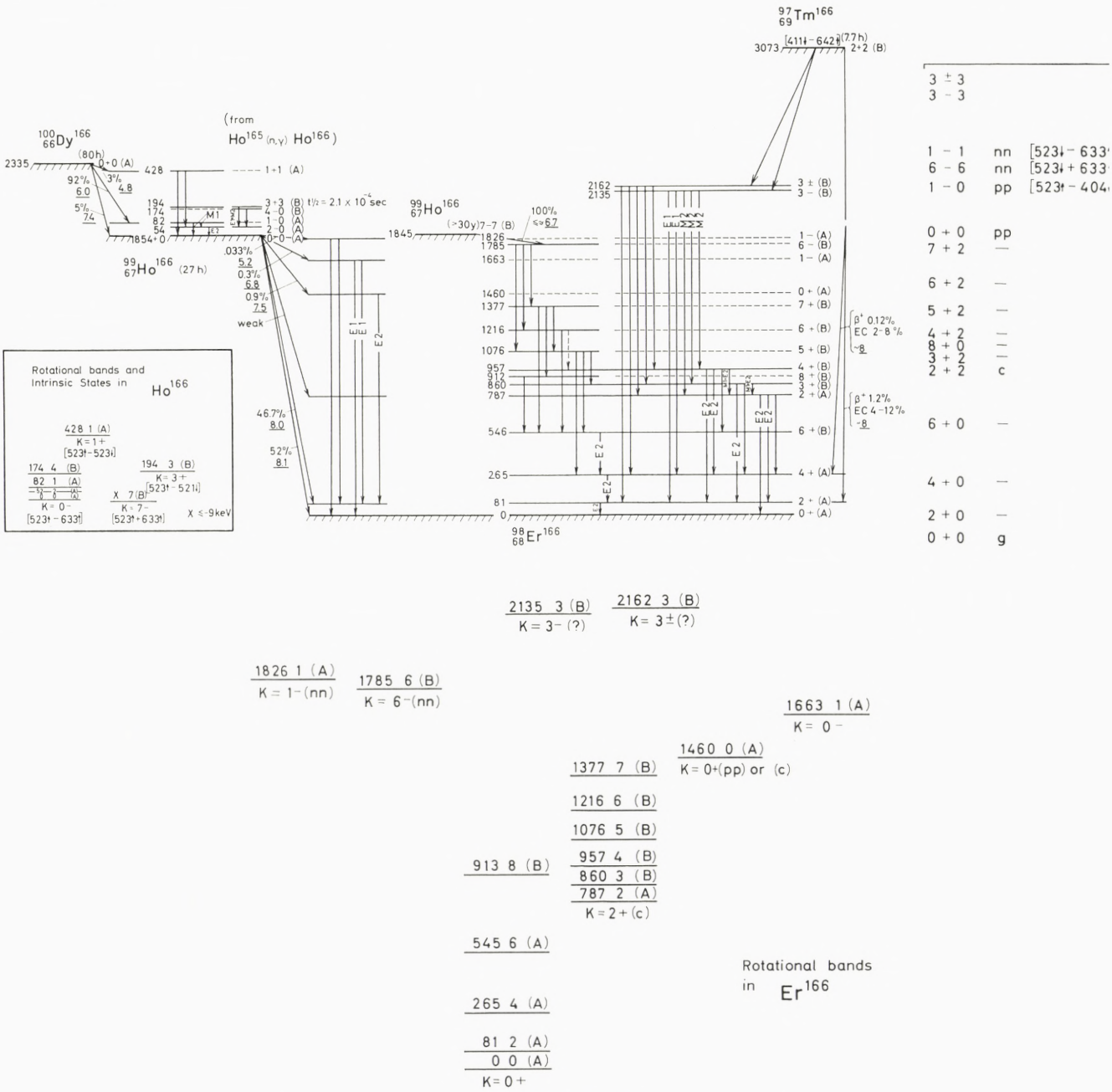

Fig. 10. A = 166.

The decay scheme of Dy^{166} is as reported by R. G. Helmer and S. B. Burson, Phys. Rev. **119**, 788 (1960); Argonne National Laboratory Report ANL 6270 (January 1961, unpublished); J. S. Geiger, R. L. Graham, and G. T. Ewan, Bull. Am. Phys. Soc. **5**, 255 (1960). The additional levels in Ho^{166} have been reported by K. Alexander and V. Bredel, Nuclear Phys. **16**, 152 (1960); I. V. Estulin, A. S. Melioransky, and L. F. Kalinkin, Nuclear Phys. **24**, 118 (1961). The decay of long-lived Ho^{166} has recently been investigated

Ho^{166} (0−0)−1
(7−7)−2

TABLE III 8 a. $^{98}_{68}Er^{166}$.

Experimental		Theoretical			1†		2†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft	Class	log ft
1−	1.826	523 ↓ − 633 ↑ n	1 − 1	1.6	au	5.2	..	..
6−	1.785	523 ↓ + 633 ↑ n	6 − 6	1.6	..	..	au	$\lesssim$6.7
1−	1.663	523 ↑ − 404 ↓ p	1 − 0	2.0	ah	6.8	..	..
		(collective)	1 − 0	..	a?	..	..	..
0+	1.460	proton	0 + 0	1.7	1 u	7.5	..	..
		(collective)	0 + 0	..	1?	..	..	..
2+	.781	523 ↓ − 521 ↓ n	2 + 2	1.7	1*F	large	..	..
		411 ↑ − 411 ↓ p	2 + 2	1.8	1*F	..	..	..
		(collective)	2 + 2	..	1*?	..	..	..
2+	.081	ground	2 + 0	..	1*u	8.0	..	..
0+	0	ground	0 + 0	..	1 u	8.1	..	..

† 1) 523 ↑ − 633 ↑ 2) 523 ↑ + 633 ↑

A = 168.

The spin coupling rules predict a 3+ ground state for Tm^{168}, the configuration 411 ↓ − 633 ↑. The assignment is supported by the Tm^{168} decay scheme.

Two low-lying 3− levels are predicted in Er^{168}, a proton level 411 ↓ − 523 ↑ at ≈ 1.3 MeV, and a neutron level 633 ↑ − 521 ↓ at ≈ 1.1 MeV, in good agreement with the observed energies of 1095 and 1543 keV. The electron capture transition

† A reanalysis of angular distributions of gamma rays from aligned Ho^{166} nuclei, assuming the long-lived Ho^{166} decay scheme shown, clearly establishes the spin of Ho^{166} as 7, and the spins of the 1785 and 1076 states as 6 and 5, respectively. (Private communication from H. POSTMA). These levels should therefore be designated (A) in the figure, as should the 2+ Tm^{166} assignment (see below).

by C. J. GALLAGHER, Jr., O. B. NIELSEN, O. SKILBREID, and A. W. SUNYAR, Phys. Rev. (to be published), who review earlier experimental results and report the decay scheme shown. The spin of 0 for 27 h Ho^{166} has been deduced from the atomic beam magnetic resonance data of L. S. GOODMAN, W. J. CHILDS, R. MARRUS, I. P. K. LINDGREN, and Y. CABEZAS, Bull. Am. Phys. Soc. **5**, 344 (1960); W. J. CHILDS and L. S. GOODMAN, Phys. Rev. **112**, 591 (1961). Negative parity is deduced from its decay to the 2+ rotational level in Er^{166}. The decay energy for the 27 h isomer is as reported by R. L. GRAHAM, J. L. WOLFSON, and M. A. CLARK, Phys. Rev. **98**, 1173 A (1955). The decay of Ho^{166} to the high lying states of Er^{166} has been reported by P. G. HANSEN, K. WILSKY, D. J. HOREN, and LUNG-WEN CHIAO, Nuclear Phys. **24**, 519 (1961). A review of earlier data can be found in this reference and in the NDS. The beta branch to the 2+ level at 787 keV has been observed in Copenhagen (C. J. GALLAGHER Jr. and O. SKILBREID, unpublished data, 1960). The spin of Tm^{166} has been measured to be 2 (J. C. WALKER and D. L. HARRIS, Phys. Rev. **121**, 224 (1961)). The magnetic moment of Tm^{166} has been measured and clearly establishes the 2+ assignment shown. (J. C. WALKER, private communication). Preliminary results on the decay scheme of Tm^{166} have recently been reported by a number of authors (P. BOSKMA and H. DE WAARD, Nuclear Phys. **12**, 533 (1959); R. G. WILSON and M. L. POOL, Bull. Am. Phys. Soc. **5**, 155 (1960); K. P. JACOB, J. W. MIHELICH, B. HARMATZ, and T. H. HANDLEY, Phys. Rev. **117**, 1102 (1960); K. GROMOV, B. S. DZHELEPOV, and V. N. POKROVSKI, Izvest. Akad. Nauk. SSSR. Ser. Fiz. **23**, 821 (1959); E. P. GRIGORIEV, K. YA. GROMOV, and B. S. DZHELEPOV, *ibid* **25**, (1961, to be published); J. ZYLICZ, Y. PREIBISZ, S. CHOJNACKI, J. WOTOWOSKI, YU. MORSEEV (priv. comm. to A. BOHR and B. MOTTELSON, Jan. 1961; HHM 61). Only the well-established features of the decay scheme are shown. There is some question whether the total decay energy shown iscorrect.

$^{98}_{68}Er^{166}$

TABLE III 8 b.

State	$K\pi$	Energy (MeV)		$^{99}_{67}Ho^{166}$ 0− $p = K$; $n = K+1$		$^{99}_{67}Ho^{166}$ 7− $p = K$; $n = K+1$		$^{97}_{69}Tm^{166}$ 2+ $p = K+1$; $n = K-1$	
		Calc.	Exper.	Class	log *ft*	Class	log *ft*	Class	log *ft*
neutron levels									
$K, K+1$	6−	1.6	1.785	..	..	*au*	⩽ 6.7 (5.1)	..	..
	1−	..	1.826	*au*	5.2 (5.1)	..	..	1 *F*	..
$K, K+2$	2+	1.7	..	1**F*	..	..	..	*aF*	large
	3+	..	..	..	..	..	..	*aF*	..
$K-1, K+1$	1+	1.8	..	1 *h*	..	..	..	*a*(2)	..
	6+	..	..	..	..	1 *h*	..	..	..
$K-1, K+2$	3−	1.9	..	..	..	..	..	1 *A* (1 *u*)	..
	2−	..	..	..	..	..	..	1 *u*	(6.4)
$K, K+3$	5+	2.1	..	..	..	1**F*	..	..	..
	0+	..	..	1 *F*	..	..	..	..	..
$K-2, K+1$	2−	2.1	..	..	..	..	..	1 *F*	..
	5−	..	..	..	..	..	..	..	..
K, K ..... $K+1, K+1$	0+	2.1	..	1 *u*	..	..	..	..	..
$K+1, K+2$	4−	2.2	..	..	..	..	..	1**F*	..
	3−	..	..	..	..	..	..	1 *F*	..
$K-1, K$	5−	2.4	..	..	..	..	..	..	..
	0−	..	..	*aF*	..	..	..	1**h*	..
$K+1, K+3$	1−	2.5	..	*ah*	(6.9)	..	..	1 *F*	..
	6−	..	..	..	..	*ah*	(6.9)	..	..

$K-2 = 521\uparrow$, $K-1 = 642\uparrow$, $K = 523\downarrow$, $K+1 = 633\uparrow$, $K+2 = 521\downarrow$, $K+3 = 512\uparrow$.

proton levels									
$K, K+1$	4−	1.3	..	..	..	..	..	1 *A* (1 *h*)	..
	3−	..	..	..	..	..	..	1 *h*	..
K, K ..... $K+1, K+1$	0+	1.7	1.460	1 *u*	7.5	..	..	..	..
$K-1, K+1$	2+	1.8	..	1**F*	..	..	..	*aA* (*ah*)	..
	1+	..	..	1 *F*	..	..	..	*ah*	..
$K, K+2$	7−	2.0	..	..	..	*ah*	(6.0)	..	..
	0−	..	1.663	*ah*	6.8 (6.0)	..	..	1**F*	..
$K-2, K+1$	2+	2.1	..	1**F*	..	..	..	*ah*	(6.6)
	3+	..	..	..	..	..	..	*aA* (*ah*)	..
$K-3, K+1$	3−	2.2	..	..	..	*aF*	..	1 *A* (1 *u*)	..
	1−	..	..	*aF*	..	..	..	1 *u*	..
$K-1, K$	2−	2.3	..	..	..	..	..	1 *F*	..
	5−	..	..	..	..	..	..	..	..
$K+1, K+2$	3+	2.4	..	..	..	..	..	*ah*	..
	4+	..	..	..	..	..	..	..	..
$K, K+3$	1−	2.4	..	*ah*	..	..	..	1 *F*	..
	6−	..	..	..	..	*ah*	..	..	..
$K-1, K+2$	5+	2.5	..	..	..	1**F*	..	..	..
	2+	..	..	1**F*	..	..	..	1 *F*	..

$K-3 = 532\uparrow$, $K-2 = 413\downarrow$, $K-1 = 411\uparrow$, $K = 523\uparrow$, $K+1 = 411\downarrow$, $K+2 = 404\downarrow$, $K+3 = 402\uparrow$.

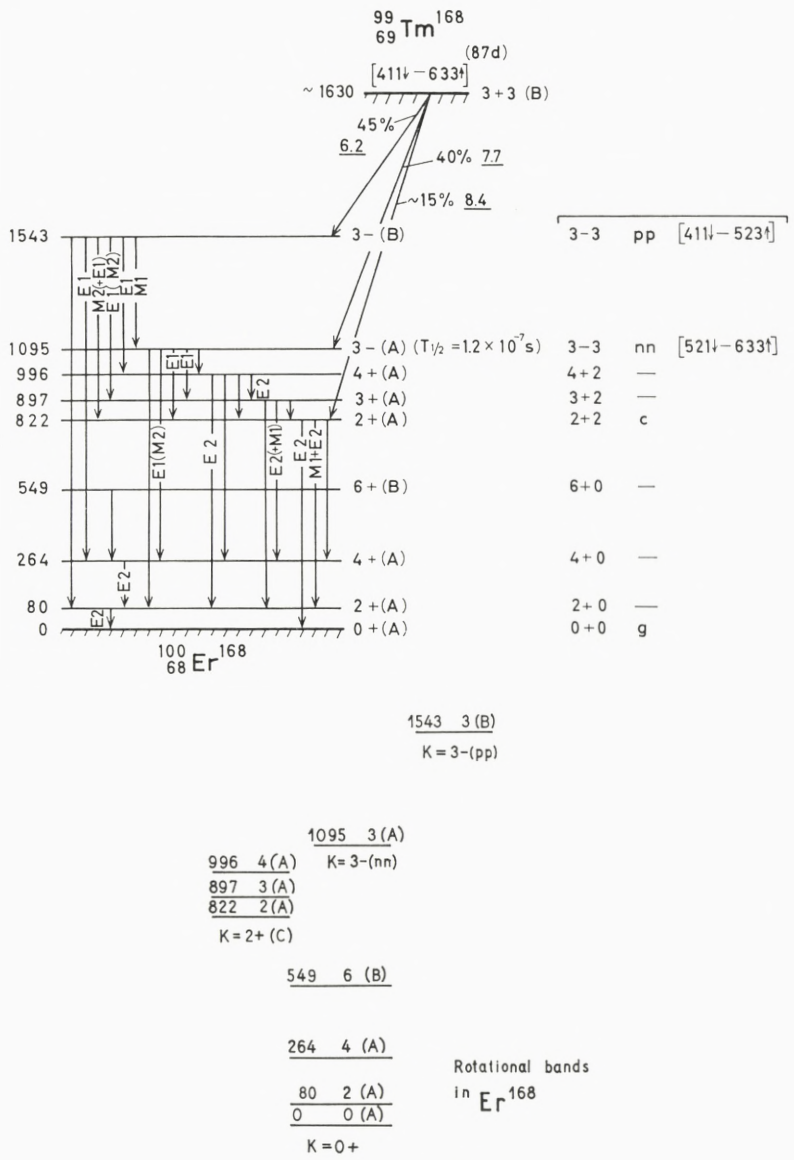

Fig. 11. A = 168.

The decay scheme of Tm^{168} is as reported by K. P. Jacob, J. W. Mihelich, B. Harmatz, and T. H. Handley, Phys. Rev. **117**, 1102 (1960). References to earlier work can be found in the NDS.

(log ft = 7.7) to the 1095 keV level is, however, retarded with respect to the same single-particle transition in odd-mass nuclei, where log ft is 6.4.

It is interesting to note that electron capture from the 3+ configuration to all states other than the two 3− states observed is theoretically forbidden. However, because both 3− states have $\Sigma = 1$, it is possible that the 4− $\Sigma = 0$ states of the two

Tm^{168} (3+3)−1 TABLE III 9a. $^{100}_{68}Er^{168}$

Experimental		Theoretical			1†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft*
3−	1.543	411 ↓ − 523 ↑ p	3 − 3	1.3	1 u	6.1 to 7.4
3−	1.095	521 ↓ − 633 ↑ n	3 − 3	1.1	1 u	7.6 to 8.0
2+	.822	521 ↓ − 512 ↑ n	2 + 2	1.6	aF	8.2 to 8.7
..	..	411 ↑ + 411 ↓ p	2 + 2	1.8	$aA(2)$	..
..	..	(collective)	2 + 2	..	a?	..

† 411 ↓ − 633 ↑

* if $1.65 \leqslant Q_{ec} \leqslant 2.0$.

doublets lie lower in energy than the 3− states, and hence may be populated by weak gamma-ray transitions from them.

The 822, 897, and 996 keV levels form a $K\pi = 2+$ rotational band. All intrinsic 2+ states are expected above ≈ 1.6 MeV, hence the low energy of the state probably indicates collective character.

A = 170.

Tm^{170} has spin 1 and a magnetic moment $|\mu| = 0.25$ nm, in good agreement with what is expected for the configuration 411 ↓ + 521 ↓. Additional support for this assignment is provided by the log $ft = 9.0$ for the beta decay to the Yb^{170} ground

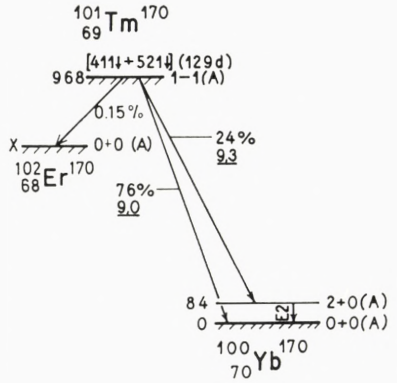

Fig. 12. A = 170.

The decay scheme of Tm^{170} to Yb^{170} is essentially as reported by R. L. GRAHAM, J. L. WOLFSON, and R. E. BELL, Can. J. Phys. **30**, 459 (1952). The 0.15% K-capture branch to Er^{170} has been reported by P. P. DAY, Phys. Rev. **102**, 1572 (1956). The spin of Tm^{170} has recently been measured as 1, the magnetic moment $|\mu| = 0.25$ nm. (I. LINDGREN, A. CABEZAS, and W. NIERENBERG, Bull. Am. Phys. Soc. **5**, 273 (1960)). Preliminary investigations of the Lu^{170} decay scheme have been made by several authors (B. HARMATZ, T. H. HANDLEY, and J. W. MIHELICH, Phys. Rev. **119**, 1345 (1960); B. S. DZHELEPOV, I. F. UCHEVATKIN, and S. A. SHESTOPALOVA, Izvest. Akad. Nauk SSSR, Ser. Fiz. **24**, 802 (1960); V. V. TUCHKEVICH, V. A. ROMANOV, and M. G. IODKO, Izvest. Akad. Nauk SSSR, Ser. Fiz. **24**, 1457 (1960)), but are not included here.

$^{100}_{63}Er^{168}$

TABLE III 9b.

State	$K\pi$	Energy (MeV)		$^{99}_{69}Tm^{168}$ $p = K+1$,	$3+$ $n = K$
		Calcul.	Exper.	Class	log ft
neutron levels					
$K, K+1$	$4-$	1.1	..	$1A(1\,u)$	..
	$3-$	..	1.095	$1\,u$	6.0 (6.2)
K, K / $K+1, K+1$	$0+$	1.2	..	..	..
$K, K+2$	$1-$	1.5	..	1^*u	..
	$6-$	..	..	..	..
$K+1, K+2$	$3+$	1.6	..	aF	..
	$2+$	..	..	aF	..
$K-1, K+1$	$2+$	2.0	..	aF	..
	$3+$	..	..	aF	..
$K-1, K$	$6-$	2.1	..	..	..
	$1-$	..	..	1^*h	..
$K-1, K+2$	$5+$	2.2	..	..	..
	$0+$	..	..	..	..
$K-2, K+1$	$3-$	2.2	..	$1\,F$	..
	$2-$	..	..	$1\,F$	..
$K-2, K$	$1+$	2.3	..	..	..
	$6+$	..	..	..	..
$K, K+3$	$7-$	2.3	..	..	..
	$0-$	..	..	..	..

$K-2 = 642\uparrow$, $K-1 = 523\downarrow$, $K = 633\uparrow$, $K+1 = 521\downarrow$, $K+2 = 512\uparrow$, $K+3 = 514\downarrow$

proton levels					
$K, K+1$	$4-$	1.3	..	$1A(1\,u)$	..
	$3-$	..	1.543	$1u$	7.7 (6.5)
K, K / $K+1, K+1$	$0+$	1.7	..	..	..
$K-1, K+1$	$2+$	1.8	..	$aA(2\,h)$	..
	$1+$	..	..	..	..
$K, K+2$	$7-$	2.1	..	..	..
	$0-$	..	..	..	..
$K-2, K+1$	$2+$	2.2	..	ah	..
	$3+$	..	..	$aA(ah)$	..
$K-1, K$	$2-$	2.3	..	$1\,F$	..
	$5-$	..	..	1^*F	..
$K+1, K+2$	$3+$	2.4	..	ah	..
	$4+$	..	..	$aA(ah)$	..

$K-2 = 413\downarrow$, $K-1 = 411\uparrow$, $K = 523\uparrow$, $K+1 = 411\downarrow$, $K+2 = 404\downarrow$.

Tm^{170} (1 −1)−1 TABLE III 10 a. $^{100}_{70}Yb^{170}$

Experimental		Theoretical			1†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft
2+	.084	ground	2+0	–	1A(1 u)	9.3
0+	0	ground	0+0	–	1A(1 u)	9.0

† 411 ↓ + 521 ↓

state, which is classified as 1 A(1 u). Because the 1 u transition 521 ↓ → 411 ↓ is usually observed to have a log ft = 6.4, the A-forbiddeness in this case results in a retardation of ≈ 400 in the transition rate.

A = 172.

The ground-state configuration of Tm^{172} is clearly established as 2− on the basis of its decay to the 0+, 2+, and 4+ members of the ground-state bands of Yb^{172}. The log ft = 8.7 for the ground-state transition is consistent with a 1*u assignment of the transition. The configuration assignment 411 ↓ − 512 ↑ is therefore unambiguously established.

The 4− configuration 404 ↓ + 521 ↓ is predicted for Lu^{172}. Recently, an extremely complex decay scheme of Lu^{172} has been proposed by B. HARMATZ, T. H. HANDLEY and J. W. MIHELICH (35). These authors have assigned 18 excited levels in the spectrum, which they have been able to analyze into 7 rotational bands, 6 based on excited intrinsic states. The electron capture decay of Lu^{172} populates only states with $K\pi$ = 4+, hence the experimental data are consistent with the assignment of Lu^{172} as 4−.

Using the rotational band analysis proposed by HARMATZ et al., the intrinsic spectrum of Yb^{172} can be interpreted very simply. Two K = 4+ states are predicted in the level spectrum, the proton state 404 ↓ + 411 ↓ and the neutron state 514 ↓ + 521 ↓, and both should be populated by 1 u transitions. We assign the 2194 keV and 2075 keV levels as these configurations, but we are unable to distinguish between them.

Both of the 4+ states have Σ = 1, consequently the Σ = 0 3+ states of the doublets might be expected somewhat lower in energy. Two 3+ intrinsic states have been identified at 1664 and 1702 keV, which we assign as these states. We are again unable to distinguish between the two, but it is not unlikely that the ordering of the configurations will be the same for both the Σ = 0 and Σ = 1 states. We have therefore arbitrarily assumed the ordering shown.

Two other intrinsic states have been identified, a 2+ state at 1468 keV and a 3+ state at 1174 keV. We assign these states as the Σ = 1 and Σ = 0 states, respectively, of the neutron configuration 512 ↑ ± 521 ↓. However, the moment of inertia of the 2+ state is about the same as those of collective 2+ states in this region, so that the interpretation of this level must be regarded as tentative.

With these configuration assignments, the apparent absence of transitions to

$^{100}_{70}Yb^{170}$ TABLE III 10 b.

State	$K\pi$	Energy (MeV)		$^{101}_{69}Tm^{170}$ 1 − $p = K$; $n = K+1$	
		Calc.	Exper.	Class	log *ft*
neutron levels					
$K, K+1$	4 −	1.1		..	
	3 −	..		..	
K, K / $K+1, K+1$	0 +	1.2		1 *F*	
$K, K+2$	1 −	1.5		*aF*	
	6 −	..		..	
$K-1, K+1$	2 +	2.0		1*A*(1**h*)	
	3 +	..		1**h*	
$K-1, K$	6 −	2.1		..	
	1 −	..		*aF*	
$K-1, K+2$	5 +	2.2		..	
	0 +	..		1 *F*	
$K-2, K+1$	3 −	2.2		..	
	2 −	..		*a*A(2)	
$K-2, K$	1 +	2.3		1 *F*	
	6 +	..		..	
$K, K+3$	7 −	2.3		..	
	0 −	..		*aF*	
$K-2 = 642\uparrow$, $K-1 = 523\downarrow$, $K = 633\uparrow$, $K+1 = 521\downarrow$, $K+2 = 512\uparrow$, $K+3 = 514\downarrow$.					
proton levels					
$K, K+1$	3 +	1.4		1*A(3)	
	4 +	..		..	
$K, K+2$	3 +	1.7		1**h*	
	2 +	..		1*A*(1**h*)	
$K, K+3$	5 −	1.8		..	
	4 −	..		..	
K, K / $K+1, K+1$	0 +	~ 1.9		1*A*(1 *u*)	
$K-1, K+1$	7 −	2.0		..	
	0 −	..		*aF*	
$K-1, K$	4 −	2.3		..	
	3 −	..		..	
$K+1, K+2$	6 +	2.3		..	
	1 +	..		1 *F*	
$K+1, K+3$	8 −	2.4		..	
	1 −	..		1 *F*	
$K-2, K+1$	5 +	2.5		..	
	2 +	..		1 *F*	
$K-2 = 411\uparrow$, $K-1 = 523\uparrow$, $K = 411\downarrow$, $K+1 = 404\downarrow$, $K+2 = 402\uparrow$, $K+3 = 514\uparrow$.					

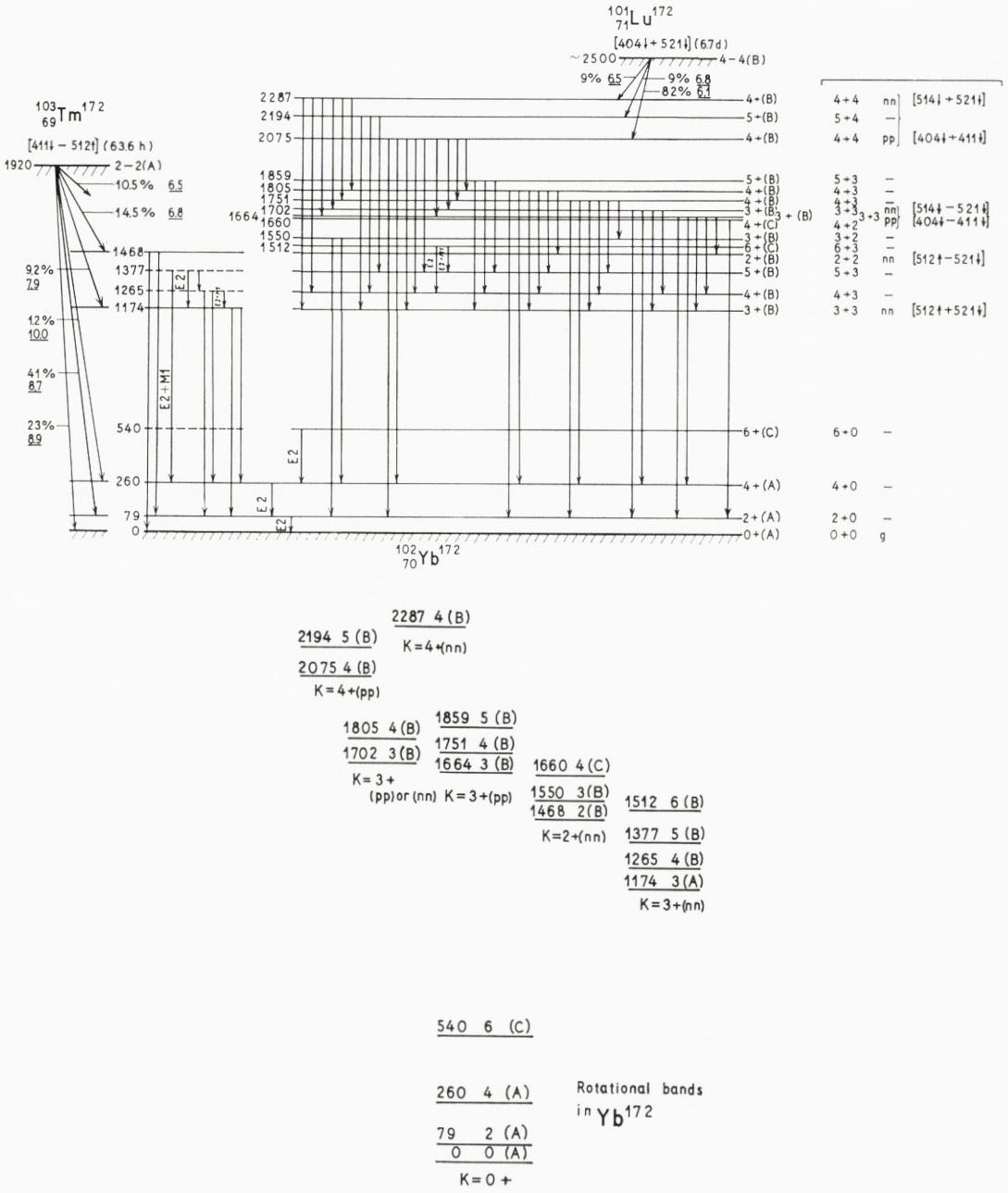

Fig. 13. A = 172.

The decay scheme of Tm^{172} has recently been reported by R. G. Helmer and S. B. Burson, Bull. Am. Phys. Soc. **6**, 72 (1961); Argonne National Laboratory Reprint, ANL-6270, January 1961 (unpublished); P. G. Hansen, O. J. Jensen, and K. Wilsky, Nuclear Phys. **27**, 516 (1961); C. J. Orth and B. J. Dropesky, Phys. Rev. **122**, 1295 (1961). These authors also report data on Er^{172} decay. The Lu^{172} decay scheme has recently been studied by a number of authors (R. G. Wilson and M. L. Pool, Phys. Rev. **118**, 1067 (1960); B. S. Dzhelepov, I. F. Uchevatkin, and S. A. Shestopalova, Izvest. Akad. Nauk SSSR Ser. Fiz. **24**, 802 (1960); V. V. Tuchkevich, V. A. Romanov, and M. G. Iodko, Izvest. Akad. Nauk SSSR, Ser. Fiz. **24**, 1457 (1960); (see also the NDS) but the results shown here are based on the recent results of HHM 61, which are consistent with the results of the above mentioned authors, but more extensive. The analysis into rotational bands was proposed by HHM 61.

Lu^{172} (4−4)−1
Tm^{172} (2−2)−2

TABLE III 11 a.

$^{102}_{70}Yb^{172}$

Experimental		Theoretical			1†		2†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft	Class	log ft
4+	2.287	514 ↓ + 521 ↓ n	4+4	1.9	$1u$	6.5	..	..
4+	2.075	411 ↓ + 404 ↓ p	4+4	1.4	$1u$	6.1	..	..
3+	1.702	514 ↓ − 521 ↓ n	3+3	1.9	$1\Lambda(1u)$	>7.7	..	..
3+	1.664	411 ↓ − 404 ↓ p	3+3	1.4	$1\Lambda(1u)$	>7.7	..	..
2+	1.468	512 ↑ − 521 ↓ n	2+2	1.2	1^*F	>8.1	$1u$	6.8
		collective(?)	2+2	..	..	..	1?	..
3+	1.174	512 ↑ + 521 ↓ n	3+3	1.2	1 F	>8.3	$1\Lambda(1u)$	7.9
4+	.260	ground	4+0	–	..	..	1^*u	10.0
2+	.079	ground	2+0	–	..	..	1^*u	8.7
0+	0	ground	0+0	–	..	..	1^*u	8.9

† 1) 404 ↓ + 521 ↓ 2) 411 ↓ − 512 ↑

the 1702 and 1664 keV levels is explained as Λ-forbiddenness. Transitions to the 1174 keV level are ah, the 404 ↓ (p) → 512 ↑ (n) being strongly hindered experimentally. The log ft's for β-decays to the 1174 and 1468 keV levels from Tm^{172} also follow naturally from the above configuration assignment*.

The theoretical analysis of the level spectrum indicates that both Lu^{172} and Tm^{172} should populate additional levels in Yb^{172} (see Table III 11.b). The 1920 keV decay energy of Tm^{172} probably inhibits some of these transitions, but low energy groups in addition to those shown have been observed. We have not included them in the figure because the low resolution employed in these studies would not have been sufficient to resolve the many transitions expected. The decay energy of Lu^{172} is large and allows population of many more states, and it is therefore not surprising that 41 transitions reported by HARMATZ et al. have *not* been assigned in the decay scheme.

A = 174.

Two isomers of Lu^{174} are observed, 1− and 6−. The coupling rules predict the 1− configuration 404 ↓ − 512 ↑ for the Lu^{174} ground state. The 6− isomeric state is most easily described as the $\Sigma = 0$ member of the ground state doublet. The half-life of the 1− state is not known, but it apparently decays only to the ground, the 76 keV 2+ state of the ground state band and a 2− level at 1321 keV. No negative parity proton states are expected as low as 1300 keV in Yb^{174}, but the 2− neutron configuration 624 ↑ − 512 ↑ has a low energy and should be populated by an ah transition. However, there is a considerable difference between the calculated and

* Possible intrinsic state assignments based on Tm^{172} decay rates have also been discussed by R. G. HELMER and S. B. BURSON[36].

$^{102}_{70}Yb^{172}$

TABLE III 11 b.

State	$K\pi$	Energy (Mev)		$^{103}_{69}Tm^{172}$ 2− $p = K$; $n = K+1$		$^{101}_{71}Lu^{172}$ 4− $p = K+1$; $n = K$	
		Calc.	Exper.	Class	log *ft*	Class	log *ft*
neutron levels							
$K, K+1$	3+	1.1	1.174	$1A(1\,u)$	7.9	$1\,h$	> 8.3
	2+	..	1.468	$1\,u$	6.8 (6.6)	$1^*A(1\,h)$	> 8.1
K, K / $K+1, K+1$	0+	~ 1.3	..	1^*F	..	..	..
$K-1, K+1$	1−	1.4	..	a (2)	..	..	..
	6−	..	..	..	..	..	..
$K-1, K$	4−	1.7	..	..	..	ah	..
	3−	..	..	aF	..	$aA(ah)$	..
$K, K+2$	3+	1.9	1.702	$1\,F$	..	$1A(1\,u)$	> 7.7
	4+	..	2.287	1^*F	..	$1\,u$	6.5 (6.3)
$K+1, K+2$	6+	2.0	..	..	..	1^*F	..
	1+	..	..	1 (3)	..	..	..
$K-1, K+2$	7−	2.1	..	..	..	..	..
	0−	..	..	..	..	..	..
$K-2, K+1$	5+	2.3	..	..	..	$1\,F$	..
	0+	..	..	1^*h	..	..	..
$K, K+3$	5−	2.4	..	..	..	ah	..
	4−	..	..	..	..	$aA(ah)$	..

$K-2 = 523\downarrow$, $K-1 = 633\uparrow$, $K = 521\downarrow$, $K+1 = 512\uparrow$, $K+2 = 514\downarrow$, $K+3 = 624\uparrow$.

proton levels							
$K, K+1$	3+	1.4	1.664	$1\,h$	(8.7)	$1A(1\,u)$	> 7.7
	4+	..	2.075	$1A(1\,h)$	..	$1\,u$	6.1 (6.6)
$K, K+2$	3+	1.7	..	$1A(1\,u)$	..	$1\,F$	..
	2+	..	..	$1\,u$	(6.0)	1^*F	..
$K, K+3$	5−	1.8	..	..	..	aF	..
	4−	..	..	..	..	aF	..
K, K / $K+1, K+1$	0+	~ 1.9	..	1^*u	..	..	..
$K-1, K+1$	7−	2.0	..	..	..	..	..
	0−	..	..	..	..	..	..
$K-1, K$	4−	2.3	..	..	..	aF	..
	3−	..	..	ah	..	aF	..
$K+1, K+2$	6+	2.3	..	..	..	..	..
	1+	..	..	$1\,F$	..	..	..
$K+1, K+3$	8−	2.4	..	..	..	..	..
	1−	..	..	aF	..	..	..
$K-2, K+1$	5+	2.5	..	..	..	$1\,u$	..
	2+	..	..	$1\,F$	..	..	..

$K-2 = 411\uparrow$, $K-1 = 523\uparrow$, $K = 411\downarrow$, $K+1 = 404\downarrow$, $K+2 = 402\uparrow$, $K+3 = 514\uparrow$.

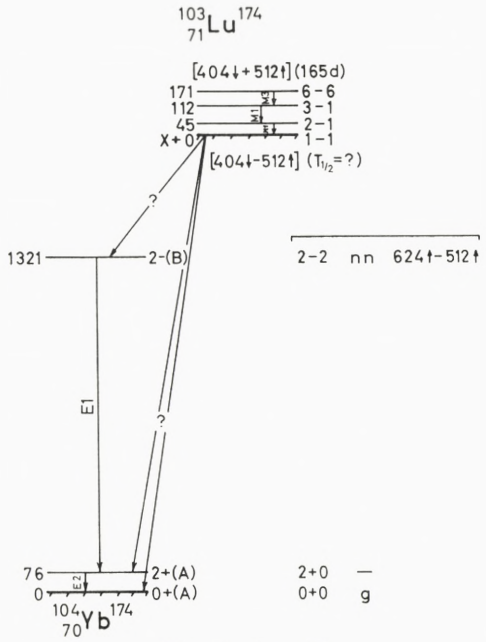

Fig. 14. A = 174.

The levels in Lu^{174} are as reported by B. Harmatz, T. H. Handley, and J. W. Mihelich, Phys. Rev. **119**, 1345 (1960); for earlier results see SHS, the NDS. The decay scheme of the Lu^{174} isomers is as reported by these authors. The level at 1321 keV has recently been established as 2− (H. J. Prask, F. G. Funk, and J. W. Mihelich, priv. comm., May 1961; J. Borggreen, P. Jastram, M. Jørgensen, and O. B. Nielsen, priv. comm., May 1961).

Lu^{174} (1−1)−1 TABLE III 12 a. $^{104}_{70}Yb^{174}$

Experimental		Theoretical			1†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft
2−	1.321	624 ↑ − 512 ↑ n	2−2	2.3	*ah*	–
2+	.076	ground	2+0	–	*ah*	–
0+	0	ground	0+0	–	*ah*	–

† 404 ↓ − 512 ↑

observed energy for this state, which may reflect the fact that the $N = 104$ level spectrum has been calculated only for the first group of level parameters, but actually $N = 104$ is the neutron number at which the transition from the first to the second group occurs. For this case some deviation might be expected.

A = 176.

The measured spin of Lu^{176} is 7, in agreement with the predicted configuration 404 ↓ + 514 ↓. The magnetic moment of the isomer calculated directly from the Nilsson wave functions is not in good agreement with the measured value, but if the

$^{104}_{70}Yb^{174}$

TABLE III 12 b.

State	$K\pi$	Energy (MeV)		$^{103}_{71}Lu^{174}$ 1 − $p = K+1$; $n = K$	
		Calc.	Exper.	Class	log ft
neutron levels					
$K, K+1$	6+	1.6	..	..	..
	1+	..	..	1 u	..
$K-1, K+1$	3+	2.0	..	1*F	..
	4+	..	..	..	..
K, K } $K+1, K+1$	0+	~ 2.2	..	1 h	..
$K, K+2$	2−	2.3	1.321	ah	..
	7−	..	..	..	..
$K-2, K+1$	7−	2.3	..	..	..
	0−	..	..	aF	..
$K, K+3$	2+	2.4	..	1(3)	..
	3+	..	..	1*A(3)	..
$K-1, K+2$	5−	2.6	..	..	..
	4−	..	..	..	..
$K-1, K$	3+	2.6	..	1*A(3)	..
	2+	..	..	1(3)	..
$K+1, K+2$	8−	2.7	..	..	..
	1−	..	..	aF	..

$K-2 = 633\uparrow$, $K-1 = 521\downarrow$, $K = 512\uparrow$, $K+1 = 514\downarrow$, $K+2 = 624\uparrow$, $K+3 = 510\uparrow$.

proton levels					
$K, K+1$	3+	1.4	..	..	..
	4+	..	..	..	..
$K, K+2$	3+	1.7	..	1*F	..
	2+	..	..	1 F	..
$K, K+3$	5−	1.8	..	..	..
	4−	..	..	..	..
K, K } $K+1, K+1$	0+	~ 1.9	..	1 F	..
$K-1, K+1$	7−	2.0	..	..	..
	0−	..	..	ah	..
$K-1, K$	4−	2.3	..	..	..
	3−	..	..	..	..
$K+1, K+2$	6+	2.3	..	..	..
	1+	..	..	1 u	..
$K+1, K+3$	8−	2.4	..	..	..
	1−	..	..	a(2)	..
$K-2, K+1$	5+	2.5	..	..	..
	2+	..	..	1 u	..

$K-2 = 411\uparrow$, $K-1 = 523\uparrow$, $K = 411\downarrow$, $K+1 = 404\downarrow$, $K+2 = 402\uparrow$, $K+3 = 514\uparrow$.

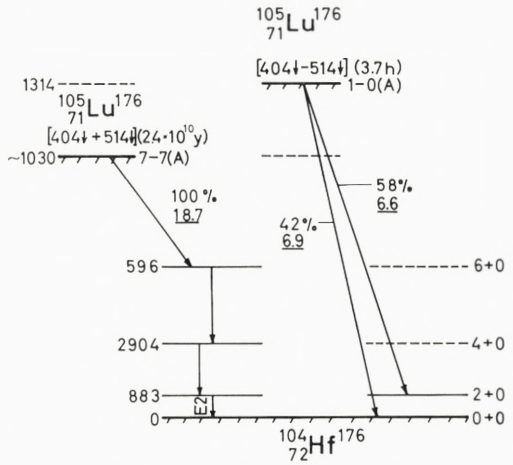

Fig. 15. A = 176.

The spin of 7 of long lived Lu^{176} is based on atomic spectroscopy and Coulomb excitation results. The magnetic moment of +2.8 is determined from atomic spectroscopic measurements. The decay scheme has been checked by several authors (see SHS, the NDS for references). The spin of 3.7 *h* Lu^{176} has recently been measured as 1 (M. B. White, S. S. Alpert, and E. Lipworth, Bull. Am. Phys. Soc. **5**, 273 (1960)). The $K = 0-$ quantum number assignment is based on the recent measurements of the beta branching of this isomer to the 0+ and 2+ levels of Hf^{176}. (I. Řezánka, J. Frána, J. Adam, and L. K. Peker, Izvest. Akad. Nauk SSSR, Ser. Fiz. **26**, 127 (1961)). The beta endpoint energies are also taken from this work. Preliminary studies of Ta^{176} decay (J. O. Rasmussen and D. A. Shirley, University of California Radiation Laboratory Report UCRL-8618 (1959) (unpublished); B. Harmatz, T. H. Handley, and J. W. Mihelich, Phys. Rev. **119**, 1345 (1960)) indicate that the decay scheme is very complex.

Lu^{176} (1−0)−1
(7−7)−2

Table III 13 a.

$^{104}_{72}Hf^{176}$

Experimental		Theoretical			1†		2†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log *ft*	Class	log *ft*
6+	.596	ground	6+0	–	..	..	$1K(1u)$	18.7
2+	.088	ground	2+0	–	$1u$	6.6	..	..
	0	ground	0+0	–	$1u$	6.9	..	..

† 1) 404 ↓ − 514 ↓ 2) 404 ↓ + 514 ↓

empirical magnetic moment of the 404 ↓ proton is substituted for the calculated 404 ↓ magnetic moment good agreement is obtained[18]. The beta decay of long-lived Lu^{176} is the classical example of *K*-forbidden beta decay.

Two possible spin 1 isomeric states are possible for the 3.7 h Lu^{176}, the $\Sigma = 0$ doublet state 404 ↓ − 514 ↓ and the $\Sigma = 1$ configuration 404 ↓ − 624 ↑. The recent measurements of the beta branching ratio for the decay of this isomer favour the $K\pi = 0-$ assignment.

$^{104}_{72}Hf^{176}$

TABLE III 13b.

State	$K\pi$	Energy (MeV)		$^{105}_{71}Lu^{176}$ $1-0$ $p=K$; $n=K+1$		$^{105}_{71}Lu^{176}$ $7-$ $p=K$; $n=K+1$	
		Calc.	Exper.	Class	log ft	Class	log ft
neutron levels							
$K, K+1$	$6+$	1.6	..	..	..	$1\,h$	..
	$1+$	..	..	$1\,h$	..	..	..
$K-1, K+1$	$3+$	2.0	..	..	..	..	..
	$4+$	..	..	..	..	..	..
K, K / $K+1, K+1$	$0+$	~2.2	..	$1\,F$	..	..	..
$K, K+2$	$2-$	2.3	..	aF	..	..	..
	$7-$	..	..	..	..	aF	..
$K-2, K+1$	$7-$	2.3	..	..	..	ah	..
	$0-$	..	..	ah	..	..	..
$K, K+3$	$2-$	..	..	aF	..	..	..
	$3-$	2.4	..	..	..	..	..
$K-1, K-2$	$5-$	2.6	..	..	..	..	..
	$4-$	..	..	..	..	..	..
$K-1, K$	$3+$	2.6	..	1^*F	..	..	..
	$2+$	..	..	$1\,F$	..	..	..
$K+1, K+2$	$8-$	2.7	..	..	..	ah	..
	$1-$	..	..	ah	..	..	..

$K-2 = 633\uparrow$, $K-1 = 521\downarrow$, $K = 512\uparrow$, $K+1 = 514\downarrow$, $K+2 = 624\uparrow$, $K+3 = 510\uparrow$.

proton levels							
$K, K+1$	$8-$	1.0	..	..	..	au	(4.7)
	$1-$	..	..	au	..	..	..
K, K / $K+1, K+1$	$0+$	~1.2	..	$1\,u$	..	..	..
$K-1, K+1$	$5-$	1.7	..	..	..	..	..
	$4-$	..	..	..	..	..	..
$K, K+2$	$6+$	1.8	..	..	..	$1\,h$	..
	$1+$	..	..	$1\,h$	..	..	..
$K-1, K$	$3+$	1.8	..	1*(3)	..	..	..
	$4+$	..	..	..	..	..	..
$K+1, K+2$	$2-$	1.9	..	aF	..	..	..
	$7-$	..	..	..	..	aF	..
$K-2, K+1$	$1+$	2.2	..	$1\,F$	..	..	..
	$8+$	..	..	..	..	$1\,F$	..
$K-2, K$	$7-$	2.3	..	..	..	ah	..
	$0-$	..	..	ah	..	..	..

$K-2 = 523\uparrow$, $K-1 = 411\downarrow$, $K = 404\downarrow$, $K+1 = 514\uparrow$, $K+2 = 402\uparrow$.

A = 178.

Two isomers of Ta^{178} are known. The 9.3 m isomer decays by transitions with log *ft* = 4.6 to the 0+ and 2+ levels in Hf^{178}, clearly indicating the 1+ configuration $514\uparrow - 514\downarrow$ for the isomer. The 2.1 h isomer decays by a transition with log *ft* = 4.9 to an 8− level at 1148 keV in Hf^{178}. The *au* transition to this 8− state and the similarity in energy to the 1142 keV 5.5 h 8− isomer in Hf^{180} suggest the assignment of the 8− state as the proton configuration $404\downarrow + 514\uparrow$ and the Ta^{178} isomer as the 7− configuration $404\downarrow + 514\downarrow$. The latter state is predicted as the Ta^{178} ground state by the spin coupling rules, hence it has been drawn below the 1+ state in the figure.

The energy of the 8− state at 1480 keV is in excellent agreement with the calculated energy of the neutron configuration $624\uparrow + 514\downarrow$. The population of this state by an electron capture branch with a log *ft* = 4.9 is, however, seriously inconsistent with the interpretation of the state as a two-neutron state, and suggests that the state contains a large amplitude of the 1148 keV two-proton state. The *M*1 transition between them is then consistent with this interpretation.

The 1+ Ta^{178} isomer populates two 0+ levels at 1197 and 1440 keV. The similarity in energy of these two levels to the 8− levels suggests their assignment as proton and neutron pair excitations, respectively. The calculated energies of the lowest-lying pair excitations are in excellent agreement with this interpretation.

The 1+ state at 1430 keV is difficult to explain, because it is populated by an *au* electron-capture transition, and we can give no simple explanation for this fast transition within the framework we discuss. Furthermore, the energy of the state is somewhat lower than the energies of the 1+ states expected in the spectrum. These isomers have previously been discussed by Gallagher and Nielsen[37].

Ta^{178} (7−7)−1
(1+1)−2

Table III 14 a. $^{106}_{72}Hf^{178}$

Experimental		Theoretical			1†		2†	
$I\pi$	*E*	Final configuration	$I\pi K$	*E*	Class	log *ft*	Class	log *ft*
8−	1.480	$624\uparrow + 514\downarrow$ *n*	8−8	1.5	*ah*	4.9	..	..
0+	1.440	neutron	0+0	1.7	..	..	*au*	4.7
1+	1.430	$512\uparrow - 514\downarrow$ *n*	1+1	2.0	..	..	*a*(2)	≈4.4
		$404\downarrow - 402\uparrow$ *p*	1+1	1.9	..	..	*aF*	..
0+	1.197	proton	0+0	1.2	..	..	*aF*	5.1
8−	1.148	$404\downarrow + 514\uparrow$ *p*	8−8	1.0	*au*	4.9	..	..
2+	.093	ground	2+0	−	..	..	*au*	4.8
0+	0	ground	0+0	−	..	..	*au*	4.6

† 1) $404\downarrow + 514\downarrow$ 2) $514\uparrow - 514\downarrow$

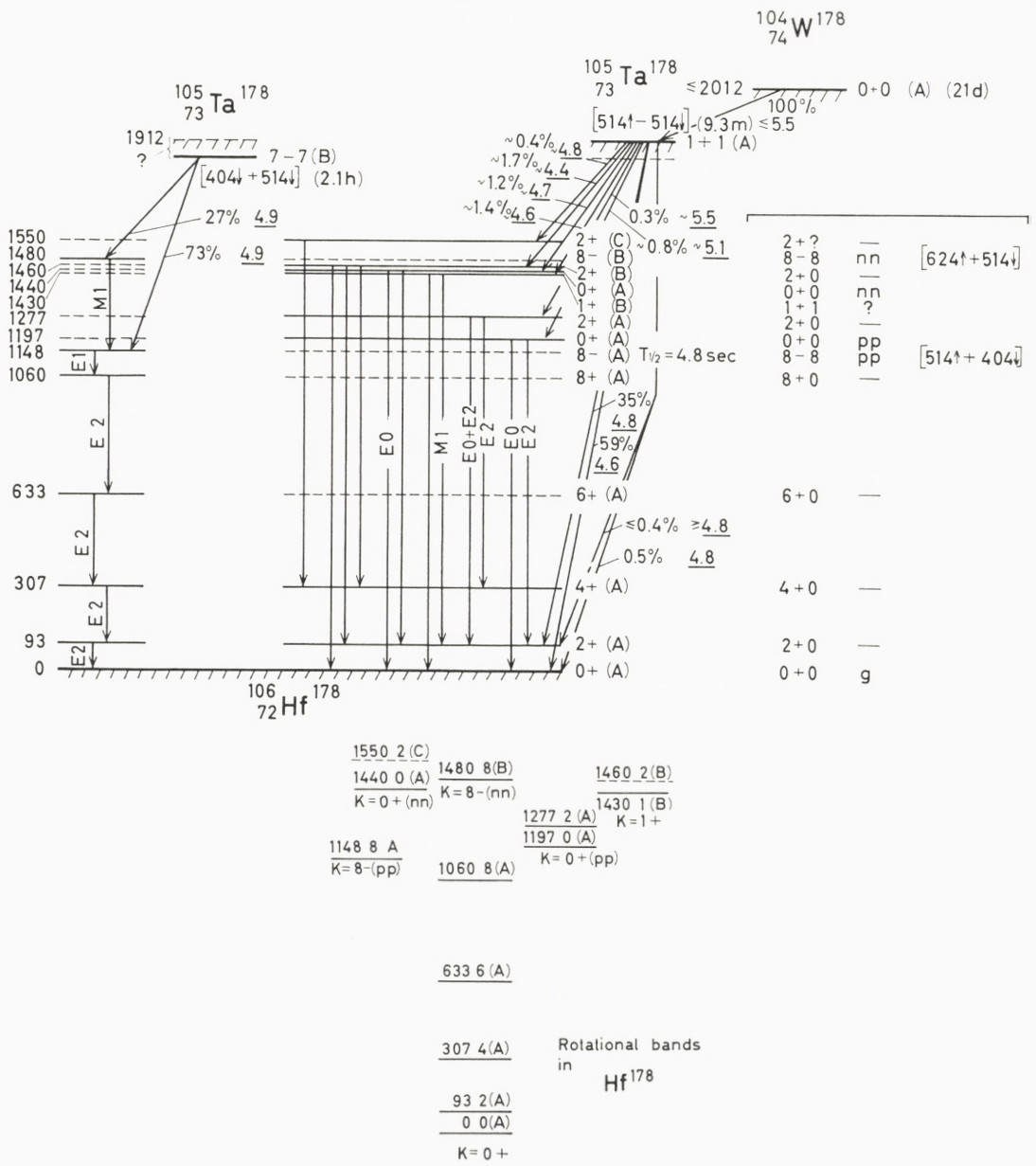

Fig. 16. A = 178.

The decay scheme of 9.3 min. Ta^{178} has recently been studied by C. J. Gallagher, Jr., H. L. Nielsen, and O. B. Nielsen, Phys. Rev. **123**, 1590 (1961); J. Borggreen, U. Bertelsen, and O. Nathan, Phys. Rev. **123**, 564 (1961). Previous experimental studies are reviewed in the former work. The decay scheme of 2.1 *h* Ta^{178} was first reported by F. F. Felber, F. S. Stephens, and F. Asaro, J. Inorg. Nuclear Chem. **7**, 153 (1958). The M1 assignment of the 331.7 keV transition is as proposed by B. Harmatz, T. H. Handley, and J. W. Mihelich, Phys. Rev. **119**, 1345 (1960). The spin 8 of the 1148 keV level has recently been established by M. Deutsch and R. W. Bauer, Nuclear Phys. **21**, 128 (1960). The analysis of the level scheme has previously been discussed (C. J. Gallagher, Jr., and H. L. Nielsen, Phys. Rev. (to be published)). The estimate of the total decay energy of W^{178} to 9.3 *m* Ta^{178} is based on a measurement of an upper limit on the K/Total-capture ratio of W^{178} (C. J. Gallagher, Jr., and H. L. Nielsen, unpublished data (1960). Other data on W^{178} decay are as reported in SHS.

$^{106}_{72}Hf^{178}$

TABLE III 14 b.

State	$K\pi$	Energy (MeV)		$^{105}_{73}Ta^{178}$ 7− $p = K+1$; $n = K$		$^{105}_{73}Ta^{178}$ 1+ $p = K$; $n = K$	
		Calc.	Exper.	Class	log ft	Class	log ft
neutron levels							
$K, K+1$	8−	1.5	1.480	ah	4.9 (6.9)	..	..
	1−	..	..	..	..	1 u	..
K, K / $K+1, K+1$	0+	1.7	1.440	..	..	au	≈ 4.6
$K-1, K+1$	2−	1.7	..	..	..	1 F	..
	7−	..	..	aF	..	..	..
$K, K+2$	4+	1.9	..	..	..	..	..
	3+	..	..	..	..	..	..
$K-1, K$	6+	2.0	..	1 h	..	..	..
	1+	..	..	..	..	ah	..
$K, K+3$	2+	2.3	..	..	..	$a(2)$	..
	5+	..	..	1*h	..	..	..
$K-2, K$	3+	2.3	..	..	..	..	..
	4+	..	..	..	..	..	..

$K-2 = 521\downarrow$, $K-1 = 512\uparrow$, $K = 514\downarrow$, $K+1 = 624\uparrow$, $K+2 = 510\uparrow$, $K+3 = 512\downarrow$.

proton levels							
$K, K+1$	8−	1.0	1.148	au	4.9 (4.7)	..	..
	1−	..	..	..	..	1 u	..
K, K / $K+1, K+1$	0+	1.2	1.197	..	..	aF	≈ 5.1
$K-1, K+1$	3+	1.7	..	..	..	..	..
	4+	..	..	..	..	..	..
$K, K+2$	2−	1.8	..	..	..	1 h	..
	7−	..	..	aF	..	..	..
$K-1, K$	5−	1.8	..	..	..	..	..
	4−	..	..	..	..	..	..
$K+1, K+2$	6+	1.9	..	1 h	..	..	..
	1+	..	..	..	..	aF	..
$K-2, K+1$	7−	2.2	..	ah	..	..	..
	0−	..	..	..	..	1 F	..
$K-2, K$	1+	2.3	..	..	..	ah	..
	8+	..	..	1 F	..	..	..

$K-2 = 523\uparrow$, $K-1 = 411\downarrow$, $K = 514\uparrow$, $K+1 = 404\downarrow$, $K+2 = 402\uparrow$.

A = 180.

The isomeric state in Hf^{180}, in analogy to that in Hf^{178}, is assigned as the proton configuration $514\uparrow + 404\downarrow$.

Two isomers of Ta^{180} are known. The spin coupling rules predict a 1+ configuration $404\downarrow - 624\uparrow$ as the ground state, a 9− configuration $514\uparrow + 624\uparrow$ as a low

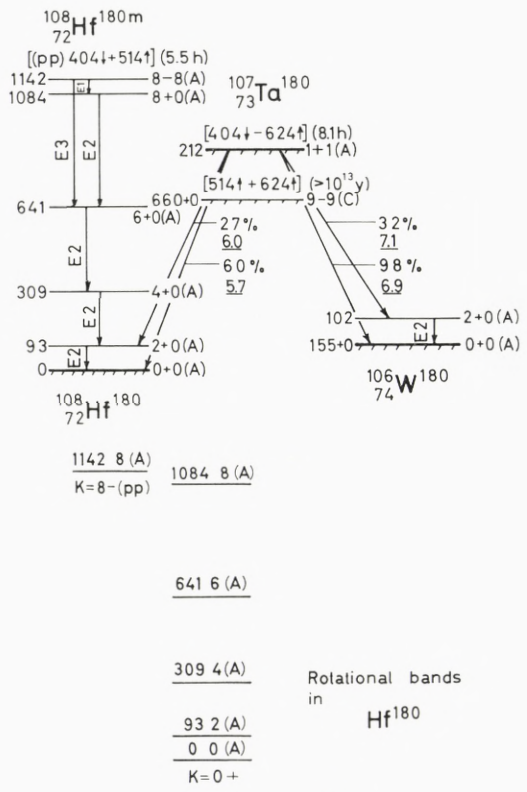

Fig. 17. A = 180.

The decay of 5.5 *h* Hf^{180} is as reported in SHS, the NDS. The spin 8 of the 1142 keV level has recently been established by M. Deutsch and R. W. Bauer, Nuclear Phys. **21**, 128 (1960). Limits on the half-life of the long-lived Ta^{180} using different methods have been set by P. Eberhardt, J. Geiss, and C. Lang, Z. Naturforsch. **10a**, 796 (1955); E. R. Bauminger and S. G. Cohen, Phys. Rev. **110**, 953 (1958). The beta and electron capture branching ratios of 8.15 hour Ta^{180} have been measured by C. J. Gallagher, Jr., M. Jørgensen, and O. Skilbreid, Nuclear Phys. (to be published), but the decay scheme of the isomer is essentially as proposed by H. N. Brown, W. L. Bendel, F. S. Store, and R. A. Becker, Phys. Rev. **84**, 292 (1951). The relative ordering of the two isomers is based on the Ta^{181} (γ, n) Ta^{180} reaction studies of K. N. Geller, J. Halpern, and E. G. Muirhead, Phys. Rev. **118**, 1302 (1960). The E.C. decay energy is based on a recent adjustment of mass values in the rare earth region (A. H. Wapstra, priv. comm. May 1961).

Ta^{180} (1+1)−1
(9−9)−2

Table III 15. $^{108}_{72}Hf^{180}$ $^{106}_{74}W^{180}$

Experimental		Theoretical			1†		2†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft*	Class	log ft
2+	.102	ground (W^{180})	2+0	–	*ah*	7.1	..	..
0+	0	ground (W^{180})	0+0	–	*ah*	6.9	..	..
2+	.093	ground (Hf^{180})	2+0	–	*ah*	6.2	..	..
0+	0	ground (Hf^{180})	0+0	–	*ah*	5.9	..	..

† 1) 404 ↓ − 624 ↑ 2) 514 ↑ + 624 ↑

* assuming $Q_{EC} = .872$.

lying isomer. The results of Ta^{181} (γ, n) Ta^{180} reactions, however, seem to indicate that the high spin isomer actually lies below the 1+ state. On the basis of measurements of the $\beta-$ and electron capture branching ratios of the 8.15 h isomer of Ta^{180}, its $K\pi = 1+$ assignment seems well established.

A = 182.

The beta decay of Ta^{182} populates 2+, 2−, 3−, and 4− states in W^{182}, suggesting 3− as the most probable configuration for the ground state of Ta^{182}, in agreement with the 3− configuration predicted by the coupling rules.

Two Re^{182} isomers are observed. On the basis of the decay schemes of the isomers a $2\pm$ or $3\pm$ assignment is possible for the 13 *h* isomer, and $7\pm$ is the most probable assignment for the 60 h isomer. A 7+ configuration, $402\uparrow + 624\uparrow$, is predicted as the Re^{182} ground state. Two possible configurations seem equally probable for the 13 h isomer if the energy level systematics in odd-mass nuclei are considered, either the $2+$ $\Sigma = 0$ state of the ground state doublet, or the $\Sigma = 1$ 3− neutron excitation state $402\uparrow + 510\uparrow$.

The W^{182} level spectrum determined from the decay of the 3 nucleides is extremely complex, but the apparent complexity is reduced considerably by analysis into rotational bands. Our tentative analysis is shown in Fig. 18.

Beginning with the decay of Ta^{182}, the 1290 keV state appears to be the base state of a $K = 2-$ band, to which belong the 1374 and 1488 keV levels. The 1554 keV state is assigned as the base state of a $K = 4-$ band. The lowest lying intrinsic proton state is the 2− configuration $514\uparrow - 402\uparrow$, and the lowest lying neutron state is the 4− configuration $624\uparrow - 510\uparrow$. Beta decay from 3− Ta^{182} to the 2− state is non-overlap forbidden, and the transitions to this state are strongly retarded (but somewhat less than might be expected). Beta decay to the 4− state at 1554 keV is *ah*, and the log *ft* = 6.8 observed for the transition is equal within experimental error to the transition rate for the $404\downarrow$ (p)→$624\downarrow$ (n) transition observed in odd-mass nuclei. The 2+ state at 1222 seems best described as a collective state. The beta transition to this state is strongly retarded. We are uncertain whether the $K = 0+$ state (unobserved) on which the 1258 keV 2+ state is based should be assigned as a collective state or as a pair excitation.

The decay of 13 h Re^{182} populates predominantly the $K\pi = 2-$ rotational band at 1290 keV. Decays to this band from the 3− state $402\uparrow + 510\uparrow$ are strongly forbidden, whereas transitions from the 2+ state $402\uparrow - 624\uparrow$ are *ah*, with log *ft* = 6.8. The 13 h Re^{182} isomer therefore seems best assigned as the $\Sigma = 0$ state of the Re^{182} ground state doublet. A 2− state at 2185 keV and a 3− state at 2024 keV are also populated by 2+ Re^{182}. On the basis of the decay ratio to these states, assignments of $624\uparrow - 512\uparrow$ and $624\uparrow - 512\downarrow$, respectively, to these states seem reasonable.

The decay of the 7+ isomer populates predominantly 6− and 7− states. A definite analysis of these states is difficult, and the analysis shown must be considered

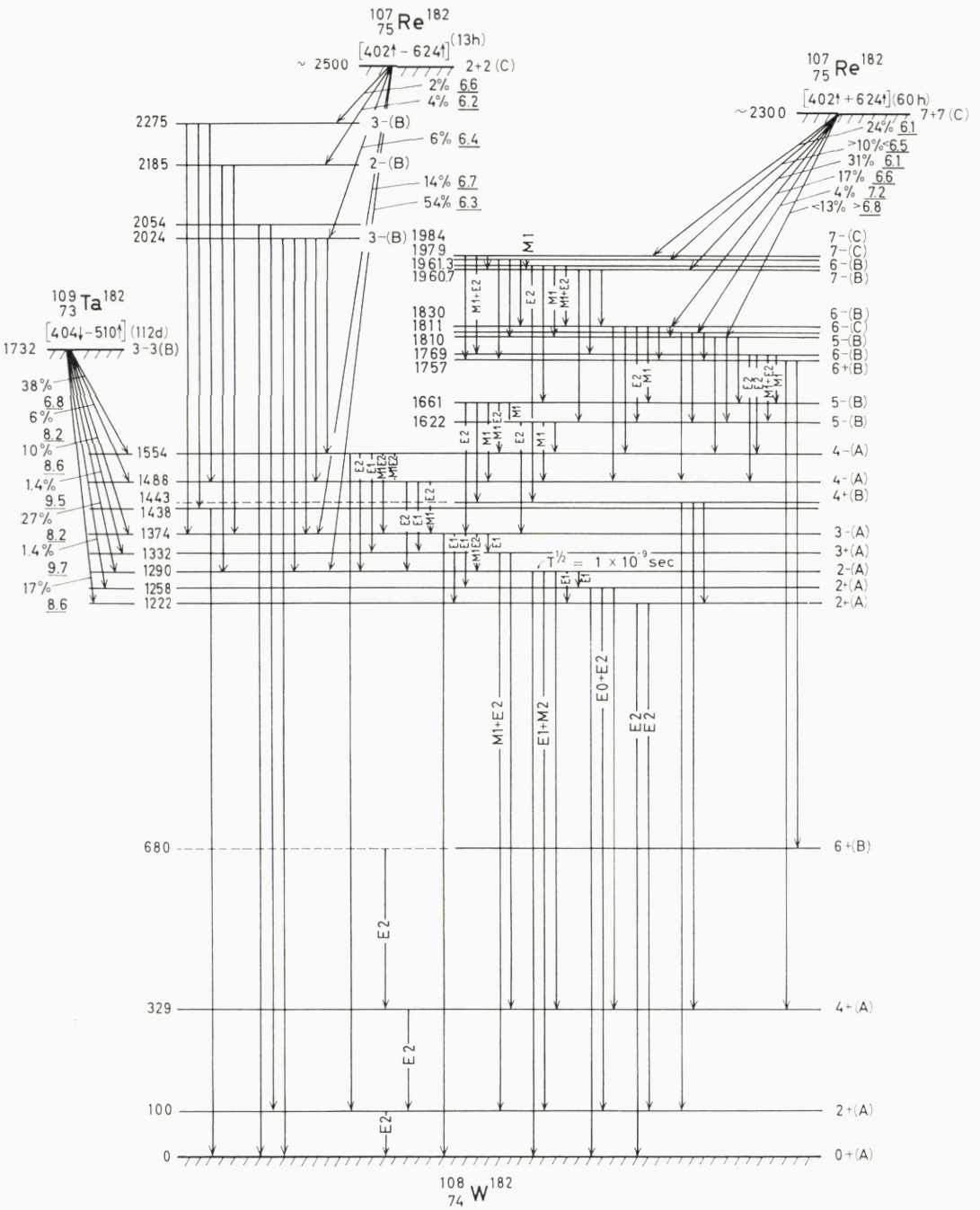
107 75 Re 182
[402↑ - 624↑] (13h)
~ 2500
2+2 (C)
2% 6.6
4% 6.2
2275
3-(B)
6% 6.4
2185
2-(B)
14% 6.7
54% 6.3
2054
2024
3-(B)
107 75 Re 182
[402↑ + 624↑] (60 h)
~ 2300
7+7 (C)
24% 6.1
>10% <6.5
31% 6.1
17% 6.6
4% 7.2
<13% >6.8
109 73 Ta 182
[404↓ - 510↑] (112d)
1732
3-3(B)
38% 6.8
6% 8.2
10% 8.6
1.4% 9.5
27% 8.2
1.4% 9.7
17% 8.6
1554
1488
1443
1438
1374
1332
1290
1258
1222
1984
1979
1961.3
1960.7
1830
1811
1810
1769
1757
1661
1622
M1
M1+E2
E2
M1
M1+E2
7-(C)
7-(C)
6-(B)
7-(B)
6-(B)
6-(C)
5-(B)
6-(B)
6+(B)
5-(B)
5-(B)
4-(A)
4-(A)
4+(B)
3-(A)
3+(A)
2-(A)
2+(A)
2+(A)
T½ = 1 × 10⁻⁹ sec
M1+E2
E1+M2
E0+E2
E2
E2
680
329
100
0
E2
E2
E2
6+(B)
4+(A)
2+(A)
0+(A)
108 74 W 182
3 − 2 —
2 − 2 nn [624↑ - 512↑]
3 − 3 nn [624↑ - 512↓]
7 − 2,7 —
7 − 6 —
6 − 5 —
7 − 7,2 {pp [402↑ + 514↑]
nn [512↑ + 624↑]
6 − 6 nn [624↑ + 512↓]
6-2,4
5 − 5 nn [624↑ + 510↑]
6 − 2 —
6 + 6 pp [404↓ + 402↑]
5 − 4 —
5 − 2 —
4 − 4 nn [624↑ - 510↑]
4 − 2 —
4
3 − 2 —
3 + 2 —
2 − 2 pp [514↑ - 402↑]
2 + 0 —
2 + 2 (c)
6 + 0 —
4 + 0 —
2 + 0 —
0 + 0 g

Fig. 18. A = 182.

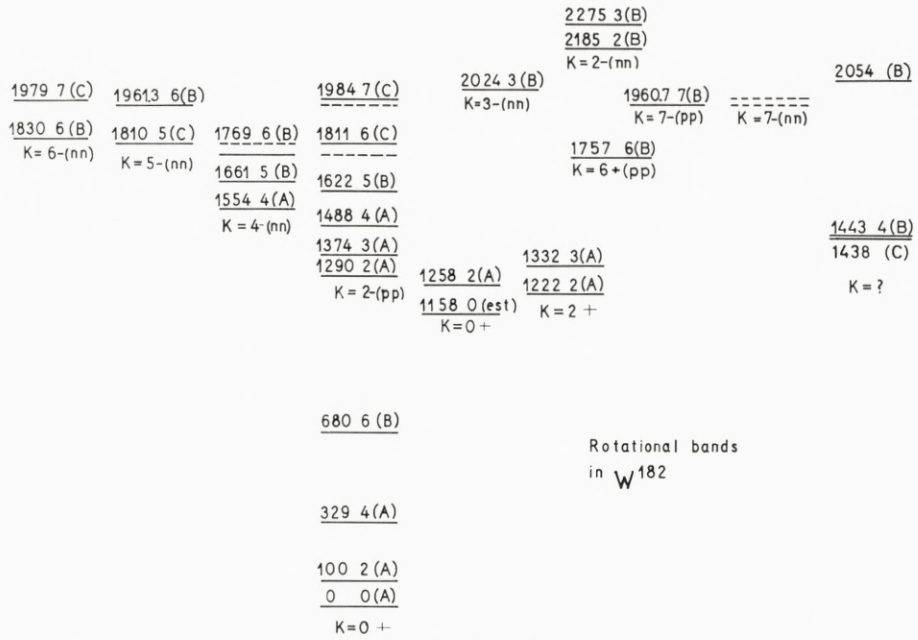

Fig. 18. A = 182.

The decay scheme of Ta^{182} has been extensively studied. The decay scheme shown is essentially that proposed by J. J. Murray, F. Boehm, P. Marmier, and J. W. M. Du Mond, Phys. Rev. **97**, 1007 (1955). It should be noted that the primary beta branchings reported by these authors have been questioned, but the values shown are theirs. (Other work which supports the decay scheme and established the level spin is reported in SHS and the NDS). The 1258 level has recently been reassigned by V. S. Grozdev, L. I. Rusinov, and Yu L. Khazov, Izvest. Akad. Nauk SSSR. Ser. Fiz. **24**, 1444 (1960) from data on Ta^{182} decay and independently by HHM 61 from data on 13 *h* Re^{182} decay. The decay of the 16 m Ta^{182} isomer has recently been studied in some detail (A. W. Sunyar and P. Axel, Phys. Rev. **121**, 1158 (1961)). However, because it is not as yet clear how the levels reported in this work fit into the Ta^{182} level spectrum, we have not included these results in the figure. The levels in W^{182} populated by 13 *h* Re^{182} are as proposed by C. J. Gallagher, Jr., J. O. Newton, and V. S. Shirley, Phys. Rev. **113**, 1298 (1959), with additional levels at $\approx$2 Mev as proposed by HHM 61. The electron capture branching ratios reported by HHM 61 are shown. The electron capture decay of 60 hour Re^{182} has been studied by C. J. Gallagher, Jr., and J. O. Rasmussen, Phys. Rev. **112**, 1730 (1958) and HHM 61. Transitions supporting several of the levels proposed in the former work have been reassigned by the latter authors on the basis of more detailed results. The electron capture branching ratios are as reported by HHM 61.

tentative at least for the 8 states beginning with the 6 – states at 1769 keV. However, the qualitative prediction of many 6 – and 7 – intrinsic states seems well borne out. On the basis of the observed branching, we tentatively assign the 1810 keV 5 – state as the neutron state $624\uparrow + 510\uparrow$, and the 6 – 1830 keV state as the neutron state $624\uparrow + 512\downarrow$. There seem to be at least three 7 – states in the observed spectrum, whereas theoretically, in addition to the two intrinsic 7 – states expected, the neutron state $624\uparrow + 512\uparrow$ and the proton state $514\uparrow + 402\uparrow$, many 7 – rotational states based on the lower-lying negative parity states should also be present.

We have assigned the 1757 keV level as the $K\pi = 6+$ proton state $404\downarrow + 402\uparrow$. This state should be populated directly by electron capture, and although Harmatz et al.[35] indicate no primary capture, the de-exciting gamma-ray intensity seems

Ta^{182} (3−3)−1
Re^{182} (7+7)−2
(2+2)−3

TABLE III 16 a. $^{108}_{74}W^{182}$

Experimental		Theoretical			1†		2†		3†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft	Class	log ft	Class	log ft
2−	2.185	624 ↑ − 512 ↑ n	2−2	2.3	..	..	..	..	1 u	6.2
3−	2.024	624 ↑ − 512 ↓ n	3−3	1.9	..	..	..	..	1 u	6.4
7−	1.984	rot. state 1.290	7−2	..	..	..	1 K(1 u)	6.1	..	..
..	..	rot. state 1.554	7−4	..	..	..	1 K(1*h)	..	..	..
..	..	rot. state 1.830	7−6	..	..	..	1 u	..	..	..
..	..	624 ↑ + 512 ↑ n	7−7	2.3	..	..	1 u	..	..	..
..	..	514 ↑ + 402 ↑ p	7−7	1.3	..	..	1 u	..	..	..
7−	1.979	same as 1.984	..	..	..	..	..	< 6.5	..	..
6−	1.9613	rot. state 1.810	7−6	..	..	..	..	> 7	..	..
..	..	624 ↑ + 512 ↓ n	6−6	1.9	..	..	1 u	..	..	..
7−	1.9607	same as 1.984	..	..	..	..	..	6.1	..	..
6−	1.830	624 ↑ + 512 ↓ n	6−6	1.9	..	..	1 u	6.6	..	..
..	..	rot. state 1.290	6−2	..	..	..	1 K(1 u)	..	..	..
..	..	rot. state 1.554	6−4	..	..	..	1 K(1*h)	..	..	..
6−	1.811	same as 1.830	..	..	..	..	..	7.2	..	..
5−	1.810	624 ↑ + 510 ↑ n	5−5	1.5	..	..	1*h	> 6.8	..	..
6+	1.757	404 ↓ + 402 ↑ p	6+6	1.4	..	..	ah	..	..	..
4−	1.554	624 ↑ − 510 ↑ n	4−4	1.5	ah	6.8	..	..	1*h	> 7
2−	1.290	514 ↑ − 402 ↑ p	2−2	1.3	aF	8.2	..	..	1 u	6.3
2+	1.258	collective	2+0	..	1 K	≈ 9.7	..	..	..	..
2+	1.222	collective	2+2	..	1?	≈ 8.6	..	..	..	..

† 1) 404 ↓ − 510 ↑ 2) 402 ↑ + 624 ↑ 3) 402 ↑ − 624 ↑

to far exceed that exciting it. Direct capture does not therefore seem ruled out by the experimental data.

It seems somewhat surprising that the $7- \Sigma = 1$ state of the 514 ↑ ± 402 ↑ doublet does not occur lower in energy than ≈ 2 MeV, because with the present assignment the energy of spin splitting for this level is ≈ 700 keV. That it does occur at such a high excitation energy seems to be borne out by the absence of any strongly populated state around 1500 keV which decays directly to the 6+ and 8+ members of the ground-state band.

A = 184.

Re^{184} electron capture populates levels with $I\pi = 3+$ and 2+, and decays only weakly, if at all, to the $K\pi = 0+$ ground state band in W^{184}, indicating 2±, 3± as the most probable spin assignments. A $K\pi = 3-$ configuration 402 ↑ + 510 ↑ is predicted as the Re^{184} ground state, in good agreement with the experimental data.

$^{108}_{74}W^{182}$

TABLE III 16 b.

State	$K\pi$	Energy (MeV)		$^{109}_{73}Ta^{182}$ 3− $p = K-1$; $n = K+1$		$^{107}_{75}Re^{182}$ 7+ $p = K+1$; $n = K$		$^{107}_{75}Re^{182}$ 2+ $p = K+1$; $n = K$	
		Calc.	Exper.	Class	log ft	Class	log ft	Class	log ft
neutron levels									
$K, K+1$	4−	1.5	1.554	ah	6.8 (6.9)	..	..	1^*h	..
	5−	..	1.810	..	..	1^*h	large	..	..
K, K ..... / $K+1, K+1$	0+	1.6	..	..	..	..	..	..	..
$K, K+2$	6−	1.9	1.830	..	..	$1\,u$	6.6 (7.3)	..	..
	3−	..	2.024	aF	..	..	..	$1\,u$	6.4 (7.3)
$K-1, K+1$	4+	1.9	..	$1\,u$	..	..	..	..	..
	3+	..	..	$1\Lambda(1\,u)$	..	..	..	aF	..
$K-1, K$	8−	2.0	..	..	..	$1\,h$	..	..	..
	1−	..	..	..	..	..	..	$1\,h$	..
$K-2, K+1$	2+	2.1	..	$1\,h$	..	..	..	aF	..
	3+	..	..	$1\Lambda(1\,h)$	..	..	..	aF	..
$K, K+3$	1−	2.2	..	..	..	..	..	$1\,u$	..
	8−	..	..	..	..	$1\,u$	..	..	..
$K+1, K+2$	2+	2.2	..	$1\Lambda(1^*h)$	..	..	..	aF	..
	1+	..	..	1^*h	..	..	..	aF	..
$K-2, K$	2−	2.3	2.184	aF	..	..	..	$1\,u$	(6.7)
	7−	..	..	..	..	$1\,u$	(6.7)	..	..

$K-2 = 512\uparrow$, $K-1 = 514\downarrow$, $K = 624\uparrow$, $K+1 = 510\uparrow$, $K+2 = 512\downarrow$, $K+3 = 503\uparrow$.

proton levels									
$K, K+1$	2−	1.3	1.290	aF	8.2	..	..	$1\,u$	6.3 (6.4)
	7−	..	..	..	..	$1\,u$	(6.4)	..	..
$K-1, K+1$	6+	1.4	1.757	..	..	ah	(6.7)	..	..
	1+	..	..	1^*h	..	..	..	ah	(6.5)
K, K ..... / $K+1, K+1$	0+	1.8	..	..	..	..	..	..	..
$K-1, K+2$	4+	2.0	..	$1\Lambda(1\,u)$	..	..	..	..	..
	3+	..	..	$1\,u$	..	..	..	aF	..
$K-1, K$	8−	2.0	..	..	..	$1\,F$	..	..	..
	1−	..	..	..	..	..	..	$1\,F$	..
$K, K+2$	4−	2.0	..	aF	..	..	..	..	..
	5−	..	..	..	..	1^*F	..	..	..
$K-2, K+1$	3+	2.1	..	$1\,F$	..	..	..	$a\Lambda(4)$	..
	2+	..	..	$1\,F$	..	..	..	$a(4)$	..
$K+1, K+2$	2+	2.2	..	$1\,F$	..	..	..	$a(4)$	..
	3+	..	..	$1\,F$	..	..	..	$a\Lambda(4)$	..
$K-3, K+1$	1−	2.5	..	..	..	..	..	$1u$	..
	6−	..	..	..	..	$1\,u$	..	..	..
$K+1, K+3$	4+	2.6	..	$1\,F$	..	..	..	..	..
	1+	..	..	..	..	..	..	$a(2)$	..

$K-3 = 523\uparrow$, $K-2 = 411\downarrow$, $K-1 = 404\downarrow$, $K = 514\uparrow$, $K+1 = 402\uparrow$, $K+2 = 400\uparrow$, $K+3 = 402\downarrow$.

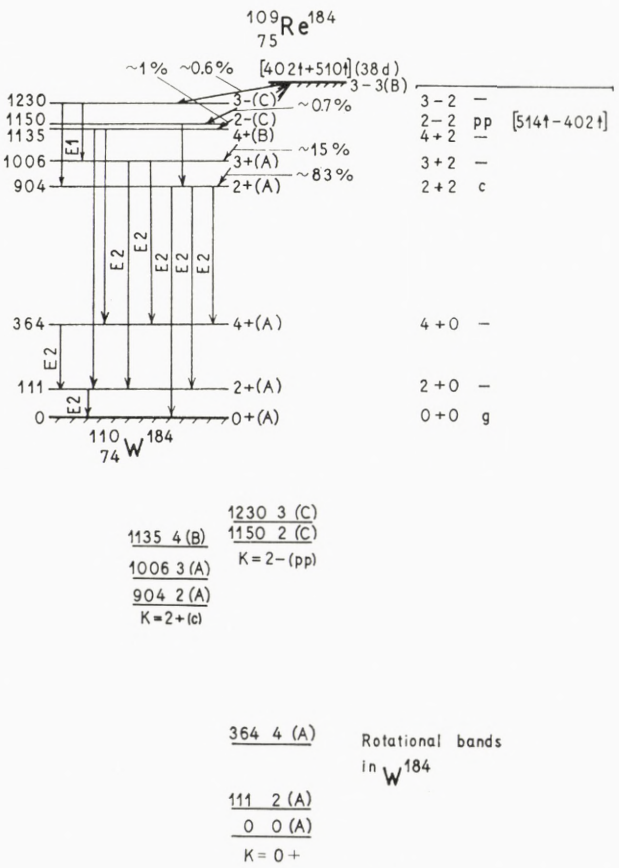

Fig. 19. A = 184.

The decay scheme of 38 *d* Re^{184} has been studied by C. J. Gallagher, Jr., D. Strominger, and J. P. Unik, Phys. Rev. **110**, 725 (1958) and HHM 61. The spins of the 904 and 1006 keV levels have been established by E. Bodenstedt, E. Matthias, H. J. Körner, E. Gerdau, F. Frisius, and D. Hovestadt, Nuclear Phys. **15**, 239 (1960), who also established the half-life of the isomer. Recently a second isomer of Re^{184} with a 165 *d* half-life has been reported by N. R. Johnson, Bull. Am. Phys. Soc. **6**, 73 (1961). Two levels at 1106 are 1101 keV proposed by HHM 61 have not been included in the figure.

Re^{184} (3–3)–1 TABLE III 17. $^{110}_{74}W^{184}$

Experimental		Theoretical			1†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log ft*
2–	1.150	514 ↑ – 402 ↑ p	2–2	1.3	$a(4)$	7.3 to 8.3
2+	.904	510 ↑ + 512 ↓ n	2+2	..	1 u	7.0 to 7.4
..	..	402 ↑ – 400 ↑ p	2+2	..	$1A(1u)$	..
..	..	collective	2+2	..	1?	..

† 402 ↑ + 510 ↑

* if $1.33 \leqslant Q_{EC} \leqslant 1.6$

Whether the $K\pi = 2+$ band in W^{184} should be assigned as a collective or intrinsic band is somewhat uncertain, because the lowest-lying neutron excitation is the $K\pi = 2+$ state $510\uparrow + 512\downarrow$, which should be populated by a 1 *u* electron capture branch. The log *ft* estimated for the branch (≈ 7.0) is somewhat larger than that expected for a 1 *u* transition, but actually less than the transition rate for the same single-particle transition in W^{185} and W^{187} decay. The calculated energy of the state is considerably higher than the experimental energy.

Weak branches to the 2− proton level $514\uparrow - 402\uparrow$ may be observed, but the assignment of the 2− level at 1150 keV is uncertain.

A = 186.

Re^{186} is clearly stablished as the 1− configuration $402\uparrow - 512\downarrow$. The log *ft* = 7.7 for the beta branch to the Os^{186} ground state is somewhat larger than ordinarily ob-

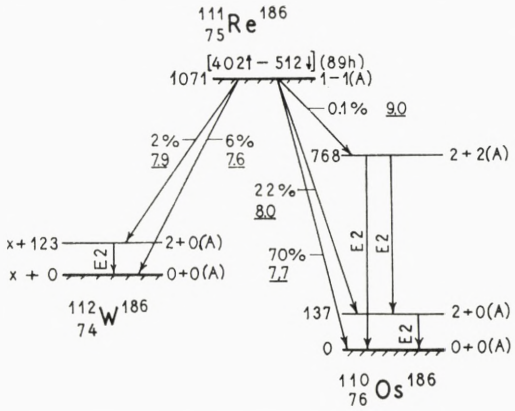

Fig. 20. A = 186.
The data on the decay of Re^{186} is as reported in SHS and the NDS. The electron capture decay energy is taken from a recent adjustment of mass values in the rare earth region (A. H. WAPSTRA, priv. comm., May 1961).

$Re^{186}(1-1)-1$ TABLE III 18. $^{102}_{74}W^{186}$

Experimental		Theoretical			1†	
$I\pi$	E	Final configuration	$I\pi K$	E	Class	log *ft**
2+	.768	collective (Os^{186})	2+2	–	1?	9.0
2+	.137	ground (Os^{186})	2+0	–	1 *u*	8.0
0+	0	ground (Os^{186})	0+0	–	1 *u*	7.7
2+	.123	ground (W^{186})	2+0	–	1 *u*	7.9
0+	0	ground (W^{186})	0+0	–	1 *u*	7.6

† $402\uparrow - 512\downarrow$.
* if $Q_{EC} = .70$.

served for a 1 u transition, although the similar log ft = 7.5 observed for the odd-particle transition in the $W^{185} \rightarrow Re^{185}$ decay suggests that the deformation may be changing rapidly here. The energy of the 768 keV 2+ state in Os^{186} suggests a collective excitation. No energies for $N = 112$ or $Z = 76$ have been calculated (see Section II).

IV. DISCUSSION AND CONCLUSIONS

A. K Selection Rules

1. *Beta decay.* The K selection rules have been found to be very important in beta decay. While such classic examples as the $\nu = 6$ ($\nu = K_f - K_i - \lambda$, where λ is the multipole order of the transition) forbidden beta decay of the high spin isomer of Lu^{176} clearly demonstrate the validity of the rules, even $\nu = 1$ forbidden transitions are appreciably retarded. A forbiddenness of $\approx 10^2$ per unit of K forbiddenness seems to be generally observed.

2. *Gamma-ray decay.* Data on gamma-ray retardations are at present somewhat scarce. The available evidence indicates that appreciable retardations due to K-forbiddenness occur. Particularly striking examples are the Hf^{178} and Hf^{180} isomers, where the $\nu = 7$ forbidden transitions are retarded by factors of $\approx 10^{13}$ and $\approx 10^{15}$, respectively.

B. K Intensity Rules

1. *Beta decay.* In Table IV 1 are presented the available experimental data on relative ft values for beta decay from an odd-odd nucleus to rotational levels in the even-even ground state band. For Ho^{162}, Ho^{164}, Tm^{170}, Tm^{172}, Ta^{178}, Re^{186}, and Re^{188} the K quantum numbers are established by the absolute values of the transition rates which establish the configurations. In these cases (with the exception of Ho^{162}, in which the experimental branching ratio has a very large experimental uncertainty) the experimental branching ratios are within experimental error of the theoretical predictions. From these data we conclude that in general the K intensity rules are valid experimentally. The K quantum numbers of Lu^{176} and Ta^{180} have therefore been assigned on the basis of the observed ratios. No theoretical values are listed for the 0− states 9.3 h Eu^{152} and 2.7 h Ho^{166}, because in these cases the matrix elements for transitions to the 0+ and 2+ rotational states are clearly not identical. The case of Eu^{156} seems to be the single exception to the generally valid rules, but in this case the spin is not clearly established.

2. *Gamma-ray Decay.* We have made no systematic effort to classify the K quantum numbers of even-even levels on the basis of the K intensity rules, nor to investigate this question in any detail. However, K intensity rules for interband transitions have been checked in a systematic way for the decay of the $K = 2+$[38] and $K = 0$

TABLE IV 1.

Initial nucleus	Initial $I\pi K$	Final nucleus	Decay fraction (%) to final state of $(I\pi)$			Total decay energy (MeV)	Total t 1/2	Ratio $\frac{ft(I_i\pi_i K_i \to 2+0)}{ft(I_i\pi_i K_i \to 0+0)} = \frac{\langle I_i L K_i K_f - K_i \mid 00\rangle^2}{\langle I_i L K_i K_f - K_i \mid 20\rangle^2}$		
			0+	2+	4+			Theor.	Exp.	Ref.
$^{89}_{63}Eu^{152m}$	0 − 0	$^{90}_{62}Sm^{152}$	.007	.004	–	1.917	9.3*h*	. .[α]	0.8 ± 0.3	a
$^{95}_{67}Ho^{162}$	1 + 1	$^{96}_{66}Dy^{162}$	44	56	–	2.160	11.8*m*	2.0	0.9 ± 0.7	b
$^{97}_{67}Ho^{164}$	1 + 1	$^{96}_{68}Er^{164}$	35	14	–	0.99	≳25*m*	2.0	1.8 ± 0.5	c, d
$^{99}_{67}Ho^{166}$	0 − 0	$^{98}_{68}Er^{166}$	52	48	–	1.854	27*h*	. .[α]	0.8 ± 0.35	e
$^{101}_{69}Tm^{170}$	1 − 1	$^{100}_{70}Yb^{170}$	76	24	–	0.969	129*d*	2.0	1.9 ± 0.2	f
$^{103}_{69}Tm^{172}$	2 − 2	$^{102}_{70}Yb^{172}$	23	41	1.2	1.920	63.6*h*	0.70:1:14[β]	0.63:1:13[β]	g
$^{105}_{71}Lu^{176}$	1 − 0	$^{104}_{72}Hf^{176}$	42	58	–	1.314	3.7*h*	0.5	0.56 ± 0.16	h
$^{105}_{73}Ta^{178}$	1 + 1	$^{106}_{72}Hf^{178}$	59	35	–	1.912	9.3*m*	2.0	1.6 ± 0.8	i
$^{107}_{73}Ta^{180}$	1 + 1	$^{108}_{72}Hf^{180}$	60	27	–	0.865	8.15*h*	2.0	2.0 ± 0.3	j, k
$^{107}_{73}Ta^{180}$	1 + 1	$^{106}_{74}W^{180}$	6.9	3.2	–	0.710	8.15*h*	2.0	1.8 ± 0.3	j
$^{111}_{75}Re^{186}$	1 − 1	$^{112}_{74}W^{186}$	6	2	–	0.700	89*h*	2.0	1.8 ± 0.5	e, k
$^{111}_{75}Re^{186}$	1 − 1	$^{110}_{76}Os^{186}$	70	22	–	1.071	89*h*	2.0	2.1 ± 0.2	l
$^{113}_{75}Re^{188}$	1 − 1	$^{112}_{76}Os^{188}$	73	24	–	2.116	17*h*	2.0	2.1 ± 0.2	m

Table IV. 1. *Comparison of theoretical and experimental relative reduced transition probabilities for beta decay of strongly deformed odd-odd nuclei.*

(a) D. ALBURGER, S. OFER, and M. GOLDHABER, Phys. Rev. **112**, 1998 (1958).
(b) M. JØRGENSEN, O. B. NIELSEN, and O. SKILBREID, Nuclear Phys. **24**, 443 (1961).
(c) M. JØRGENSEN, O. B. NIELSEN, and O. SKILBREID, Nuclear Phys. (to be published).
(d) H. N. BROWN and R. A. BECKER, Phys. Rev. **96**, 1372 (1954).
(e) R. L. GRAHAM, J. L. WOLFSON, and M. A. CLARK, Phys. Rev. **98**, 1173A (1955).
(f) R. L. GRAHAM, J. L. WOLFSON, and R. E. BELL, Can. J. Phys. **30**, 459 (1952).
(g) P. G. HANSEN, O. J. JENSEN, and K. WILSKY, Nuclear Phys. **27**, 516 (1961).
(h) I. ŘEZÁNKA, J. FRÁNA, J. ADAM, and L. K. PEKER, Izvest. Akad. Nauk SSSR, Ser. Fiz., **26**, 127 (1961).
(i) C. J. GALLAGHER, Jr., H. L. NIELSEN, and O. B. NIELSEN, Phys. Rev. **123**, 1590 (1961).
(j) C. J. GALLAGHER, Jr., M. JØRGENSEN, and O. SKILBREID, Nuclear Phys. (to be published).
(k) A. H. WAPSTRA, priv. comm., May 1961.
(l) F. T. PORTER, M. S. FREEDMAN, T. B. NOVEY, and F. WAGNER, Jr., Phys. Rev. **103**, 921 (1956).
(m) K. O. NIELSEN and O. B. NIELSEN, Nuclear Phys. **5**, 319 (1958).

(α) Different matrix elements in transitions to 0+ and 2+ states.
(β) $ft(2-2\to 2+0)$: $ft(2-2\to 0+0)$: $ft(2-2\to 4+0)$.

bands[22] to the ground-state band. In order to understand the branchings for the $K = 2+$ bands it has been necessary to postulate appreciable band mixing[38]. Branchings from the $K = 0-$ levels, however, (for the $A > 220$ mass region) have shown a remarkable consistency with theoretical prediction.[22] The branchings for the 963 keV level in Sm^{152} and the 1663 keV level in Er^{166} are also consistent with the $K = 0$ interpretation of these levels. In general the data on the decay of other types of levels are not sufficiently precise to test the predictions in detail. Similarly, data on interband transitions, which have been found to agree well with theory in the odd-mass nuclei, are scarce in even-mass nuclei and we therefore do not consider these questions here.

C. Log ft Values

In Tables IV 2a, b and c we summarize the log ft's for single-particle transitions between two quasi-particle states. The data are tabulated so that all cases of the same transition are listed together. The single-particle transition rate used to determine the magnitude of the matrix element is also listed. The data indicate that the transition rates lie within the same range in odd and even-mass nuclei if no additional selection

TABLE IV 2a

Transition	Initial state		Final state		R	log $(ft)_e$	log $(ft)_c$	log $[(ft)_c R\eta]$
	$I\pi K$	Configuration	$I\pi K$	Configuration				
allowed unhindered								
$Ho^{167} \rightarrow Er^{167}$	7/2 − 7/2	523 ↑	5/2 − 5/2	523 ↓	0.52	*4.8*	4.8[a]	4.6
$Ho^{160} \rightarrow Dy^{160}$	5 + 5	523 ↑ + 521 ↑	4 + 4	523 ↓ + 521 ↑ (n)	0.36	4.8	4.9	4.4
$Ho^{162} \rightarrow Dy^{162}$	1 + 1	523 ↑ − 523 ↓	0 + 0	ground	0.25	4.7	5.3	3.9
$Ho^{162} \rightarrow Dy^{162}$	6 − 6	523 ↑ + 642 ↑	5 − 5	523 ↓ + 642 ↑ (n)	0.20	4.6	5.2	4.0
$Ho^{164} \rightarrow Dy^{164}$	1 + 1	523 ↑ − 523 ↓	0 + 0	ground	0.35	~ 5.3	5.3	4.3
$Ho^{164} \rightarrow Er^{164}$	1 + 1	523 ↑ − 523 ↓	0 + 0	ground	0.20	5.4	5.5	4.3
$Tm^{164} \rightarrow Er^{164}$	1 + 1	523 ↑ − 523 ↓	0 + 0	ground	0.61	≤ 5.0	5.1	4.2
$Yb^{164} \rightarrow Tm^{164}$	0 + 0	ground	1 + 1	523 ↑ − 523 ↓	0.08	≲ 5.0	5.5	3.8
$Dy^{166} \rightarrow Ho^{166}$	0 + 0	ground	1 + 1	523 ↑ − 523 ↓	0.44	4.9	5.0	4.5
$Ho^{166} \rightarrow Er^{166}$	0 − 0	523 ↑ − 633 ↑	1 − 1	523 ↓ − 633 ↑ (n)	0.38	5.2	5.1	4.8
$Ho^{166} \rightarrow Er^{166}$	7 − 7	523 ↑ + 633 ↑	6 − 6	523 ↓ + 633 ↑ (n)	0.38	≲ 6.7	5.1	..
$Yb^{175} \rightarrow Lu^{175}$	7/2 − 7/2	514 ↓	9/2 − 9/2	514 ↑	0.32	*4.7*	4.7[b]	4.2
$Ta^{178} \rightarrow Hf^{178}$	1 + 1	514 ↑ − 514 ↓	0 + 0	ground	0.22	4.6	5.4	3.6
$Ta^{178} \rightarrow Hf^{178}$	7 − 7	404 ↓ + 514 ↓	8 − 8	404 ↓ + 514 ↑ (p)	0.34	4.9	4.7	4.4
$W^{178} \rightarrow Ta^{178}$	0 + 0	ground	1 + 1	514 ↑ − 514 ↓	0.36	≤ 5.5	4.8	..

(a) See ref. 6.
(b) See NDS.

TABLE IV 2b

Transition	Initial state		Final State		R	log $(ft)_e$	log $(ft)_c$	log $[(ft)_c R\eta]$
	$I\pi K$	Configuration	$I\pi K$	Configuration				
allowed hindered								
$W^{181} \rightarrow Ta^{181}$	9/2 + 9/2	624 ↑	7/2 + 7/2	404 ↓	0.34	*6.6*[a]	6.6[a]	6.2
$Ta^{178} \rightarrow Hf^{178}$	7 − 7	404 ↓ + 514 ↓	8 − 8	624 ↑ + 514 ↓ (n)	0.21	4.9	6.9	4.2
$Ta^{180} \rightarrow Hf^{180}$	1 + 1	404 ↓ − 624 ↑	0 + 0	ground	0.23	6.0	7.1	5.0
$Ta^{180} \rightarrow W^{180}$	1 + 1	404 ↓ − 624 ↑	0 + 0	ground	0.38	6.8	6.9	6.1
$Ta^{182} \rightarrow W^{182}$	3 − 3	404 ↓ − 510 ↑	4 − 4	624 ↑ − 510 ↑ (n)	0.22	6.9	6.9	6.2

(a) See NDS.

TABLE IV 2c.

Transition	Initial state		Final state		R	log $(ft)_e$	log $(ft)_c$	log $[(ft)_e R\eta]$
	$I\pi K$	Configuration	$I\pi K$	Configuration				
first forbidden unhindered								
$Dy^{165} \rightarrow Ho^{165}$	$7/2+7/2$	$633\uparrow$	$7/2-7/2$	$523\uparrow$	0.33	*6.2*[a]	6.2[a]	5.7
$Dy^{166} \rightarrow Ho^{166}$	$0+0$	ground	$0-0$	$523\uparrow - 633\uparrow$	0.19	7.1[b]	6.4	6.4
$Ho^{166} \rightarrow Er^{166}$	$0-0$	$523\uparrow - 633\uparrow$	$0+0$	ground	0.33	8.1[b]	6.1	7.7
$Tm^{168} \rightarrow Er^{168}$	$3+3$	$411\downarrow - 633\uparrow$	$3-3$	$411\downarrow - 523\uparrow$ (p)	0.30	6.0	6.2	5.5
$Tm^{167} \rightarrow Er^{167}$	$1/2+1/2$	$411\downarrow$	$1/2-1/2$	$521\downarrow$	0.37	*6.5*[c]	6.5[c]	6.1
$Tm^{168} \rightarrow Er^{168}$	$3+3$	$411\downarrow - 633\uparrow$	$3-3$	$521\downarrow - 633\uparrow$ (n)	0.36	7.7	6.5	7.2
$Tm^{172} \rightarrow Yb^{172}$	$2-2$	$411\downarrow - 512\uparrow$	$2+2$	$521\downarrow - 512\uparrow$ (n)	0.29	6.8	6.6	6.3
$Lu^{172} \rightarrow Yb^{172}$	$4-4$	$404\downarrow + 521\downarrow$	$4+4$	$404\downarrow + 411\downarrow$ (p)	0.38	6.1	6.5	5.3
$Ta^{175} \rightarrow Hf^{175}$	$7/2+7/2$	$404\downarrow$	$7/2-7/2$	$514\downarrow$	0.31	*6.4*[d]	6.4[d]	5.8
$Lu^{172} \rightarrow Yb^{172}$	$4-4$	$404\downarrow + 521\downarrow$	$4+4$	$514\downarrow + 521\downarrow$ (n)	0.40	6.5	6.3	6.1
$W^{181} \rightarrow Ta^{181}$	$9/2+9/2$	$624\uparrow$	$9/2-9/2$	$514\uparrow$	0.37	*6.8*[c]	6.8[c]	6.4
$Re^{182} \rightarrow W^{182}$	$2+2$	$402\uparrow - 624\uparrow$	$2-2$	$402\uparrow - 514\uparrow$ (p)	0.28	6.3	6.9	5.7
$W^{185} \rightarrow Re^{185}$	$3/2-3/2$	$512\downarrow$	$5/2+5/2$	$402\uparrow$	0.38	*7.5*[a]	7.5[a]	7.1
$Re^{186} \rightarrow W^{186}$	$1-1$	$402\uparrow - 512\downarrow$	$0+0$	ground	0.23	7.6	8.2	6.5
$Re^{186} \rightarrow Os^{186}$	$1-1$	$402\uparrow - 512\downarrow$	$0+0$	ground	0.38	7.7	7.9	6.8
$Re^{188} \rightarrow Os^{188}$	$1-1$	$402\uparrow - 512\downarrow$	$0+0$	ground	0.30	8.0	8.1	7.0

(a) See ref. 6.

(b) Different operators are probably responsible for the transition in this case because of the $0- \rightarrow 0+$ transition.

(c) See NDS.

(d) B. HARMATZ, T. H. HANDLEY, and J. W. MIHELICH, Phys. Rev. **119**, 1345 (1960).

Table IV. 2. Comparison of beta decay transition rates for single-particle transitions between two-quasi-particle states. Log $(ft)_e$ is the experimental log ft reported in Section III. $R = R_Z R_N$ is the correction which accounts for the different distribution of paired-particle amplitudes in the proton and neutron cores in the final and initial states (i. e. the superfluid correction). The calculated log $(ft)_c$ is discussed in Section II. Log $[(ft)_e R\eta]$ is the single-particle transition rate from which the superfluid (R) and statistical (η) corrections have been excluded. a) allowed unhindered beta transitions; b) allowed hindered beta transitions; c) first forbidden unhindered beta transitions.

rules arising from the two-particle system apply. These results support the validity of the conclusion previously obtained from a less extensive classification.[8]

The range of rates applying to the various Alaga-selection rule-classifications in odd-mass nuclei is (cf. MOTTELSON and NILSSON)

$$4.5 \lesssim \log ft \lesssim 5.0 \quad au$$

$$6.0 \lesssim \log ft \lesssim 7.5 \quad ah$$

$$6.0 \lesssim \log ft \lesssim 7.5 \quad 1\,u$$

$$7.5 \lesssim \log ft \lesssim 8.5 \quad 1\,h.$$

The effect of excluding pairing correlation corrections from the single-particle transition probabilities tends to increase the transition rates and decrease the spread of the separate cases, so that after correction the range of rates for the various classes is

$$4.0 < \log [(ft)_e R\eta] < 4.7 \quad au$$
$$5.5 < \log [(ft)_e R\eta] < 6.5 \quad ah$$
$$5.5 < \log [(ft)_e R\eta] < 6.5 \quad 1\ u.$$

No data on 1 h transitions are included in this compilation because the available data are few. This investigation of the β-decay rates thus shows that at least to first order the concept of independent quasi-particles is correct. In addition, the correction terms for beta decay rates calculated on the basis of the pairing correlation calculations which take into account the differences in properties between odd and even-mass systems produce a greater consistency in the observed single-particle rates than is possible to achieve without them.

D. Level Energies

A comparison of the experimental data discussed in Section III with the calculated level spectra leads us to several conclusions. First of all, the qualitative agreement of the predicted and observed level spectra shows the general validity of the concept of two-quasi-particle excitations in deformed even-even nuclei.

A feature of these spectra that becomes apparent from the comparison is that the degeneracy of the $\Omega_1 \pm \Omega_2$ doublet is removed at least partly as a result of spin splitting, in analogy to deformed odd-odd nuclei, and the $\Sigma = 0$ state of the configuration appears lower, as expected. In the best established case (Er^{166}), the splitting of the doublet is only ≈ 40 keV; in other cases, if the postulated analyses are correct, the splitting is as large as ≈ 800 keV.

A particularly important experimental fact is that the energy of at least one member of the $(K, K+1)$ configuration is observed at energies considerably less than the formal gap. Table IV 3 summarizes the information on the $(K, K+1)$ class of levels. Where both the $\Sigma = 0$ and $\Sigma = 1$ states are known, both are listed. We have also included the level rating (A, B, C) in the table, as all the data are not equally reliable. In this table are listed three energies for each configuration: the formal gap 2C, the degenerate doublet energy calculated assuming blocking, and the experimental energy. It can be clearly seen from the table that all experimental energies are within calculational error of the calculated energies. This would appear to be a conclusive proof for the existence of blocking, except for the fact that the forces which split the states of the $\Omega_1 \pm \Omega_2$ doublet are not clearly understood. A further complication is that the energy splittings of the doublets are not well known experimentally either. For these reasons it does not seem possible at present to decide definitely what the strength of the blocking is relative to other residual interactions. However, we can

TABLE IV 3.

Nucleus	System	$K\pi$	Classification	Gap 2 C (MeV)	Energy (MeV)	
					Calculated	Observed
W^{184}	proton	2−	C	1.61	1.3	1.150
	neutron	2+	A^a	1.97	1.8	.904
W^{182}	proton	2−	A	1.61	1.3	1.290
	proton ($\Sigma = 1$) ...	7−	B	1.61	1.3	1.961
	neutron	4−	A	1.89	1.5	1.554
	neutron ($\Sigma = 1$) ..	5−	C	1.89	1.5	1.810
Hf^{180}	proton	8−	A	1.66	1.0	1.142
Hf^{178}	proton	8−	A	1.66	1.0	1.148
	neutron	8−	B	1.85	1.5	1.480
Yb^{172}	proton	3+	B	1.80	1.4	1.664
	proton ($\Sigma = 1$) ...	4+	B	1.80	1.4	2.075
	neutron	3+	B	1.65	1.3	1.174
	neutron ($\Sigma = 1$) ..	2+	B^a	1.65	1.3	1.468
Er^{168}	proton ($\Sigma = 1$) ...	3−	B	1.82	1.3	1.543
	neutron ($\Sigma = 1$) ..	3−	A	1.64	1.1	1.095
Er^{166}	neutron	6−	B	1.63	1.6	1.785
	neutron ($\Sigma = 1$) ..	1−	A	1.63	1.6	1.826
Dy^{162}	neutron	5−	A	1.83	1.3	1.485
Dy^{160}	proton	2−	A^b	1.90	1.4	1.260
	neutron	4+	A	..	1.6	1.694
Gd^{156}	proton	4+	A^b	2.0	1.45	1.511
	proton ($\Sigma = 1$) ...	1+	B	2.0	1.45	1.966
	neutron	1−	A^b	2.0	1.5	1.240
	neutron ($\Sigma = 1$) ..	4−	A^b	2.0	1.5	2.042

(a) May be collective state.
(b) Experimental data excellent but configuration assignment not definite.

Table IV. 3. Energy of $(K, K+1)$ states in deformed even-even nuclei. Unless otherwise indicated the observed state is the $\Sigma = 0$ state of the $(K, K+1)$ configuration. The classification of states is as in Section III. The gap, or correlation, energy $2C$ is the energy of the formal gap. The calculated energy includes the effect of blocking.

conclude on the basis of the experimental data that, if an average spin splitting of $\leqslant 500$ keV is assumed and if there is no shift in the center of gravity of the configuration, blocking does exist.

E. Evidence for Collective Excitations

The classification of the intrinsic spectrum made possible by the present model provides us with means of deciding whether there are states which have properties clearly different from two-quasi-particle states. In this category are particularly the well-known 2+ states at ≈ 1 Mev which are known to occur systematically. The energies of these states are consistently less than those calculated for intrinsic 2+

excitations, thus providing further support for their classification as collective excitations. However, the variation in energy of these 2+ states (once the deformation has stabilized) as a function of mass number seems to follow to some extent the energies of the intrinsic 2+ levels. With the exception of the Sm-Gd region, 0+ states which unambiguously have energies less than the energies calculated for the pair excitations have *not* systematically been observed. Little can be said about the 1− states which have been interpreted as collective octupole excitations, except that the two 1− states that can be assigned in this category, in Sm^{152} and Er^{166}, both appear where intrinsic excitations of the same nature are expected, but at energies somewhat lower than calculated.

F. General Conclusions

The most important results that appear from the present analysis are that the intrinsic states of deformed even-even nuclei can be consistently described as two-quasi-particle excitations, and that beta decay selection rules based on two-quasi-particle wave functions can describe the beta decay rates observed. In general, the assignments are clearest where the data are most comprehensive. In addition, the general fit of the calculated excitation energies of the two-quasi-particle states with the experimental energies supports the inherent validity of the model and makes it appear to be a useful basis for further studies of other properties of the two-quasi-particle system.

In addition to the calculation of properties calculable within the framework of the model, there is already clearly a need for the introduction of a term to account for the splitting of the $\Omega_1 \pm \Omega_2$ doublets; also, the presence of certain exceptions to the expected behaviour (like that of the 8− states in Hf^{178}) indicates greater complexity than is accounted for by the model. From these apparent discrepancies it is thus clear that more experimental information is needed before more detailed conclusions can be drawn about the strength of residual quasi-particle interactions.

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BY

H. J. MANG AND J. O. RASMUSSEN

København 1962
i kommission hos Ejnar Munksgaard

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CONTENTS

Synopsis

The formulation of the alpha decay rate theory based on the independent-particle shell model wave functions, which has earlier been successfully applied to spherical nuclei, is here extended to apply to spheroidally deformed nuclei. This method essentially projects out of the shell model wave function of the most lightly bound neutrons and protons a finite-sized Gaussian, singlet-spin alpha-particle internal wave function, resulting in a wave function in the center-of-mass coordinate of the alpha cluster. This wave function serves to fix the boundary condition on the nuclear surface for the irregular type Coulomb wave solution through the anisotropic barrier. The independent-particle formulation is generalized to include correlation effects arising from the pairing interaction.

Numerical calculations of relative alpha intensities to rotational states of several even nuclei of elements 92–100 are carried out using Nilsson's numerical wave functions. The theoretical results nicely show the essential features of the relative intensity patterns, although the theoretical intensity of the decay to the first excited 2+ state is too high.

The absolute transition probability calculated for Cm^{242} is about a factor of 60 too low assuming IGO's optical model potential for the barrier, but the factor is extremely sensitive to this latter assumption.

The essential role of the configuration mixing induced by the pairing force in smoothing the decay rate trends from nucleus to nucleus and in giving a large enhancement of the absolute rate is pointed out in the discussion.

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Introduction

For some time it has been realized that there is a close connection between α-decay rates and the shell-model orbitals of the more lightly bound nucleons. Formulations of the problem have been made (MANG, 1957, 1959; BRUSSAARD and TOLHOEK, 1958) and quite a number of numerical calculations for spherical nuclei near doubly magic Pb^{208} have been carried out and compared with experiment (MANG, 1960).

There are extensive data on α-decay of spheroidally deformed nuclei, and the classification of nucleon states of odd-mass nuclei according to the Nilsson scheme (1955) has been carried out rather satisfactorily throughout the region of heavy deformed nuclei ($A \geq 229$) (MOTTELSON and NILSSON, 1959; STEPHENS, ASARO, and PERLMAN, 1959).

Despite the formidable computational difficulties involved, it appeared worth while to make an attempt at applying MANG's shell model formulation of α-decay to the spheroidal nuclear region, using the IBM-709 computer at the Lawrence Radiation Laboratory.

It has long appeared probable that α-decay to the ground rotational band of even-even nuclei involves an averaging of participation of many nucleon orbitals near the Fermi surface, since reduced widths and hindrance factors vary smoothly with nucleon numbers. From the outset it was clear that a meaningful calculation for even nuclei must involve repeated calculations of the contribution of various Nilsson orbital combinations followed by a weighted averaging process, weighting combinations according to the probability that a given orbital is occupied in the parent and vacant in the daughter. The Belyaev pairing interaction method (BELYAEV, 1959) was chosen, and we have drawn heavily on the analysis of NILSSON and PRIOR (1961) for numerical values of the energy gap parameter Δ as well as best values of the quadrupole deformation for given nuclei.

After a theoretical calculation of α-wave amplitudes in the region of the nuclear surface it was necessary to treat their propagation through the anisotropic barrier. The matrix method of FRÖMAN (1957) was used with certain important modifications which bring better agreement with the numerical work of RASMUSSEN and HANSEN (1958) on Cm^{242}. Preliminary results of the calculations herein described have been given previously in a brief report (MANG and RASMUSSEN, 1961).

I. Basic Formulas for the Decay Constant

Slightly generalizing a method (Mang, 1957, 1959, 1960) which has been described earlier, we obtain expressions for the asymptotic form of the total wave function of the α-decaying system* (Casimir, 1934) and for the decay constant

$$\left.\begin{aligned} \Psi_{R\to\infty} &\to \sum_{\sigma} \left[\left(\frac{N}{2}\right)\left(\frac{Z}{2}\right)\right]^{1/2} \frac{\hbar^2}{2M} \int dS\, d\xi_\alpha\, d\xi_K \left[\overset{*}{\Phi}{}_J^{M K_0 q} \overset{\leftrightarrow}{\frac{\partial}{\partial n}} \Psi^M_{\sigma E J} \right]_{E=E_0} \Psi^{+M}_{\sigma E J} \\ \lambda &= \frac{2\pi}{\hbar}\left(\frac{N}{2}\right)\left(\frac{Z}{2}\right) \sum_{\sigma} \left| \frac{\hbar^2}{2M} \int dS\, d\xi_\alpha\, d\xi_K \left[\overset{*}{\Phi}{}_J^{M K_0 q} \overset{\leftrightarrow}{\frac{\partial}{\partial n}} \Psi^M_{\sigma E J} \right]_{E=E_0} \right|^2, \end{aligned}\right\} \quad \text{(I. 1)}$$

where

$$\Psi^{+M}_{\sigma E J} = \text{outgoing part of } \Psi^M_{\sigma E J}.$$

In (I. 1), $\Phi_J^{M K_0 q}$ is the wave function of the parent nucleus and E_0 is its total energy. $\Psi^M_{\sigma E J}$ describes the final state α-particle plus daughter nucleus. The index σ is a shorthand notation for all quantum numbers specifying the final state, except the total energy and the angular momentum J, M. The coordinates ξ_α and ξ_K are internal coordinates of the α-particle and daughter nucleus. The closed surface S in the space of the vector R, the distance between α-particle and daughter nucleus, is so chosen that outside S the interaction between an α-particle and the daughter nucleus may be described by a potential $V(R)$, whereas inside S an individual nucleon, shell model type representation should be valid. As will be seen later, it is of essential importance that the pairing force effects be added to the Nilsson model.

As will be discussed again later, there is uncertainty as to the effective potential experienced by the α-particle close to the nucleus. We suppose the outer tail of the effective nuclear potential to be not too different from the real part of Igo's optical model potential (Igo, 1959) derived from α-scattering. Of course, by introducing an anisotropic nuclear potential we have gone beyond the Igo potential and introduced a mechanism for exchange of energy between the α-particle and the rotational degrees of freedom of the nucleus. The region of validity of the outer representation (α-particle + daughter nucleus) can, in principle, be brought inward further and further by introduction of additional couplings between α-particle and internal degrees of freedom of the daughter nucleus. Likewise, the region of validity of the inner representation (individual nucleon product wave function) can be extended outward by improvements in the Hamiltonian, especially with regard to representing the tendency toward nucleon clustering, expected to be most important in the surface region (cf. Wilkinson, 1961). The addition of the pairing interaction is an important improvement in this direction, but there is not yet a clear way to include the specific neutron-proton cor-

* The symbol $\left[\overset{*}{\Phi} \overset{\leftrightarrow}{\frac{\partial}{\partial n}} \Psi\right]$ is defined as $\overset{*}{\Phi} \frac{\partial}{\partial n} \Psi - \frac{\partial}{\partial n} \overset{*}{\Phi} \Psi$, where $\frac{\partial}{\partial n}$ is the derivative normal to the surface S.

relations expected from the special stability of the α-cluster. The leveling off of the Nilsson oscillator potential in the surface region is another needed improvement, for the oscillator potential attenuates the wave function much too drastically in the outermost region of main interest here. If, by such improvements to the Hamiltonians in both the inner and the outer region, the regions can be made to overlap, then the connection surface may be chosen anywhere within the region of overlap, and the theoretical decay constant will be independent of the exact choice. Of course, neither Hamiltonian can ever be perfect and the connecting surface will always be located as a compromise where both inner and outer descriptions are still fairly good. It would seem that the best choice of S will be along a surface of constant nuclear density. Serious problems arise in carrying the external α-wave solutions inward through an inner classical turning point with an anisotropic potential. Thus, one is compelled to locate the connection surface within the α-barrier. We shall choose it along a surface of constant nuclear density somewhat more than 1×10^{-13} cm beyond the effective charge radius $1.2\times10^{-13}\,A^{1/3}$ cm.

In a next step of the development we shall define the wave functions which enter into Eq. (I. 1). The wave function $\Phi_J^{MK_0q}$ will be a solution of the strong-coupling Hamiltonian of BOHR and MOTTELSON (1953)

$$\left.\begin{aligned} \{H_{\mathrm{rot}}(\Theta_i)+H_{\mathrm{intrinsic}}-E_0\}\,\Phi_J^{MK_0q}&=0\\ \Phi_J^{MK_0q}&=\sqrt{\frac{2J+1}{16\pi^2}}\{D^J_{MK_0}X_{K_0}+(-1)^{J-q-K_0}D^J_{M-K_0}X_{-K_0}\}. \end{aligned}\right\} \qquad \text{(I. 2)}$$

The functions $D^J_{MK_0}$, the eigenfunctions to the symmetric top, are eigenfunctions of the rotational Hamiltonian H_{rot}. The Eulerian angles Θ_i connect the "body-fixed" nuclear coordinate system with a "space-fixed" frame of reference. The wave functions X_{K_0} are eigenfunctions of the intrinsic Hamiltonian $H_{\mathrm{intrinsic}}$. We shall use NILSSON's model Hamiltonian with a pairing interaction included to approximate H_{intr}. The phase factor $(-1)^{J-q-K_0}$, where $(-1)^q$ is the parity of the state, differs somewhat from the one given by BOHR and MOTTELSON, but this is due to a different phase choice for X_{-K_0} which will later turn out to be convenient. The wave functions $\Psi^M_{\sigma EJ}$ describing the final state of the system are solutions of

$$\left\{H_{\mathrm{rot}}+H_{\mathrm{intr}}(\mathrm{daughter})+H_\alpha(\xi_\alpha)-\frac{\hbar^2}{2M}\Delta_{\mathrm{R}}+V(R,\,\Theta_i)-E\right\}\Psi^M_{\sigma EJ}=0. \qquad \text{(I. 3)}$$

The Eulerian angles Θ_i have been inserted in $V(R,\,\Theta_i)$ to exhibit the dependence of the anisotropic potential on the nuclear orientation. It should be pointed out that the Eulerian angles Θ_i are included in the coordinates ξ_K of Eq. (I. 1).

The $\Psi^M_{\sigma EM}$ are regular everywhere (standing-wave solutions) and *normalized* as follows:

$$\int d\xi_\alpha \, d\xi_K \, d^3R \, \overset{*}{\Psi}{}^{M'}_{\sigma' E' J'} \, \Psi^{M}_{\sigma E J} = \delta_{\sigma\sigma'} \, \delta_{MM'} \, \delta_{JJ'} \, \delta(E - E'), \tag{I. 4}$$

where E is the total energy of the system.

We shall also need the irregular (standing-wave) solutions of (I. 3), irregular as functions of R. They will be denoted by $\Phi^{M}_{\sigma E J}$ and we note the important relation which normalizes these functions

$$\int dS \, d\xi_\alpha \, d\xi_K \, \overset{*}{\Psi}{}^{M}_{\sigma E J} \overleftrightarrow{\frac{\partial}{\partial n}} \Phi^{M}_{\sigma' E J} = \frac{2M}{\pi \hbar^2} \, \delta_{\sigma\sigma'} \tag{I. 5}$$

where S may be any closed surface around the origin, in particular the connection surface mentioned earlier.

At this point some words should be said about the terms "regular and irregular solutions". To define such solutions the potential $V(R)$ must be defined throughout the nuclear volume, a procedure which seems to be somewhat arbitrary. But, because of the small penetrability, the potential inside the nucleus may be changed somewhat without changing the solutions in the barrier region. It is well known from the simple case of a central potential when the W-K-B approximation is valid that the regular solution is the one which increases in the barrier region with increasing distance R and is linearly independent of the irregular solution which continually decreases throughout the barrier and that this behaviour is rather independent of the potential inside the nucleus. In such a sense the terms irregular and regular will be used from now on.

We write $\Phi^{M}_{\sigma E J}$ in general as follows:

$$\Phi^{PKM}_{\sigma E J} = \chi_\alpha \sqrt{\frac{2M}{\pi \hbar^2 k_0}} \sum_{l' m'} a^{\sigma}_{l' m'} \sum_{lm} \frac{g^{l' m'}_{lm}(R)}{R} \varphi^{PKM}_{mlJ}, \tag{I. 6}$$

where

$$\varphi^{PKM}_{mlJ} = \sqrt{\frac{2J+1}{16\pi^2}} \left\{ D^{J}_{MK+m} \, X_K \, Y^{m}_{l}(\vartheta' \varphi') + (-1)^{J-L-P-K} \, D^{J}_{M-K-m} \, X_{-K} \, Y^{-m}_{l}(\vartheta' \varphi') \right\},$$

$\frac{\hbar^2}{2M} k_0^2 = \varepsilon_{\max}$, $\varepsilon_{\max}$ being the maximum kinetic energy of an α-particle involved in the process. In (I. 6) χ_α is the internal α-particle wave function, X_K the intrinsic wave function of the daughter nucleus, and $(-1)^P$ its parity. The quantum numbers K and P were originally included in the set σ, but from now on it is convenient to exhibit the dependence of the wave function on them explicitly. The functions $g^{l' m'}_{lm}(R)$ constitute dimensionless components, indexed lm, of a set, indexed $l'm'$, of linearly independent solutions of the coupled α-wave equations.

$$\left\{-\frac{\hbar^2}{2M}\frac{d^2}{dR^2}+V(R)+\frac{\hbar^2}{2M}\frac{l(l+1)}{R^2}-\varepsilon\right\} g_{lm}^{l'm'}(R) = -\sum_{l''} V_{ll''}^{m}(R)\, g_{l''m}^{l'm'}(R) - \sum_{m''} A_{m}^{m''}(KlJ)\, g_{lm''}^{l'm'}(R), \tag{I. 7}$$

where

$$A_{m}^{m''}(KlJ) = \sum_{j} E_{\mathrm{rot}}(jK)(-1)^{m-m''} C(Jlj;\, K+m-m)\, C(Jlj;\, K+m''-m''),$$

reducing for even-even nuclear decay to $\frac{\hbar^2}{2\Im} l(l+1)$

$$V_{ll''}^{m} = \int \overset{*}{Y}_{l}^{m}\, V(R, \vartheta', \varphi')\, Y_{l''}^{m}\, d\Omega'.$$

The potential $V(R\vartheta'\varphi')$ is the non-central part of $V(R\Theta_i)$. An analogous expansion to (I. 6) could be written down for the regular functions $\Psi_{\sigma EJ}^{PKM}$, but it will turn out later that we do not need explicit expressions for regular solutions. The boundary conditions determining the various solutions $(l'm')$ are imposed along a connection surface of cylindrical symmetry $R_s(\vartheta')$. Firstly, the wave amplitude of solution $(l'm')$ should vary as $Y_l^{m'}(\vartheta'\varphi')$ along the surface $R_s(\vartheta')$. Secondly, the first derivative normal to the surface is to be fixed such that the solution should not go into exponentially increasing behaviour anywhere within the barrier. This gives exactly the irregular solution, as has been explained earlier.

Formally we may write the first condition as

$$\sum_{lm} g_{lm}^{l'm'}(R_s(\vartheta'))\, \varphi_{mlJ}^{PKM} = \varphi_{m'l'J}^{PKM}.$$

If the connection surface were a sphere, this normalization would mean a value of unity for diagonal elements $g_{l'm'}^{l'm'}(R_s)$ and zero for off-diagonal. The condition on the derivatives will, for practical purposes, be satisfied by constructing solutions in the barrier region from linear combinations of irregular Coulomb functions or decreasing W-K-B solutions.

The expansion coefficients $a_{l'm'}^{\sigma}$ are free to be determined by the boundary conditions at the nuclear surface subject to the restriction that the normalization conditions (I. 4) and (I. 5) are fulfilled.

We shall now discuss the boundary condition which actually will be imposed on our solutions $\Phi_{\sigma EJ}^{PKM}$. If the inner and outer region Hamiltonians are both correct at the connection surface S, as has been assumed in the context of Eq. (I. 1), then there are particular irregular solutions $\Phi_{E_0K_0-KJ}^{PKM}$ and $\Phi_{E_0K_0+KJ}^{PKM}$ for any quantum number K, characterizing a rotational band in the daughter nucleus, and these solutions have the following properties:

$$\left.\begin{aligned}
\Phi^{PKM}_{E_0 K_0 - KJ} &\overset{\text{at } S}{=} \chi_\alpha \sqrt{\frac{2M}{\pi\hbar^2 k_0}} \sum_{l'} \frac{a_{l' K_0 - K}}{R_s} \varphi^{PKM}_{K_0 - K l' J} \\
&\overset{\text{at } S}{=} C_{K_0 - K} \chi_\alpha \sqrt{\frac{2M}{\pi\hbar^2 k_0}} \sum_{L} R_s^{-3/2} G_{L K_0 - K}(R_s) \varphi^{PKM}_{K_0 - K LJ} \\
\Phi^{PKM}_{E_0 K_0 + KJ} &\overset{\text{at } S}{=} \chi_\alpha \sqrt{\frac{2M}{\pi\hbar^2 k_0}} \sum_{l'} \frac{a_{l' K_0 + K}}{R_s} \varphi^{PKM}_{-K_0 - K l' J} \\
&\overset{\text{at } S}{=} C_{K_0 + K} \chi_\alpha \sqrt{\frac{2M}{\pi\hbar^2 k_0}} \sum_{L} R_s^{-3/2} G_{L K_0 + K}(R_s) \varphi^{PKM}_{-K_0 - K LJ}
\end{aligned}\right\} \quad \text{(I. 8)}$$

where

$$\frac{a_{l' m'}}{C_{m'}} = \sum_{L} \int \overset{*}{Y}{}^{m'}_{l'}(\vartheta' \varphi') R_s^{-1/2} G_{L m'}(R_s) Y^{m'}_{L}(\vartheta' \varphi') \, d\Omega'$$

$$G_{L K_0 - K}(R) = R^{3/2} \left[\binom{N}{2}\binom{Z}{2}\right]^{1/2} \int \overset{*}{X}_{K_0} \chi_\alpha X_K \, Y_L^{K_0 - K} \, d\xi_\alpha \, d\xi_K \, d\Omega'$$

$$G_{L K_0 + K}(R) = R^{3/2} \left[\binom{N}{2}\binom{Z}{2}\right]^{1/2} (-1)^P \int \overset{*}{X}_{K_0} \chi_\alpha X_{-K} \, Y_L^{K_0 + K} \, d\xi_\alpha \, d\xi_K \, d\Omega'.$$

Analogous relations to (I. 8) are valid for the derivatives normal to S. The constants $C_{K_0 - K}$, $C_{K_0 + K}$ (of dimension $R^{1/2}$) are introduced so that the $\Phi^{PKM}_{E_0 mJ}$ are properly normalized according to (I. 5) and (I. 4). The factor $\left[\binom{N}{2}\binom{Z}{2}\right]^{1/2}$ in the definition of $G_{Lm}(R)$ has been introduced so that G_{Lm} is the probability amplitude for finding an α-particle with angular momentum L at a radial distance R. G_{Lm} is defined in dimensionless fashion, so the identification as an effective one-dimensional internal radial wave function requires it to be divided by $R^{1/2}$. The boundary condition (I. 8) is the usual one made in resonance theory when dealing with a quasi-stationary state (THOMAS, 1954). The solution in the inner region joins smoothly to the irregular solution in the outer region. In the case of a purely central Coulomb potential this would be the well-known irregular Coulomb wave function. If, later on, the functions G_{Lm} calculated from model wave functions should not fulfill exactly the boundary condition (I. 8), this will be due to the fact that our model is not accurate enough. One of the improvements mentioned in connection with the definition of the surface should then be made. Actual calculations for spherical nuclei (ZEH and MANG, 1961) show that in the nuclear surface region the logarithmic derivative of G_{Lm} deviates by less than $20\,\%$ from that of the irregular Coulomb function.

The two particular solutions which have been selected by Eq. (I. 8) may now be considered as the first two of a whole set which of course must fulfill the condition (I. 5).

If we now consider that part of the parent wave function $\Phi_J^{MK_0q}$ that is proportional to χ_α (i.e. contains an α-particle), it may be expanded at the nuclear surface in terms of functions $\Phi_{E_0mJ}^{PKM}$. Therefore, the sum on σ in (I. 1) contains only a sum on K and for each K the two terms defined in (I. 8), and we get

$$\left.\begin{aligned}
&\left[\binom{N}{2}\binom{Z}{2}\right]^{1/2}\int\left[\overset{*}{\Phi}{}_J^{MK_0q}\overset{\leftrightarrow}{\frac{\partial}{\partial n}}\Psi_{E_0mJ}^{PKM}\right]dS\,d\xi_\alpha\,d\xi_K\\
&=\sqrt{\frac{\pi\hbar^2k_0}{2M}}\left\{\frac{\delta_{m,\,K_0-K}}{C_{K_0-K}}\int\left[\overset{*}{\Phi}{}_{E_0K_0-KJ}^{PKM}\overset{\leftrightarrow}{\frac{\partial}{\partial n}}\Psi_{E_0K_0-KJ}^{PKM}\right]dS\,d\xi_\alpha\,d\xi_K\right.\\
&\left.+\frac{\delta_{m,\,K_0+K}}{C_{K_0+K}}(-1)^{J-q-P-K}\int\left[\overset{*}{\Phi}{}_{E_0K_0+KJ}^{PKM}\overset{\leftrightarrow}{\frac{\partial}{\partial n}}\Psi_{E_0K_0+KJ}^{PKM}\right]dS\,d\xi_\alpha\,d\xi_K\right\}\\
&=\sqrt{\frac{2Mk_0}{\pi\hbar^2}}\left[\frac{\delta_{m,\,K_0-K}}{C_{K_0-K}}+\frac{(-1)^{J-q-P-K}\,\delta_{m,\,K_0+K}}{C_{K_0+K}}\right].
\end{aligned}\right\}\qquad\text{(I. 9)}$$

Eq. (I. 9) is strictly correct as long as the projection of the angular momentum on the nuclear symmetry axis is a constant of motion or, in other words, as long as K_0 and K are good quantum numbers. If we allow for Coriolis mixing of rotational bands, for instance, then (I. 9) has to be slightly generalized.

It is now easy to construct the asymptotic wave function using (I. 9).

$$\Psi_{R\to\infty}\sqrt{\frac{\pi\hbar^2k_0}{2M}}\sum_{KP}\left\{\frac{1}{C_{K_0-K}}\Psi_{E_0K_0-KJ}^{+\,PKM}+\frac{(-1)^{J-q-P-K}}{C_{K_0+K}}\Psi_{E_0K_0+KJ}^{+\,PKM}\right\}.\qquad\text{(I. 10)}$$

Of course, we may use the outgoing part of $\Phi_{E_0K_0-KJ}^{PKM}$ and $\Phi_{E_0K_0+KJ}^{PKM}$ as well, and indeed we shall make use of this possibility. We now consider the asymptotic behaviour of $\Phi_{E_0m'J}^{+\,PKM}$.

$$\Phi_{E_0m'J}^{+\,KPM}{}_{R\to\infty}\chi_\alpha\sqrt{\frac{2M}{\pi\hbar^2k_0}}\sum_{l'lm}a_{l'm'}\frac{g_{lm}^{+\,l'm'}(R)}{R}\varphi_{mlJ}^{PKM},\qquad\text{(I. 11)}$$

where

$$m'=\begin{cases}K_0-K\\K_0+K\end{cases}.$$

The $g_{lm}^{+\,l'm'}$ are the outgoing parts of the $g_{lm}^{l'm'}$ and follow from a solution of the α-wave equation. The meaning of the "matrix" $g_{lm}^{+\,l'm'}(R\to\infty)$ may be easily visualized: An α-particle which is formed in a state $l'm'$ at the nuclear surface may be scattered by the anisotropic potential into states lm at infinity.

After transforming the $Y_l^m(\vartheta'\varphi')$ which are contained in φ_{mlJ}^{PKM} to the space-fixed coordinate system we get

$$\left.\begin{aligned}\Phi^{+PKM}_{E_0 m' J} &= \sum_{l' l m} a_{l' m'} \frac{g^{+l' m'}_{lm}(R)}{R} \sum_{\nu} \sqrt{\frac{2j+1}{2J+1}}\, C(ljJ;\, mK) \\ &\times \sum_{\nu} C(ljJ;\, \nu M-\nu)\, Y^{\nu}_{l}(\vartheta\varphi) \sqrt{\frac{2j+1}{16\pi^2}} \left\{ D^{j}_{M-\nu K} X_K + (-1)^{j-P-K} D^{j}_{M-\nu-K} X_{-K} \right\}.\end{aligned}\right\} \tag{I. 12}$$

We easily recognize the sum on ν as a properly normalized wave function of an α-particle with angular momentum l coupled to a rotational state of the daughter nucleus with angular momentum j to give the total angular momentum J. The transition probability to such a state is exactly what we are interested in. We now define a matrix $B^{l'm'}_{lj}$ through

$$\sum_{m} g^{+l' m'}_{lm} \sqrt{\frac{2j+1}{2J+1}}\, C(ljJ;\, mK) = B^{l' m'}_{lj}\, e^{i(k_j R + \delta^{\text{COULOMB}}_{ljK})}, \tag{I. 13}$$

where $k_j = \sqrt{\frac{2M}{\hbar^2}\varepsilon_j}$, ε_j being the kinetic energy of the α-transition leading to the state j.

The matrix $B^{l'm'}_{lj}$ has essentially the same meaning as $g^{l'm'}_{lm}$, only the states labeled by lm have been replaced by states labeled by lj. These states are indeed the appropriate ones to use because they belong to a definite energy of the emitted α-particle. Finally, we arrive at a formula for the asymptotic wave function which contains the desired information.

$$\left.\begin{aligned}\Psi_{R\to\infty} &\to \sum_{ljK} \sqrt{\frac{2M}{\pi\hbar^2 k_j}} \frac{e^{i(k_j R + \delta^{\text{COULOMB}}_{ljK})}}{R} \chi_\alpha \\ &\sum_{\nu} C(ljJ;\, \nu M-\nu)\, Y^{\nu}_{l}(\vartheta,\varphi) \sqrt{\frac{2j+1}{16\pi^2}} \left\{ D^{j}_{M-\nu K} X_K \right. \\ &\left. + (-1)^{j-P-K} D^{j}_{M-\nu-K} X_{-K} \right\} \sum_{l'} \left[B^{l' K_0 - K}_{lj} \frac{a_{l' K_0 - K}}{C_{K_0 - K}} \right. \\ &\left. + (-1)^{J-L-K} B^{l' K_0 + K}_{lj} \frac{a_{l' K_0 + K}}{C_{K_0 + K}} \right] \sqrt{\frac{\hbar}{2\pi}} v_j,\end{aligned}\right\} \tag{I. 14}$$

where

$$v_j = \sqrt{\frac{2\varepsilon_j}{M}}.$$

Eq. (I. 14) gives the decomposition of the asymptotic wave function into definite final states ljK. It follows therefore from Eq. (I. 14) that the transition rate from a state of the parent labeled by JK_0q to a state jKp of the daughter via emission of an α-particle with angular momentum l equals

$$\lambda_{ljKP}^{JK_0q} = v_j \left| \sum_{l'L} \left[B_{lj}^{l'K_0-K} \int d\Omega' \overset{*}{Y}_{l'}^{K_0-K} \frac{G_{LK_0-K}(R_s)}{R_s^{1/2}} Y_L^{K_0-K} \right. \right.$$
$$\left. \left. + (-1)^{J-L-K} B_{lj}^{l'K_0+K} \int d\Omega' \overset{*}{Y}_{l'}^{K_0+K} \frac{G_{LK_0+K}(R_s)}{R_s^{1/2}} Y_L^{K_0+K} \right] \right|^2 . \qquad \text{(I. 15)}$$

Of course, the total decay constant is given by

$$\lambda = \sum_{ljKP} \lambda_{LJKP}^{JK_0q} = \sum_{KP} \left(\frac{1}{C_{K_0-K}^2} + \frac{1}{C_{K_0+K}^2} \right) \frac{2Mk_0}{\pi\hbar^2} . \qquad \text{(I. 16)}$$

The last equality follows from the fact that, according to (I. 5),

$$\int \overset{*}{\Phi}_{E_0 m' J}^{+PKM} \overleftrightarrow{\frac{\partial}{\partial n}} \Phi_{E_0 m'' J}^{+P''K''M} d\xi_\alpha \, d\xi_K \, dS = 2i \frac{2M}{\pi\hbar^2} \delta_{m'm''} \delta_{pp''} \delta_{KK''} \qquad \text{(I. 17)}$$

for any closed surface S around the origin. This relation, when applied to the asymptotic wave function, implies

$$\frac{2M}{\pi\hbar^2 k_0} \sum_{l'l''lj} k_j \overset{*}{a}_{l'm'} a_{l''m''} \overset{*}{B}_{lj}^{l'm'} B_{lj}^{l''m''} = \frac{2M}{\pi\hbar^2} \delta_{m'm''} . \qquad \text{(I. 18)}$$

From this equation (I. 18) the given result for the total decay constant follows immediately. On the other hand, this result could have been also obtained by inserting (I. 9) into (I. 1).

Before going on and treating special cases of (I. 16), we shall once more explain the meaning of the quantities appearing in the above equation. The function $R_s^{-1/2} G_{LM}(R_s)$ is, as already pointed out in connection with the boundary condition, the probability amplitude for forming an α-particle and a daughter nucleus out of the wave function of the parent. $R_s^{-1/2} G_{LM}$ depends essentially on the specific nuclear properties of the parent and daughter nucleus and is closely related to the reduced width of the transition (MANG, 1959a). On the other hand, $B_{lj}^{l'm'}$ depends mainly on gross nuclear properties as atomic weight A, charge Z, and quadrupole moment Q_0, the dependence on the angular momenta jKK_0 being nearly purely geometrical. In fact, $B_{lj}^{l'm'}$ tells us how an α-partial wave $l'm'$ of unit amplitude at the nuclear surface penetrates through the anisotropic potential barrier to give rise to an outgoing partial wave (lj) at large distances.

It may be useful here to give the expression for the matrix $B_{lj}^{l'm'}$ in the Fröman approximation (FRÖMAN, 1957) for the special case of even-even nuclear decay to the ground band of the daughter. In this case, $l = j$, $m' = 0$ and the coupled radial equations can be expressed like the standard Coulomb form as

$$\frac{d^2 u_l}{d\varrho^2} - \left[\frac{2\eta}{\varrho} - 1 + V_N(\varrho) + l(l+1)\left(\frac{1}{\varrho^2} + \varepsilon\right)\right] u_l = \frac{q}{\varrho^3} \sum_{l'} u_{l'} \langle Y_{l'}^0 \mid P_2 \mid Y_l^0 \rangle, \qquad \text{(I. 19)}$$

where $\eta = \dfrac{2Ze^2}{\hbar v_0}$ with v_0 the velocity of the ground alpha group,

$$\varepsilon = \frac{M}{\Im k_0}, \quad \varrho = k_0 R,$$

$q = \eta \dfrac{k_0^2 Q_0}{Z}$ with $\Im$ the nuclear moment of inertia, k_0 the ground alpha wave number, Q_0 the intrinsic quadrupole moment, $V_N(\varrho)$ is the short-range, attractive nuclear potential, and we have omitted coupling terms in $V_N(\varrho)$.

Then,

$$B_{ll}^{l'0}\,(\text{even-even}) = \frac{1}{G_l(\eta\varrho)}\, k_{ll'}(B), \qquad \text{(I. 20)}$$

where $G_l(\eta\varrho)$ is the irregular solution of the uncoupled equation for u_l with the right side set to zero. The reciprocal of the irregular function at the inner turning point is equivalent to the square root of the barrier penetrability factor.

We might mention that, inserting $\delta_{ll'}$ for $k_{ll'}$ and the WKB approximation for $G_l(\eta\varrho)$, we get results for spherical nuclei that have been derived earlier (Mang, 1960).

II. Formulas for Calculation of *G*-functions from the Shell Model

To calculate G_{LK_0-K} and G_{LK_0+K} explicitly we assume that the intrinsic properties of a deformed nucleus follow from a Hamiltonian of the type (Belyaev, 1958)

$$\left.\begin{aligned} H = &\sum_{\Omega_p} \varepsilon_{\Omega_p} \{a_{\Omega_p}^+ a_{\Omega_p} + a_{-\Omega_p}^+ a_{-\Omega_p}\} \\ &+ \sum_{\Omega_N} \varepsilon_{\Omega_N} \{a_{\Omega_N}^+ a_{\Omega_N} + a_{-\Omega_N}^+ a_{-\Omega_N}\} \\ &+ G_p \sum_{\Omega_p \Omega'_p} a_{\Omega_p}^+ a_{-\Omega_p}^+ a_{\Omega' p} a_{-\Omega' p} \\ &+ G_N \sum_{\Omega_N \Omega'_N} a_{\Omega_N}^+ a_{-\Omega_N}^+ a_{-\Omega' N} a_{-\Omega'}. \end{aligned}\right\} \qquad \text{(II. 1)}$$

The index p or N refers to protons and neutrons, respectively. The quantum number Ω labels the Nilsson orbits and the summation runs over all the orbits outside closed shells. The operator a_Ω^+ creates a particle in a state $\mid \varphi_\Omega \rangle$. The representation is that used by Nilsson (1955)

$$\varphi_\Omega = \sum_{l\Lambda} \alpha_{l\Lambda}\, \varphi_{nl}^{\Lambda}(\vec{r})\, \chi_{\pm 1/2}^{\Omega-\Lambda}. \qquad \text{(II. 2)}$$

Nilsson's nucleon wave functions are given in the isotropic harmonic oscillator representation with basis functions

$$\varphi_{nl}^{\Lambda}(\vec{r}) = (-1)^n \left[\frac{2\,n!\,\alpha^{3/2}}{(n+l+1/2)!}\right]^{1/2} (\alpha r^2)^{l/2} e^{-\frac{\alpha r^2}{2}} L_n^{l+1/2}(\alpha r^2)\, Y_l^{\Lambda}(\vartheta, \varphi), \qquad \text{(II. 3)}$$

where n is the number of radial nodes and equal to $(N-l)/2$, and $\alpha = \dfrac{m\omega_0}{\hbar}$ with m the nucleon mass and $\hbar\omega_0 = 41\,A^{-1/3}$ MeV chosen by NILSSON to give the proper nuclear size. $L_n^{l+1/2}$ is an associated Laguerre polynomial satisfying the equation

$$L_n^{l+1/2}(x) = \sum_k{}' (-1)^k \binom{n+l+1/2}{n-k} \frac{x^k}{k!},$$

where the $\binom{a}{b}$ quantity is a binomial coefficient in the usual notation. Ω is the projection of total angular momentum of the nucleon. Where a negative Ω value is involved, we will use the time-reversed wave function of positive Ω in order to have the correct phases for use with the pairing interaction formalism.

Approximate solutions of $(H-E)\,X = 0$ are

$$X_0 = \prod_{\Omega_p}{}' \prod_{\Omega_N}{}' (U_{\Omega_p} + V_{\Omega_p} a_{\Omega_p}^{+} a_{-\Omega_p}^{+}) \times (U_{\Omega_N} + V_{\Omega_N} a_{\Omega_N}^{+} a_{-\Omega_N}^{+}) \,|\, 0\rangle \qquad \text{(II. 4)}$$

in the case of an even-even nucleus, and the constants $U_{\Omega_p} V_{\Omega_p} U_{\Omega_N} V_{\Omega_N}$ are determined by the equations

$$U_{\Omega}^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_{\Omega} - \lambda}{\sqrt{(\varepsilon_{\Omega} - \lambda)^2 + \Delta^2}}\right) \qquad \text{(II. 5a)}$$

$$V_{\Omega}^2 = 1 - U_{\Omega}^2 \qquad \text{(II. 5b)}$$

$$\frac{2}{G} = \frac{2}{\Delta} \sum_{\Omega>0}{}' U_{\Omega} V_{\Omega} = \sum_{\Omega>0}{}' \frac{1}{\sqrt{(\varepsilon_{\Omega} - \lambda)^2 + \Delta^2}} \qquad \text{(II. 5c)}$$

$$n = 2 \sum_{\Omega>0}{}' V_{\Omega}^2 = \sum_{\Omega>0}{}' \left[1 - \frac{\varepsilon_{\Omega} - \lambda}{\sqrt{(\varepsilon_{\Omega} - \lambda)^2 + \Delta^2}}\right], \qquad \text{(II. 5d)}$$

where n is the average number of particles (neutrons or protons) outside closed shells.

From (II. 4) we are able to calculate the functions G_{L0} for the decay of the ground state of an even-even nucleus to the ground-state band of the daughter nucleus.

$$G_{LO}(\mathrm{R}) = \prod_{\Omega_p} \prod_{\Omega_N} (U^i_{\Omega_p} U^f_{\Omega_p} + V^i_{\Omega_p} V^f_{\Omega_p}) \times (U^i_{\Omega_N} U^f_{\Omega_N} + V^i_{\Omega_N} V^f_{\Omega_N}) \sum_{\Omega_p \Omega_N}{}' \frac{V^i_{\Omega_p} U^f_{\Omega_p}}{U^i_{\Omega_p} U^f_{\Omega_p} + V^i_{\Omega_p} V^f_{\Omega_p}} \times \frac{V^i_{\Omega_N} U^f_{\Omega_N}}{U^i_{\Omega_N} U^f_{\Omega_N} + V^i_{\Omega_N} V^f_{\Omega_N}} \Gamma_{LO}^{\Omega_p - \Omega_p \, \Omega_N - \Omega_N}(\alpha, \beta, R) \qquad \text{(II. 6)}$$

$$\Gamma_{Lm}^{\Omega_1 \Omega_2 \Omega_3 \Omega_4} = R^{3/2} \int \mathfrak{A}(\varphi^{(1)}_{\Omega_1} \varphi^{(2)}_{\Omega_2}) \mathfrak{A}(\varphi^{(3)}_{\Omega_3} \varphi^{(4)}_{\Omega_4}) \times \chi_\alpha(\beta, \xi_\alpha) \, Y^m_L(\vartheta' \varphi') \, d\xi_\alpha \, d\Omega', \qquad \text{(II. 7)}$$

where $\mathfrak{A}$ means an antisymmetrization operator. The index i refers to the parent and f to the daughter nucleus.

Here we have written equation (II. 7) in a general manner that will apply also to unfavoured alpha decay. For favoured decay we are dealing only with paired nucleons, and the proton function $\varphi(2)$ is just the time-reversed wave function for $\varphi(1)$; similarly, for the neutron function $\varphi(3)$ and $\varphi(4)$. The first bracketed factor in (II. 6) together with the denominator of the next factor essentially brings in a decrease associated with the incomplete overlap between parent and daughter of the various pairs other than the pairs contributing to the sum. This "core overlap" factor will presumably not vary rapidly from nucleus to nucleus and will not affect relative intensities very much, unless one is at some discontinuity in orbital level spacing where there is a large change in the Fermi energy between parent and daughter. In deriving this factor it has been further assumed that the deformations of parent and daughter nucleus are the same. At any rate, in the numerical work to be reported in this paper, we have set all $U^i U^f + V^i V^f$ factors of (II. 6) to unity.

The numerators $V^i_{\Omega_p} U^f_{\Omega_p} V^i_{\Omega_N} U^f_{\Omega_N}$ provide the essential weighting factor for the contributions of the various orbital combinations to the sum $G_{LO}(R)$. This weighting factor is a measure of the probability that the given orbitals are occupied in the parent and vacant in the daughter. The factor attains a maximum value for orbitals with energies nearest the average of the parent and daughter chemical potentials, λ_i, λ_f, and the factor decreases for orbitals with greater or lesser energies.

Equations (II. 6) are quite general and define the $G_{LO}(R)$ functions throughout the nuclear volume. Thus, the $G_{LO}(R)$ functions along any desired connection surface S and their derivatives normal to that surface are calculable.

A Gaussian wave function is substituted for the alpha particle internal wave function and the integration over the internal coordinates is carried out as described in earlier work (Mang, 1960). The alpha size parameter β is related to the mean square radius of the alpha particle by the relation $\beta = \frac{9}{8} \frac{1}{\langle r^2 \rangle}$. The resulting formulas are the same as in an earlier report (Mang, 1959a) except that the angular momentum

factors are modified in the present use of the $|\,l\Lambda\Omega\,\rangle$ representation, whereas an $|\,lj\Omega\,\rangle$ scheme was previously used.

The integral of Eq. (II. 7), corresponding to a particular set of Nilsson orbital assignments for the protons (1, 2) and the neutrons (3, 4), has the following values:

$$\left.\begin{aligned} I_{Lm}^{\Omega_1\Omega_2\Omega_3\Omega_4}(\alpha,\beta,R) &= (-1)^f\left(\frac{2}{\alpha+\beta}\right)^{\frac{9}{2}}(\alpha\beta)^{\frac{9}{4}}\left(\frac{2\alpha}{\alpha+\beta}\right)^{\varrho_{\max}+\frac{L}{2}}\sqrt{2} \\ &\times\left(\frac{1}{2}!\right)^{-\frac{1}{2}}(\alpha R^2)^{\frac{3}{4}}e^{-2\alpha R^2}[2(\alpha+\beta)R^2]^{\frac{L}{2}}\sum_{\varrho}\left(\frac{\beta-\alpha}{2\alpha}\right)^{\varrho_{\max}-\varrho}C_{\varrho}^{L} \\ &\times L_{\varrho}^{L+\frac{1}{2}}(2(\alpha+\beta)R^2), \end{aligned}\right\} \qquad \text{(II. 8)}$$

where the Ω_i are the angular momentum projections and imply all additional indices needed to specify the particular Nilsson orbital. $\varrho_{\max}=\dfrac{(N_1+N_2+N_3+N_4-L)}{2}$, and the phase factor exponent f is the sum of $|\,\Omega_i\,|-1/2$ values for all orbitals with Ω_i negative.

The C_{ϱ}^{L} expansion coefficients do not depend upon α, β or R and are determined solely by the four nucleon wave functions as follows:

$$\left.\begin{aligned} C_{\varrho}^{L} &= \varrho!\,(2L+1)^{-\frac{1}{2}}2^{-(2\varrho+L)}\left(\frac{1}{2}!\right)^2\sum_{l_1l_2l_3l_4}[(2l_1+1)(2l_2+1) \\ &\times(2l_3+1)(2l_4+1)]^{\frac{1}{2}}\left[n_1!\,n_2!\,n_3!\,n_4!\left(n_1+l_1+\frac{1}{2}\right)!\left(n_2+l_2+\frac{1}{2}\right)!\left(n_3+l_3+\frac{1}{2}\right)!\right. \\ &\left.\times\left(n_4+l_4+\frac{1}{2}\right)!\right]^{-\frac{1}{2}}B_{\varrho}^{L}(n_i\,l_i)\sum_{\Sigma_1\Sigma_2\Sigma_3\Sigma_4}(-1)^{1-\Sigma_1-\Sigma_3+n_1+n_2+n_3+n_4} \\ &\delta_{\Sigma_1,-\Sigma_2}\,\delta_{\Sigma_3,-\Sigma_4}\,\alpha_{l_1|\Lambda_1|}\,\alpha_{l_2|\Lambda_2|}\,\alpha_{l_3|\Lambda_3|}\,\alpha_{l_4|\Lambda_4|}\,D(l_1\,l_2\,l_3\,l_4\,\Lambda_1\,\Lambda_2\,\Lambda_3\,\Lambda_4\,L) \end{aligned}\right\} \qquad \text{(II. 9)}$$

with

$$\Lambda_i+\Sigma_i=\Omega_i.$$

Our convention here is to take the Nilsson expansion coefficients $\alpha_{l\Lambda}$ for an orbital of negative Ω as identical (no sign change) to the corresponding coefficient in an orbital of positive Ω. There is no separate summation over the radial quantum numbers n, since the Nilsson wave functions do not have configuration admixture from other oscillator shells.

The D factor comes from the vector coupling conditions and is a sum over products of six Clebsch-Gordan coefficients.

$$\left.\begin{aligned} D(l_1 l_2 l_3 l_4 \Lambda_1 \Lambda_2 \Lambda_3 \Lambda_4 L) = \sum_{l_p l_N} & C(l_1 l_2 l_p;\ \Lambda_1 \Lambda_2) \\ & C(l_1 l_2 l_p;\ 00)\, C(l_3 l_4 l_N;\ \Lambda_3 \Lambda_4)\, C(l_3 l_4 l_N;\ 00) \\ & C(l_p l_N L;\ \Lambda_1 + \Lambda_2\ \Lambda_3 + \Lambda_4)\, C(l_p l_N L;\ 00). \end{aligned}\right\} \quad \text{(II. 10)}$$

It is interesting to note that the D function has just the value of the integral

$$\int Y_L^{*\Lambda_1 + \Lambda_2 + \Lambda_3 + \Lambda_4}\, Y_{l_1}^{\Lambda_1}\, Y_{l_2}^{\Lambda_2}\, Y_{l_3}^{\Lambda_3}\, Y_{l_4}^{\Lambda_4}\, d\Omega .$$

The B factor comes from the radial functions and is as follows:

$$\left.\begin{aligned} B_\varrho^L(n_i l_i) = (-1)^\varrho\, n_1!\, n_2!\, n_3!\, n_4! \sum_{\nu_1 \nu_2 \nu_3 \nu_4} & \frac{(-1)^{\nu_1 + \nu_2 + \nu_3 + \nu_4}}{\nu_1!\, \nu_2!\, \nu_3!\, \nu_4!} \\ \times \binom{n_1 + l_1 + \frac{1}{2}}{n_1 - \nu_1} & \binom{n_2 + l_2 + \frac{1}{2}}{n_2 - \nu_2} \binom{n_3 + l_4 + \frac{1}{2}}{n_3 - \nu_3} \binom{n_4 + l_4 + \frac{1}{2}}{n_4 - \nu_4}, \end{aligned}\right\} \quad \text{(II. 11)}$$

where the summation is restricted by

$$2\varrho + L = 2(\nu_1 + \nu_2 + \nu_3 + \nu_4) + l_1 + l_2 + l_3 + l_4 .$$

III. Numerical Computations: Input parameters and methods

In order to treat the alpha decay of Cm^{242} and its neighbours throughout the deformed region and yet keep the computing time on the IBM-709 computer reasonable we made a compromise choice of a set of 10 proton- and 10 neutron-orbitals centered about the Fermi energies appropriate to Cm^{242}. In Mottelson and Nilsson's (1959) proton level diagram (their Fig. 5) the orbitals chosen are the $1/2 + (660)$, $3/2 + (651)$ and successively higher orbitals at deformation $\eta = 5$ up through $7/2 - (514)$ and $9/2 + (624)$. For the neutrons (their Fig. 6) they are orbitals $3/2 - (761)$, $3/2 + (631)$, $5/2 - (752)$ and higher up to the gap at 152 neutrons.

In the first stage of computation the C_ϱ^L coefficients were evaluated according to Eq. (II. 9) and punched into cards. The only input data were the Nilsson coefficients which were taken, as a compromise, as the deformation $\eta = 4$ entries in the tables. It would have been desirable to have $\eta = 5$ wave functions, since this is a more typical deformation for the alpha emitters treated, but it was felt somewhat risky to attempt an interpolation of the Nilsson coefficients because of the probable need for more than two-point interpolation with greater chance for errors.

Computer programming was entirely in the FORTRAN II system except for use of a Clebsch-Gordan coefficient subroutine, kindly supplied by the Los Alamos Scientific Laboratory. Subroutines were written for Eqs. (II. 10) and (II. 11). In order to save computer time, factorials and binomial coefficients were stored in tables within

the memory. The coefficients were computed for L of 0,2, and 4 and for all 100 combinations of the 10×10 set of orbitals. The total computing time required for the approximately 3000 C_{ϱ}^{L} coefficients was about eight hours, not counting many times this amount of time spent testing, correcting, and retesting the programs.

The computer programs were thoroughly checked at many stages. One satisfying final check involved hand calculation of the $11/2-(505)$, $13/2+(606)$ combination. The program for C_{ϱ}^{L} coefficients was at first made to transform the Nilsson functions into an $|lj\Omega\rangle$ representation before calculations were performed using formulas based on Eq. (A 32) of MANG (1959a). This program was brought to completion and verified to give correct answers, but it was intolerably slow. Then, extensive reprogramming to treat the original Nilsson representation by Eq. (II. 9) of this paper was carried out. Ultimately, an order of magnitude improvement in program running speed was attained. The earlier slow program provided a valuable check against the new program, for a number of complicated orbital combinations were treated with both programs and found to give identical results at least to five significant figures.

To determine the quantities U and V of the pairing interaction, we have used mainly the Δ values determined by NILSSON and PRIOR (1961) from an analysis of odd-even mass differences. Orbital energy values were interpolated values for deformation $\eta = 5$ used by NILSSON and PRIOR in their moment of inertia calculations, and we are grateful to Dr. NILSSON for providing us with these unpublished tables of interpolated eigenvalues. The values of the chemical potentials, λ_p and λ_N, for various nuclei were calculated by an iterative computer program solving Eq. (II. 5d). The U and V values were then calculated from Eqs. (II. 5a) and (II. 5b). The orbitals and their energies assumed in this work are tabulated in Table I. The energies are given in units of $\varkappa\hbar\omega_0$ as in Nilsson's tables.

The evaluation of Eq. (II. 6) for $G_{LO}(R)$ was also carried out by the Lawrence Radiation Laboratory IBM-709 computer. In the calculation of G_{LO} for a particular nucleus the input quantities were as follows: (1) the 1000 C_{ϱ}^{L} coefficients on 300 cards, (2) the α value, (3) the β value, (4) the twenty orbital energies, and (5) four λ values and four Δ values for neutrons and protons in the parent and daughter nucleus. The program computed and printed out the 100 Γ_{LO} values from Eq. (II. 7), and also calculated the U and V values and the grand summation of (II. 6). The computing time for each G_{LO} was about two minutes.

We believe the best value for β to be $0.47 \times 10^{26}\,\mathrm{cm}^{-2}$, corresponding to the mean square radius of the He^4 nucleus of 1.55×10^{-13} cm, as measured by electron scattering (cf. HERMAN and HOFSTADTER, 1960). By mistake, a value of $\beta = 0.625$ was used for most of the computations. Several nuclei were recalculated with the value 0.47 with only small changes in the results, as can be seen in Tables V and VI.

The α value, which determines the nuclear size, is given by the equation

$$\alpha = \frac{m\omega_0}{\hbar}$$

TABLE I. Orbitals and their Energies Used for Calculations.

	Energy (units of $\varkappa\hbar\omega_0$)
Protons	
11/2 − (505)	− 20.000
1/2 + (660)	− 21.170
3/2 + (651)	− 19.833
1/2 − (530)	− 18.815
5/2 + (642)	− 17.705
5/2 − (523)	− 17.006
3/2 − (521)	− 14.753
7/2 + (633)	− 14.406
7/2 − (514)	− 12.328
9/2 + (624)	− 10.679
Neutrons	
13/2 + (606)	− 16.400
3/2 − (761)	− 20.013
3/2 + (631)	− 18.090
5/2 − (752)	− 17.958
5/2 + (633)	− 16.300
7/2 − (743)	− 15.176
1/2 + (631)	− 14.611
5/2 + (622)	− 13.278
7/2 + (624)	− 12.540
9/2 − (734)	− 11.789

with m the nucleon mass and $\hbar\omega_0$ the quantum energy in the harmonic nuclear potential well. We have chosen $\hbar\omega_0$ using NILSSON's (1955) relation $\hbar\omega_0 = 41\,A^{-1/3}$ Mev. For $A = 238$, the $\varkappa$ value is $0.1597\times10^{26}\,\mathrm{cm}^{-2}$. For simplicity, we have used this $\varkappa$ value for all the nuclei. The relevant parameter is $\varkappa R^2$ for the nuclear surface which should stay nearly constant for the various nuclei. A few calculations were run for a too small nuclear size ($\varkappa = .175$) in order to give insight into the sensitivity of the results on $\varkappa$.

Calculations were run at several R values for Th^{228} and Cm^{242}, and all other nuclei were calculated only at $R = 8.25\times10^{-13}$ cm (corresponding to the apparent inflection point in the $R^{-\frac{1}{2}}G_{LO}$ *vs.* R curves).

IV. Numerical Values of the G_{LO} Functions

Some interesting insight into the theoretical alpha probability functions G_{LO} are to be gained by examining the intermediate results $\Gamma_{LO}(\varkappa\beta R)$ for the contributions of the 100 different orbital combinations. Table II lists the relative values of Γ_{LO} for $L = 0$, $\varkappa = 0.1597$, $\beta = 0.47$, and $R = 8.25$. The entries of successive columns refer

TABLE II. Γ_{00} Relative Values.

L = O R = 8.25 $\beta = 0.47$ $\alpha = 0.1597$

Prot. $\Omega\,\Pi$ \ Neut. $\Omega\,\Pi$	$\frac{13}{2}+$	$\frac{3}{2}-$	$\frac{3}{2}+$	$\frac{5}{2}-$	$\frac{5}{2}+$	$\frac{7}{2}-$	$\frac{1}{2}+$	$\frac{5}{2}+$	$\frac{7}{2}+$	$\frac{9}{2}-$
$\frac{9}{2}+$	6	5	22	7	17	10	24	36	20	15
$\frac{7}{2}-$	7	4	13	5	10	7	14	24	13	9
$\frac{7}{2}+$	4	10	40	15	30	20	51	32	19	19
$\frac{3}{2}-$	9	27	77	34	58	39	103	72	42	37
$\frac{5}{2}-$	4	9	31	12	23	16	40	32	18	16
$\frac{5}{2}+$	3	23	43	29	33	24	72	22	13	14
$\frac{1}{2}-$	5	77	76	62	58	42	159	35	21	23
$\frac{3}{2}+$	2	46	31	34	25	17	76	14	9	8
$\frac{1}{2}+$	2	49	22	23	17	12	70	12	7	7
$\frac{11}{2}-$	16	2	5	2	4	3	6	10	6	4

to neutron orbitals and the rows to proton orbitals. We note that all entries are positive, a consequence of the time-reversal definition of relative phases of paired orbitals to insure all U and V values positive. It is to be seen that the lowest contributions generally come from the combination of an orbital of low Ω value (wave function large in polar region) with an orbital of high Ω value (large in equatorial region). Intuitively, we associate these low intrinsic contributions with the poor overlap of these functions.

Table III lists the corresponding values of Γ_{20} at the above α, β and R values. Here we note that all combinations are positive, except those involving the high-Ω strongly equatorial proton orbital 11/2-(505) and the neutron orbital 13/2+(606). This observation, too, is intuitively understood; those orbitals predominantly overlapping at polar latitudes $\vartheta' < \cos^{-1}\sqrt{1/3}$, where the Legendre function $P_2(\cos\vartheta')$ is positive, make positive contributions. In fact, the slope of an orbital in the Nilsson diagram measures a similar property. Roughly we may expect down-sloping orbitals to contribute positively to Γ_{20}, and vice versa.

TABLE III. Γ_{20} Relative Values.

L = 2 R = 8.25 $\beta = 0.47$ $\alpha = 0.1597$

Prot. $\Omega\,\Pi$ \ Neut. $\Omega\,\Pi$	$\frac{13}{2}+$	$\frac{3}{2}-$	$\frac{3}{2}+$	$\frac{5}{2}-$	$\frac{5}{2}+$	$\frac{7}{2}-$	$\frac{1}{2}+$	$\frac{5}{2}+$	$\frac{7}{2}+$	$\frac{9}{2}-$
$\frac{9}{2}+$	−10	5	27	8	20	12	33	11	7	11
$\frac{7}{2}-$	−11	1	9	2	6	4	12	1	1	0
$\frac{7}{2}+$	−7	24	74	37	55	41	108	36	22	25
$\frac{3}{2}-$	−16	74	146	88	109	79	238	61	38	47
$\frac{5}{2}-$	−6	21	56	29	41	30	85	25	15	19
$\frac{5}{2}+$	−5	83	110	92	84	63	210	34	22	26
$\frac{1}{2}-$	−10	310	201	215	155	115	528	58	36	43
$\frac{3}{2}+$	−4	188	93	124	74	52	274	20	13	15
$\frac{1}{2}+$	−3	218	62	88	49	33	277	15	10	11
$\frac{11}{2}-$	−37	−3	−8	−3	−6	−5	−9	−15	−8	−6

Table IV lists the relative Γ_{40} values taken from a calculation at the same α, β, and R values as for Tables II and III. We now note that combinations in the lower left-hand part of the table give positive contributions, and those in the upper right-hand part contribute negative Γ_{40} values. It is immediately apparent that $L = 4$ intensities will be determined in large measure by a cancellation of contributions that may vary rapidly with changing nucleon numbers. From Table IV we can note that a combination of extreme polar orbitals (any of the $\Omega_p = 1/2$, $\Omega_N = 1/2$ combinations) always gives a positive value, and a combination of extreme equatorial orbitals (e.g. 11/2 −, 13/2 +) gives a positive Γ_{40}. These results follow from the fact that the Legendre function is positive in the vicinity of $\vartheta' = 0$ and also $\vartheta' = \frac{\pi}{2}$.

Fig. 1 shows bar graphs of the weighting factors V_Ω (parent) U_Ω (daughter) for the contributions of the various neutron and proton orbitals. The orbital energies are to scale vertically, and the parent and daughter λ values are marked by dashed lines. It

TABLE IV. Γ_{40} Relative Values.

L = 4 R = 8.25 $\beta = 8.25$ $\alpha = 0.1597$

Prot. $\Omega\,\Pi$ \ Neut. $\Omega\,\Pi$	$\frac{13}{2}^+$	$\frac{3}{2}^-$	$\frac{3}{2}^+$	$\frac{5}{2}^-$	$\frac{5}{2}^+$	$\frac{7}{2}^-$	$\frac{1}{2}^+$	$\frac{5}{2}^+$	$\frac{7}{2}^+$	$\frac{9}{2}^-$
$\frac{9}{2}^+$	69	−241	−1235	−286	−937	−512	−1196	−2015	−1145	−884
$\frac{7}{2}^-$	15	−135	−607	−169	−470	−280	−588	−1295	−709	−486
$\frac{7}{2}^+$	64	−158	−1768	−286	−1312	−803	−1756	−1859	−1082	−1009
$\frac{3}{2}^-$	195	184	−3223	−342	−2384	−1427	−2731	−3969	−2260	−2028
$\frac{5}{2}^-$	71	−110	−1465	−242	−1080	−649	−1408	−1832	−1024	−929
$\frac{5}{2}^+$	47	788	−924	25	−670	−469	−261	−900	−533	−533
$\frac{1}{2}^-$	105	5212	−962	1631	−632	−506	3835	−1437	−825	−839
$\frac{3}{2}^+$	36	3278	124	1300	144	72	2931	−535	−296	−253
$\frac{1}{2}^+$	31	4822	−33	1192	33	−34	4743	−506	−284	−268
$\frac{11}{2}^-$	665	20	55	25	43	32	70	37	18	34

is apparent that the results for the lighter nuclei, such as Th^{228}, need improvement by inclusion of lower-lying orbitals, and we have eliminated Th from our final analyses. These calculations used mostly the orbitals that have been identified in the energy level systems of odd-A nuclei and hence appear on the simplified diagrams of the MOTTELSON-NILSSON work (1959). These diagrams fail to show many of the levels from adjacent major shells. The neglect of these primarily equatorial orbitals may well produce a systematic error of too great theoretical $L = 2$ intensities.

The function $R^{-1/2} G_{LO}$ as defined by Eq. (II. 5) may be considered the partial wave amplitude in the nuclear interior of the alpha particle of maximum kinetic energy (daughter nucleus ground state pairing function assumed) which must go over smoothly into the penetrating alpha wave of the decay process. In the simplest view of the Nilsson functions in the isotropic harmonic oscillator representation, the functions would define the α-wave function on a spherical surface as $\sum_L R^{-1/2} G_{LO} Y_L^0$. In our alpha decay calculations it is very important that we consider the Nilsson

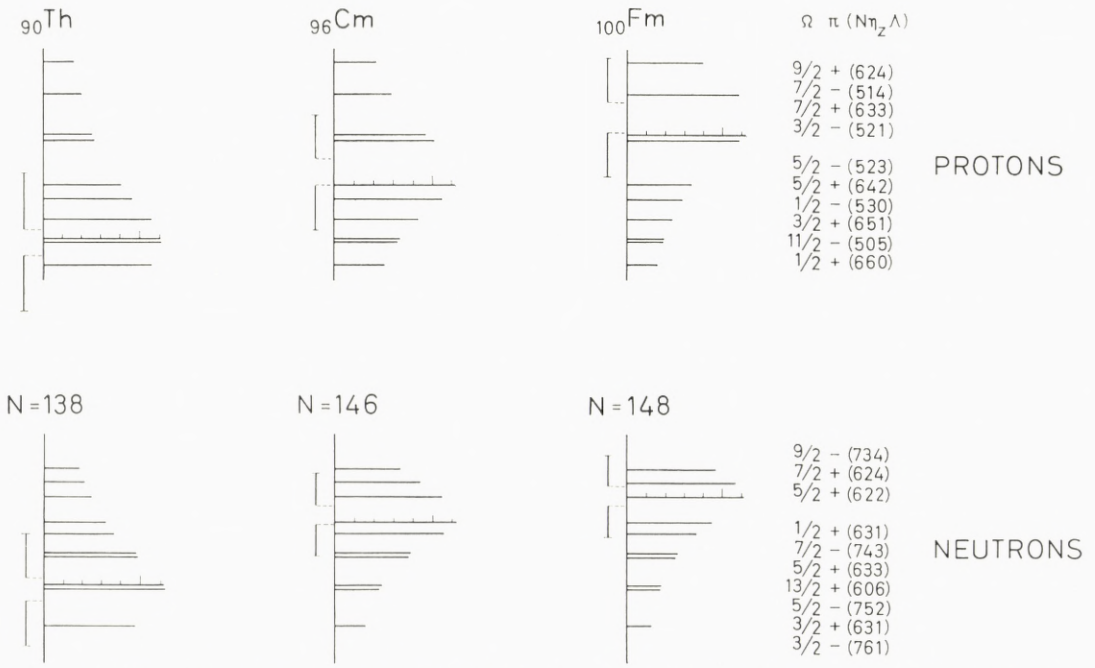

Fig. 1. Diagrams for three sample proton numbers and three sample neutron numbers where the energy of the Nilsson orbital is plotted to scale vertically and the lengths of the horizontal bars give the $u_i' v_i$ weighting factor for each orbital. (This factor is the square root of the probability that the orbital is occupied in the parent and vacant in the daughter.) The horizontal scale is indicated on the longest bar by marks every 0.1 unit. The vertical energy scale can be deduced from the vertical base lines which go from ε values of -22 to -10. The orbital energy for a proton orbital is then $(5+3/2+0.05\,\varepsilon_i)\,\hbar\omega_0$ and for a neutron $(6+3/2+.05\,\varepsilon_i)\,\hbar\omega_0$ with $\hbar\omega_0 = 41\,A^{-1/3}$ Mev. The orbital energies correspond to a deformation $\delta \sim 0.24$. To the left of the base line are dashed lines showing the positions of the chemical potential (or Fermi energy) for parent and daughter used in the calculation. The vertical bars extending from the ends of these reference lines are of length equal to the gap parameter Δ used for parent (upper) and daughter (lower). The size of Δ essentially establishes the energy width of the envelope of the $u_i' v_i$ values, with the envelope tending toward an asymptotic limit of

$$\frac{\Delta}{\sqrt{2}\,|\,\varepsilon_i - \lambda\,|}\,.$$

The orbitals used are listed with the usual asymptotic indices.

functions in the alternative representation described in his appendix *A* (Nilsson, 1955). This representation is superior in that Nilsson's neglect of wave function components from other major shells is much better justified. In the alternative representation, the radial coordinate surfaces are spheroids of half the deformation of the isopotential nuclear surface. For a nucleus of deformation δ we have to lowest order (where the subscript a denotes coordinates of a point (x, y, z) in the alternate representation) the following relations:

$$x_a = x\,(1 + \delta/6)$$
$$y_a = y\,(1 + \delta/6)$$
$$z_a = z\,(1 - \delta/3).$$

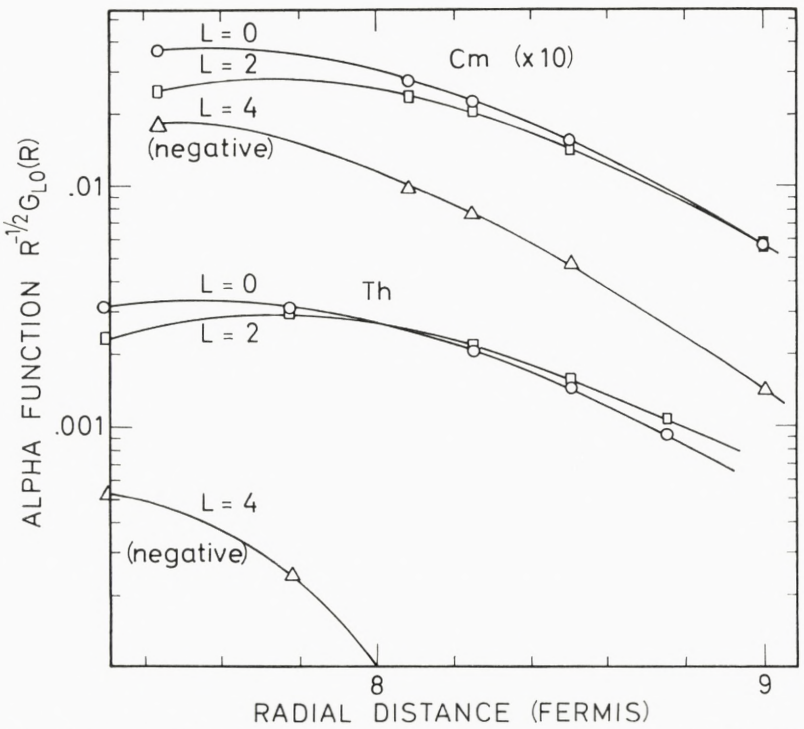

Fig. 2. Semi-logarithmic plot of the radial behaviour of the computed "internal" alpha-particle wave function $R^{-1/2}G_{LO}(R)$ for Cm^{242} and Th^{228} ($L=0$, ○; $L=2$, □; $L=4$, △). For the calculation were used $\alpha=0.1597$ and $\beta=0.625$. The values slightly differ from the functions and ratios tabulated in the text, because the radial behaviour here plotted comes from early calculations, using guessed values for the Fermi energies λ. The values in the text are later calculations using λ values as plotted in Fig. 1, which are solutions of the Belyaev equation $N=2\sum_i v_i^2$. The radial behaviour would be little affected by the slightly wrong λ values although the magnitudes of the functions are somewhat affected.
For Th^{228} the $L=4$ function is not graphed at large distance because it becomes too small to show and even changes sign.
A linear plot shows that the inflection points (zero curvature) are around $R=8.25$ f.

The first calculations to be made investigated the radial dependence of $G_{LO}(R)$ for Th^{228} and Cm^{242}. The G_{LO} functions were calculated at several different radii and at two different values of the nuclear size parameter α. Fig. 2 shows the variation of the $R^{-\frac{1}{2}}G_{LO}$ functions with distance for $\alpha=0.1597$ and $\beta=0.625$. The calculations at $\alpha=0.175$, corresponding to a nuclear size 5 % too small, are not plotted, but the results are very nearly the same at the same values of αR^2. Thus, a change of α mainly affects the distance scale. We have in general performed our calculations over a range of nuclei using constant values of α and R with this justification.

The larger functions $R^{-1/2}G_{00}$ and $R^{-1/2}G_{20}$ at the outermost distances show a radial behaviour similar to that of the most lightly bound nucleon wave functions. The outer inflection points $\sim 8.2\times10^{-13}$ cm occur at about the distance of the classical turning points of these nucleon orbitals in the harmonic potential. The fall-off outside the

Table V. G_{LO} Value Ratios.

Alpha ..... Emitter.....		G_{20}/G_{00} G_{40}/G_{00}	
	α = .1597 β = .47 R = 8.25	α = .1597 β = .625 R = 8.25	α = .1597 β = .625 R = 8.5
Th^{228}	1.110	1.092	1.133
	.049	.058	.095
U^{230}	..	1.075	..
	..	+.004	..
U^{232}	..	1.040	..
	..	−.047	..
U^{234}	..	1.013	..
	..	−.085	..
U^{236}	..	1.004	..
	..	−.113	..
Pu^{238}	..	.976	..
	..	−.187	..
Pu^{240}	..	.945	..
	..	−.240	..
Cm^{242}	.919	.887	.926
	−.340	−.352	−.318
Cm^{244}	.848	.818	..
	−.428	−.438	..
Cf^{246}	.786	.758	..
	−.525	−.531	..
Fm^{248}	.736	.708	..
	−.575	−.580	..

inflection points is more rapid than exponential, like the behaviour of the nucleon functions in the rapidly rising harmonic potential. In fact, this overly-rapid, Gaussian-like fall-off is an unrealistic property of the harmonic oscillator wave functions. Radial wave functions in a more realistic square well-like potential show more nearly a simple exponential fall-off at outer distances. Harada (1961) has investigated this question and the effects on alpha decay rate calculations of spherical nuclei.

For two reasons we prefer to modify and approximate the calculated outermost radial dependence of $R^{-1/2}G_{LO}$ functions by a simple exponential dependence as it would be with a square well potential. First of all, this modification offers a means of approximately remedying the too-repulsive harmonic potential at large distances, and secondly, the exponential dependence simplifies the transformation of the G_{LO} vector from the spheroidal surface of constant radial parameter R_0 over to the more eccentric spheroidal surface of constant nuclear density at which the external solution is to be joined.

We have made a comparison between rounded square well wave functions

Table VI. Absolute G_{00} Values.

Alpha emitter	$G_{00}\times 10^2$		
	$\alpha = .1597$ $\beta = .47$ $R = 8.25$	$\alpha = .1597$ $\beta = .625$ $R = 8.25$	$\alpha = .1597$ $\beta = .625$ $R = 8.5$
Pu^{238}	..	.67	..
Pu^{240}	..	.64	..
Cm^{242}	.67	.628	.439

(Blomqvist and Wahlborn, 1960) and the harmonic oscillator wave functions and have concluded that a reasonable way to improve the H.O. wave functions would be to smoothly join a simple exponential to the H.O. wave function at its inflection point. Thus, we shall adopt the procedure of replacing the $R^{-1/2}G_{LO}$ functions by a simple exponential, tangent to the H.O. wave function at its inflection point (near $R = 8.2$).

Of course, the behaviour of the small G_{40} in Th^{228} which changes sign at $R = 8.2$ is not well approximated by an exponential, but its small magnitude, relative to G_{00} and G_{20}, makes the errors produced by the exponential approximation in the final answers quite unimportant.

Table V lists the G_{LO} values relative to G_{00}; it is only the ratios that enter into the calculations of final relative intensity of alpha groups to various rotational states. Fortunately, it appears that the results are not too sensitive to the exact choice of parameters. Thus, we shall use the most complete set of calculations, that of the middle column, for our further calculations, although the β value of 0.47 of the first column of results actually corresponds best to the size of the alpha particle in free space. The ratios are seen to have a smooth behaviour from one nucleus to the next heavier nucleus.

Table VI lists the absolute G_{00} values for a few nuclei whose Fermi energies lie toward the middle of the energy range of the nucleon orbitals used in the calculation. The absolute values and their trends can only be expected to have meaning for such nuclei.

V. Theoretical Intensity Values

Before we can calculate theoretical alpha decay intensities we must transform the G_{LO} expansion into a Legendre expansion on the spheroidal connection surface. That is, we must evaluate the integral of Eq. (I. 16). For this it is most convenient to have a simple approximate functional form for the radial dependence of the functions just beyond their inflection points.

We shall assume that the radial dependence in the vicinity of $R = 8.375f$ is just a simple exponential joining the calculated functions smoothly at this distance. Such

behaviour means a slower fall-off than calculated at large distance, but is really more appropriate for a finite-well nuclear potential

$$R^{-1/2} G_{LO}(R) = R_0^{-1/2} G_{LO}(R_0) \exp\left[-\gamma_L \cdot \frac{R - R_0}{R_0}\right]. \tag{V. 1}$$

To join smoothly we take γ_L as a dimensionless logarithmic derivative of $R^{-1/2} G_{LO}$ at $R = 8.375$. From the calculated G_{LO} values for Cm^{242} at $R = 8.25$ and $R = 8.5$ we get by finite difference $\gamma_0 = +12.6$, $\gamma_2 = +11.3$, and $\gamma_4 = +16.4$. We shall use these γ_L values also for other nuclei, though we only have investigated radial variations for one other, Th^{228}, with nearly the same result for γ_0 and γ_2 and somewhat different for the small G_{40}.

Let us consider that the nuclear surface on which connection is to be made is given by the equation

$$\left.\begin{aligned} R_s(\vartheta') &= R_c\left[1 + \frac{2\delta}{3} P_2(\cos\vartheta')\right] + R_0 - R_c \\ &= R_0\left[1 + \frac{2\delta_f}{3} P_2(\cos\vartheta')\right], \end{aligned}\right\} \tag{V. 2}$$

where

$$\delta_f = \frac{R_c}{R_0}\,\delta.$$

R_c is the equivalent radius $1.2 \times 10^{-13} A^{1/3}$ cm for which the δ values of Prior and Nilsson (1961) were calculated using experimental Q_0 values. R_0 is the radius $1.37 \times 10^{-13} A^{1/3}$ cm (i.e., $8.5f$ for Cm^{242}) slightly beyond the inflection point of the G_{LO} functions at $8.25f$, the radius at which most of our calculations were made. We feel that the above choice of the connection surface is a good estimate of the surface on which the effective alpha-particle potential is constant, aside from $P_4(\cos\vartheta')$ deformations discussed later. The assumption is essentially that the effects, such as diffuseness of the nuclear density distribution and finite range of nuclear forces, act to position the beginning of the alpha barrier at a constant distance $(R_0 - R_c)$ from the surface of the uniformly charged spheroid giving the proper experimental mean square radius and intrinsic quadrupole moment. It is troublesome that the real part of the Igo optical-model potential would make the barrier begin still about one Fermi further out than our R_0. We feel that this discrepancy is due to remaining defects in the Hamiltonians describing both inner and outer regions. In order to apply our formulations of Section I we need to alter the external potential from the Igo potential so that the alpha barrier begins at the inflection point of our G_{LO} functions. Fortunately, the theoretical *relative* intensities we calculate will be nearly independent of the detailed way in which the Igo potential is altered, but the absolute transition probabilities we calculate will be subject to uncertainty.

As pointed out in the first section, it is desirable to carry out the connection of

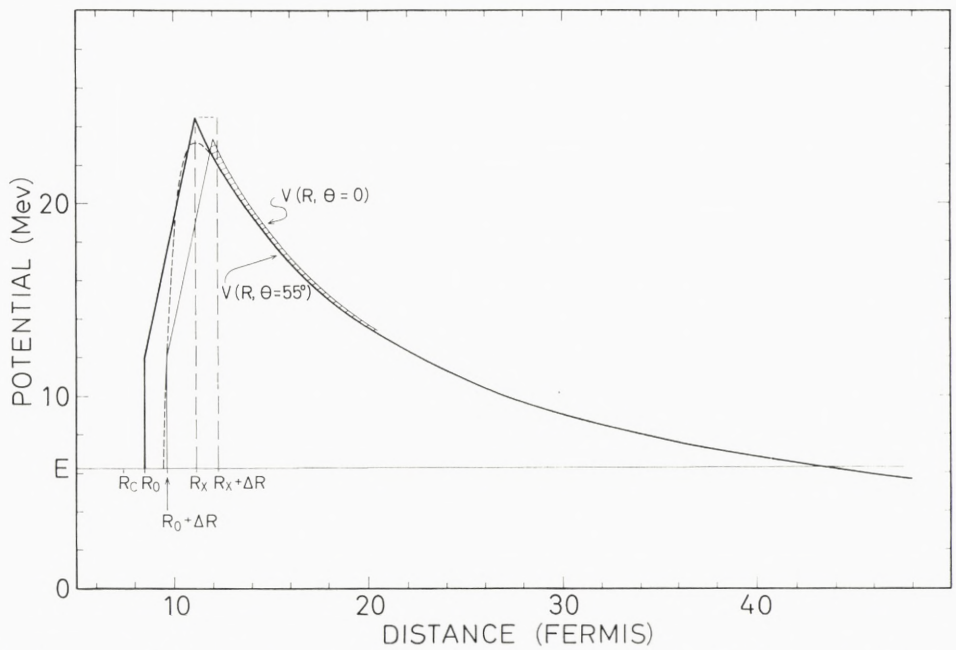

Fig. 3. Plots to scale of the potential profiles of the assumed barrier for Cm^{242} along $\theta = 55°$ (i.e. the zero of $P_2(\cos\theta)$) and along the polar axis $\theta = 0°$. The continuous curve gives the Igo real potential for comparison. Several radial distances are noted, R_c, the effective charge radius $1.2\times10^{-13}A^{1/3}$.
R_0, the chosen connection radius between internal and external solutions.
$R_0+\Delta R$, the distance of the connection surface at $\theta = 0$.
$\left(\Delta R = \frac{2}{3}\delta Rc\right)$.
R_x is the barrier peak along $\theta = 55°$, chosen to match the Igo barrier peak.
The horizontal line E marks the alpha distintegration energy.

inner and outer solutions within the barrier region, because one wishes the WKB approximation to be valid for the external solution and wishes to be able to neglect centrifugal barrier effects near the nucleus in treating the anisotropic barrier problem.

We shall make use of the Fröman matrix method (1957) in dealing with the barrier transmission, but we shall carefully reexamine the problem to determine the arguments of the matrices, using a diffuse nuclear potential and basing the relationship between experimentally determined Q_0 values and inferred deformation parameters on nuclear charge distributions of the correct size. In order to have a definite diffuse anistropic potential for analysis we assume, based on the curvature of the G_{LO} functions at R_0, that the potential energy is 12 Mev on the surface $R_s(\vartheta')$ defined by (V. 2) and that the barrier maximum comes at the average distance $11.1f$, which is the barrier top obtained using the Igo potential. (Fortunately the barrier treatment here is quite independent of the constant potential assumed at R_s.) We let the potential experienced by the alpha particle rise linearly with distance from $R_s(\vartheta')$ for all angles ϑ' until it intersects the pure Coulomb potential

$$V_c - \frac{2\,Ze^2}{R} + \frac{Q_0\,e^2}{R^3}\,P_2(\cos\vartheta').$$

From the intersection surface outward the potential is taken as purely coulombic.

Fig. 3 plots the potential profiles along $\vartheta' = 55°$ (where $P_2(\cos\vartheta')$ vanishes) and along $\vartheta' = 0$. The Fröman matrix method divides the wave propagation through the barrier into two stages, first, the propagation from the spheroidal surface $R_s(\vartheta')$ to a spherical surface and, second, the propagation from the sphere outward to infinity. We shall choose the spherical surface to be just beyond the range of the nuclear force, i.e., $R_x + \Delta R$ in Fig. 3. The appropriate argument B for the Fröman matrix is just the value of the WKB barrier integral along $\vartheta' = 55°$ minus the value of the integral along 0°.

Before considering the Fröman matrix further let us consider the transformation from the coordinate system of the nucleon to the isopotential connection surface.

The surface integral of Eq. (I. 16) accomplishes this transformation and may now be evaluated using (V. 1) and (V. 2)

$$\int Y_{l'}^{0\,*}\frac{G_{LO}}{R_s^{1/2}}\,Y_L^0\,d\Omega' = \int Y_{l'}^{0\,*}\exp\left[-\frac{2}{3}\,\delta_f\gamma_L P_2(\cos\vartheta')\right]Y_L^0\,d\Omega' \times R_0^{-1/2}\,G_{LO}(R_0). \qquad \text{(V. 3)}$$

The exponent above would be obtained if the G_{LO} were expansion coefficients in spherical polar coordinates. As we have pointed out in the preceding section, it is important to consider that the expansion is in Nilsson's alternate representation of modified scale parameter. Taking this into account and noting that the integrals are now just identical to the definition of a Fröman matrix element, we have

$$\int Y_{l'}^{0\,*}\frac{G_{LO}(R_s)}{R_s^{1/2}}\,Y_L^0\,d\Omega' = k_{l'L}(B_L)\,R_0^{-1/2}\,G_{LO}(R_0) \qquad \text{(V. 4)}$$

with

$$B_L = -\frac{\gamma_L}{3}(2\,\delta_f - \delta) = -0.27\,\delta\gamma_L.$$

If we take a weighted average γ value of about 12, we have the approximate expression

$$B_L \approx -3.2\,\delta.$$

At the end of Section I it was pointed out that the matrix element $B_{lj}^{l'm'}$ simplified in the even-even case to a Fröman matrix element times a reciprocal irregular Coulomb function. Since the product of two Fröman matrices is the matrix whose argument is the sum of those of the factors, we shall be able to write Eq. (I. 16) in a simple form:

$$\lambda_l = \frac{v_l}{R_0\,G_l^2(\eta_l, \varrho_{lo})}\left|\sum_L k_{lL}(B_q + B_s + B_L)\,G_{LO}(R_0)\right|^2. \qquad \text{(V. 5)}$$

B_s is the argument of the matrix that transforms the expansion on the connection surface (V. 2) to the spherical surface at $R_x + \Delta R$ just beyond the range of nuclear forces. B_q is the argument of the matrix transforming the expansion on the sphere to the expansion near the classical turning point. In analogous fashion to FRÖMAN we get the following expression:

$$B_s \approx \frac{2}{3} \delta k_0 R_c \left(\frac{2\eta}{k_0 R_x} - 1 \right)^{1/2}, \tag{V. 6}$$

where R_x is the radial distance at the barrier maximum

$$B_q \approx -\frac{q}{6\eta^2} \left(\frac{2\eta}{k_0 (R_x + \Delta R)} - 1 \right)^{1/2} \left(1 + \frac{\eta}{k_0 (R_x + \Delta R)} \right), \tag{V. 7}$$

where the symbols have been defined in connection with Eq. (I. 19). The parameter q, the dimensionless quadrupole coupling constant, can be rewritten

$$q = \eta \frac{k_0^2 Q_0}{Z} = \frac{2 M k_0 Q_0 e^2}{\hbar^2}.$$

Thus, we may rewrite B_q

$$B_q = -\frac{k_0^2 Q_0}{6 Z} \left(\frac{2\eta}{k_0 (R_x + \Delta R)} - 1 \right)^{1/2} \left(\frac{1}{\eta} + \frac{1}{k_0 (R_x + \Delta R)} \right).$$

In Fig. 3 the nature of the approximation can be seen. B_s is the WKB integral over the rectangular region of width ΔR and height the coulombic potential at R_x. B_q is the integral over the barrier difference shown by the small shaded region. To get a simpler approximate expression for B arguments we may substitute parameters for our average alpha emitter Cm^{242}.

$$\eta = 23.7$$

$$k_0 = 1.085 f^{-1}$$

$$R_c = 7.45 f$$

$R_x = 11.1 f$, using the real part of IGO's potential.

Then,

$$B_s \approx 9.30 \delta$$

$$B_q \approx -0.045 Q_0.$$

The total argument is

$$B = B_q + B_s + B_L \approx 6.1 \delta - 0.045 Q_0. \tag{V. 8}$$

We have used Eqs. (V. 5) and (V. 8) to calculate relative intensities from the G_{LO} relations of the central column of Table V.

Table VII. Experimental and Theoretical Reduced Wave Amplitudes assuming only Quadrupole Surface Deformation.

Alpha emitter	δ daughter	Q_0 daughter (10^{-24}cm^2)	B	Theory				Experiment	
				b_2	b_4	b_{4i}	b_4	b_2	b_4
U^{230}	.195	8.20	0.82	1.26	0.34	−.130	.37	1.36	.70
U^{232}	.199	8.47	0.83	1.23	0.29	−.112	.31	1.31	.60
U^{234}	.205	8.74	0.86	1.22	0.27	−.106	.29	1.23	.63
U^{236}	.214	9.26	0.89	1.21	0.25	−.107	.27	1.22	.62
Pu^{238} ...	.219	9.80	0.90	1.18	0.18	−.105	.21	1.08	.22
Pu^{240} ...	.229	10.35	0.93	1.16	0.14	−.121	.19	1.02	.26
Cm^{242}...	.236	10.96	0.95	1.10	+0.022	−.112	.114	0.99	.12
Cm^{244}...	.240	11.20	0.96	1.02	−0.08	−.100	.13	0.93	.08
Cf^{246}....	.243	11.70	0.95	0.97	−0.20	−.105	.226	0.84	.19
Fm^{248}...	.243	12.00	0.94	0.91	−0.28	−.103	.30	..	..
Fm^{254}...	..	..	..	..	..	..	..	.70	0.30

Table VII lists the final calculations of reduced relative intensities b_2 and b_4 compared with experiment. These quantities are defined exactly in accordance with Fröman

$$b_l = \frac{\sum_L k_{lL} G_{LO}(R_0)}{\sum_L k_{OL} G_{LO}(R_0)}. \qquad \text{(V. 9)}$$

They are the square roots of reciprocals of the reduced hindrance factors. The δ values are taken from Nilsson and Prior (1961) and the Q_0 values calculated by their quadratic relationship with these values, using the nuclear radius $1.2A^{1/3}f$.

There is a further correction which is not negligible for very weak groups. That is essentially the Coulomb excitation process occurring primarily beyond the classical turning point. The effect may be approximated by a small imaginary component in the argument of the Fröman matrix as Nosov (1957) has done. The calculation of this correction is discussed in the Appendix. The b_{4i} of Table VII is given as follows:

$b_{4i} = b_2 \hat{k}_{24} \times$ (penetrability factor of $L = 2$ divided by the penetrability of $L = 4)^{1/2}$ with $\hat{k}_{24}$ given by the equation of the Appendix, including the correction for finite nuclear rotational energy.

The proper $|b_4|$ reduced amplitude to compare with the experimental is

$$|b_4| = \sqrt{b_4^2 + b_{4i}^2}.$$

The Coulomb excitation components of the abundant $L = 0$ and $L = 2$ groups are quite negligible and have not been calculated.

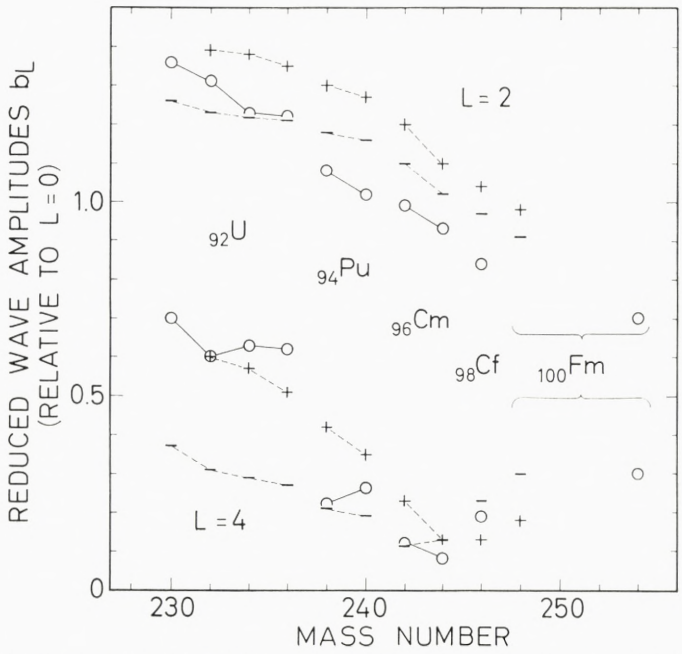

Fig. 4. Comparison of experimental (○) and theoretical reduced wave amplitudes $|b_L|$. The values for a given element are connected by lines, solid for experiment, dashed for theoretical. The theoretical values marked by bars (−) are for no $P_4(\cos\vartheta')$ deformation and those with crosses (+) are corrected for such deformation.

There is also a second set of theoretical points plotted in Fig. 4. These points correspond to values approximately corrected for 2^4-pole deformation of the nuclear surface. KJÄLLQVIST (1958) has calculated theoretically the magnitude of the surface deformation term $\beta_4 Y_{40}(\Theta')$. To treat the higher order deformation properly would involve a Fröman-type matrix with elements of the form

$$\int Y_l^{0*} \exp\left[BP_2(\cos\vartheta') + DP_4(\cos\vartheta')\right] Y_L^0 \, d\Omega',$$

and this matrix would not exactly factor into a product of matrices depending separately on quadrupole and 2^4-pole deformation. To first order in β_4, and following similar considerations to FRÖMAN (1957) and those used earlier here in deriving approximate expressions for B_L and B_s, we make a correction for P_4 deformation by multiplying the G_{LO} (real) vector by a square matrix whose elements are

$$f_{lL} = \delta_{lL} + \frac{9.15\,\beta_4}{\sqrt{4\pi}} C^2(l\,4\,L;\,00) \sqrt{\frac{9\cdot(2l+1)}{2l+1}}.$$

The corresponding corrected wave amplitudes are given in Table VIII.

Table VIII. Theoretical Reduced Wave Amplitudes Corrected for $P_4(\cos\vartheta')$ Deformation of the Nuclear Surface.

Alpha emitter	(theo.) β_4	b_2	b_4	b_{4i}	$\lvert b_4 \rvert$
U^{230}	No β_4 value available for daughter				
U^{232}	.062	1.39	.59	−.12	.60
U^{234}	.061	1.38	.56	−.12	.57
U^{236}	.053	1.35	.50	−.12	.51
Pu^{238}	.048	1.30	.40	−.12	.42
Pu^{240}	.043	1.27	.33	−.13	.35
Cm^{242}	.042	1.20	.20	−.12	.23
Cm^{244}	.038	1.10	.07	−.11	.13
Cf^{246}	.035	1.04	−.07	−.11	.13
Fm^{248}	.036	0.98	−.15	−.11	.18

The Kjällqvist β_4 values are all positive and range monotonically downward from 0.062 at Th^{228} to 0.022 at Cf^{250}. The correction matrix element of most importance to us is the f_{04}, which acts to add a positive contribution to the $l = 4$ amplitude.

Since there are no direct experimental measurements of 2^4-pole deformation, it is satisfying to see that the effects of such a deformation on our calculations are not so drastic as to invalidate it. Nevertheless, the effects of 2^4-pole deformation of the isopotential surface clearly cannot be neglected for really quantitative future theoretical calculations.

Fig. 4 plots the magnitudes of the relative reduced amplitudes. The theoretical results reproduce the essential features of the experimental values with the minimum in $|b_4|$ and with the gradual fall-off of $|b_2|$.

If the results of Fig. 4 are compared with the figure of the preliminary paper on this work (Mang and Rasmussen, 1961), some differences are noted. The preliminary results did not take into account the Coulomb excitation component of $l = 4$, which is significant for the cases of nearly vanishing b_4. More important, the preliminary results were calculated using larger arguments for the Fröman matrix based on the formula $B \approx 6.0\,\delta$ rather than Eq. (V. 8) of $B = 6.1\,\delta - 0.045\,Q_0$. The larger B values threw the minimum in b_4 into element 98, at a higher atomic number than experimental. The results of Fig. 4 show the theoretical minimum to be now somewhat on the other side of experimental. The theoretical $|b_2|$ values of Fig. 4 show generally some reduction as a consequence of the lowered B value.

In part the smaller B value expression of Eq. (V. 8) results from the consideration of a sloping nuclear potential, but the difference comes mainly from our inexact procedure in the preliminary work of using the deformation values of Nilsson and

Prior (1961), based on a charge radius of $1.2 \times 10^{-13} A^{1/3}$ cm with Fröman's Eq. (VIII-6), which was derived on the basis of a charge radius of $1.44 \times 10^{-13} A^{1/3}$ cm. The relative intensities of $l = 4$ are seen to be rather sensitive to the anisotropic barrier penetration effects dealt with by the Fröman matrix. Of course, there are still uncertainties with our present formula (V. 8), but it is probably more nearly correct than the expression used in the preliminary paper.

The agreement of theory with experiment in Fig. 4 is clearly so encouraging that we feel it established that the wave function of alpha particles contributing to alpha decay undergoes angular variation over the deformed surface in essentially the same way as the nucleon orbitals near the Fermi surface.

We may confidently use the results of our calculations to decide in most cases which is the correct one of the several possible results of inward integrations based on experimental intensities, deciding the phase ambiguity through $L = 0$, 2, and 4. For example, in Pennington and Preston (1958), four possible phase cases are depicted from inward numerical integrations of several nuclei from U^{234} through Fm^{254}. Our work would now categorically rule out cases III and IV, with their large negative $L = 2$ amplitudes. Further, we would select case I for the nuclei below Cm^{242} and case II for those heavier than Cm^{242}, with the choice between cases I and II being uncertain for Cm^{242} itself. Our theoretical prediction of positive $L = 2$ phase is indirectly confirmed by several angular correlation experiments involving favoured decay of odd-mass nuclei, but no experiments have yet measured our prediction that $L = 4$ is in phase below curium and out-of-phase for heavier elements.

That the $L = 4$ minima of theory and experiment coincide at element Cm is somewhat fortuitous; the inclusion of more $\Omega = 1/2$ orbitals at lower energy might displace the minimum toward higher Z. Also the inclusion of G_{60} in future calculations will probably affect the location of the $L = 4$ minimum.

The inclusion of the above-mentioned $\Omega = 1/2$ orbitals would probably also increase somewhat the $| b_2 |$ values mostly for uranium. The inclusion of more of the orbitals from the next lower major shell (only one $h\,11/2$ proton orbital and one $i\,13/2$ neutron orbital were used here) would tend to lower the $L = 2$ amplitudes.

Perhaps the contribution to the alpha-decay amplitude from orbitals in neighbouring closed shells would tend to contribute rather uniformly over the nuclear surface and enhance $L = 0$ relative to $L = 2$.

In contradistinction to the interpretation of spheroidal nuclear alpha intensity patterns as arising from a non-uniform alpha amplitude over a constant-matter-density surface, there has been an alternative approach relating the patterns uniquely to the shape of the nuclear surface (Fröman, 1957; Gol'din, Novikova, and Ter-Martirosyan, 1959; Gol'din, Adel'son-Velskii, Birzgal, Pilia, and Ter-Martirosyan (1958); Nosov, 1957; Strutinsky, 1957). Such theories are based on the assumption that the alpha amplitude over the nuclear surface is constant. These treatments give the correct $L = 2$ phase and nearly the correct magnitude for the quadrupole deformations, since the dominant influence on the alpha penetration is the thin barrier in the

polar region. When calculating finer details, the assumption of a strictly constant alpha wave function over the surface (i.e., over the isopotential surface for alpha) may cause difficulties. These treatments generally lead to quadrupole deformation parameters that decrease with mass number through the region of deformed nuclei, in conflict with experimental and theoretical evidence as shown, for example, by Szymański (1961). Small amounts of P_4 deformation of the spheroidal surface are also needed to explain the intensity patterns observed, but the negative β_4 values required near Curium seem in complete conflict with the shell model β_4 estimates (Kjällqvist, 1958).

We would suggest a modified version for an alpha decay model solely related to shape parameters—one which is more in line with the spirit of our shell model treatment and is more likely to give reasonable results. That is, the alpha wave function over the deformed isopotential surface should vary in accordance with the *change* in nuclear matter density between parent and daughter. That is, the Y_{20} component of the alpha wave on the surface should be proportional to the change in quadrupole deformation and the Y_{40} component to the change in β_4 between parent and daughter. It is beyond the scope of this paper to make here a quantitative test of such a new model, but it does seem physically reasonable and could relate alpha relative intensities and shape parameters so as to be consistent with Szymański's β_2 and Kjällquist's β_4 values.

Our theoretical computations may be used also to calculate absolute decay rates, although such calculations depend much more sensitively than the relative rates upon detailed assumptions about the attractive nuclear potential felt by the alpha within the inmost part of the barrier. We make a rough estimate for the ground state decay of Cm^{242} by assuming the penetrability 2.16×10^{-27} from calculations using the Igo potential (Rasmussen, 1958). From Table VI we have $G_{00} = 0.0063$ at its inflection point at $R = 8.25$. Using Eq. (III. 4) we calculate an absolute decay rate 65 times less than experimentally observed. This absolute rate calculation is really uncertain. If we were to be consistent with the barrier assumptions made for the analysis of the relative transition rates, we would be thickening the barrier by bringing it in closer by about one fermi compared with the Igo potential, and the discrepancy with experiment would be greater than the factor 65 quoted above.

Qualitatively, it seems clear that our shell model formulation of alpha decay is giving us absolute decay rates too low, but it is quite uncertain just how much we fall short. Because of the great sensitivity of rate to barrier thickness it may be difficult ever to test a model of alpha decay really quantitatively in absolute rates. It would be of great value in this respect to have more optical-model analyses of alpha elastic (and rotational inelastic) scattering, particularly at energies below 40 Mev. Then the alpha decay theorist might have a potential he could extrapolate with greater confidence into the energy region of alpha decay.

The pairing interaction was an important addition in bringing in neutron correlations and proton correlations separately, but influence of neutron-proton forces

in bringing about correlations enhancing the alpha cluster is as yet not included. The proton motion in our treatment is completely uncorrelated with neutron motion.

We have examined the effect of the pairing correlation on absolute decay rate by comparing the G_{00} for Cm^{242} with the average of the G_{00} values which would replace G_{00} values in the limit $\Delta \to 0$, no pairing interaction. The actual G_{00} is 18 times the average and even 2.9 times the Γ_0 corresponding to the most favourable combination of orbitals considered (i.e., $1/2-(530)$ protons, $1/2+(631)$ neutrons). The effect of pairing on the decay rate is the square of the above number, an enhancement of a factor of 320. Thus, we see clearly that the pairing correlation not only smooths out the great fluctuations in decay rate for various nuclei that would obtain in the absence of pairing, but it also greatly enhances the decay rate. We have made a rough estimate of the further enhancement to be obtained by using all orbitals of three oscillator shells, as NILSSON and PRIOR (1961) did, and find about an additional factor of 4. This rough estimate is based on a suggestion by MOTTELSON to use the relationship $\frac{\Delta}{G} = \sum_{\Omega} u_\Omega v_\Omega$. There is perhaps also to be expected some increase if the harmonic oscillator radial wave functions were to be replaced by more realistic functions in a WOODS-SAXON potential (1954); (BLOMQVIST and WAHLBORN, 1960). We have partially corrected our work in this regard by fitting exponentials to the G functions at their outermost inflection points.

Perhaps the external Hamiltonian is at fault, too. It is well known that the optical-model potentials for neutrons and protons are energy-dependent, with the real part becoming less attractive with increasing kinetic energy. If the same trend were to hold for alpha particles, the barrier might be thinner than is given by the optical potential for 40 Mev alphas. Also we have in the external Hamiltonian neglected all coupling between alpha particle and nuclear internal degrees of freedom aside from nuclear rotation. Inclusion of further couplings can also effectively enhance the barrier penetrability for the ground-band decay.

Despite the failure to match experimental decay rates absolutely, can anything be said from our results about trends of absolute transition probabilities from nucleus to nucleus? We must be cautious about drawing conclusions from the trends of the G_{00} values at constant αR^2 in Table VI, because of the limited span of orbital energies compared to Δ. Because of the great G_{00} enhancement due to pairing correlation we should expect to see a spurious fall-off of G_{00} as the Fermi energy approaches any of the outer limits of our range of orbital energies. The decrease with mass number seen in Table VI probably comes mainly from the use of Δ values decreasing with proton and with neutron number.

We cannot make quantitative calculations, but with some of our results as a guide we can discuss matters qualitatively. Thus, the Nilsson orbital density near the Fermi energy should directly affect the absolute alpha transition probabilities in that a high density results in a larger Δ and the participation of more orbitals in the collective enhancement of the alpha amplitude.

A second factor may be inferred from examination of Γ_{00} and Γ_{20} values in Tables II and III. The $\Omega = 1/2$ orbitals seem especially effective in contributing to alpha decay in exhibiting large Γ_{00} values. A third general factor has been discussed by several authors and involves the increased penetrability expected for increasing deformation.

The first-factor dependence would suggest that there might be a direct correlation between the odd-even mass difference (which measures Δ) and the reduced alpha transition probability to ground. For the deformed nuclei there does appear to be the same general dependence of these quantities, namely a systematic decrease from Ra and Th through the heaviest elements. For a plot of alpha reduced widths, see Fig. 1 of RASMUSSEN (1958). For plots of the odd-even mass differences, see Figs. 2 and 3 of NILSSON and PRIOR (1961). There are not enough data beyond $N = 152$ to determine whether the predicted minimum in Δ and reduced alpha decay rates exist.

The second factor, involvement of $\Omega = 1/2$ orbitals, should act in the same direction, the lighter deformed nuclei receiving heavier contributions from these favourable orbitals.

The third factor should operate in a contrary fashion, and in the overall dependence of reduced alpha transition probabilities the first two factors apparently dominate.

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V. G. SOLOVIEV (Physics Letters **1**, 202, 1962) has recently published some studies of the alpha-decay enhancement due to the superfluidity properties of nuclei, finding also a very large enhancement given to favoured decay. Soloviev found an enhancement factor of 1700 for the alpha decay of Cm^{244}. This factor is to be compared with our factor of 320 for Cm^{242} when the sum runs over ten proton and ten neutron orbitals; our factor would go roughly to $\sim$ 1300 for summation over all orbitals in three oscillator shells. It is not clear to us how many orbitals are included in Soloviev's summation and it is important to note that the wide fluctuation of our Γ_{00} entries in Table II calls for caution regarding Soloviev's assumption of constancy (his eq. (5)). In view of the differences in our calculations the enhancement factors of 1700 and $\sim$ 1300 would seem to be in satisfactory agreement.

Appendix

Coulomb Excitation Corrections

Consider equations governing the barrier transmission of alpha waves in the presence of a nuclear quadrupole potential

$$\frac{d^2 u_l}{d\varrho^2} - \left[\frac{2\eta}{\varrho} - 1 + l(l+1)\left(\frac{1}{\varrho^2} + \varepsilon\right)\right] u_l = \frac{q}{\varrho^3} \sum_{l'} \langle l' \mid P_2 \mid l \rangle u_{l'} \tag{A. 1}$$

and the effects of quadrupole coupling on the wave equation in the region near and outside the classical turning point. JACOBSOHN and MILLER (1959) have pointed out the connection between Coulomb excitation matrix elements and the imaginary components of the matrix transforming the alpha wave vector from the barrier region to the vector at infinity. Using this result and the symbols of ALDER *et al* (1956) we may write the matrix elements in lowest order as

$$\left.\begin{aligned} \hat{k}_{ll'} &= \delta_{ll'} - iq\, M_{ll'}^{-3} \langle l' \mid P_2 \mid l \rangle, \\ \text{where} \quad M_{ll'}^{-3} &= \int_0^\infty I_l(\eta_l \varrho)\, I_{l'}(\eta_l \varrho)\, \varrho^{-3}\, d\varrho, \quad \text{where} \quad \eta_l = \eta(1-\varepsilon)^{-1/2}. \end{aligned}\right\} \tag{A. 2}$$

Nosov's formula for the imaginary component, in these units, is equivalent to setting

$$M_{ll'}^{-3} = \frac{1}{6\eta^2} \tag{A. 3}$$

and this is just the limit of the radial integral for $\eta \gg l$ and $\varepsilon = 0$. The approximation is a fairly good one for the cases of practical interest in alpha decay.

A more general formula for all l but $\varepsilon = 0$ is (II. E. 75) of ALDER et al. (1956)

$$M_{ll+2}^{-3} = \frac{1}{6\,|\,l+1+i\eta\,|\,|\,l+2+i\eta\,|}\,. \tag{A. 4}$$

They give a somewhat more complicated formula for M_{ll}^{-3} which is not repeated here. Correction for $\varepsilon \neq 0$ can be made on the matrix element from the tables of the semi-classical Coulomb excitation integrals of ALDER et al. (1956).

The phase shift approximation method of CHASMAN and RASMUSSEN (1958) can be used to calculate the imaginary matrix elements and yields values exactly 3/2 that of Nosov (1957). The error arises from taking the interaction as a $\frac{1}{\varrho^2}$ instead of a $\frac{1}{\varrho^3}$ dependence.

For example, the $\hat{k}_{24}$ matrix element for Cm^{242} with $Q_0 = 10.96 \times 10^{-24}$ cm^2, $q = 320$, $\eta = 23.7$. $\varepsilon = 0.0011$ has an angular matrix element $6/7\sqrt{5}$, a radial factor (assuming $\varepsilon = 0$) of 0.093, a correction for finite ε of 0.87 for a value $\hat{k}_{24} = -0.031$ i. Nosov's formula yields a value about 15% too high. This matrix element should establish a lower limit on the ratio of intensities of $l = 4$ to $l = 2$ groups near Cm^{242}. That is

$$\frac{\text{Intensity}\,(l=4)}{\text{Intensity}\,(l=2)} \geq (0.031)^2 \frac{v_4}{v_2} = 9.5 \times 10^{-4},$$

where v_2 and v_4 are alpha velocities at infinity.

The experimental ratios in Cm^{242} and Cm^{244}, respectively, are 11.4×10^{-4} and 7.3×10^{-4}. Cm^{244} falls slightly below the limit, suggesting that the quadrupole moment of daughter Pu^{240} should be at least 15% lower than the 11 barns assumed or that the experimental intensity of the $l = 4$ group is in error on the low side.

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C. PELLEGRINI AND J. PLEBANSKI

København 1963
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CONTENTS

Synopsis

The consequences of the hypothesis – recently advanced by C. Møller – that gravitation may be described by a tetrad field, are examined by studying the most general Lagrangian obtained as a linear combination of invariants. A particular choice of these can be made on the basis of correspondence with the Newtonian theory. The field equations obtained from this particular Lagrangian, although somewhat different from those of Møller, give rise, in the case of a static, spherically symmetric system, to the usual Schwarzschild metric. Moreover, in the cases considered explicitly by Møller the solutions of the field equations are the same.

A conserved energy-momentum complex having the property that the energy density is localizable is also derived. The use of a tetrad field to describe the structure of space-time allows the introduction of spinor fields, and in particular of the neutrino field, in a natural way. A new coupling between fermions and gravitation also follows from this theory.

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I. Introduction

The concepts of energy and momentum and of conservation laws, which have played a very important part in all physics, have some peculiar features in the theory of general relativity. Owing to the general covariance of the theory, there exist an infinite number of conservation laws, all equally valid[1].

The selection from these of what may be called the "energy-momentum" conservation law is essentially a matter of physical interpretation. Various "complexes", each with certain definite properties, have therefore been proposed[2]. In particular, MØLLER[3] introduced some conditions which must be satisfied in order that a complex be the energy-momentum complex. Especially he required that the energy density be localizable, i. e. a scalar under the group of purely spatial coordinate transformations, and that the total energy and momentum be transformed like a four-vector with respect to the Lorentz group. Subsequently MØLLER[4] was able to show that no complex satisfying both these conditions can be formed within the framework of Einstein's theory.

To come out of this situation, he proposed a new formulation of the theory [4] [5], in which the fundamental variables of the gravitational field were assumed to be the 16 components of a tetrad field, connected by ten relations with the metric tensor.

There are two possible approaches to tetrad fields. The usual one consists in regarding additional degrees of freedom associated with tetrads as non-physical. In the framework of this philosophy tetrads may be used as working tools in the same way as one uses potentials in electrodynamics. However, similarly as in electrodynamics, where physically meaningful quantities have to be gauge-invariant, the entire physical content of the theory must, in the usual approach to tetrads in general relativity, stay invariant with respect to arbitrary Lorentz rotations of tetrads (which may change from point to point). When using tetrads in this spirit, one remains strictly on the level of orthodox general relativity.*

The second approach to tetrads, which is closer in spirit to that advocated by MØLLER, is based on the hypothesis that *all* 16 degrees of freedom of tetrads may be physically meaningful; here one demands of the theory that its physical quantities are invariant only with respect to *constant* tetrad rotations.

* The question how convenient tetrads are in the treatment of *global* conserved quantities (and in other problems of the usual theory) is discussed by one of us (J. P.) in Proceedings of the Warsaw Conference on Relativistic Theories of Gravity.

Once this assumption is made, it is possible to obtain an energy-momentum complex satisfying both conditions. Since, for a given physical situation, the determination of the tetrad field requires sixteen equations, MØLLER added to the usual Einstein equations a set of six equations $\varphi_{\alpha\beta} = 0$, where $\varphi_{\alpha\beta}$ is a skew tensor function of the tetrads and their derivatives. He was then able to show that, in the linearized case, his equations

$$\left.\begin{aligned} G_{\alpha\beta} &= -\chi T_{\alpha\beta} \\ \varphi_{\alpha\beta} &= 0 \end{aligned}\right\} \tag{1.1}$$

are equivalent to the Einstein weak-field equations, and that the solution of (1.1) for a static, spherically symmetric system gives rise to the usual Schwarzschild metric. The new theory is thus in agreement with all known experimental facts. However, the general expression for $\varphi_{\alpha\beta}$ contains a certain arbitrariness, which it would seem interesting to try to eliminate by attempting a variational-principle formulation of the Møller theory. This is what we will try to do in the present paper.

In other words, we intend to investigate the theory that follows from these assumptions: (1) the Møller hypothesis that all 16 degrees of freedom of tetrads are physically meaningful (invariance only with respect to constant tetrad rotations); (2) that a canonical formulation of the theory in terms of an action principle is possible.

We see that in this way we investigate a theory that from a heuristic point of view is wider than orthodox general relativity, which so beautifully solves all problems meaningful in the framework of its philosophy. Nevertheless we are of opinion that a generalization of this type is worthy of investigation.

It is of importance to realize that even the dynamical laws determining in this theory the metric tensor may be slightly different from the usual Einstein equations; nevertheless the usual philosophy of general relativity (including the principle of equivalence) here remains the same.

Some misunderstanding may arise in connection with the possibility of Fernparallelismus in this theory, which might be taken to be contradictory to the orthodox interpretation of general relativity. We would point out that when, in the usual theory, there exists a physical vectorial field, e. g. potentials of the vectorial mesonic field, the notion of Fernparallelismus to that vector may be introduced without violation of any first principles of the theory. When one understands tetrads as four physical vectorial fields fixed by consistent dynamical laws, and the metric as a secondary concept defined in terms of these fields, there is no need to change the usual interpretation. There is, however, the possibility that the dynamical laws governing tetrads are different from the usual ones, which determine tetrads only up to x-dependent Lorentz rotations.

The chief purpose of this paper is precisely to investigate the possibilities associated with the small latitude that can be allowed in the choice of the dynamics determining tetrad quantities. The interpretation of the theory, however, stays the same as in orthodox general relativity.

In the next section the tetrad formalism is briefly introduced, and our notations fixed. In section III the general structure of the Lagrangian $\mathfrak{L}$ of the tetrad field is studied. The actual construction of the most general $\mathfrak{L}$ by means of the invariants formed of tetrads is made in section IV.

As noted by Møller, the space-time continuum used in this theory differs from the usual Riemannian space by the existence of a tetrad in every point. This fact has interesting consequences in geometry; for instance it allows the introduction of the concept of absolute parallelism of two vectors at distant points.

For the definition of absolute parallelism and its developments, such as the absolute derivation, the reader is referred to the work of MØLLER [5]. Here we only want to point out that the most important geometrical notion in this space is that of torsion, characterized by a tensor $A_{[\alpha\beta]\gamma}$ such that when $A_{[\alpha\beta]\gamma} \equiv 0$, space-time is flat. In accordance with this the torsion tensor is used in section IV to build up the invariants. The Lagrangian is written as a linear combination of four of these invariants; hence it will contain four arbitrary constants; these are determined in section V, which deals with the linearized form of the theory. The result is that if we choose two constants equal to zero, the linearized theory is equivalent to that of Einstein.

Since we assume this to be a necessary condition, we obtain in this way a Lagrangian $\mathfrak{L}$ depending on two constants k_1 and k_2 only; the further development of the theory will be based on this $\mathfrak{L}$. From the linear approximation it also follows — which is interesting to note — that k_1^{-1} is equal to the Einstein gravitational constant. Although the constant k_2 will remain undetermined in this work, it seems possible that further developments will be able to give us some information on it.

Another characteristic of a theory of this type is that, together with the group of coordinate transformations, there is another group leaving the Lagrangian invariant, i. e. a simultaneous and equal rotation of all the tetrads. This is shown in section VI and is also used in appendix B to introduce spinors by means of the representations of these rotations. This simple and natural way of defining spinors has two noteworthy consequences: (a) the derivative of a spinor can be consistently defined as the partial derivative; (b) since the theory is invariant only with respect to the group of proper tetrad rotations, the neutrino has its own place in the theory, and its existence is related to the fundamental structure of space-time.

The field equations are derived from the Lagrangian in section VII. They turn out to be different from those proposed by Møller. This is due to the fact that the possibility of using the Levi-Civita tensor in the construction of $\varphi_{\alpha\beta}$ was overlooked, whereas the same tensor plays a fundamental part in this work. The field equations derived in section VII are

$$\left.\begin{aligned} k_1 G_{\alpha\beta} + k_2 F_{<\alpha\beta>} &= -T^{(b)}{}_{\alpha\beta} - T^{(f)}{}_{<\alpha\beta>} \\ k_2 F_{[\alpha\beta]} &= -T^{(f)}{}_{[\alpha\beta]}, \end{aligned}\right\} \qquad (I.2)$$

where again $G_{\alpha\beta}$ is the Einstein tensor and $F_{\alpha\beta}$ is analogous to $\varphi_{\alpha\beta}$. In our case, anyway $F_{\alpha\beta}$ has a symmetric as well as an antisymmetric part. The matter tensor has been

divided, in (I.2), into a boson part and a fermion part. The existence of the new "skew" equation $k_2 F_{[\alpha\beta]} = -T^{(f)}_{[\alpha\beta]}$ is interpreted to mean that the space-time structure is determined by matter not only through the symmetric energy-momentum tensor, but also through the skew part $T^{(f)}_{[\alpha\beta]}$ which is connected with the spin angular-momentum tensor. All the physical content of the theory now becomes clearer: the usual Riemannian space-time is not general enough to describe classical matter as well as spinor fields; this deficiency is shown in the lack of a satisfactory (in the Møller sense) energy-momentum complex and of a natural way to introduce spinors [6].

If we assume that the influence of a boson and that of a fermion on the space-time structure are qualitatively different, we need a scheme wider than that of Einstein, and this might be a space with a built-in tetrad lattice. For the theory to be in agreement with experimental facts it is further necessary that the tetrad field obtained by solving eqs. (I.2) in the case of a static, spherically symmetric system, gives rise to the Schwarzschild metric. That it is so, is shown in section VIII. It is interesting that this particular tetrad field is just identical with that obtained by MØLLER [5] for the same case.

Finally, in section IX, the energy-momentum conservation law is discussed. It is shown that the energy-momentum complex we derive satisfies both Møller conditions. In addition to a conservation law $\mathsf{T}_{\alpha,\beta}^{\ \beta} = 0$, a tensorial conservation law is seen to follow from the structure of the field equations. In general, $\mathsf{T}_{\alpha}^{\ \beta}$ can be written in the same form as the Møller energy-momemtum complex:

$$\mathsf{T}_{\alpha}^{\ \beta} = \Theta_{\alpha}^{\ \beta} + \mathfrak{U}_{\mu}^{\ [\beta\nu]} \Delta^{\mu}_{\ \alpha\nu}, \tag{I.3}$$

$$\mathsf{T}_{\alpha}^{\ \beta} = \mathfrak{U}_{\alpha}^{\ [\beta\gamma]}{}_{,\gamma}, \tag{I.4}$$

and the only non-tensorial term in (I.3) is $\Delta^{\mu}_{\ \alpha\nu}$. Both the superpotential $\mathfrak{U}_{\alpha}^{\ [\beta\gamma]}$ and $\mathsf{T}_{\alpha}^{\ \beta}$ can be written as a linear combination of the corresponding Møller term and a new one:

$$\mathsf{T}_{\alpha}^{\ \beta} = \mathsf{T}_{\alpha\ (M)}^{\ \beta} + \mathsf{T}'_{\alpha}{}^{\beta}.$$

In the case of a static, spherically symmetric system the new term vanishes, while in the linearized case it can be written as a divergence and is moreover symmetric.

The use of tetrads in general relativity was already proposed by EINSTEIN in 1928 [7]. He tried, however, to use the six new degrees of freedom contained in the tetrad field to describe electromagnetism. The equations derived by Einstein were shown to be incompatible with the Schwarzschild solution [8].

II. Preliminaries and Notations

Let V_4 be a normal hyperbolic Riemannian space characterized, in arbitrary coordinates x^{α}, by the symmetric metric tensor $g_{\alpha\beta}(x)$. Greek indices take the values $0, 1, 2, 3$. The signature $(+, -, -, -)$ is assumed for the metric. The indices labelling the vectors of a tetrad will also be denoted by Greek letters, but with a "roof" above

them, so that the index $\hat{\alpha}$ takes the values $\hat{0}, \hat{1}, \hat{2}, \hat{3}$. The Einstein summation convention is assumed.

Now, because of the normal character of V_4, one may always construct at a given point four vectors orthogonal to each other, one of them being time-like and normalized to plus one, the remaining ones space-like and normalized to minus one. Denoting the covariant components of these vectors by $g_{\alpha}^{\hat{\alpha}}(x)$, we may summarize their orthonormality properties in

$$g^{\alpha\beta}\, g_{\alpha}^{\hat{\alpha}}\, g_{\beta}^{\hat{\beta}} = g^{\hat{\alpha}\hat{\beta}}, \tag{II.1}$$

where $g^{\hat{\alpha}\hat{\beta}}$ is the numerical matrix of special relativity,

$$g^{\hat{\alpha}\hat{\beta}} = g_{\hat{\alpha}\hat{\beta}} = \begin{vmatrix} 1 & & & \\ & -1 & & 0 \\ & & -1 & \\ & 0 & & -1 \end{vmatrix}. \tag{II.2}$$

Note that the existence of such vectors is equivalent to Hilbert's condition. We will also assume that the $g_{\alpha}^{\hat{\alpha}}(x)$ as functions of x are differentiable, i. e. that they change from point to point in a regular way. The normal and roofed indices may be raised or lowered by means of the quantities $g_{\alpha\beta}, g^{\alpha\beta}, g_{\hat{\alpha}\hat{\beta}}, g^{\hat{\alpha}\hat{\beta}}$ respectively. (II.1) may now be written as

$$g_{\varrho}^{\hat{\alpha}}\, g_{\hat{\beta}}^{\varrho} = \delta_{\hat{\beta}}^{\hat{\alpha}}. \tag{II.3}$$

Multiplying (II.3) by four arbitrary scalars $A_{\hat{\alpha}}$ and by $g_{\sigma}^{\hat{\beta}}$, one obtains

$$\left(A_{\hat{\alpha}}\, g_{\varrho}^{\hat{\alpha}}\right) g_{\sigma}^{\hat{\beta}}\, g_{\hat{\beta}}^{\varrho} = A_{\hat{\alpha}}\, g_{\sigma}^{\hat{\alpha}},$$

and from this follows

$$g_{\sigma}^{\hat{\beta}}\, g_{\hat{\beta}}^{\varrho} = \delta_{\sigma}^{\varrho}, \tag{II.4}$$

$$g_{\varrho}^{\hat{\beta}}\, g_{\hat{\beta}\sigma} = g_{\varrho\sigma}. \tag{II.5}$$

Eq. (II.5) is the fundamental relation between the ten components of the metric tensor and the sixteen components of tetrads. While the tetrads completely determine the metric, the reverse is not true.

A Lorentz transformation of the roofed indices, i. e. a tetrad rotation

$$g'^{\hat{\alpha}}_{\alpha}(x) = L^{\hat{\alpha}}{}_{\hat{\beta}}(x)\, g^{\hat{\beta}}{}_{\alpha}(x) \tag{II.6}$$

with

$$g_{\hat{\varrho}\hat{\sigma}}\, L^{\hat{\varrho}}{}_{\hat{\alpha}}(x)\, L^{\hat{\sigma}}{}_{\hat{\beta}}(x) = g_{\hat{\alpha}\hat{\beta}}, \tag{II.7}$$

leaves the metric tensor invariant.

Adopting the notation

$$\left.\begin{aligned} g_{..} &= \det\left|g_{\alpha\beta}\right|, \qquad g^{\cdot\cdot} = \det\left|g^{\alpha\beta}\right|, \\ g^{\hat{:}} &= \det\left|g^{\hat{\alpha}}_{\hat{\beta}}\right|, \qquad g^{:}_{\hat{:}} = \det\left|g^{\alpha}_{\hat{\beta}}\right|, \end{aligned}\right\} \tag{II.8}$$

one obtains

$$\left.\begin{aligned} g^{\hat{:}}\, g^{:}_{\hat{:}} &= 1 \\ g_{..} &= -(g^{\hat{:}})^2 \\ g^{\cdot\cdot} &= -(g^{:}_{\hat{:}})^2. \end{aligned}\right\} \tag{II.9}$$

Therefore, if one understands as $\sqrt{-g_{..}}$ the positive branch of $\sqrt{\quad}$, one gets

$$\sqrt{-g_{..}} = \left|g^{\hat{:}}\right|. \tag{II.10}$$

We conclude this section with the remark that, considering all metric quantities as known, one may attribute to a vector A four different kinds of component: A^{α}, A_{α}, $A^{\hat{\alpha}}$, $A_{\hat{\alpha}}$. The table below explains how one of them can be expressed through the others.

TABLE 1

$$\begin{aligned} A^{\alpha} &= A^{\alpha} \qquad = g^{\alpha\beta} A_{\beta} = g^{\alpha}_{\hat{\beta}}\ A^{\hat{\beta}} = g^{\alpha\hat{\beta}} A_{\hat{\beta}} \\ A_{\alpha} &= g_{\alpha\beta} A^{\beta} = \qquad A_{\alpha} = g_{\alpha\hat{\beta}} A^{\hat{\beta}} = g^{\hat{\beta}}_{\alpha}\ A_{\hat{\beta}} \\ A^{\hat{\alpha}} &= g^{\hat{\alpha}}_{\beta}\ A^{\beta} = g^{\hat{\alpha}\beta} A_{\beta} = \qquad A^{\hat{\alpha}} = g^{\hat{\alpha}\hat{\beta}} A_{\hat{\beta}} \\ A_{\hat{\alpha}} &= g_{\hat{\alpha}\beta} A^{\beta} = g_{\hat{\alpha}}^{\ \beta} A_{\beta} = g_{\hat{\alpha}\hat{\beta}} A^{\hat{\beta}} = \qquad A_{\hat{\alpha}}. \end{aligned}$$

III. The Lagrangian of the Tetrad Field

The principal aim of this work is the formulation of an action principle

$$\delta A = \delta \int \mathfrak{L}\left(g^{\hat{\alpha}}_{\alpha}(x),\ g^{\hat{\alpha}}_{\alpha,\beta}(x)\right) d^4x = 0$$

for the tetrad field. We assume that the Lagrangian satisfies the following conditions:

(I) it must be a scalar (or pseudoscalar) density with respect to the group of coordinate transformations;

(II) it must be a scalar or pseudoscalar density with respect to the subgroup of constant Lorentz rotations of the tetrads, i. e. the rotations for which

$$\frac{\partial L^{\hat{\alpha}}_{\hat{\beta}}(x)}{\partial x^{\mu}} = 0;$$

(III) it must be a function of the $g^{\hat{\alpha}}_{\alpha}(x)$ and their first derivatives, and further it must be bilinear in the $g^{\hat{\alpha}}_{\alpha,\beta}(x)$.

This is sufficient to determine the general form of $\mathfrak{L}$. In fact, because of the covariance requirement, the first derivatives of the tetrads can appear in $\mathfrak{L}$ only in the form of covariant derivatives, i. e. as

$$g^{\hat{\alpha}}_{\alpha;\beta} = g^{\hat{\alpha}}_{\alpha,\beta} - \Gamma^{\varrho}_{\alpha\beta}\, g^{\hat{\alpha}}_{\varrho}. \tag{III.1}$$

Expressing the metric tensor in terms of tetrads and substituting in the Christofell symbol, we obtain the relation between the covariant and non-covariant derivatives of $g^{\hat{\alpha}}_{\alpha}$*

$$g_{\hat{\alpha}\beta;\gamma} = g^{\alpha}_{\hat{\alpha}}\, P^{[\nu\mu]\,\hat{\sigma}}_{[\alpha\beta]\,\gamma}\,(g_{\hat{\sigma}\nu,\mu} - g_{\hat{\sigma}\mu,\nu}), \tag{III.2}$$

where

$$4\, P^{[\nu\mu]\,\hat{\sigma}}_{[\alpha\beta]\,\gamma} = g^{\hat{\sigma}}_{\alpha}(\delta^{\nu}_{\beta}\,\delta^{\mu}_{\gamma} - \delta^{\nu}_{\gamma}\,\delta^{\mu}_{\beta}) + g^{\hat{\sigma}}_{\beta}(\delta^{\nu}_{\gamma}\,\delta^{\mu}_{\alpha} - \delta^{\nu}_{\alpha}\,\delta^{\mu}_{\gamma}) + g^{\hat{\sigma}}_{\gamma}(\delta^{\nu}_{\beta}\,\delta^{\mu}_{\alpha} - \delta^{\nu}_{\alpha}\,\delta^{\mu}_{\beta}). \tag{III.3}$$

Therefore we can get a Lagrangian satisfying (I), (II) and (III) if we write it in the form

$$\mathfrak{L} = \frac{1}{4}\, g\hat{:}\, L^{[\alpha\beta]\,[\mu\nu]}_{\hat{\gamma}\quad\hat{\varrho}}\,(g^{\hat{\gamma}}_{\alpha,\beta} - g^{\hat{\gamma}}_{\beta,\alpha})\,(g^{\hat{\varrho}}_{\mu,\nu} - g^{\hat{\varrho}}_{\nu,\mu}). \tag{III.4}$$

The quantity $L^{[\alpha\beta]\,[\mu\nu]}_{\hat{\gamma}\quad\hat{\varrho}} = L^{[\mu\nu]\,[\alpha\beta]}_{\hat{\varrho}\quad\hat{\gamma}}$ must be a tensor with respect to coordinate transformations. It is clear that it can be constructed only from quantities like the tetrads and the Levi-Civita tensor.

Without specifying the form of $L^{[\alpha\beta]\,[\mu\nu]}_{\hat{\gamma}\quad\hat{\varrho}}$ it is already possible to draw some results from the form (III.4) of the Lagrangian. By varying the tetrad field in (III.4) we obtain the equations of motion

$$-2\left[g\hat{:}\, L^{[\lambda\delta]\,[\mu\nu]}_{\hat{\lambda}\quad\hat{\varrho}}\, g^{\hat{\varrho}}_{\mu,\nu}\right]_{,\delta} + \frac{\partial}{\partial g^{\hat{\lambda}}_{\hat{\lambda}}}\left[g\hat{:}\, L^{[\alpha\beta]\,[\mu\nu]}_{\hat{\gamma}\quad\hat{\varrho}}\right]\cdot g^{\hat{\gamma}}_{\alpha;\beta}\, g^{\hat{\varrho}}_{\mu;\nu} = -\,g\hat{:}\, T^{\lambda}_{\hat{\lambda}}. \tag{III.5}$$

To derive (III.5) we have added to (III.4) the Lagrangian of an external field and have introduced the notation

$$g\hat{:}\, T^{\lambda}_{\hat{\lambda}} = \frac{\delta \mathfrak{L}_{\text{ext.}}}{\delta\, g^{\hat{\lambda}}_{\hat{\lambda}}}.$$

From (III.5) a conservation law follows immediately:

$$\left[g\hat{:}\, T^{\lambda}_{\hat{\lambda}} + \frac{\partial}{\partial\, g^{\hat{\lambda}}_{\hat{\lambda}}}(g\hat{:}\, L^{[\alpha\beta]\,[\mu\nu]}_{\hat{\gamma}\quad\hat{\varrho}})\, g^{\hat{\gamma}}_{\alpha;\beta}\, g^{\hat{\gamma}}_{\mu;\nu}\right]_{,\lambda} = 0. \tag{III.6}$$

* By $[\alpha\beta]$ and $<\alpha\beta>$ we will indicate antisymmetry and symmetry with respect to the indices α, β.

Note that both terms in (III.6) are vector densities. Introducing the notation

$$g\hat{:}\, t_{\hat{\lambda}}^{\lambda} = \frac{\partial}{\partial g_{\hat{\lambda}}^{\hat{\lambda}}} (g\hat{:}\, L_{\hat{\gamma}}^{[\alpha\beta]\,[\mu\nu]}_{\hat{\varrho}})\, g_{\alpha;\beta}^{\hat{\gamma}}\, g_{\mu;\nu}^{\hat{\varrho}} \tag{III.7}$$

$$\Theta_{\hat{\lambda}}^{\lambda} = t_{\hat{\lambda}}^{\lambda} + T_{\hat{\lambda}}^{\lambda}, \tag{III.8}$$

we may write (III.6) as

$$g\hat{:}\, \Theta_{\hat{\lambda};\lambda}^{\lambda} = 0, \tag{III.9}$$

which is a completely covariant equation. Furthermore, from (III.5) it is easily seen that

$$g\hat{:}\, \Theta_{\hat{\lambda}}^{\lambda} = g\hat{:}\, U_{\hat{\lambda};\delta}^{[\lambda\delta]} \tag{III.10}$$

$$g\hat{:}\, U_{\hat{\lambda}}^{[\lambda\delta]} = 2\, g\hat{:}\, L_{\hat{\lambda}}^{[\lambda\delta]\,[\mu\nu]}_{\hat{\varrho}}\, g_{\mu;\nu}^{\hat{\varrho}}. \tag{III.11}$$

These results will be used in section IX to obtain a conserved energy-momentum complex.

IV. Construction of the Lagrangian from the Invariants of the Tetrad Field

In section III the general structure of the Lagrangian has been studied. Now the most general form of $\mathfrak{L}$ satisfying our conditions will be written explicitly as a linear combination of the invariants bilinear in the first derivatives of the tetrad field.

In order to construct the invariants we introduce the tensors

$$\gamma_{[\alpha\beta]\,\gamma} = g_{\alpha}^{\hat{\alpha}}\, g_{\hat{\alpha}\beta;\,\gamma}, \tag{IV.1}$$

$$\Lambda_{[\alpha\beta]\,\gamma} = (g_{\alpha,\,\beta}^{\hat{\alpha}} - g_{\beta,\,\alpha}^{\hat{\alpha}})\, g_{\hat{\alpha}\gamma} = (g_{\alpha;\,\beta}^{\hat{\alpha}} - g_{\beta;\,\alpha}^{\hat{\alpha}})\, g_{\hat{\alpha}\gamma}, \tag{IV.2}$$

$$\Phi_{\alpha} = \Lambda_{[\alpha\beta]}{}^{\beta} = \gamma^{\beta}{}_{\alpha\beta}, \tag{IV.3}$$

$$\check{\Lambda}^{\alpha} = \eta^{\alpha\beta\gamma\delta}\, \Lambda_{[\beta\gamma]\,\delta}, \tag{IV.4}$$

$$\check{\Lambda}_{\alpha} = \eta_{\alpha\beta\gamma\delta}\, \Lambda^{[\beta\gamma]\,\delta}, \tag{IV.5}$$

$$\check{\Lambda}^{[\varrho\sigma]}{}_{\tau} = \frac{i}{2}\, \eta^{\varrho\sigma\lambda\nu}\, \Lambda_{[\lambda\nu]\,\tau}, \tag{IV.6}$$

$$\check{\Lambda}_{[\varrho\sigma]\,\tau} = \frac{i}{2}\, \eta_{\varrho\sigma\lambda\nu}\, \Lambda^{[\lambda\nu]}{}_{\tau}, \tag{IV.7}$$

where the tensor η is defined by

$$\eta^{\alpha\beta\gamma\delta} = -g\,\varepsilon^{\alpha\beta\gamma\delta}$$

$$\eta_{\alpha\beta\gamma\delta} = g\,\varepsilon_{\alpha\beta\gamma\delta}$$

and $\varepsilon^{\alpha\beta\gamma\delta}$, $\varepsilon_{\alpha\beta\gamma\delta}$ are the numerical Levi-Civita symbols.

$A_{[\alpha\beta]\gamma}$ is the fundamental torsion tensor in our Riemannian space with a built-in tetrad lattice [5].

All the invariants bilinear in the $g^{\hat{\alpha}}_{\alpha;\beta}$ can now be written in the form

$$I = T^{\alpha\beta\gamma}_{\lambda\mu\nu} A_{[\alpha\beta]\gamma} A^{[\lambda\mu]\nu}.$$

The use of the conditions I and II gives us the following seven invariants:

$$I_1 = g\, A_{[\varrho\sigma]}{}^{\sigma} A^{[\varrho\tau]}{}_{\tau}, \tag{IV.8}$$

$$I_2 = g\, A_{[\alpha\beta]\gamma} A^{[\gamma\beta]\alpha}, \tag{IV.9}$$

$$I_3 = g\, A_{[\alpha\beta]\gamma} A^{[\alpha\beta]\gamma}, \tag{IV.10}$$

$$\check{I}_1 = \varepsilon^{\beta\gamma\nu\mu}\, g^{\alpha\lambda}\, A_{[\alpha\beta]\gamma} A_{[\lambda\nu]\mu}, \tag{IV.11}$$

$$\check{I}_2 = \varepsilon^{\alpha\beta\nu\mu}\, g^{\gamma\lambda}\, A_{[\alpha\beta]\gamma} A_{[\lambda\nu]\mu}, \tag{IV.12}$$

$$\check{I}_3 = \varepsilon^{\alpha\lambda\nu\mu}\, g^{\beta\gamma}\, A_{[\alpha\beta]\gamma} A_{[\lambda\nu]\mu}, \tag{IV.13}$$

$$\check{I}_4 = \varepsilon^{\alpha\beta\lambda\nu}\, g^{\gamma\mu}\, A_{[\alpha\beta]\gamma} A_{[\lambda\nu]\mu}. \tag{IV.14}$$

All these are pseudoscalar densities with respect to the group of coordinate transformations. I_1, I_2, I_3 are pseudoscalar also with respect to constant Lorentz rotations of tetrads, while $\check{I}_1, \cdots, \check{I}_4$ are scalar with respect to this group (see section VI).

The term $\check{I}_4$ can be written as a full divergence; in fact

$$\left.\begin{aligned} \check{I}_4 &= 4\,\varepsilon^{\alpha\beta\lambda\nu}\, g^{\gamma\mu}\, g_{\hat{\varrho}\gamma}\, g_{\hat{\sigma}\mu}\, g^{\hat{\varrho}}_{\alpha,\beta}\, g^{\hat{\sigma}}_{\lambda,\nu} \\ &= 4\left[\varepsilon^{\alpha\beta\lambda\nu}\, g_{\hat{\varrho}\hat{\sigma}}\, g^{\hat{\varrho}}_{\alpha,\beta}\, g^{\hat{\sigma}}_{\lambda}\right]_{,\nu}. \end{aligned}\right\} \tag{IV.15}$$

Using the inverse relation of (IV.6)

$$A_{[\lambda\nu]\mu} = \frac{i}{2}\, g\, \varepsilon_{\lambda\nu\varrho\sigma} \check{A}^{[\varrho\sigma]}{}_{\mu} \tag{IV.16}$$

and the relation

$$A_{[\lambda\nu]\mu} + A_{[\nu\mu]\lambda} + A_{[\mu\lambda]\nu} = ig\, \varepsilon_{\varrho\lambda\nu\mu} \check{A}^{[\varrho\sigma]}{}_{\sigma}, \tag{IV.17}$$

we find

$$\left.\begin{aligned} \check{I}_3 &= \varepsilon^{\alpha\lambda\nu\mu}\, g^{\gamma\beta}\, A_{[\alpha\beta]\gamma}\left(\frac{i}{2}\, g\, \varepsilon_{\varrho\sigma\lambda\nu} \check{A}^{[\varrho\sigma]}{}_{\mu}\right) \\ &= 2\,i\, g^{\gamma\beta}\, \check{A}^{[\varrho\sigma]}{}_{\sigma}\, A_{[\varrho\beta]\gamma}, \end{aligned}\right\} \tag{IV.18}$$

$$\left.\begin{aligned}\check{I}_2 &= \frac{1}{2}\,\varepsilon^{\alpha\beta\nu\mu}\,g^{\gamma\lambda}\,\Lambda_{[\alpha\beta]\gamma}\,(\Lambda_{[\lambda\nu]\mu}-\Lambda_{[\lambda\mu]\nu}+\Lambda_{[\nu\mu]\lambda}-\Lambda_{[\nu\mu]\lambda})\\ &= 2\,i\,g^{\lambda\gamma}\,\check{\Lambda}^{[\varrho\sigma]}{}_{\sigma}\,\Lambda_{[\varrho\lambda]\gamma}-\frac{1}{2}\,\check{I}_4\\ &= \check{I}_3-\frac{1}{2}\,\check{I}_4,\end{aligned}\right\}\qquad\text{(IV.19)}$$

$$\left.\begin{aligned}\check{I}_1 &= \frac{1}{2}\,\varepsilon^{\beta\gamma\nu\mu}\,g^{\alpha\lambda}\,\Lambda_{[\alpha\beta]\gamma}\,(\Lambda_{[\lambda\nu]\mu}-\Lambda_{[\lambda\mu]\nu}+\Lambda_{[\nu\mu]\lambda}-\Lambda_{[\nu\mu]\lambda})\\ &= -\frac{1}{2}\,\check{I}_2-\frac{1}{2}\,\check{I}_3\\ &= -\check{I}_3+\frac{1}{4}\,\check{I}_4.\end{aligned}\right\}\qquad\text{(IV.20)}$$

It is clear that of the invariants $\check{I}_1,\cdots,\check{I}_4$ only one among the first three need be considered in the Lagrangian; we select for later use the term $\check{I}_3$.

Let us now turn to the other invariants, I_1, I_2, I_3. It will be useful to introduce some linear combination of them, such as

$$P_1=\frac{1}{2}\,I_2+\frac{1}{4}\,I_3-I_1=\hat{g\colon}\,[\gamma_{\alpha\beta\gamma}\,\gamma^{\alpha\gamma\beta}-\Phi_\alpha\,\Phi^\alpha],\qquad\text{(IV.21)}$$

$$P_2=I_2-\frac{1}{2}\,I_3=-\frac{1}{16}\,\hat{g\colon}\,\check{\Lambda}^\alpha\,\check{\Lambda}_\alpha\qquad\text{(IV.22)}$$

$$P_3=\frac{1}{2}\,I_2+\frac{3}{4}\,I_3=\hat{g\colon}\,\gamma_{\alpha\beta\gamma}\,\gamma^{\alpha\beta\gamma}.\qquad\text{(IV.23)}$$

It is easy to see that P_1 is equal to $\mathfrak{L}_M$, the Møller gravitational Lagrangian, differing from $\sqrt{-g}\,R$ only by a divergence (see appendix A). Our general Lagrangian now takes the form

$$\mathfrak{L}=\sum_1^3{}_i\,a_i\,P_i+a_4\,\check{I}_3,\qquad\text{(IV.24)}$$

and in it we have four arbitrary constants.

V. The Linear Approximation and the Complete Determination of the Lagrangian

We shall study in this section some consequences derivable from the Lagrangian (IV.24) in order to get information on the constants $a_1,\cdots,a_4$. The approach used is the study of the linear form of the theory; in particular we require that the linearized field equations are the same as the Einstein ones plus, of course, a set of six

equations. To put it in a different form, we ask that our theory contains the Newtonian theory of gravitation as a limiting case.

To perform the linearization we consider an "insular" system of matter and assume that space-time is asymptotically flat and that cartesian coordinates are used at infinity. Then the tetrad can be written in the form

$$g_{\underset{\varrho}{\hat{\varrho}}} = \delta_{\underset{\varrho}{\hat{\varrho}}} + \frac{1}{2} h_{\underset{\varrho}{\hat{\varrho}}}. \tag{V.1}$$

The term $h_{\underset{\varrho}{\hat{\varrho}}}$, describing the deviation of space-time from flatness, is assumed to be everywhere small of the first order. In all the following calculations terms of orders higher than the first in $h_{\underset{\varrho}{\hat{\varrho}}}$ will be neglected. Introducing the quantity

$$h_{\alpha\beta} = g_{\hat{\alpha}\hat{\beta}}\, \delta^{\hat{\alpha}}_{\alpha}\, h^{\hat{\beta}}_{\beta} \tag{V.2}$$

and substituting (V.1), (V.2) in (II.5), we find that

$$g_{\alpha\beta} = \eta_{\alpha\beta} + h_{<\alpha\beta>}, \tag{V.3}$$

where $\eta_{\alpha\beta}$ is the special-relativity metric tensor.

Hence, in the linear approximation, the tetrad field is described by the tensor $h_{\alpha\beta}$, whose symmetric part gives the metric tensor while the antisymmetric part describes the new degrees of freedom of the theory.

The torsion tensor obtained from (V.1) is

$$A_{[\alpha\beta]\gamma} = \frac{1}{2} [h_{\gamma\alpha,\beta} - h_{\gamma\beta,\alpha}]. \tag{V.4}$$

Substituting (V.4) in (IV.13), (IV.21), (IV.22), (IV.23) and introducing the notation

$$h = h_{<\alpha}{}^{\alpha>} \tag{V.5}$$

and the dual

$$\check{h}^{[\alpha\beta]} = -\frac{i}{2} \varepsilon^{\varrho\sigma\alpha\beta}\, h_{[\varrho\sigma]}, \tag{V.6}$$

we obtain

$$\left.\begin{aligned} \mathfrak{L}_M \equiv P_1 = \frac{1}{4} h_{<\alpha\beta>,\gamma}\, h^{<\alpha\beta>,\gamma} - \frac{1}{2} h_{<\alpha\beta>}{}^{,\alpha}\, h^{<\gamma\beta>}{}_{,\gamma} \\ + \frac{1}{2} h_{,\alpha}\, h^{<\alpha\beta>}{}_{,\beta} - \frac{1}{4} h_{,\alpha}\, h^{,\alpha}, \end{aligned}\right\} \tag{V.7}$$

$$P_2 = \check{h}^{[\alpha\beta]}{}_{,\beta}\, \check{h}_{[\alpha\gamma]}{}^{,\gamma}, \tag{V.8}$$

$$P_3 = \frac{1}{2} h_{<\alpha\beta>,\gamma} h^{<\alpha\beta>,\gamma} - \frac{1}{2} h_{<\alpha\beta>}{}^{,\alpha} h^{<\gamma\beta>}{}_{,\gamma} + \frac{1}{4} h_{[\alpha\beta],\gamma} h^{[\alpha\beta],\gamma} + h_{<\alpha\beta>}{}^{,\alpha} h^{[\gamma\beta]}{}_{,\gamma}, \tag{V.9}$$

$$\check{I}_3 = 4\, i\, \check{h}^{[\alpha\beta]}{}_{,\beta} [h_{<\alpha\gamma>}{}^{,\gamma} - h_{[\alpha\gamma]}{}^{,\gamma}]. \tag{V.10}$$

In writing down (V.7), . . . , (V.10), we have neglected divergences; in particular, the expansion of $\mathfrak{L}_M$ has been replaced by that of $\sqrt{-g}\, R$ since, of course, they can only differ by a divergence.

The equations obtained by varying $\mathfrak{L}_M$ with respect to $h_{<\alpha\beta>}$ are just the Einstein weak-field equations. This means that the constants a_2, a_3, a_4 must be so chosen that in the equation obtained by varying the Lagrangian with respect to $h_{<\alpha\beta>}$ all terms depending on $h_{<\alpha\beta>}$ itself come only from $\mathfrak{L}_M$. The first thing one would think of is then to assume

$$a_3 = a_4 = 0$$

so that the Langrangian becomes

$$\mathfrak{L} = a_1\, \mathfrak{L}_M + a_2\, P_2 .$$

The linearized field equations, in the absence of matter, are then

$$\frac{1}{2} \{ - \Box \varphi_{\alpha\beta} - \eta_{\alpha\beta}\, \varphi^{\varrho\sigma}{}_{,\varrho,\sigma} + (\eta_{\alpha\varrho}\, \delta^{\gamma}_{\beta} + \eta_{\beta\varrho}\, \delta^{\gamma}_{\alpha})\, \varphi^{\varrho\sigma}{}_{,\sigma,\gamma} \} = 0, \tag{V.11}$$

$$\check{h}^{[\alpha\beta]}{}_{,\beta}{}^{,\gamma} - \check{h}^{[\gamma\beta]}{}_{,\beta}{}^{,\alpha} = 0, \tag{V.12}$$

$$\varphi_{\alpha\beta} = h_{<\alpha\beta>} - \frac{1}{2} \eta_{\alpha\beta}\, h . \tag{V.13}$$

Equations (V.11), (V.12) cannot be solved unless we specify the boundary conditions. To derive the linear approximation we have assumed an asymptotically flat space-time in which cartesian coordinates are used at infinity. Hence we can introduce the "outgoing waves" boundary conditions [5]

(a) $$\lim_{r \to \infty} g^{\hat{\alpha}}_{\alpha} = \delta^{\hat{\alpha}}_{\alpha};$$

(b) if ψ is any of the quantities $g^{\alpha}_{\hat{\alpha}} - \delta^{\alpha}_{\hat{\alpha}}$ or $g_{\alpha\beta} - \eta_{\alpha\beta}$, it must satisfy the condition

$$\lim_{r \to \infty} \left\{ \frac{\partial (r\psi)}{\partial r} + \frac{1}{c} \frac{\partial (r\psi)}{\partial t} \right\} = 0$$

for all values of $t_0 = t + \dfrac{r}{c}$ in an arbitrary fixed interval; the ψ and the first-order derivatives must also be bounded everywhere and must go to zero at least like $1/r$ for $r \to \infty$.

The conditions a, b require the matter system to be an insular system, but they do not exclude the presence of gravitational waves emitted by it. An important consequence [5] of a, b is that, given a quantity ψ satisfying b, the only solution of the equation

$$\Box\, \psi = 0 \tag{V.14}$$

is

$$\psi = 0\,. \tag{V.15}$$

This result allows us to solve equation (V.12); in fact we obtain from it by derivation

$$\Box\, \check{h}^{[\alpha\beta]}{}_{,\beta} = 0$$

and, using (V.14), (V.15),

$$\check{h}^{[\alpha\beta]}{}_{,\beta} = 0\,. \tag{V.16}$$

Equation (V.16) just says that $h_{[\mu\nu]}$ can be written by means of a vector potential A_μ as

$$h_{[\mu\nu]} = A_{\mu,\nu} - A_{\nu,\mu}\,. \tag{V.17}$$

For an arbitrary vector field A_μ the $h_{[\mu\nu]}$ given by (V.17) satisfy the field equations (V.12); hence these cannot determine the skew degrees of freedom of the tetrad field.

In this situation it is impossible to attribute any physical meaning to the $h_{[\mu\nu]}$. The Lagrangian we obtain when choosing $a_3 = a_4 = 0$ is thus completely unsatisfactory, although we can derive the linearized Einstein equations from it.

A choice of constants giving a better result is

$$a_2 = a_3 = 0 \qquad a_1 \neq 0 \qquad a_4 \neq 0\,.$$

In this case the field equations are

$$\left.\begin{aligned} &\frac{a_1}{2}\Big\{-\Box\,\varphi^{\mu\nu} - \eta^{\mu\nu}\,\varphi^{\alpha\beta}{}_{,\alpha,\beta} + (\delta^\mu_\alpha\,\eta^{\gamma\nu} + \delta^\nu_\alpha\,\eta^{\gamma\mu})\,\varphi^{\alpha\beta}{}_{,\beta,\gamma}\Big\} \\ &\qquad - 2\,i a_4\Big\{\check{h}^{[\nu\beta]}{}_{,\beta}{}^{,\mu} + \check{h}^{[\mu\beta]}{}_{,\beta}{}^{,\nu}\Big\} = -\,T^{<\mu\nu>}, \end{aligned}\right\} \tag{V.18}$$

$$-\,2\,\varepsilon^{\mu\nu\alpha\beta}\Big\{h_{<\alpha\gamma>,\beta}{}^{,\gamma} - h_{[\alpha\gamma],\beta}{}^{,\gamma}\Big\} + 2\,i\Big\{\check{h}^{[\mu\beta]}{}_{,\beta}{}^{,\nu} - \check{h}^{[\nu\beta]}{}_{,\beta}{}^{,\mu}\Big\} = 0\,. \tag{V.19}$$

To derive (V.18) we added to our Lagrangian a matter term $\mathfrak{L}_m$ depending on the $g^\alpha_{\dot\alpha}$ only through the metric tensor, so that

$$\frac{\delta\,\mathfrak{L}_m}{\delta\,h_{<\mu\nu>}} = T^{<\mu\nu>}$$

$$\frac{\delta\,\mathfrak{L}_m}{\delta\,h_{[\mu\nu]}} = 0\,.$$

All the macroscopic physical systems are of this type, so that equations (V.18), (V.19) are what we need in order to see whether the linear form of our theory contains the Newtonian theory of gravitation.

Taking the derivative with respect to x^ν of (V.19), we obtain

$$\Box \check{h}^{[\mu\beta]}{}_{,\beta} = 0 \tag{V.20}$$

and, using (V.14), (V.15),

$$\check{h}^{[\mu\beta]}{}_{,\beta} = 0\,. \tag{V.21}$$

This result reduces (V.18) to the Einstein weak-field equations. The other equation, (V.19), still contains both the symmetric and the skew part of $h_{\mu\nu}$.

A complete separation can be achieved in harmonic coordinates, where the de Donder condition

$$\varphi^{\alpha\beta}{}_{,\beta} = 0 \tag{V.22}$$

holds. This, together with (V.21), allows us to write (V.18), (V.19) as

$$-a_1 \Box \varphi^{\mu\nu} = 2\, T^{<\mu\nu>}, \tag{V.23}$$

$$h_{[\alpha\beta],\beta}{}^{,\gamma} - h_{[\beta\gamma],\alpha}{}^{,\gamma} = 0\,. \tag{V.24}$$

Since from (V.21) it follows again that

$$h^{[\alpha\beta]} = A_{\alpha,\beta} - A_{\beta,\alpha},$$

(V.24) becomes simply

$$\Box h_{[\alpha\beta]} = 0 \tag{V.25}$$

so that eventually our field equations are reduced to

$$-a_1 \Box \varphi^{\mu\nu} = 2\, T^{<\mu\nu>}, \tag{V.23}$$

$$h_{[\mu\nu]} = 0\,. \tag{V.26}$$

This is the same result as that obtained by Møller[5]. From (V.23) we can determine the value of the constant a_1:

$$a_1^{-1} = \frac{8\pi k}{c^4}, \tag{V.27}$$

where k is the Newtonian gravitational constant. These results allow us to assume as Lagrangian of the tetrad field

$$\mathfrak{L} = k_1 \mathfrak{L}_M + k_2 \check{I}_3 \tag{V.28}$$

with $k_1 = a_1$ given by (V.27).

About the other constant, k_2, we have no information; since k_2 drops out of the equations also in the case of a spherically symmetric system, for which the solution of the field equations derivable from (V.28) will be given in section VIII, we shall not be able to give its value in this paper. We have a feeling that k_2 is related to some

non-classical aspect of the gravitational field and that it might become important in a quantized version of this theory.

We would also point out that the results (V.23), (V.26), and also those obtained in section VIII for the Schwarzschild case, are left unchanged if we add to the Lagrangian (V.28) the term $a_2 P_2$. For simplicity we assume $a_2 = 0$, but the possibility of adding the term $a_2 P_2$ to our Lagrangian is worth noting.

VI. The Invariance Properties of the Lagrangian with Respect to the Group of Tetrad Rotations

In this section we want to study the behaviour of the Lagrangian

$$\mathfrak{L} = k_1 \mathfrak{L}_M + k_2 \check{I}_3 \tag{VI.1}$$

with respect to the group of tetrad rotations, defined by

$$g'^{\hat{\alpha}}_{\alpha}(x) = L^{\hat{\alpha}}_{\hat{\beta}}(x)\, g^{\hat{\beta}}_{\alpha}(x), \tag{VI.2}$$

$$g_{\hat{\varrho}\hat{\sigma}}\, L^{\hat{\varrho}}_{\hat{\alpha}}(x)\, L^{\hat{\sigma}}_{\hat{\beta}}(x) = g_{\hat{\alpha}\hat{\beta}} \tag{VI.3}$$

and already introduced in section II.

The matrix $L^{\hat{\alpha}}_{\hat{\beta}}$ can in general be a function of the coordinates. We have already noted that the metric tensor is invariant under the substitution (VI.2). The same is true of the Ricci tensor $R^{\alpha\beta}$ and of the scalar curvature R, in accordance with the fact that the Einstein field equations cannot alone fix the tetrad field.

Let us now consider the Lagrangian (VI.1). It is clear that under constant tetrad rotations, i. e. when $L^{\hat{\alpha}}_{\hat{\beta},\mu} = 0$, all the tensors not containing tetrad indices, like $A_{[\alpha\beta]\gamma}$, will be transformed like scalars. On the other hand, the quantity $g\hat{:}$ is transformed like a density:

$$g'\hat{:} = g\hat{:} \quad \det \left| L^{\hat{\alpha}}_{\hat{\beta}} \right|. \tag{VI.4}$$

It follows that the two terms $\mathfrak{L}_M$ and $\hat{I}_3$ definde by (IV.21) and (IV.13) are transformed like a pseudoscalar and a scalar density respectively under the whole rotation group. The Lagrangian $\mathfrak{L}$ is invariant only with respect to the subgroup of proper tetrad rotations.

Let us now look into the general case $L^{\hat{\alpha}}_{\hat{\beta},\mu} \neq 0$, but limiting ourselves to the subgroup of proper rotations. For simplicity, the infinitesimal transformation

$$L^{\hat{\alpha}}_{\hat{\beta}} = \delta^{\hat{\alpha}}_{\hat{\beta}} + \varepsilon^{\hat{\alpha}}_{\hat{\beta}}, \tag{VI.5}$$

for which the condition (VI.3) becomes

$$\varepsilon_{\hat{\alpha}\hat{\beta}} = -\varepsilon_{\hat{\beta}\hat{\alpha}}, \tag{VI.6}$$

will be considered.

After a somewhat long but simple calculation the variation of $\mathfrak{L}$ can be written as

$$\delta\,\mathfrak{L} = 2\,k_1\,g\hat{:}\,(W^{\mu}_{\hat{\alpha}\hat{\beta}}\,\varepsilon^{\hat{\alpha}\hat{\beta}})_{;\,\mu} + k_2\,Z^{\mu}_{\hat{\alpha}\hat{\beta}}\,\varepsilon^{\hat{\alpha}\hat{\beta}}{}_{,\,\mu}, \tag{VI.7}$$

where

$$W^{\mu}_{\hat{\alpha}\hat{\beta}} = (g^{\mu}_{\hat{\alpha};\,\lambda} - g^{\nu}_{\hat{\alpha};\,\nu}\,\delta^{\mu}_{\lambda})\,g^{\lambda}_{\hat{\beta}} - (g^{\mu}_{\hat{\beta};\,\lambda} - g^{\nu}_{\hat{\beta};\,\nu}\,\delta^{\mu}_{\lambda})\,g^{\lambda}_{\hat{\alpha}} \tag{VI.8}$$

and

$$\left.\begin{aligned} Z^{\mu}_{\hat{\alpha}\hat{\beta}} = \varepsilon^{\alpha\beta\gamma\delta}\,g^{\lambda\nu}\{&A_{[\alpha\lambda]\,\nu}\,g_{\hat{\beta}\delta}\,(\delta^{\varrho}_{\beta}\,\delta^{\mu}_{\gamma} - \delta^{\varrho}_{\gamma}\,\delta^{\mu}_{\beta}) \\ &+ A_{[\beta\gamma]\,\delta}\,g_{\hat{\beta}\lambda}\,(\delta^{\varrho}_{\alpha}\,\delta^{\mu}_{\nu} - \delta^{\varrho}_{\nu}\,\delta^{\mu}_{\alpha})\}\,g_{\hat{\alpha}\varrho}. \end{aligned}\right\} \tag{VI.9}$$

Note that the variation of $\mathfrak{L}_M$ is a four-divergence, as it should be, since the theory deduced only from this term is equivalent to the Einstein theory.

The quantity $W^{\mu}_{\hat{\alpha}\hat{\beta}}$ has the property that

$$W^{\mu}_{\hat{\alpha}\hat{\beta};\,\mu} = 0\,. \tag{VI.10}$$

This can be seen more easily if we use absolute derivatives and the identity [5]

$$A_{[\alpha\beta]}{}^{\mu}{}_{/\mu} + \Phi_{\beta/\alpha} - \Phi_{\alpha/\beta} - A_{[\alpha\beta]\,\mu}\,\Phi^{\mu} = 0\,. \tag{VI.11}$$

A stroke, $A_{\alpha/\beta}$, here means absolute derivative. In fact, from the connection between the absolute and the covariant derivative [5] we obtain

$$\left.\begin{aligned} W^{\mu}_{\hat{\alpha}\hat{\beta};\,\mu} &= W_{\hat{\alpha}\hat{\beta}}{}^{\mu}{}_{/\mu} - W_{\hat{\alpha}\hat{\beta}}{}^{\mu}\,\Phi_{\mu} \\ &= g^{\alpha}_{\hat{\alpha}}\,g^{\beta}_{\hat{\beta}}\,(W_{\alpha\beta}{}^{\mu}{}_{/\mu} - W_{\alpha\beta}{}^{\mu}\,\Phi_{\mu})\,. \end{aligned}\right\} \tag{VI.12}$$

From the definition (VI.8) of $W^{\mu}_{\hat{\alpha}\hat{\beta}}$ we find that

$$W_{\alpha\beta}{}^{\mu} = -A_{[\alpha\beta]}{}^{\mu} + \delta^{\mu}_{\beta}\,\Phi_{\alpha} - \delta^{\mu}_{\alpha}\,\Phi_{\beta}. \tag{VI.13}$$

Substituting (VI.13) in (VI.12) and using the identity (VI.11), we find the result (VI.10).

The variation of the Lagrangian can now be written simply as

$$\delta\,\mathfrak{L} = (2\,k_1\,g\hat{:}\,W^{\mu}_{\hat{\alpha}\hat{\beta}} + k_2\,Z^{\mu}_{\hat{\alpha}\hat{\beta}})\,\varepsilon^{\hat{\alpha}\hat{\beta}}{}_{,\,\mu}. \tag{VI.14}$$

We see that $\mathfrak{L}$, contrary to the Einstein Lagrangian, is not invariant under a position-dependent tetrad rotation. The condition

$$\delta\,\mathfrak{L} = 0 \tag{VI.15}$$

can be satisfied only when we assume

$$\varepsilon_{\hat{\alpha}\hat{\beta},\,\mu} = 0\,. \tag{VI.16}$$

It follows that the Lagrangian (VI.1) is invariant only with respect to the group of proper constant tetrad rotations. The existence of this "gauge" group will be used in appendix B to introduce spinors.

VII. The Field Equations

In this section we want to derive explicitly the field equations from our Lagrangian, which we now write as

$$\mathfrak{L} = \frac{1}{2}\,k_1\,\mathfrak{L}_M + k_2\,\check{I}_3 + \frac{1}{2}\,\mathfrak{L}_m^{(b)} + \mathfrak{L}_m^{(f)}. \tag{VII.1}$$

The Lagrangian of matter has been divided into two parts; the first, $\mathfrak{L}_m^{(b)}$, depends on the tetrads only through the metric tensor, whereas this assumption does not apply to the second, $\mathfrak{L}_m^{(f)}$.

Examples of physical systems of the first kind are all the classical systems, such as the electromagnetic field, a hydrodynamical system and a field of boson particles. To the second type belongs the Lagrangian of fermions, like electrons and neutrinos, which must be written in terms of spinors.

To evalute the variation of the action integral we first consider the terms $\mathfrak{L}_M$ and $\mathfrak{L}_m^{(b)}$ of the Lagrangian. Since

$$\delta\int_\Omega (k_1\,\mathfrak{L}_M + \mathfrak{L}_m^{(b)})\,d^4x = \delta\int_\Omega (k_1\,\mathfrak{R} + \mathfrak{L}_m^{(b)})\,d^4x\,, \tag{VII.2}$$

we have

$$\left.\begin{aligned}&\int_\Omega \frac{\delta}{\delta g_{\hat{\varrho}}^{\hat{\varrho}}}\left\{k_1\,\mathfrak{L}_M + \mathfrak{L}_m^{(b)}\right\}\delta g_{\hat{\varrho}}^{\hat{\varrho}}\,d^4x\\ =&\int_\Omega \frac{\delta}{\delta g_{\varrho\sigma}}\left\{k_1\,\mathfrak{R} + \mathfrak{L}_m^{(b)}\right\}\delta g_{\varrho\sigma}\,d^4x\,.\end{aligned}\right\} \tag{VII.3}$$

But

$$\delta g_{\alpha\beta} = g_{\hat{\varrho}\beta}\,\delta g_{\alpha}^{\hat{\varrho}} + g_{\hat{\varrho}\alpha}\,\delta g_{\beta}^{\hat{\varrho}} \tag{VII.4}$$

so that we obtain

$$\delta\int_\Omega (k_1\,\mathfrak{L}_M + \mathfrak{L}_m^{(b)})\,d^4x = 2\int_\Omega \hat{g}\,(k_1\,G^{\alpha\beta} + T^{(b)\,\alpha\beta})\,g_{\hat{\varrho}\beta}\,\delta g_{\alpha}^{\hat{\varrho}}\,d^4x\,, \tag{VII.5}$$

where

$$\left.\begin{aligned} G^{\alpha\beta} &= R^{\alpha\beta} - \frac{1}{2} g^{\alpha\beta} R, \\ g\hat{:}\, T^{(b)\,\alpha\beta} &= \frac{\delta \mathfrak{L}_m^{(b)}}{\delta g_{\alpha\beta}}, \end{aligned}\right\} \tag{VII.6}$$

and $R^{\alpha\beta}$ is the Ricci tensor.

On introduction of the quantities

$$g\hat{:}\, F_{\hat{\varrho}}^{\ \varrho} = \frac{\delta \check{I}_3}{\delta g_{\varrho}^{\ \hat{\varrho}}} \tag{VII.7}$$

$$g\hat{:}\, T^{(f)}{}_{\hat{\varrho}}^{\ \varrho} = \frac{\delta \mathfrak{L}_m^{(f)}}{\delta g_{\varrho}^{\ \hat{\varrho}}} \tag{VII.8}$$

the variational principle can be written as

$$\left.\begin{aligned} 0 &= \delta \int_{\Omega} \left(\frac{1}{2} k_1 \mathfrak{L}_M + k_2 \check{I}_3 + \frac{1}{2} \mathfrak{L}_m^{(b)} + \mathfrak{L}_m^{(f)} \right) d^4 x \\ &= \int_{\Omega} g\hat{:}\, (k_1 G_{\hat{\varrho}}^{\ \varrho} + k_2 F_{\hat{\varrho}}^{\ \varrho} + T^{(b)}{}_{\hat{\varrho}}^{\ \varrho} + T^{(f)}{}_{\hat{\varrho}}^{\ \varrho})\, \delta g_{\varrho}^{\hat{\varrho}}\, d^4 x, \end{aligned}\right\} \tag{VII.9}$$

and the resulting field equations are

$$k_1 G_{\hat{\varrho}}^{\ \varrho} + k_2 F_{\hat{\varrho}}^{\ \varrho} + T^{(b)}{}_{\hat{\varrho}}^{\ \varrho} + T^{(f)}{}_{\hat{\varrho}}^{\ \varrho} = 0\,. \tag{VII.10}$$

The evaluation of $F_{\hat{\varrho}}^{\ \varrho}$ and of $F^{\alpha\beta} = g^{\hat{\varrho}\alpha} F_{\hat{\varrho}}^{\ \beta}$ is performed in appendix A.

Multiplying (VII.10) by $g^{\hat{\varrho}\alpha}$ and using (A.24), (A.25), we obtain another form of the field equations:

$$\left.\begin{aligned} & k_1 G^{\alpha\beta} + k_2 \Big\{ \check{\Lambda}^{\beta;\,\alpha} + 2\, \eta^{\beta\alpha\varrho\sigma}\, \Phi_{\varrho;\,\sigma} - \Phi^{\alpha}\, \check{\Lambda}^{\beta} \\ & + \check{\Lambda}^{\gamma}\, \gamma^{\beta\alpha}{}_{\gamma} + 2\, \eta^{\beta\varrho\sigma\tau}\, \Phi_{\varrho}\, \Lambda_{[\sigma\tau]}{}^{\alpha} + \check{\Lambda}^{\varrho}\, \Lambda_{[\varrho\cdot]}{}^{\alpha\beta} \\ & + \frac{1}{2} g^{\alpha\beta}\, \eta^{\varrho\sigma\tau\zeta}\, \Lambda_{[\tau\zeta]\,\omega}\, \Lambda_{[\varrho\sigma]}{}^{\omega} \Big\} \\ & = - T^{(b)\,\alpha\beta} - T^{(f)\,\alpha\beta}. \end{aligned}\right\} \tag{VII.11}$$

While $G^{\alpha\beta}$ and $T^{(b)\,\alpha\beta}$ are symmetric tensors, $F^{\alpha\beta}$ and $T^{(f)\,\alpha\beta}$ have no well-defined symmetry property. Both $T^{(b)\,\alpha\beta}$ and $T^{(f)\,\alpha\beta}$ differ from the canonical energy-momentum matter tensor by a four-divergence.

Since our theory is generally covariant, the field equations must contain a set of four identities, in the same way as the Einstein equations are supplemented by the

Bianchi identities. To obtain these identities we apply the method of infinitesimal coordinate transformations to the scalar density $\mathfrak{L}^*$.

Therefore, under an arbitrary infinitesimal coordinate transformation

$$x'^{\alpha} = x^{\alpha} + \xi^{\alpha}(x) \tag{VII.12}$$

the local variation of $\mathfrak{L}$ is given by

$$\delta \mathfrak{L} = -(\mathfrak{L}\,\xi^{\alpha})_{,\alpha}. \tag{VII.13}$$

Integrating (VII.13) over a finite region Ω in space-time, we obtain, for all functions ξ^{α} which vanish on the boundary of Ω together with their first-order derivatives,

$$\int_{\Omega} \delta \mathfrak{L}\, d^4 x = \int_{\Omega} \frac{\delta \mathfrak{L}}{\delta g_{\hat{\alpha}\alpha}}\, \delta g_{\hat{\alpha}\alpha}\, d^4 x = 0, \tag{VII.14}$$

where

$$\frac{\delta \mathfrak{L}}{\delta g_{\hat{\alpha}\alpha}} = \frac{\partial \mathfrak{L}}{\partial g_{\hat{\alpha}\alpha}} - \left(\frac{\partial \mathfrak{L}}{\partial g_{\hat{\alpha}\alpha,\beta}}\right)_{,\beta}.$$

Substituting

$$\delta g_{\hat{\alpha}\alpha} = -g_{\hat{\alpha}\beta}\,\xi^{\beta}{}_{,\alpha} - g_{\hat{\alpha}\alpha,\beta}\,\xi^{\beta} \tag{VII.15}$$

in (VII.14), we obtain, after a partial integration,

$$\int_{\Omega} \left[\left(\frac{\delta \mathfrak{L}}{\delta g_{\hat{\alpha}\alpha}}\, g_{\hat{\alpha}\beta}\right)_{,\alpha} - \frac{\delta \mathfrak{L}}{\delta g_{\hat{\alpha}\alpha}}\, g_{\hat{\alpha}\alpha,\beta}\right] \xi^{\beta}\, d^4 x = 0. \tag{VII.16}$$

As the functions ξ^{β} are arbitrary inside Ω, the identities

$$\left(\frac{\delta \mathfrak{L}}{\delta g_{\hat{\alpha}\alpha}}\, g_{\hat{\alpha}\beta}\right)_{,\alpha} - \frac{\delta \mathfrak{L}}{\delta g_{\hat{\alpha}\alpha}}\, g_{\hat{\alpha}\alpha,\beta} = 0 \tag{VII.17}$$

must hold.

Since in our case $\mathfrak{L} = \frac{1}{2} k_1 \mathfrak{L}_M + k_2 \check{I}_3$, (VII.17) can be written as

$$[g\hat{:}\,(k_1 G^{\hat{\alpha}\alpha} + k_2 F^{\hat{\alpha}\alpha})\, g_{\hat{\alpha}\beta}]_{,\alpha} - g\hat{:}\,(k_1 G^{\hat{\alpha}\alpha} + k_2 F^{\hat{\alpha}\alpha})\, g_{\hat{\alpha}\alpha,\beta} = 0$$

or, on introduction of the quantity

$$\Delta^{\varrho}{}_{\alpha\beta} = g^{\varrho}_{\hat{\alpha}}\, g^{\hat{\alpha}}{}_{\alpha,\beta}, \tag{VII.18}$$

as

$$[g\hat{:}\,(k_1 G_{\beta}{}^{\alpha} + k_2 F_{\beta}{}^{\alpha})]_{,\alpha} - g\hat{:}\,(k_1 G_{\varrho}{}^{\alpha} + k_2 F_{\varrho}{}^{\alpha})\, \Delta^{\varrho}{}_{\alpha\beta} = 0. \tag{VII.19}$$

* See, for instance, reference 10 and also C. Møller, Proceedings of the Warsaw Conference on General Relativity.

Using the relation[5]

$$\Delta^{\alpha}{}_{\beta\gamma} = \Gamma^{\alpha}{}_{\beta\gamma} + \gamma^{\alpha}{}_{\beta\gamma}, \tag{VII.20}$$

we have from (VII.19)

$$(k_1 G_{\beta}{}^{\alpha} + k_2 F_{\beta}{}^{\alpha})_{;\alpha} - (k_1 G_{\varrho}{}^{\alpha} + k_2 F_{\varrho}{}^{\alpha})\,\gamma^{\varrho}{}_{\alpha\beta} = 0\,,$$

or, taking into account the symmetry properties of $G^{\alpha\beta}$ and $\gamma_{\varrho\alpha\beta}$,

$$k_1 G^{\alpha\beta}{}_{;\alpha} + k_2 [F^{\beta\alpha}{}_{;\alpha} - F^{\varrho\alpha}\,\gamma_{\varrho\alpha}{}^{\beta}] = 0\,. \tag{VII.21}$$

In case $k_2 = 0$, (VII.21) becomes the usual Bianchi identities.

An analogous result can be derived for the matter tensor, i. e.

$$T^{(b)\,\alpha\beta}{}_{;\beta} = 0 \tag{VII.22}$$

$$T^{(f)\,\alpha\beta}{}_{;\beta} - T^{(f)\,\varrho\beta}\,\gamma_{\varrho\beta}{}^{\alpha} = 0\,. \tag{VII.23}$$

That this is true can be seen by applying the method used to derive (VII.21) to the scalar densities $\mathfrak{L}_m^{(b)}$ and $\mathfrak{L}_m^{(f)}$ and keeping in mind that the variation of $\mathfrak{L}_m$ with respect to the matter field variables vanishes when the field equations are satisfied.

Going back to the field equations, we note that it is possible to separate them into two independent sets, viz

$$\left\{\begin{array}{c} k_1 G^{\alpha\beta} + k_2 F^{<\alpha\beta>} = -T^{(b)\,\alpha\beta} - T^{(f)\,<\alpha\beta>} \\ k_2 F^{[\alpha\beta]} = -T^{(f)\,[\alpha\beta]}. \end{array}\right. \tag{VII.24}$$

We saw already in the linearized case the usefulness of this separation.

In general (VII.24) shows that, contrary to what happens in the standard Einstein theory, the space-time structure is determined by matter not only through the symmetric energy-momentum tensors $T^{(b)\,\alpha\beta}$ and $T^{(f)\,<\alpha\beta>}$ but also through the skew term $T^{(f)\,[\alpha\beta]}$.

To acquire an insight into the meaning of this fact, let us consider explicitly a system formed by a Dirac particle with its own gravitational field. The Lagrangian of this system can be written as

$$\mathfrak{L} = \frac{1}{2} k_1 \mathfrak{L}_M + k_2 I_3 + \mathfrak{L}_D; \tag{VII.25}$$

$\mathfrak{L}_D$ is assumed to be given by

$$\mathfrak{L}_D = \frac{i}{2} g \{\psi^{+} (\alpha^{\mu} \psi_{,\mu} - im\beta\psi) - (\psi^{+}_{,\mu} \alpha^{\mu} + im\psi^{+}\beta)\psi\} \tag{VII.26}$$

(see appendix B).

Note that in our formalism $\psi_{,\mu}$ is simply the usual derivative $\dfrac{\partial\psi}{\partial x^{\mu}}$.

Performing the variation of $\mathfrak{L}_D$ with respect to ψ^+ and ψ, we arrive at the field equations

$$\left.\begin{aligned} &\alpha^\mu \psi_{,\mu} - im\,\beta\psi - \frac{1}{2}\alpha^\mu \Phi_\mu \psi = 0 \\ &\psi^+{}_{,\mu}\,\alpha^\mu + im\,\psi^+\beta - \frac{1}{2}\psi^+\alpha^\mu \Phi_\mu = 0\,. \end{aligned}\right\} \tag{VII.27}$$

To obtain (VII.27) the identity

$$g_{\hat{\alpha}}{}^{\mu}{}_{;\mu} = g_{\hat{\alpha}}{}^{\varrho}\, g_{\hat{\beta}\varrho}\, g^{\hat{\beta}\mu}{}_{;\mu} = -\, g_{\hat{\alpha}}{}^{\varrho}\, \Phi_\varrho \tag{VII.28}$$

has been used.

From the form (VII.26) of $\mathfrak{L}_D$, the continuity equation

$$J^\mu{}_{;\mu} \equiv (\psi^+ \alpha^\mu \psi)_{;\mu} = 0 \tag{VII.29}$$

is easily seen to hold.

Equations (VII.27) are reduced to the usual Dirac equations in the case of a flat space, since here we have $A_{[\alpha\beta]\gamma} \equiv 0$, $\Phi_\alpha \equiv 0$. In a space with torsion the extra term $-\frac{1}{2}\alpha^\mu \Phi_\mu \psi$ represents the interaction between the fermion and gravitation. The similarity of this term to the one introduced in the same equations by the coupling with the electromagnetic field is worth noting.

The tensor $T^{(f)\,\alpha\beta}$ appearing in (VII.11) can easily be derived; in fact

$$\left.\begin{aligned} g\hat{:}\; T_D{}^{\alpha\beta} &= g_{\hat{\alpha}}{}^{\alpha}\frac{\delta \mathfrak{L}_D}{\delta g_{\hat{\alpha}\beta}} \\ &= g^{\alpha\beta}\,\mathfrak{L}_D - \frac{i}{2}\, g\hat{:}\,\{\psi^+\alpha^\alpha \psi^{,\beta} - \psi^{+,\beta}\alpha^\alpha\psi\}. \end{aligned}\right\} \tag{VII.30}$$

As a consequence of the field equations (VII.27), $\mathfrak{L}_D$ vanishes so that only the second term of (VII.30) has to be taken into account.

We now consider the weak-field limit of the equation

$$k_1 G^{\alpha\beta} + k_2 F^{\alpha\beta} = -\, T_D{}^{\alpha\beta}. \tag{VII.31}$$

In harmonic coordinates, i. e. when we use the coordinate condition (V.22), this is

$$-\frac{1}{2}k_1 \Box\, \varphi^{\alpha\beta} + k_2\{\varepsilon^{\alpha\gamma\mu\nu}\, h_{[\nu\mu],\gamma}{}^{,\beta} - \varepsilon^{\alpha\beta\varrho\sigma}\, h_{[\tau\varrho],\sigma}{}^{,\tau}\} = -\, T_{D0}^{\alpha\beta}, \tag{VII.32}$$

where

$$T_{D0}^{\alpha\beta} = \frac{i}{2}\{\psi^+\tilde{\alpha}^\alpha \psi^{,\beta} - \psi^{+,\beta}\tilde{\alpha}^\alpha\psi\} \tag{VII.33}$$

and

$$\tilde{\alpha}^\alpha = \delta^\alpha_{\hat{\beta}}\,\alpha^{\hat{\beta}}. \tag{VII.34}$$

The quantity $T_{D0}^{\alpha\beta}$ is the special-relativity energy-momentum tensor of a Dirac particle. It satisfies the relation

$$T_{D0}^{\alpha\beta}{}_{,\beta} = 0\,, \tag{VII.35}$$

as can easily be verified by means of the zero-order Dirac equations

$$\left.\begin{aligned} &\tilde{\alpha}^{\mu}\,\psi_{,\mu} - im\,\beta\psi = 0 \\ &\psi^{+}{}_{,\mu}\,\tilde{\alpha}^{\mu} + im\,\psi^{+}\beta = 0\,. \end{aligned}\right\} \tag{VII.36}$$

Taking the derivative with respect to x^{β} of (VII.32) and using (VII.35), we find

$$\Box\,\varepsilon^{\alpha\lambda\nu\mu}\,h_{[\mu\nu],\,\lambda} \equiv -\frac{i}{2}\Box\,\check{h}^{[\alpha\lambda]}{}_{,\,\lambda} = 0\,. \tag{VII.37}$$

If again we supplement equations (VII.32) with the boundary conditions *a*, *b* used in section V, it follows from (VII.37) that

$$\check{h}^{[\alpha\lambda]}{}_{,\,\lambda} = 0\,, \tag{VII.38}$$

$$h_{[\mu\nu]} = A_{\mu,\,\nu} - A_{\nu,\,\mu}\,. \tag{VII.39}$$

If we use (VII.38), (VII.39) and separate the symmetric and the skew part of (VII.32), the field equations become

$$k_1\,\Box\,\varphi^{\alpha\beta} = 2\,T_{D0}^{<\alpha\beta>} \tag{VII.40}$$

$$\frac{1}{2}\,k_2\,\varepsilon^{\alpha\beta\varrho\sigma}\,\Box\,h_{[\varrho\sigma]} \equiv ik_2\,\Box\,\check{h}^{[\alpha\beta]} = -\,T_{D0}^{[\alpha\beta]}. \tag{VII.41}$$

It is well known[9] that the antisymmetric part of $T_{D0}^{\alpha\beta}$ is related to the spin angular-momentum tensor $\Im^{\alpha\beta\gamma}$ of a Dirac particle. In fact

$$T^{D}{}_{0}^{[\alpha\beta]} = \frac{1}{2}\,\Im^{\alpha\beta\gamma}{}_{,\gamma}$$

and (VII.40), (VII.41) tell us that while the symmetric part of the field is coupled to the symmetric energy-momentum tensor of matter, the antisymmetric part is coupled to the spin angular momentum.

The solution of equations (VII.40), (VII.41) may give us some information about the constant k_2, but it is clear that a meaningful solution can be obtained only within the framework of a quantized theory.

To conclude this section we want to add the remark that equations similar to (VII.27), i. e. with the same coupling term $\alpha^{\mu}\,\Phi_{\mu}$, are valid also for the neutrino field. Using the two-spinor formalism (see appendix B), we can write the neutrino Lagrangian as

$$\mathfrak{L}_{\nu} = \frac{i}{2}\,g\,\{\psi_A\,g^{\mu\,\dot{A}B}\,\psi_{B,\,\mu} - \psi_{A,\,\mu}\,g^{\mu\,\dot{A}B}\,\psi_B\}\,. \tag{VII.42}$$

Again $\psi_{A,\,\mu}$ is simply the partial derivative.

Performing the variation with respect to ψ_A and ψ_B and using (VII.28), we obtain from (VII.42) the equations

$$\left.\begin{aligned} &g^{\mu\dot{A}B}\,\psi_{B,\mu} - \frac{1}{2}\,g^{\mu\dot{A}B}\,\Phi_\mu\,\psi_B = 0 \\ &\psi_{\dot{A},\mu}\,g^{\mu\dot{A}B} - \frac{1}{2}\,\psi_{\dot{A}}\,g^{\mu\dot{A}B}\,\Phi_\mu = 0 \end{aligned}\right\} \tag{VII.43}$$

and the continuity equation

$$J^\mu{}_{;\mu} = (\psi_{\dot{A}}\,g^{\mu\dot{A}B}\,\psi_B)_{;\mu} = 0\,. \tag{VII.44}$$

VIII. Solution of the Field Equations for a Static, Spherically Symmetric System

In the case of a static, spherically symmetric system, the field equations are

$$k_1\,G^{\alpha\beta} + k_2\,F^{<\alpha\beta>} = -\,T^{(b)\,\alpha\beta} \tag{VIII.1}$$

$$k_2\,F^{[\alpha\beta]} = 0\,. \tag{VIII.2}$$

Let us introduce an isotropic coordinate system, where the line element is of the type

$$ds^2 = b\,(r)\,(dx^0)^2 - a\,(r)\sum_1^3{}_\alpha\,(dx^\alpha)^2 \tag{VIII.3}$$

and

$$r^2 = (x^1)^2 + (x^2)^2 + (x^3)^2\,.$$

A solution of (VIII.2), satisfying also the relation (II.5), is then given by

$$g^\alpha_{\hat{\alpha}} = \frac{\delta^\alpha_{\hat{\alpha}}}{\sqrt{\varepsilon_{\alpha)}\,g_{\alpha\alpha}}}, \tag{VIII.4}$$

where $\varepsilon_\alpha = (1, -1, -1, -1)$ and the bracket after the index α means that no summation over α should be performed.

In fact, using (VIII.4) and the notation

$$A' = \frac{dA\,(r)}{ds}, \quad n_\alpha = \frac{\partial r}{\partial x^\alpha} = \left(0\,, \frac{x^i}{r}\right),$$

we have

$$\left.\begin{aligned} \Lambda_{[\alpha\beta]}{}^{\gamma} &= \frac{1}{2}\,[ln\,(\varepsilon_{\alpha})\,g_{\alpha\alpha})]'\,\delta^{\gamma}_{\alpha}\,n^{\beta} \\ &\quad - \frac{1}{2}\,[ln\,(\varepsilon_{\beta})\,g_{\beta\beta})]'\,\delta^{\gamma}_{\beta}\,n_{\alpha}, \end{aligned}\right\} \tag{VIII.5}$$

$$\Phi_{\alpha} = -\,[ln\,a\sqrt{b}]'\,n_{\alpha}. \tag{VIII.6}$$

From (VIII.5), (VIII.6) it follows that

$$\check{\Lambda}_{\alpha} = 0\,, \tag{VIII.7}$$

$$\Phi_{\alpha,\,\beta} - \Phi_{\beta,\,\alpha} = 0\,. \tag{VIII.8}$$

When we use this last result, the tensor $F^{\alpha\beta}$ becomes simply

$$F^{\alpha\beta} = 2\,\eta^{\alpha\varrho\sigma\tau}\,\Phi_{\varrho}\,\Lambda_{[\sigma\tau]}{}^{\beta} + \frac{1}{2}\,g^{\alpha\beta}\,\eta^{\varrho\sigma\lambda\mu}\,\Lambda_{[\varrho\sigma]\,\nu}\,\Lambda_{[\lambda\mu]}{}^{\nu},$$

and by means of (VIII.5), (VIII.6) we have

$$\left.\begin{aligned} F^{\alpha\beta} = &-\eta^{\alpha\varrho\sigma\tau}\,(ln\,a\sqrt{b})'\,\{[ln\,(\varepsilon_{\sigma})\,g_{\sigma\sigma})]'\,\delta^{\beta}_{\sigma}\,n_{\tau} \\ &\quad - [ln\,(\varepsilon_{\tau})\,g_{\tau\tau})]'\,\delta^{\beta}_{\tau}\,n_{\sigma}\}\,n_{\varrho} \\ &+ \frac{1}{4}\,g^{\alpha\beta}\,\eta^{\varrho\sigma\lambda\mu}\,\{[ln\,(\varepsilon_{\varrho})\,g_{\varrho\varrho})]'\,g_{\varrho\nu}\,n_{\sigma} \\ &- [ln\,(\varepsilon_{\sigma})\,g_{\sigma\sigma})]'\,g_{\sigma\nu}\,n_{\varrho}\}\,\{[ln\,(\varepsilon_{\lambda})\,g_{\lambda\lambda})]'\,\delta^{\nu}_{\lambda}\,n_{\mu} - [ln\,(\varepsilon_{\mu})\,g_{\mu\mu})]'\,\delta^{\nu}_{\mu}\,n_{\lambda}\} \equiv 0\,. \end{aligned}\right\} \tag{VIII.9}$$

Since the tensor $F^{\alpha\beta}$ vanishes, we are left with the equation

$$k_1\,G_{\alpha\beta} = -\,T^{(b)}_{\alpha\beta}, \tag{VIII.10}$$

which determines in the usual way the two functions $a(r)$, $b(r)$.

The fact that the Schwarzschild metric holds for a static, spherically symmetric system is of course very important, since it allows us to say that this theory predicts correctly the results of the three experimental tests of the theory of general relativity.

IX. The Energy–Momentum Conservation Law

In section III the conservation law

$$g\hat{:}\ \Theta^{\lambda}_{\hat{\lambda};\,\lambda} = 0 \tag{IX.1}$$

was obtained, and it was further shown that a superpotential $g\hat{:}\ U^{[\lambda\delta]}_{\hat{\lambda}}$ exists such that

$$\Theta^{\lambda}_{\hat{\lambda}} = U^{[\lambda\delta]}_{\hat{\lambda};\,\delta}. \tag{IX.2}$$

From (A.11), (A.20) it is easy to see that

$$\left.\begin{aligned} U_{\hat{\lambda}}^{[\lambda\mu]} &= k_1 \left\{ g_{\hat{\lambda}\sigma}\, \gamma^{\lambda\mu\sigma} + g_{\hat{\lambda}}^{\ \mu}\, \Phi^{\lambda} - g_{\hat{\lambda}}^{\lambda}\, \Phi^{\mu} \right\} \\ &+ k_2 \left\{ \Lambda^{\mu}\, g_{\hat{\lambda}}^{\lambda} - \Lambda^{\lambda}\, g_{\hat{\lambda}}^{\mu} - 2\, \eta^{\lambda\mu\alpha\beta}\, \Phi_{\alpha}\, g_{\hat{\lambda}\beta} \right\}. \end{aligned}\right\} \tag{IX.3}$$

In the case of a static closed system, and in the absence of fermions, the metric is asymptotically of the Schwarzschild type, and the gravitational part of $\Theta_{\hat{\lambda}}^{\lambda}$, which is bilinear in the first derivatives of $g_{\hat{\lambda}}^{\lambda}$, behaves at infinity like $1/r^4$. Hence the four quantities

$$P_{\hat{\lambda}} = \int_{x_0 = \text{const}} g\hat{:}\, \Theta_{\hat{\lambda}}^{0}\, d^3 x \tag{IX.4}$$

are constant in time and invariant under coordinate transformations. We can write (IX.4) in a manifestly covariant form, substituting for the surface $x_0 = \text{const}$ a general three-dimensional, time-like surface Σ, as

$$P_{\hat{\lambda}} = \int_{\Sigma} \Theta_{\hat{\lambda}}^{\lambda}\, n_{\lambda}\, d\Sigma, \tag{IX.5}$$

where n_{λ} is the unit vector orthogonal to Σ, and $d\Sigma$ is the invariant volume element.

Using (IX.2), we can also express $P_{\hat{\lambda}}$ as an integral over a two-dimensional, space-like surface S, the boundary of $x_0 = \text{const}$:

$$P_{\hat{\lambda}} = \int_{S} g\hat{:}\, U_{\hat{\lambda}}^{[0k]}\, n_k\, dS, \tag{IX.6}$$

where n_k is a unit three-vector orthogonal to the surface element dS.

The relation between the four scalars $P_{\hat{\lambda}}$ and the total energy and momentum can easily be seen in the case of a closed system. We now want to introduce a conservation law of the usual form. To do this we introduce the tensor density

$$\mathfrak{U}_{\nu}^{[\lambda\mu]} = g\hat{:}\, g_{\nu}^{\hat{\lambda}}\, U_{\hat{\lambda}}^{[\lambda\mu]} \tag{IX.7}$$

and the quantity

$$\mathsf{T}_{\nu}^{\ \lambda} = \mathfrak{U}_{\nu}^{[\lambda\mu]}{}_{,\mu}. \tag{IX.8}$$

Clearly $\mathsf{T}_{\nu}^{\ \lambda}$ satisfies the conservation law

$$\mathsf{T}_{\nu}^{\ \lambda}{}_{,\lambda} = 0. \tag{IX.9}$$

From (IX.3), (IX.7) it follows that

$$\mathfrak{U}_{\nu}^{[\lambda\mu]} = \mathfrak{U}_{1\nu}^{[\lambda\mu]} + \mathfrak{U}_{2\nu}^{[\lambda\mu]}, \tag{IX.10}$$

where

$$\mathfrak{U}_{1\,\nu}^{[\lambda\mu]} = k_1\, g\hat{:}\, [\gamma_\nu^{\lambda\mu} + \delta_\nu^\mu\, \Phi^\lambda - \delta_\nu^\lambda\, \Phi^\mu] \tag{IX.11}$$

is the Møller superpotential[5], and

$$\mathfrak{U}_{2\,\nu}^{[\lambda\mu]} = k_2\, g\hat{:}\, [\check{A}^\mu\, \delta_\nu^\lambda - \check{A}^\lambda\, \delta_\nu^\mu - 2\, \eta^{\lambda\mu\alpha\beta}\, \Phi_\alpha\, g_{\beta\nu}]\,. \tag{IX.12}$$

In the case of a static, spherically symmetric system and in isotropic coordinates the Møller superpotential is given by[5]

$$\mathfrak{U}_{1\,\nu}^{[\lambda\mu]} = k_1 \sqrt{ab}\left[ln \frac{a\sqrt{b}}{\sqrt{|\,g_{\mu\mu}\,|}}\right]' (\delta_\nu^\lambda\, n^\mu - \delta_\nu^\mu\, n^\lambda), \tag{IX.13}$$

where the notations of section VIII have been used. For the second term of $\mathfrak{U}_\nu^{[\lambda\mu]}$ we obtain

$$\mathfrak{U}_{2\,\nu}^{[\lambda\mu]} = k_2\, \eta^{\alpha\beta\lambda\mu}\, [ln\, a\sqrt{b}]'\, g_{\beta\nu}\, n_\alpha \tag{IX.14}$$

and, as an immediate consequence,

$$\mathfrak{U}_{2\,\nu}^{[\lambda\mu]}{}_{,\,\mu} = 0\,. \tag{IX.15}$$

The quantity $\mathsf{T}_\nu^{\,\lambda}$ is now given by

$$\mathsf{T}_\nu^{\,\lambda} = \mathfrak{U}_{1\,\nu}^{[\lambda\mu]}{}_{,\,\mu} \tag{IX.16}$$

and is equal to the Møller energy-momentum complex. It is worth remembering that in isotropic coordinates the Møller complex $\mathsf{T}_\nu^{M\lambda}$ is equal to the Einstein complex $\Theta_\nu^{E\lambda}$ so that we have in this case

$$\mathsf{T}_\nu^{\,\lambda} = \mathsf{T}^M{}_\nu^{\,\lambda} = \Theta^E{}_\nu^{\,\lambda}. \tag{IX.17}$$

This result allows us to identify $\mathsf{T}_\nu^{\,\lambda}$, defined by (IX.8), as the energy-momentum complex.

We can now introduce the total energy and momentum for a closed system

$$P_\nu = \int_{x_0 = \text{const}} \mathsf{T}_\nu^{\,0}\, d^3 x\,. \tag{IX.18}$$

The relation between P_ν and $P_{\hat{\nu}}$ can be found if we write P_ν in the form

$$P_\nu = \int_S \mathfrak{U}_\nu^{0i}\, n_i\, dS, \tag{IX.19}$$

where n_i, dS and S have the same meaning as in (IX.6). Then, using the fact that, in isotropic coordinates and for $r \to \infty$, $\mathfrak{U}_{1\,\nu}^{0i} \sim 0\left(\frac{1}{r^2}\right)$ and $g_\nu^{\hat{\lambda}} = \delta_\nu^{\hat{\lambda}} + 0\left(\frac{1}{r}\right)$, and further that $\int_S \mathfrak{U}_{2\,\nu}^{0i}\, n_i\, dS = 0$, we have

$$\left.\begin{aligned} P_\nu &= \int_S \mathfrak{U}_\nu^{[0i]}\, n_i\, dS = \int_S g\hat{:}\, g_\nu^{\hat{\lambda}}\, U_{\hat{\lambda}}^{[0i]}\, n_i\, dS \\ &= \int_S g\hat{:}\, \delta_\nu^{\hat{\lambda}}\, U_{\hat{\lambda}}^{[0i]}\, n_i\, dS = \delta_\nu^{\hat{\lambda}}\, P_{\hat{\lambda}}\,. \end{aligned}\right\} \tag{IX.20}$$

The superpotential defined by (IX.7) is a true tensor density; hence $\mathfrak{U}_0{}^{[\lambda\mu]}$ is transformed like an antisymmetric tensor under the group of purely spatial transformations

$$\left.\begin{aligned} x'^0 &= x^0 \\ x'^i &= x'^i(x^k). \end{aligned}\right\} \tag{IX.21}$$

Then $\mathfrak{U}_0{}^{[\lambda\mu]}{}_{,\mu}$ will be transformed like a vector density under the same group, and in particular $\mathfrak{U}_0{}^{[0\mu]}{}_{,\mu}$ will be a scalar so that it is possible to give to $\mathsf{T}_0{}^0 = \mathfrak{U}_0{}^{[0\mu]}{}_{,\mu}$ the meaning of an energy density.

In contrast to $\Theta_{\hat{\lambda}}^{\lambda}$, $\mathsf{T}_\nu{}^\lambda$ is not a tensor. On the other hand $\mathsf{T}_\nu{}^\lambda$ is a scalar under the "gauge" group of the constant tetrad rotations, while $\Theta_{\hat{\lambda}}^{\lambda}$ is a vector with respect to that group. The same is true of P_ν and $P_{\hat{\nu}}$. The situation does not lead to difficulties for the total energy and momentum (IX.4), since the tetrad rotations can be interpreted, for $r \to \infty$, as Lorentz transformations. In fact, to write the total energy momentum in the form (IX.6) is a compact way of saying that this quantity is transformed like a four-vector under Lorentz transformations.

When we consider the local properties of the field instead of the global quantity $P_{\hat{\lambda}}$, we are not allowed to use $\Theta_{\hat{\lambda}}^{\lambda}$ and $\mathsf{T}_\nu{}^\lambda$ in the same way. In particular, $\mathsf{T}_0{}^0$ and not $\Theta_{\hat{0}}^{0}$ is the energy density, since it is not possible in general to give to the tetrad rotations the meaning of Lorentz transformations.

The explicit form of $\mathsf{T}_\nu{}^\lambda$ can be evaluated from its definition (IX.8):

$$\left.\begin{aligned} \mathsf{T}_\nu{}^\lambda &= \mathfrak{U}_\nu^{[\lambda\mu]}{}_{,\mu} = \left(g\hat{:}\, g_\nu^{\hat{\lambda}}\, U^{[\lambda\mu]}_{\hat{\lambda}}\right)_{,\mu} \\ &= g_\nu^{\hat{\lambda}}\, g\hat{:}\, U^{[\lambda\mu]}_{\hat{\lambda}\,;\mu} + g\hat{:}\, U^{[\lambda\mu]}_{\hat{\lambda}}\, g^{\hat{\lambda}}_{\nu,\mu} \\ &= g\hat{:}\, \Theta_\nu{}^\lambda + \mathfrak{U}_{\varrho}^{[\lambda\mu]}\, \Delta^{\varrho}_{\nu\mu}. \end{aligned}\right\} \tag{IX.22}$$

Since

$$\Theta_\nu{}^\lambda = g_\nu{}^{\hat{\lambda}} \left\{ k_1\, U_{1\hat{\lambda}}^{\lambda} + k_2\, U_{2\hat{\lambda}}^{\lambda} + T^{(b)}{}_{\hat{\lambda}}^{\lambda} + T^{(f)}{}_{\hat{\lambda}}^{\lambda} \right\}, \tag{IX.23}$$

we have from (A.14), (A.21), (IX.11), (IX.12), (IX.23)

$$\mathsf{T}_\nu{}^\lambda = g\hat{:}\, [t_\nu{}^\lambda + T^{(b)}{}_\nu{}^\lambda + T^{(f)}{}_\nu{}^\lambda] \tag{IX.24}$$

$$\left.\begin{aligned} t_\nu^{\ \lambda} = k_1 \Big[& \gamma^{\lambda\varrho\sigma} \Lambda_{[\varrho\nu]\,\sigma} + \Phi^\sigma \Lambda_{[\nu\sigma]}^{\ \ \lambda} \\ & - \Phi_\nu \Phi^\lambda - \frac{1}{2} g\vdots\ \delta_\nu^{\ \lambda}\, \mathfrak{L}_M + U_{1\,\varrho}^{\ [\lambda\mu]} \Delta^\varrho_{\ \nu\mu} \Big] \\ & + k_2 \left[\check{\Lambda}^\varrho \Lambda_{[\varrho\nu]}^{\ \ \lambda} - \eta^{\alpha\beta\gamma\lambda} \Phi_\gamma \Lambda_{[\alpha\beta]\,\nu} + U_{2\,\varrho}^{\ [\lambda\mu]} \Delta^\varrho_{\ \nu\mu} \right]. \end{aligned}\right\} \qquad \text{(IX.25)}$$

The form (IX.22) of $\mathsf{T}_\nu^{\ \lambda}$, which was already derived by Møller [5] for his complex, allows us to establish the transformation properties of our complex. In fact they are the same as for $\mathsf{T}^M{}_\nu^{\ \lambda}$, namely

$$t'_\alpha{}^\beta = \frac{\partial x'^\beta}{\partial x^\mu} \left\{ \frac{\partial x^\lambda}{\partial x'^\alpha}\, t'^\mu_\lambda + \frac{\partial}{\partial x^\nu} \left(\frac{\partial x^\varrho}{\partial x'^\alpha} \right)_{\rfloor} \mathfrak{U}_\varrho^{[\mu\nu]} \right\}. \qquad \text{(IX.26)}$$

Now we want to examine our energy-momentum complex in the weak-field case, and for simplicity we will assume that the coordinate condition (V.22) holds. Using again the expression (V.1) for $g^\alpha_{\hat\alpha}$, we have

$$\gamma_{\alpha\beta}^{\ \ \gamma} = \frac{1}{2} \left(h_{<\beta\cdot>,\,\alpha} - h_{<\alpha\cdot>,\,\beta} \right)$$

$$\Phi_\alpha = -\frac{1}{4} h_{,\,\alpha}$$

$$h_{[\alpha\beta]} = 0\,,$$

so that

$$\left.\begin{aligned} \mathfrak{U}_\nu^{[\varrho\sigma]} = \frac{1}{2} k_1 \Big\{ & h_{<\nu\cdot>}^{\ \ \sigma\,,\,\varrho} - h_{<\nu\cdot>}^{\ \ \varrho\,,\,\sigma} \\ & + \frac{1}{2} \left(\delta_\nu^\varrho\, h'^{,\,\sigma} - \delta_\nu^\sigma\, h'^{,\,\varrho} \right) \Big\} + \frac{1}{2} k_2\, \varepsilon^{\varrho\sigma\alpha\beta}\, \eta_{\beta\nu}\, h_{,\,\alpha}. \end{aligned}\right\} \qquad \text{(IX.27)}$$

From (IX.8) we find, using the coordinate condition,

$$\mathsf{T}_\nu^{\ \lambda} = -\frac{1}{2} k_1 \Box \varphi_\nu^{\ \lambda} = \mathsf{T}^{(b)}{}_\nu^{\ \lambda}, \qquad \text{(IX.28)}$$

so that $\mathsf{T}_\nu^{\ \lambda}$ is equal to the matter tensor, in agreement with the fact that the gravitational complex is of the second order.

If we perform the evaluation of $t_\alpha^{\ \beta}$ to the second order, using the $h_{<\alpha\beta>}$ as determined from the first-order approximation, the tensor

$$t_\alpha^{\ \beta} = t^M{}_\alpha^{\ \beta} + t'_\alpha{}^\beta \qquad \text{(IX.29)}$$

with

$$t^{M}{}_{\alpha}{}^{\beta} = \frac{1}{4} k_1 \left\{ (h_{<\lambda\cdot>}{}^{\mu}{}_{,\beta} - h_{<\lambda\cdot>}{}^{\beta}{}_{,\mu})\, h^{<\lambda\cdot>}{}_{\mu,\alpha} \right. \\ \left. + \frac{1}{2} (h_{,\lambda}\, h^{<\lambda\beta>}{}_{,\alpha} - h_{,\alpha}\, h^{,\beta}) - \delta_{\alpha}{}^{\beta}\, \mathfrak{L}_{M} \right\} \tag{IX.30}$$

$$\mathfrak{L}_{M} = \frac{1}{4} h_{<\alpha\beta>,\gamma}\, h^{<\alpha\beta>,\gamma} - \frac{1}{8} h_{,\alpha}\, h^{,\alpha} \tag{IX.31}$$

and

$$t'_{\alpha}{}^{\beta} = X_{\alpha}{}^{[\beta\lambda]}{}_{,\lambda} + X^{\beta}{}_{\alpha}{}^{[\cdot\,\lambda]}{}_{,\lambda} \tag{IX.32}$$

$$X_{\alpha}{}^{[\beta\lambda]} = \frac{1}{4} k_2\, \varepsilon^{\beta\mu\lambda\nu}\, h\, h_{<\nu\alpha>,\mu} \tag{IX.33}$$

is obtained.

The tensor $t^{M}{}_{\alpha}{}^{\beta}$ is just the Møller weak-field gravitational complex. It is noteworthy that the symmetric term $t'_{\alpha}{}^{\beta}$ can be written as a divergence.

We want to thank Professor C. Møller for many illuminating discussions. One of us (C. P.) wants to express his gratitude to Professor C. Møller for the generous hospitality accorded to him by NORDITA.

Appendix A

The Einstein Tensor, the Tensor $F^{\alpha\beta}$ and the Evaluation of the Superpotential

We will recall here the connection, first discovered by Møller [4] [5], between the tetrads and the curvature tensor.

Replacing in the basic formula

$$A_{\beta;\gamma;\delta} - A_{\beta;\delta;\gamma} = - A_{\alpha} R^{\alpha}{}_{\beta\gamma\delta}$$

the vector A_{α} by $g^{\hat{\alpha}}_{\alpha}$ and multiplying by $g_{\hat{\alpha}}{}^{\varrho}$, we get

$$R^{\varrho}{}_{\beta\gamma\delta} = - g^{\varrho}_{\hat{\alpha}} \left(g^{\hat{\alpha}}{}_{\beta;\gamma;\delta} - g^{\hat{\alpha}}{}_{\beta;\delta;\gamma} \right). \tag{A.1}$$

By contracting this we obtain

$$R_{\alpha\beta} = R^{\varrho}{}_{\alpha\varrho\beta} = - g^{\varrho}_{\hat{\alpha}} \left(g^{\hat{\alpha}}_{\alpha;\varrho;\beta} - g^{\hat{\alpha}}_{\alpha;\beta;\varrho} \right), \tag{A.2}$$

$$R = R^{\alpha}_{\alpha} = - g^{\alpha\beta}\, g_{\hat{\alpha}}{}^{\varrho} \left(g^{\hat{\alpha}}_{\alpha;\varrho;\beta} - g^{\hat{\alpha}}_{\alpha;\beta;\varrho} \right). \tag{A.3}$$

The last formula can easily be rewritten as

$$\begin{aligned} g^{\hat{}}: R = & \left[g^{\hat{}}: \left(g^{\sigma}_{\hat{\varrho}} g^{\hat{\varrho}\varrho}{}_{;\varrho} - g^{\varrho}_{\hat{\varrho}} g^{\hat{\varrho}\sigma}{}_{;\varrho} \right) \right]_{,\sigma} \\ & + g^{\hat{}}: \left(g^{\varrho}_{\hat{\varrho}}{}_{;\sigma} g^{\hat{\varrho}\sigma}{}_{;\varrho} - g^{\varrho}_{\hat{\varrho}}{}_{;\varrho} g^{\hat{\varrho}\sigma}{}_{;\sigma} \right) \\ & - 2 \left(g^{\hat{}}: \Phi^{\sigma} \right)_{,\sigma} + g^{\hat{}}: \left(\gamma_{\tau\varrho\sigma} \gamma^{\tau\sigma\varrho} - \Phi_{\varrho} \Phi^{\varrho} \right) \\ & = H^{\sigma}{}_{,\sigma} + \mathfrak{L}_{M}. \end{aligned} \tag{A.4}$$

The importance of this decomposition, as compared with the usual one, which can for example be written as[11]

$$\sqrt{-g}\, R = - \left\{ \frac{1}{\sqrt{-g}} \left(- g g^{\varrho\sigma} \right)_{,\sigma} \right\}_{,\varrho} + \sqrt{-g}\, g^{\alpha\beta} \left\{ \Gamma^{\varrho}_{\alpha\sigma} \Gamma^{\sigma}_{\varrho\beta} - \Gamma^{\varrho}_{\alpha\beta} \Gamma^{\sigma}_{\varrho\sigma} \right\},$$

lies in the fact that $\mathfrak{L}_M$ is a scalar with respect to coordinate transformations, so that the action principle is of the type used in other field theories.

By means of (A.2), (A.4) the Ricci tensor can be written as

$$\begin{aligned} G_{\alpha\beta} = & g^{\varrho}_{\hat{\alpha}} \left(g^{\hat{\alpha}}_{\alpha;\beta;\varrho} - g^{\hat{\alpha}}_{\alpha;\varrho;\beta} \right) \\ & - \frac{1}{2} g_{\alpha\beta} g^{\varrho}_{\hat{\alpha}} \left(g^{\hat{\alpha}\sigma}{}_{;\sigma;\varrho} - g^{\hat{\alpha}\sigma}{}_{;\varrho;\sigma} \right), \end{aligned} \tag{A.5}$$

and, multiplying by $g_{\hat{\beta}\alpha}$, we have

$$\begin{aligned} G^{\beta}_{\hat{\beta}} = g_{\hat{\beta}\alpha} G^{\alpha\beta} = & g_{\hat{\beta}\alpha} g^{\varrho}_{\hat{\alpha}} \left(g^{\hat{\alpha}\alpha;\beta}{}_{;\varrho} - g^{\hat{\alpha}\alpha}{}_{;\varrho}{}^{;\beta} \right) \\ & - \frac{1}{2} g^{\beta}_{\hat{\beta}} g^{\varrho}_{\hat{\alpha}} \left(g^{\hat{\alpha}\sigma}{}_{;\sigma;\varrho} - g^{\hat{\alpha}\sigma}{}_{;\varrho;\sigma} \right). \end{aligned} \tag{A.6}$$

The mixed expression $G^{\beta}_{\hat{\beta}}$ can be decomposed in the form

$$G^{\beta}_{\hat{\beta}} = - \mathfrak{U}_1{}^{[\beta\gamma]}_{\hat{\beta}}{}_{;\gamma} + \mathfrak{U}_1{}^{\beta}_{\hat{\beta}}, \tag{A.7}$$

where $\mathfrak{U}_1{}^{\beta}_{\hat{\beta}}$ is bilinear and $\mathfrak{U}_1{}^{[\beta\gamma]}_{\hat{\beta}}$ linear in the first derivatives of $g^{\alpha}_{\hat{\alpha}}$.

To establish the form (A.7) of $G^{\beta}_{\hat{\beta}}$ it is better to start from the alternative expression of $R_{\alpha\beta}$ and R given by Møller[5]:

$$R^{\alpha\beta} = \gamma^{\varrho\alpha\beta}{}_{|\varrho} - \Phi^{\alpha|\beta} - \gamma^{\varrho\alpha\beta} \Phi_{\varrho} + \gamma^{\varrho\alpha}{}_{\sigma} \gamma^{\sigma\beta}{}_{\varrho}, \tag{A.8}$$

$$R = - 2 \Phi^{\varrho}{}_{|\varrho} + \gamma_{\varrho\sigma\tau} \gamma^{\varrho\tau\sigma} - \Phi_{\varrho} \Phi^{\varrho}. \tag{A.9}$$

Using the fact that the absolute derivative $g^{\alpha}_{\hat{\alpha}/\beta} = 0$, we obtain

$$\left.\begin{aligned} G_{\hat{\beta}}^{\ \beta} &= g_{\hat{\beta}\alpha}\, G^{\alpha\beta} = g_{\hat{\beta}\alpha}\, G^{\beta\alpha} \\ &= \left(g_{\hat{\beta}\alpha}\, \gamma^{\varrho\beta\alpha} + g_{\hat{\beta}}^{\ \beta}\, \Phi^{\varrho} - g_{\hat{\beta}}^{\ \varrho}\, \Phi^{\beta}\right)_{/\varrho} + g_{\hat{\beta}\alpha}\left(\gamma^{\varrho\beta}{}_{\sigma}\, \gamma^{\sigma\alpha}{}_{\varrho}\right. \\ &\quad \left. - \Phi_{\varrho}\, \gamma^{\varrho\beta\alpha}\right) - \frac{1}{2}\, g_{\hat{\beta}}^{\ \beta}\left(\gamma_{\varrho\sigma\tau}\, \gamma^{\varrho\tau\sigma} + \Phi_{\varrho}\, \Phi^{\varrho}\right). \end{aligned}\right\} \tag{A.10}$$

Defining

$$U_{1\,\hat{\beta}}^{[\beta\varrho]} = g_{\hat{\beta}\alpha}\, \gamma^{\beta\varrho\alpha} + g_{\hat{\beta}}^{\ \varrho}\, \Phi^{\beta} - g_{\hat{\beta}}^{\ \beta}\, \Phi^{\varrho} \tag{A.11}$$

and using the connection between the absolute and the covariant derivative[5]

$$U_{1\,\hat{\beta}/\varrho}^{[\beta\varrho]} = U_{1\,\hat{\beta};\,\varrho}^{[\beta\varrho]} + U_{1\,\hat{\beta}}^{[\sigma\beta]}\, \gamma^{\beta}_{\sigma\varrho} + U_{1\,\hat{\beta}}^{[\beta\sigma]}\, \gamma^{\varrho}_{\sigma\varrho}, \tag{A.12}$$

we easily find from (A.10), (A.11), (A.12)

$$\left.\begin{aligned} G_{\hat{\beta}}^{\ \beta} &= -\,U_{1\,\hat{\beta};\,\varrho}^{[\beta\varrho]} - U_{1\,\hat{\beta}}^{[\sigma\varrho]}\, \gamma^{\beta}_{\sigma\varrho} + g_{\hat{\beta}}^{\ \sigma}\, \Phi^{\beta}\, \Phi_{\sigma} \\ &\quad + g_{\hat{\beta}\alpha}\, \gamma^{\varrho\beta}{}_{\sigma}\, \gamma^{\sigma\alpha}{}_{\varrho} - \frac{1}{2}\, g_{\hat{\beta}}^{\ \beta}\, g\hat{:}\, \mathfrak{L}_M \end{aligned}\right\} \tag{A.13}$$

and

$$U_{1\,\hat{\beta}}^{\beta} = -\,U_{1\,\hat{\beta}}^{[\sigma\varrho]}\, \gamma^{\beta}_{\sigma\varrho} - g_{\hat{\beta}}^{\ \sigma}\, \Phi_{\sigma}\, \Phi^{\beta} + g_{\hat{\beta}\alpha}\, \gamma^{\varrho\beta}{}_{\sigma}\, \gamma^{\sigma\alpha}{}_{\varrho} - \frac{1}{2}\, g_{\hat{\beta}}^{\ \beta}\, g\hat{:}\, \mathfrak{L}_M. \tag{A.14}$$

A decomposition similar to (A.7) can be found for

$$g\hat{:}\, F_{\hat{\varrho}}^{\ \varrho} = \frac{\delta \check{I}_3}{\delta g_{\hat{\varrho}}^{\ \varrho}}. \tag{A.15}$$

The term $\check{I}_3$ of our Lagrangian can be written as

$$\left.\begin{aligned} \check{I}_3 &= -\frac{1}{2}\, g\hat{:}\left\{\eta^{\alpha\lambda\nu\mu}\, g_{\hat{\gamma}}^{\ \beta} - \eta^{\beta\lambda\nu\mu}\, g_{\hat{\gamma}}^{\ \alpha}\right\} g_{\hat{\mu}\mu} \\ &\quad \cdot \left(g_{\alpha,\,\beta}^{\hat{\gamma}} - g_{\beta,\,\alpha}^{\hat{\gamma}}\right)\left(g_{\lambda,\,\nu}^{\hat{\mu}} - g_{\nu,\,\lambda}^{\hat{\mu}}\right). \end{aligned}\right\} \tag{A.16}$$

Performing the variation of $\check{I}_3$, we have

$$g\hat{:}\, F_{\hat{\varrho}}^{\ \varrho} = \frac{\delta \check{I}_3}{\delta g_{\hat{\varrho}}^{\ \varrho}} = -\,g\hat{:}\, U_{2\,\hat{\varrho};\,\sigma}^{[\varrho\sigma]} + g\hat{:}\, U_{2\,\hat{\varrho}}^{\ \varrho}, \tag{A.17}$$

$$\left.\begin{aligned} -\,g\hat{:}\, U_{2\,\hat{\varrho};\,\sigma}^{[\varrho\sigma]} &= \frac{1}{2}\left\{g\hat{:}\left(\eta^{\alpha\lambda\nu\mu}\, g_{\hat{\gamma}}^{\ \beta} - \eta^{\beta\lambda\nu\mu}\, g_{\hat{\gamma}}^{\ \alpha}\right) g_{\hat{\mu}\mu}\right. \\ &\quad \left. \cdot \frac{\partial}{\partial\, g_{\varrho,\,\sigma}^{\hat{\varrho}}}\left[\left(g_{\alpha,\,\beta}^{\hat{\gamma}} - g_{\beta,\,\alpha}^{\hat{\gamma}}\right)\left(g_{\lambda,\,\nu}^{\hat{\mu}} - g_{\nu,\,\lambda}^{\hat{\mu}}\right)\right]\right\}_{,\,\sigma}, \end{aligned}\right\} \tag{A.18}$$

$$
\left.\begin{aligned}
g\hat{:}\, U_{2\,\hat{\varrho}}^{\ \ \varrho} = -\frac{1}{2}\frac{\partial}{\partial g_{\varrho}^{\hat{\varrho}}}\Big\{ & g\hat{:}\left(\eta^{\alpha\lambda\nu\mu}\, g_{\hat{\gamma}}^{\beta} - \eta^{\beta\lambda\nu\mu}\, g_{\hat{\gamma}}^{\alpha}\right) g_{\hat{\mu}\mu}\Big\} \\
& \cdot \left(g_{\alpha,\,\beta}^{\hat{\gamma}} - g_{\beta,\,\alpha}^{\hat{\gamma}}\right)\left(g_{\lambda,\,\nu}^{\hat{\mu}} - g_{\nu,\,\lambda}^{\hat{\mu}}\right).
\end{aligned}\right\} \tag{A.19}
$$

Evaluating (A.17), (A.18), we obtain

$$
-\, U_{2\,\hat{\varrho}}^{[\varrho\sigma]} = \check{\Lambda}^{\varrho}\, g_{\hat{\varrho}}^{\sigma} - \check{\Lambda}^{\sigma}\, g_{\hat{\varrho}}^{\varrho} + 2\,\eta^{\varrho\sigma\alpha\beta}\,\Phi_{\alpha}\, g_{\hat{\varrho}\beta}, \tag{A.20}
$$

$$
U_{2\,\hat{\varrho}}^{\ \ \varrho} = \check{\Lambda}^{\alpha}\, \Lambda_{[\alpha\beta]}^{\ \ \ \ \varrho}\, g_{\hat{\varrho}}^{\beta} - \eta^{\alpha\lambda\nu\varrho}\,\Phi_{\alpha}\left(g_{\hat{\varrho}\lambda,\,\nu} - g_{\hat{\varrho}\nu,\,\lambda}\right). \tag{A.21}
$$

From (A.17), (A.20), (A.21) it follows that

$$
\left.\begin{aligned}
F_{\hat{\varrho}}^{\ \ \varrho} = & \left[\check{\Lambda}^{\varrho}\, g_{\hat{\varrho}}^{\sigma} - \check{\Lambda}^{\sigma}\, g_{\hat{\varrho}}^{\varrho} + 2\,\eta^{\varrho\sigma\alpha\beta}\,\Phi_{\alpha}\, g_{\hat{\varrho}\beta}\right]_{;\,\sigma} \\
& + \check{\Lambda}^{\alpha}\, \Lambda_{[\alpha\beta]}^{\ \ \ \ \varrho}\, g_{\hat{\varrho}}^{\beta} - \eta^{\alpha\lambda\nu\varrho}\,\Phi_{\alpha}\left(g_{\hat{\varrho}\lambda,\,\nu} - g_{\hat{\varrho}\nu,\,\lambda}\right).
\end{aligned}\right\} \tag{A.22}
$$

We can now define the tensor

$$
F^{\sigma\varrho} = g^{\hat{\varrho}\sigma}\, F_{\hat{\varrho}}^{\ \ \varrho}. \tag{A.23}
$$

By means of (A.22) this is easily seen to be

$$
\left.\begin{aligned}
F^{\sigma\varrho} = & \left\{\check{\Lambda}^{\varrho}\, g^{\tau\sigma} - \check{\Lambda}^{\tau}\, g^{\sigma\varrho} + 2\,\eta^{\tau\alpha\varrho\sigma}\,\Phi_{\alpha}\right\}_{;\,\tau} \\
& - \left\{\check{\Lambda}^{\varrho}\,\gamma^{\tau\sigma}{}_{\tau} - \check{\Lambda}^{\tau}\,\gamma^{\varrho\sigma}{}_{\tau} + 2\,\eta^{\varrho\tau\alpha\beta}\,\Phi_{\alpha}\,\gamma_{\beta}{}^{\sigma}{}_{\tau}\right\} \\
& + \check{\Lambda}^{\alpha}\, \Lambda_{[\alpha\,\cdot]}^{\ \ \sigma\ \ \varrho} - \eta^{\alpha\lambda\nu\varrho}\,\Phi_{\alpha}\,\Lambda_{[\lambda\nu]}{}^{\sigma} \\
= & \ \check{\Lambda}^{\varrho;\,\sigma} - g^{\varrho\sigma}\,\check{\Lambda}^{\tau}{}_{;\,\tau} + 2\,\eta^{\varrho\sigma\alpha\beta}\,\Phi_{\alpha;\,\beta} \\
& - \Phi^{\sigma}\,\check{\Lambda}^{\varrho} + \gamma^{\varrho\sigma}{}_{\tau}\,\check{\Lambda}^{\tau} + \eta^{\varrho\alpha\beta\gamma}\,\Phi_{\alpha}\,\Lambda_{[\beta\gamma]}{}^{\sigma} \\
& + \check{\Lambda}^{\alpha}\,\Lambda_{[\alpha\,\cdot]}^{\ \ \sigma\ \ \varrho} - \eta^{\lambda\nu\mu\varrho}\,\Phi_{\mu}\,\Lambda_{[\lambda\nu]}{}^{\sigma}.
\end{aligned}\right\} \tag{A.24}
$$

The term $\check{\Lambda}^{\tau}{}_{;\,\tau}$ can be written in a form showing explicitly that it depends only on the first derivatives of the tetrad field. In fact

$$
\left.\begin{aligned}
g\hat{:}\,\check{\Lambda}^{\tau}{}_{;\,\tau} &= g\hat{:}\,\eta^{\tau\alpha\beta\gamma}\,\Lambda_{[\alpha\beta]\gamma;\,\tau} \\
&= 2\left[g\hat{:}\,\eta^{\tau\alpha\beta\gamma}\, g_{\gamma}^{\hat{\alpha}}\, g_{\hat{\alpha}\alpha,\,\beta}\right]_{,\,\tau} \\
&= -\,2\,\varepsilon^{\tau\alpha\beta\gamma}\, g_{\gamma,\,\tau}^{\hat{\alpha}}\, g_{\hat{\alpha}\alpha,\,\beta} \\
&= \frac{1}{2}\, g\hat{:}\,\eta^{\tau\alpha\beta\gamma}\,\Lambda_{[\gamma\tau]\,\delta}\,\Lambda_{[\alpha\beta]}{}^{\delta} \\
&= -\frac{1}{2}\,\check{I}_{4}.
\end{aligned}\right\} \tag{A.25}
$$

Appendix B

Tensors and Spinors

Here we want to discuss how the concepts of tensor and spinor can be introduced in our theory.

It is well known that in the special theory of relativity the definition of tensors can be given from two different points of view. One can define a vector as an object that is transformed like the coordinates under a Lorentz transformation, and a tensor as an object that is transformed like a product of vectors; or one can consider the representations of the Lorentz group and introduce in this way both tensors and spinors as quantities that are transformed in a well-defined way under a Lorentz transformation.

Clearly the second approach is more fundamental, since it allows us to introduce both spinors and tensors in a very natural way.

When we go from the special to the general theory of relativity, we can use only the first point of view. In consequence, the spinor fields are not, in the general case, on the same basis as tensor fields, which is quite unsatisfactory[6].

In the framework of our theory it seems possible instead to re-establish the connection between tensors and spinors, as representations of the Lorentz group, and the usual non-group-theoretical definition.

Let us consider a Riemannian four-space V_4 in which a coordinate system $x^0, \cdots, x^3$ has been introduced. In each point of this space we have a tetrad whose components are $g_{\hat{\alpha}}^{\alpha}(x)$. The representation of the group L of the proper tetrad rotations gives us quantities

$$T_{\hat{\beta}\cdots}^{\hat{\alpha}\cdots}$$

and

$$\psi_{B\cdots}^{A\cdots} \qquad (A, B = 1, 2)$$

which are tensors or spinors with respect to L. The connection between the "local" tensor $T_{\hat{\beta}\cdots}^{\hat{\alpha}\cdots}$ and a "world" tensor $T_{\beta\cdots}^{\alpha\cdots}$ (as defined from the first point of view) is easily established with the help of the $g_{\alpha}^{\hat{\alpha}}$:

$$T_{\beta\cdots}^{\alpha\cdots} = g_{\hat{\alpha}}^{\alpha} g_{\beta}^{\hat{\beta}} \cdots T_{\hat{\beta}\cdots}^{\hat{\alpha}\cdots}.$$

The spinors, which have no "roofed" index, are simply equivalent to "world" scalars, while the connection between the "local" Dirac matrices $\gamma^{\hat{\alpha}}$ and the "world" matrices is again given by $g_{\hat{\alpha}}^{\alpha}$:

$$\gamma^{\alpha} = g_{\hat{\alpha}}^{\alpha} \gamma^{\hat{\alpha}}.$$

From this point of view the constant tetrad rotations, which leave our theory invariant, play a part analogous to that of the Lorentz transformation of special relativity. In general there exists no relation between tetrad rotations and coordinate transformations, as there does between "local" tensors and spinors and "world" tensors. Only in the limit of flat space-time and when we use cartesian coordinates are tetrad rotations equivalent to Lorentz transformations so that we obtain the formalism of special relativity as a limiting case.

Since we need it in section VI, we will now review the essential steps of the introduction of spinors, at the same time establishing our notations.

In this paper we consider three types of transformation:

(a) coordinate transformations $x'^{\alpha} = x'^{\alpha}(x^{\beta})$ (group C);

(b) tetrad rotations $A'^{\hat{\alpha}} = L^{\hat{\alpha}}{}_{\hat{\beta}} A^{\hat{\beta}}$ (group L);

(c) linear or antilinear unimodular transformations in the two-dimensional complex spin space, induced by proper or improper tetrad rotations (group T).

Objects that are transformed appropriately with respect to all groups will be called tensors and spinors.

We remember that to the group L belong, in our theory, only the constant tetrad rotations.

A general tensor density $\mathfrak{T}^{\alpha\cdots\hat{\alpha}\cdots}_{\beta\cdots\hat{\beta}\cdots}$ is transformed like

$$\left.\begin{aligned} \mathfrak{T}'^{\alpha\cdots\hat{\alpha}\cdots}_{\beta\cdots\hat{\beta}\cdots} = {} & \left\{ \det \left| \frac{\partial x'^{\varrho}}{\partial x^{\sigma}} \right| \right\}^{w} \left\{ \det \left| L^{\hat{\varrho}}{}_{\hat{\sigma}} \right| \right\}^{\hat{w}} \\ & \frac{\partial x'^{\alpha}}{\partial x^{\lambda}} \cdots \frac{\partial x^{\mu}}{\partial x'^{\beta}} \cdots L^{\hat{\alpha}}{}_{\hat{\lambda}} \cdots L^{-1\,\hat{\mu}}{}_{\hat{\beta}} \cdots T^{\lambda\cdots\hat{\lambda}\cdots}_{\mu\cdots\hat{\lambda}\cdots}, \end{aligned} \right\} \tag{B.1}$$

where w, $\hat{w}$ are the weights of the (a) and (b) transformations, $L^{\hat{\alpha}}{}_{\hat{\lambda}}$ is submitted to the condition (II.7) and $L^{-1\,\hat{\mu}}{}_{\hat{\beta}}$ is defined by $L^{\hat{\alpha}}{}_{\hat{\varrho}} L^{-1\,\hat{\varrho}}{}_{\hat{\beta}} = \delta^{\hat{\alpha}}_{\hat{\beta}}$.* Note that $\det \left| L^{\hat{\alpha}}{}_{\hat{\beta}} \right|$ is equal to one in the case of proper tetrad rotations and to minus one in the case of improper rotations.

We give the name contravariant spinor to the quantity ψ^{A} $(A = 1, 2)$, which under linear, unimodular transformations $l^{A}{}_{B}$, $\det | l^{A}{}_{B} | = 1$, is transformed like**

$$\psi'^{A} = l^{A}{}_{B} \psi^{B}. \tag{B.2}$$

* From this definition and (II. 7) it follows that

$$L^{-1\,\hat{\alpha}}{}_{\hat{\varrho}} = g^{\hat{\alpha}\hat{\delta}} g_{\hat{\beta}\hat{\gamma}} L^{\hat{\gamma}}{}_{\hat{\delta}}.$$

** In order to simplify the notations we shall not here discuss spinor density. For a more general formulation see for instance the book by Corson (reference 9).

Spin indices may be raised or lowered with the help of the metrical spinors

$$g_{AB} = g^{AB} = \begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix} \tag{B.3}$$

so that

$$\left.\begin{aligned} \psi^A &= \psi_B\, g^{BA} = -\, g^{AB}\, \psi_B \\ \psi_A &= g_{AB}\, \psi^B. \end{aligned}\right\} \tag{B.4}$$

The isomorphism between the groups L and T may be established with the help of the numerical spin matrices

$$g_{\hat{\alpha}\dot{A}B} = \left(\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}, \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \begin{vmatrix} 0 & i \\ -i & 0 \end{vmatrix}, \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \right). \tag{B.5}$$

We have, in the case of proper tetrad rotations,

$$L^{\hat{\alpha}}{}_{\hat{\beta}} = \frac{1}{2}\, g^{\hat{\alpha}\dot{A}B}\, g_{\hat{\beta}\dot{C}D}\, t^{\dot{C}}{}_{\dot{A}}\, t^{D}{}_{B}, \tag{B.6}$$

where

$$t^{\dot{A}}{}_{\dot{B}} = \left(t^{A}{}_{B}\right)^{*}$$

(the asterisk means complex conjugation).
The space of the spinors ψ_A is the space of the representation $D(1/2, 0)$ of the proper rotation group. The conjugate representation

$$\psi^{\dot{A}} = t^{\dot{A}}{}_{\dot{B}}\, \psi^{\dot{B}}, \quad \psi^{\dot{A}} = \left(\psi^{A}\right)^{*} \tag{B.7}$$

is transformed like the representation $D(0, 1/2)$.

Under improper Lorentz rotations the spinors are transformed by means of the antilinear operators $t^{A}{}_{\dot{B}}$, $\det |t^{A}{}_{\dot{B}}| = 1$,

$$\psi^{A} = t^{A}{}_{\dot{B}}\, \psi^{\dot{B}}, \tag{B.8}$$

which mix the representations $D\left(\frac{1}{2}, 0\right)$ and $D\left(0, \frac{1}{2}\right)$. The isomorphism between the improper rotations and the antilinear operators $t^{A}{}_{\dot{B}}$ is given by

$$L^{\hat{\alpha}}{}_{\hat{\beta}} = \frac{1}{2}\, g^{\hat{\alpha}\dot{A}B}\, g_{\hat{\beta}\dot{C}D}\, t^{\dot{C}}{}_{B}\, t^{D}{}_{\dot{A}}. \tag{B.9}$$

The spin matrices $g_{\hat{\alpha}\dot{A}B}$ can be defined in a general way by the relations

$$\left(g^{\hat{\alpha}}{}_{\dot{A}B}\right)^{*} = g^{\hat{\alpha}}{}_{\dot{B}A}, \tag{B.10}$$

$$g_{\hat{\alpha}}^{\dot{B}A}\, g_{\hat{\beta}\dot{B}C} = g_{\hat{\alpha}\hat{\beta}}\, \delta^{A}{}_{C} + \frac{1}{2}\, \varepsilon_{\hat{\alpha}\hat{\beta}\hat{\gamma}\hat{\delta}}\, g^{\hat{\gamma}\dot{B}A}\, g^{\hat{\delta}}{}_{\dot{B}C}. \tag{B.11}$$

The four spinors ψ can be introduced as the direct sum of the two representations $D\left(\frac{1}{2}, 0\right)$, $D\left(0, \frac{1}{2}\right)$,

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \Phi^{\dot{1}} \\ \Phi^{\dot{2}} \end{pmatrix}.$$

The γ matrices can be given by the definition

$$\gamma^{\hat{\mu}\alpha}{}_{\beta} = \begin{vmatrix} 0 & -i\left| g^{\hat{\mu}}{}_{\dot{B}A} \right| \\ i\left| g^{\hat{\mu}\,\dot{A}B} \right| & 0 \end{vmatrix}$$

and satisfy the relation

$$\gamma^{\hat{\mu}}\,\gamma^{\hat{\nu}} + \gamma^{\hat{\nu}}\,\gamma^{\hat{\mu}} = 2\,g^{\hat{\mu}\hat{\nu}}.$$

Instead of the $\gamma^{\hat{\mu}}$ we will use the matrices $\alpha^{\hat{\mu}}$, β, which are all Hermitian, while $\gamma^{\hat{0}}$ is Hermitian and $\gamma^{\hat{1}}$, $\gamma^{\hat{2}}$, $\gamma^{\hat{3}}$ are anti-Hermitian[12]. The relation between the γ and the α is

$$\begin{aligned} \gamma^{\hat{0}} &= \beta \\ \beta\gamma^{\hat{i}} &= \alpha^{\hat{i}} \qquad (i = 1, 2, 3) \\ \alpha^{\hat{0}} &= 1\,. \end{aligned}$$

Together with spinors we must define their derivatives. In contrast to what is the case in the usual theory, this can be done quite simply. In fact, since ψ_A is a scalar with respect to the group C, $\psi_{A,\mu}$ is transformed like a vector. Further, with respect to the group L $\psi_{A,\mu}$ is transformed like a spinor, as follows from the fact that only constant tetrad rotations belong to L. So we can simply define the derivative of a two- or four-spinor as $\psi_{A,\mu}$ or $\Psi_{,\mu}$, and there is no need to introduce additive terms, as we must do in the Einstein theory.

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BY

N. E. NÖRLUND

København 1963
i kommission hos Ejnar Munksgaard

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Synopsis

Logarithmic solutions of the hypergeometric differential equation of the second order are considered at length. In the two first chapters linear and quadratic transformations of these solutions are given. Chapter III deals with RIEMANN's P-function in the cases in which one or more of the exponent differences are integers, and the last chapter is devoted to the confluent hypergeometric differential equation.

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Introduction

§ 1. The Differential Equation

$$z(1-z)\frac{d^2y}{dz^2}+[\gamma-(\alpha+\beta+1)z]\frac{dy}{dz}-\alpha\beta y=0 \tag{1}$$

has been discussed in detail since the memorable papers of GAUSS, RIEMANN and KUMMER on the subject. KUMMER obtained twenty-four solutions represented by hypergeometric series if $\gamma-1$, $\alpha-\beta$ and $\gamma-\alpha-\beta$ are not integers. It seems worth while to consider more closely than has hitherto been done, the cases in which one or more of these numbers are integers. Logarithmic solutions of the equation (1) have been considered already by GAUSS, GOURSAT, LINDELÖF and BARNES. From more recent time may be mentioned Vol. I of *Higher Transcendental Functions* compiled by the staff of the Bateman Manuscript Project under the direction of ARTHUR ERDÉLYI. The logarithmic solutions will be investigated at length on the following pages.

In Chapter I we shall consider linear transformations of the logarithmic and other exceptional solutions of Euler's hypergeometric differential equation (1). In Chapter II some examples of quadratic transformations are given. Chapter III deals with Riemann's P-function and the last chapter is devoted to the confluent hypergeometric differential equation.

If γ is neither zero nor a negative integer and if $|z|<1$ the hypergeometric function is defined by the series

$$F(\alpha,\beta,\gamma;z)=\sum_{\nu=0}^{\infty}\frac{(\alpha)_\nu(\beta)_\nu}{\nu!\,(\gamma)_\nu}z^\nu,$$

where

$$(\alpha)_\nu=\frac{\Gamma(\alpha+\nu)}{\Gamma(\alpha)}.$$

Thus

$$(\alpha)_\nu=\alpha(\alpha+1)(\alpha+2)\ldots(\alpha+\nu-1),$$

$$(\alpha)_{-\nu}=\frac{1}{(\alpha-1)(\alpha-2)(\alpha-3)\ldots(\alpha-\nu)},$$

when ν is a positive integer.

Chapter I

Euler's hypergeometric differential equation

§ 2. Using Frobenius' method we put

$$y = \sum_{\nu=0}^{\infty} c_\nu(\varrho)\, z^{\varrho+\nu}. \tag{2}$$

Substitution into the differential equation (1) yields the identity

$$\varrho(\varrho+\gamma-1)\, c_0\, z^{\varrho-1} + \sum_{\nu=0}^{\infty} [(\varrho+1+\nu)(\varrho+\gamma+\nu)\, c_{\nu+1}(\varrho) - (\varrho+\alpha+\nu)(\varrho+\beta+\nu)\, c_\nu(\varrho)]\, z^{\varrho+\nu} = 0.$$

If we determine the $c_\nu(\varrho)$'s such that

$$(\varrho+1+\nu)(\varrho+\gamma+\nu)\, c_{\nu+1}(\varrho) = (\varrho+\alpha+\nu)(\varrho+\beta+\nu)\, c_\nu(\varrho), \quad \nu = 0, 1, 2, \ldots \tag{3}$$

the series (2) will be a solution of the non-homogeneous equation

$$z(1-z)\frac{d^2y}{dz^2} + [\gamma - (\alpha+\beta+1)z]\frac{dy}{dz} - \alpha\beta y = \varrho(\varrho+\gamma-1)\, c_0(\varrho)\, z^{\varrho-1}. \tag{4}$$

From (3) we get

$$c_\nu(\varrho) = \frac{(\varrho+\alpha)_\nu\,(\varrho+\beta)_\nu}{(\varrho+1)_\nu\,(\varrho+\gamma)_\nu}\, c_0(\varrho), \quad \nu = 1, 2, 3, \ldots \tag{5}$$

By setting $\varrho = 0$ or $\varrho = 1-\gamma$ and taking $c_0 = 1$ we see that (1) has the solutions

$$F(\alpha, \beta, \gamma; z), \tag{6}$$

$$z^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z). \tag{7}$$

If γ is nonintegral, both of these solutions are applicable and they are linearly independent. If $\gamma = 1$ the two solutions become identical and if γ tends to an integer different from 1, one of them becomes meaningless.

1°. We suppose, first, that γ is an integer < 1 and that one at least of the parameters α and β is equal to one of the numbers $0, -1, -2, \ldots \gamma$. Setting $\varrho = 0$ the equations (3) leave c_0 and $c_{1-\gamma}$ indeterminate and (1) has the solution

$$c_0 \sum_{\nu=0}^{-\gamma} \frac{(\alpha)_\nu\,(\beta)_\nu}{\nu!\,(\gamma)_\nu}\, z^\nu + c_{1-\gamma}\, z^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z)$$

containing the two arbitrary constants c_0 and $c_{1-\gamma}$. For brevity we put

$$f(\alpha, \beta, \gamma; z) = \sum_{\nu=0}^{-\gamma} \frac{(\alpha)_\nu\,(\beta)_\nu}{\nu!\,(\gamma)_\nu}\, z^\nu. \tag{8}$$

Besides (7) we have then the rational solution $f(\alpha, \beta, \gamma; z)$.

2°. Next, we suppose that γ is an integer >1 and that one at least of the parameters α and β is a positive integer $<\gamma$. Taking $\varrho = 1-\gamma$, the equations (3) leave c_0 and $c_{\gamma-1}$ indeterminate. It follows that (1) has the solution

$$c_0 z^{1-\gamma} \sum_{\nu=0}^{\gamma-2} \frac{(\alpha-\gamma+1)_\nu (\beta-\gamma+1)_\nu}{\nu!\,(2-\gamma)_\nu} z^\nu + c_{\gamma-1} F(\alpha, \beta, \gamma; z),$$

where c_0 and $c_{\gamma-1}$ are arbitrary constants. Besides (6) we then have the rational solution $z^{1-\gamma} f(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z)$.

3°. Now it is assumed that γ is a positive integer and neither α nor β is one of the numbers $1, 2, \ldots \gamma-1$. Putting $\varrho = 1-\gamma$ we can give $c_{\gamma-1}$ any value, and we get again the solution (6). The two roots of the indical equation then give the same solution. To obtain a second solution we observe that if we take $c_{\gamma-1} = 1$, the right-hand side of (4) has a zero of second order at $\varrho = 1-\gamma$. The function

$$\frac{\partial}{\partial \varrho} \sum_{\nu=0}^{\infty} c_\nu(\varrho)\, z^{\varrho+\nu}$$

therefore will satisfy the equation (1) when $\varrho = 1-\gamma$.

It has been shown by FROBENIUS that if $|z|<1$, the series (2) converges uniformly with respect to ϱ in any finite domain. The second solution can therefore be represented by the series

$$\sum_{\nu=0}^{\infty} (c_\nu'(\varrho) + c_\nu(\varrho) \log z)\, z^{\varrho+\nu}. \tag{9}$$

We denote it by $G(\alpha, \beta, \gamma; z)$. Hence for $|z|<1$

$$\left.\begin{aligned} G(\alpha, \beta, \gamma; z) &= \sum_{\nu=1}^{\gamma-1} (-1)^{\nu-1} (\nu-1)!\, \frac{(\alpha)_{-\nu}(\beta)_{-\nu}}{(\gamma)_{-\nu}} z^{-\nu} \\ &+ \sum_{\nu=0}^{\infty} \frac{(\alpha)_\nu (\beta)_\nu}{\nu!\,(\gamma)_\nu} ([\alpha, \beta, \gamma; \nu] + \log z)\, z^\nu, \end{aligned}\right\} \tag{10}$$

where for $\nu = 1, 2, 3, \ldots$

$$[\alpha, \beta, \gamma; \nu] = \sum_{r=0}^{\nu-1} \left(\frac{1}{\alpha+r} + \frac{1}{\beta+r} - \frac{1}{\gamma+r} - \frac{1}{1+r}\right) =$$

$$\Psi(\alpha+r) - \Psi(\alpha) + \Psi(\beta+r) - \Psi(\beta) - \Psi(\gamma+r) + \Psi(\gamma) - \Psi(1+r) + \Psi(1)$$

and

$$[\alpha, \beta, \gamma; 0] = 0.$$

Here $\sum_{\nu=1}^{\gamma-1}$ denotes zero if $\gamma = 1$.

The first term on the right-hand side of (10) may be written

$$(-1)^\gamma \frac{\Gamma(\gamma)\,\Gamma(\gamma-1)\,\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(\alpha)\,\Gamma(\beta)} z^{1-\gamma} \sum_{\nu=0}^{\gamma-2} \frac{(\alpha-\gamma+1)_\nu (\beta-\gamma+1)_\nu}{\nu!\,(2-\gamma)_\nu} z^\nu.$$

If α tends to zero (10) reduces to

$$G(0, \beta, \gamma; z) = -\sum_{\nu=1}^{\gamma-1} \frac{(\beta)_{-\nu} z^{-\nu}}{\nu (\gamma)_{-\nu}} + \sum_{\nu=1}^{\infty} \frac{(\beta)_\nu z^\nu}{\nu (\gamma)_\nu} + \log z,$$

and if α tends to a negative integer, say $-p$, we get

$$\left.\begin{aligned} G(-p, \beta, \gamma; z) = -\sum_{\nu=1}^{\gamma-1} \frac{p!\,(\beta)_{-\nu}}{(\nu)_{p+1} (\gamma)_{-\nu}} z^{-\nu} + \sum_{\nu=1}^{p} \frac{(-p)_\nu (\beta)_\nu}{\nu!\,(\gamma)_\nu} [-p, \beta, \gamma; \nu] z^\nu \\ + (-1)^p p! \sum_{\nu=p+1}^{\infty} \frac{(\beta)_\nu z^\nu}{\nu(\nu-1)\dots(\nu-p)(\gamma)_\nu} + F(-p, \beta, \gamma; z) \log z. \end{aligned}\right\} \quad (11)$$

Another solution is obtained if c_0 is chosen in the following manner

$$c_0(\varrho) = \frac{\Gamma(\varrho+\alpha)\,\Gamma(\varrho+\beta)}{\Gamma(\varrho+1)\,\Gamma(\varrho+\gamma)}. \quad (12)$$

From (5) it now follows that

$$c_\nu(\varrho) = \frac{\Gamma(\varrho+\alpha+\nu)\,\Gamma(\varrho+\beta+\nu)}{\Gamma(\varrho+1+\nu)\,\Gamma(\varrho+\gamma+\nu)}.$$

If neither α nor β is an integer $<\gamma$, the right hand side of (4) has again a zero of the second order at $\varrho = 1-\gamma$ and (9) is a solution of (1). We denote this solution by $c_0(0)\, g(\alpha, \beta, \gamma; z)$, where

$$\left.\begin{aligned} g(\alpha, \beta, \gamma; z) = \sum_{\nu=1}^{\gamma-1} (-1)^{\nu-1} (\nu-1)! \frac{(\alpha)_{-\nu} (\beta)_{-\nu}}{(\gamma)_{-\nu}} z^{-\nu} + \\ \sum_{\nu=0}^{\infty} \frac{(\alpha)_\nu (\beta)_\nu}{\nu!\,(\gamma)_\nu} [\Psi(\alpha+\nu) + \Psi(\beta+\nu) - \Psi(\gamma+\nu) - \Psi(1+\nu) + \log z] z^\nu. \end{aligned}\right\} \quad (13)$$

If α or β is a non-positive integer, (13) becomes meaningless as $\Psi(\alpha)$ has poles at $\alpha = 0, -1, -2, \dots$ To be able to give α and β all possible values it is convenient to consider two other solutions of (1). These are obtained in the same manner if for $c_0(\varrho)$ instead of (12) we take one of the following fractions

$$\frac{1}{\Gamma(1-\varrho-\alpha)\,\Gamma(1-\varrho-\beta)\,\Gamma(\varrho+1)\,\Gamma(\varrho+\gamma)} \quad \text{or} \quad \frac{\Gamma(\varrho+\beta)}{\Gamma(1-\varrho-\alpha)\,\Gamma(\varrho+1)\,\Gamma(\varrho+\gamma)}.$$

We thus get two solutions denoted g_0 and g_1 respectively and defined by

$$\left.\begin{aligned} g_0(\alpha, \beta, \gamma; z) = \sum_{\nu=1}^{\gamma-1} (-1)^{\nu-1} (\nu-1)! \frac{(\alpha)_{-\nu} (\beta)_{-\nu}}{(\gamma)_{-\nu}} z^{-\nu} + \\ \sum_{\nu=0}^{\infty} \frac{(\alpha)_\nu (\beta)_\nu}{\nu!\,(\gamma)_\nu} [\Psi(1-\alpha-\nu) + \Psi(1-\beta-\nu) - \Psi(\gamma+\nu) - \Psi(1+\nu) + \log z] z^\nu, \end{aligned}\right\} \quad (14)$$

$$\left.\begin{aligned} g_1(\alpha, \beta, \gamma; z) = \sum_{\nu=1}^{\gamma-1} (-1)^{\nu-1} (\nu-1)! \frac{(\alpha)_{-\nu} (\beta)_{-\nu}}{(\gamma)_{-\nu}} z^{-\nu} + \\ \sum_{\nu=0}^{\infty} \frac{(\alpha)_\nu (\beta)_\nu}{\nu! (\gamma)_\nu} [\Psi(1-\alpha-\nu) + \Psi(\beta+\nu) - \Psi(\gamma+\nu) - \Psi(1+\nu) + \log(-z)] z^\nu, \end{aligned}\right\} \quad (15)$$

where in (13) and (14) $\log z$ is negative for $0 < z < 1$, whereas in (15) $\log(-z)$ is negative for $-1 < z < 0$. The series on the right of (13), (14) and (15) converges for $0 < |z| < 1$. For large positive values of ν we have by Stirling's formula the asymptotic expansion

$$\Psi(\alpha+\nu) = \log \nu + \frac{B_1(\alpha)}{\nu} - \frac{B_2(\alpha)}{2\nu^2} + \ldots,$$

where $B_1(\alpha)$, $B_2(\alpha)$, ... are the Bernoulli polynomials. Hence

$$\Psi(\alpha+\nu) + \Psi(\beta+\nu) - \Psi(\gamma+\nu) - \Psi(1+\nu) = \frac{\alpha+\beta-\gamma-1}{\nu} + O\left(\frac{1}{\nu^2}\right).$$

It follows that for $z = 1$ the series (13) e. g. is convergent if $\Re(\gamma-\alpha-\beta) > -1$, or if $\gamma-\alpha-\beta = -1$.

In (14) we suppose that neither α nor β is a positive integer.

In (15) we suppose that α is not a positive integer and β not an integer $< \gamma$. (15) remains valid after a passage to the limit (cf. (11)) if α tends to a negative integer, as

$$\Psi(1-\alpha-\nu) = \Psi(1-\alpha) + \sum_{s=0}^{\nu-1} \frac{1}{\alpha+s}.$$

(14) remains valid if α or β tends to a negative integer or zero.

$G(\alpha, \beta, \gamma; z)$, $g(\alpha, \beta, \gamma; z)$ and $g_0(\alpha, \beta, \gamma; z)$ are symmetrical functions of the two first parameters α and β. But $g_1(\alpha, \beta, \gamma; z)$ and $g_1(\beta, \alpha, \gamma; z)$ are two different solutions of (1) unless $\alpha-\beta$ is an integer, in which case they are coincident. Any of these logarithmic solutions forms a fundamental system with $F(\alpha, \beta, \gamma; z)$.

4°. If γ is a non-positive integer and neither α nor β is one of the numbers $0, -1, -2, \ldots \gamma$, it is seen in the same manner that (1) has the solutions $z^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z)$ and $z^{1-\gamma} G(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z)$.

§ 3. If we make the substitution $z' = 1-z$ in (1) it is transformed into a hypergeometric differential equation with parameters α, β and $\alpha+\beta-\gamma+1$. It follows that (1) has the linearly independent solutions

$$F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad (16)$$

$$(1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad (17)$$

provided that $\alpha+\beta-\gamma$ is nonintegral. If $\alpha+\beta-\gamma = 0$, $F(\alpha, \beta, 1; 1-z)$ and $G(\alpha, \beta, 1; 1-z)$ are two independent solutions. If $\alpha+\beta-\gamma$ is a positive integer and one at least of the parameters α and β is a positive integer $\leqq \alpha+\beta-\gamma$, then (1) has the solutions

(16) and $(1-z)^{\gamma-\alpha-\beta} f(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z)$. If $\alpha+\beta-\gamma$ is a positive integer and neither α nor β is a positive integer $\leq \alpha+\beta-\gamma$, then (1) has the solutions (16) and $G(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z)$.

If $\alpha+\beta-\gamma$ is a negative integer and one at least of the parameters α and β is equal to a non-positive integer $> \alpha+\beta-\gamma$, then (17) and $f(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z)$ are linearly independent solutions of (1).

If $\alpha+\beta-\gamma$ is a negative integer and neither α nor β equals a non-positive integer $> \alpha+\beta-\gamma$, then (1) has the solutions (17) and $(1-z)^{\gamma-\alpha-\beta} G(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z)$.

§ 4. If we make the substitutions $z = \frac{1}{z_1}$, $y = z^{-\alpha} y_1$ in (1), it is transformed into a hypergeometric differential equation with parameters $\alpha, \alpha-\gamma+1, \alpha-\beta+1$. It follows that (1) has the linearly independent solutions

$$z^{-\alpha} F\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right), \tag{18}$$

$$z^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \tag{19}$$

provided that $\alpha-\beta$ is nonintegral. If $\alpha = \beta$, they are coincident and we have the solutions (18) and $z^{-\alpha} G\left(\alpha, \alpha-\gamma+1, 1; \frac{1}{z}\right)$.

If $\alpha-\beta$ is a positive integer and one at least of the numbers α and $\alpha-\gamma+1$ is equal to a positive integer $\leq \alpha-\beta$, them (18) and $z^{-\beta} f\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right)$ are linearly independent solutions of (1). If $\alpha-\beta$ is a positive integer and neither α nor $\alpha-\gamma+1$ equals a positive integer $\leq \alpha-\beta$, then $z^{-\alpha} G\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right)$ and (18) are independent solutions of (1).

G can of course be replaced by g, g_0, or g_1, except in the cases where one or more of these functions become meaningless.

§ 5. From the expansions in powers of z it follows immediately that the solutions defined in § 2 are connected by the following linear relations

$$g(\alpha, \beta, \gamma; z) = G(\alpha, \beta, \gamma; z) + [\Psi(\alpha) + \Psi(\beta) - \Psi(\gamma) - \Psi(1)] F(\alpha, \beta, \gamma; z), \tag{20}$$

$$g_0(\alpha, \beta, \gamma; z) = G(\alpha, \beta, \gamma; z) + [\Psi(1-\alpha) + \Psi(1-\beta) - \Psi(\gamma) - \Psi(1)] F(\alpha, \beta, \gamma; z), \tag{21}$$

$$g_1(\alpha, \beta, \gamma; z) = G(\alpha, \beta, \gamma; z) + [\Psi(1-\alpha) + \Psi(\beta) - \Psi(\gamma) - \Psi(1) \mp \pi i] F(\alpha, \beta, \gamma; z). \tag{22}$$

As

$$\Psi(1-\alpha) = \Psi(\alpha) + \pi \cot \pi\alpha,$$

it follows that

$$g_0(\alpha, \beta, \gamma; z) - g(\alpha, \beta, \gamma; z) = \frac{\pi \sin \pi(\alpha+\beta)}{\sin \pi\alpha \sin \pi\beta} F(\alpha, \beta, \gamma; z), \tag{23}$$

$$g_1(\alpha, \beta, \gamma; z) - g(\alpha, \beta, \gamma; z) = \frac{\pi e^{\mp \pi i \alpha}}{\sin \pi\alpha} F(\alpha, \beta, \gamma; z), \tag{24}$$

$$g_0(\alpha, \beta, \gamma; z) - g_1(\alpha, \beta, \gamma; z) = \frac{\pi e^{\pm \pi i \beta}}{\sin \pi\beta} F(\alpha, \beta, \gamma; z). \tag{25}$$

In each case the upper or lower sign is taken according as $I(z)$ is positive or negative. $g(\alpha, \beta, \gamma; z)$ is a one-valued analytic function of z within the domain $|\arg z| < \pi$ with a cross-cut along the real axis from $-\infty$ to 0; $g_1(\alpha, \beta, \gamma; z)$ is one-valued within the domain $|\arg(-z)| < \pi$ with a cross-cut along the real axis from 0 to $+\infty$. But $g_0(\alpha, \beta, \gamma; z)$ needs a cross-cut from $-\infty$ to 0 and another from 1 to ∞ to make it one-valued.

It was pointed out by GAUSS that

$$\frac{d^n}{dz^n} F(\alpha, \beta, \gamma; z) = \frac{(\alpha)_n (\beta)_n}{(\gamma)_n} F(\alpha+n, \beta+n, \gamma+n; z).$$

Also

$$\frac{d^n}{dz^n} g(\alpha, \beta, \gamma; z) = \frac{(\alpha)_n (\beta)_n}{(\gamma)_n} g(\alpha+n, \beta+n, \gamma+n; z),$$

$$\frac{d^n}{dz^n} [z^{\gamma-1} g(\alpha, \beta, \gamma; z)] = (-1)^n (1-\gamma)_n z^{\gamma-n-1} g(\alpha, \beta, \gamma-n; z),$$

$$\frac{d^n}{dz^n} [z^{\alpha+n-1} g(\alpha, \beta, \gamma; z)] = (\alpha)_n z^{\alpha-1} g(\alpha+n, \beta, \gamma; z),$$

as is obvious by differentiation of the power series.

The hypergeometric function $F(\alpha, \beta, \gamma; z)$ satisfies the following fundamental relations due to EULER and GAUSS:

$$F(\alpha, \beta, \gamma; z) = (1-z)^{-\beta} F\left(\gamma-\alpha, \beta, \gamma; \frac{z}{z-1}\right), \tag{26}$$

$$F(\alpha, \beta, \gamma; z) = (1-z)^{-\alpha} F\left(\alpha, \gamma-\beta, \gamma; \frac{z}{z-1}\right), \tag{27}$$

$$F(\alpha, \beta, \gamma; z) = (1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta, \gamma; z). \tag{28}$$

The logarithmic solutions satisfy similar relations, but not quite the same. By changing the dependent and the independent variable it is easily verified that if (1) has the solution $G(\alpha, \beta, \gamma; z)$, the function $(1-z)^{-\beta} G\left(\gamma-\alpha, \beta, \gamma; \frac{z}{z-1}\right)$ is also a solution,

and the first term in the expansions in powers of z is the same for both solutions. We therefore have a linear relation of the form

$$(1-z)^{-\beta} G\left(\gamma-\alpha, \beta, \gamma; \frac{z}{z-1}\right) - G(\alpha, \beta, \gamma; z) = CF(\alpha, \beta, \gamma; z),$$

C being a constant. Expanding in powers of z, we get, if we equate the constant terms on both sides,

$$C = \mp \pi i + \sum_{s=1}^{\gamma-1} \frac{1}{s} \frac{(\gamma-1)(\gamma-2)\ldots(\gamma-s)}{(\alpha-1)(\alpha-2)\ldots(\alpha-s)}.$$

But it is known that

$$\Psi(1-\alpha) - \Psi(\gamma-\alpha) = \sum_{s=1}^{\infty} \frac{1}{s} \frac{(\gamma-1)(\gamma-2)\ldots(\gamma-s)}{(\alpha-1)(\alpha-2)\ldots(\alpha-s)},$$

if $\Re(\gamma-\alpha) > 0$. As in the actual case γ is a positive integer, the series reduces to the first $\gamma-1$ terms and we get

$$\begin{aligned} C &= \mp \pi i + \Psi(1-\alpha) - \Psi(\gamma-\alpha) \\ &= \mp \pi i + \sum_{s=1}^{\gamma-1} \frac{1}{\alpha-s}. \end{aligned}$$

We thus obtain the formula

$$G(\alpha, \beta, \gamma; z) = (1-z)^{-\beta} G\left(\gamma-\alpha, \beta, \gamma; \frac{z}{z-1}\right) + \left(\pm \pi i + \sum_{s=1}^{\gamma-1} \frac{1}{s-\alpha}\right) F(\alpha, \beta, \gamma; z) \quad (29)$$

where the upper or lower sign is taken according as $I(z) \gtrless 0$. As $G(\alpha, \beta, \gamma; z)$ is a symmetrical function of the two first parameters α and β, it follows that

$$G(\alpha, \beta, \gamma; z) = (1-z)^{-\alpha} G\left(\alpha, \gamma-\beta, \gamma; \frac{z}{z-1}\right) + \left(\pm \pi i + \sum_{s=1}^{\gamma-1} \frac{1}{s-\beta}\right) F(\alpha, \beta, \gamma; z). \quad (30)$$

Combining these two formulae we get

$$G(\alpha, \beta, \gamma; z) = (1-z)^{\gamma-\alpha-\beta} G(\gamma-\alpha, \gamma-\beta, \gamma; z) - \sum_{s=1}^{\gamma-1} \left(\frac{1}{\alpha-s} + \frac{1}{\beta-s}\right) F(\alpha, \beta, \gamma; z). \quad (31)$$

It will be remembered that $G(\alpha, \beta, \gamma; z)$ only exists when α and β are different from $1, 2, \ldots \gamma-1$. The constants figuring in (29), (30) and (31) therefore are always finite. If $\gamma = 1$, (31) reduces to

$$G(\alpha, \beta, 1; z) = (1-z)^{1-\alpha-\beta} G(1-\alpha, 1-\beta, 1; z).$$

From (29) and (20) it now follows that

$$g(\alpha, \beta, \gamma; z) = (1-z)^{-\beta} g\left(\gamma-\alpha, \beta, \gamma; \frac{z}{z-1}\right) + (\pm \pi i - \pi \cot \pi\alpha) F(\alpha, \beta, \gamma; z). \quad (32)$$

If we use (24), this formula reduces to

$$g_1(\alpha, \beta, \gamma; z) = (1-z)^{-\beta} g\left(\gamma-\alpha, \beta, \gamma; \frac{z}{z-1}\right). \tag{33}$$

In the same way we see that

$$g_1(\beta, \alpha, \gamma; z) = (1-z)^{-\alpha} g\left(\alpha, \gamma-\beta, \gamma; \frac{z}{z-1}\right), \tag{34}$$

$$g_1(\alpha, \beta, \gamma; z) = (1-z)^{-\alpha} g_0\left(\alpha, \gamma-\beta, \gamma; \frac{z}{z-1}\right), \tag{35}$$

$$g_1(\beta, \alpha, \gamma; z) = (1-z)^{-\beta} g_0\left(\gamma-\alpha, \beta, \gamma; \frac{z}{z-1}\right), \tag{36}$$

$$g(\alpha, \beta, \gamma; z) = (1-z)^{-\beta} g_1\left(\gamma-\alpha, \beta, \gamma; \frac{z}{z-1}\right), \tag{37}$$

$$g_0(\alpha, \beta, \gamma; z) = (1-z)^{-\alpha} g_1\left(\alpha, \gamma-\beta, \gamma; \frac{z}{z-1}\right). \tag{38}$$

Combining these formulae we obtain

$$g(\alpha, \beta, \gamma; z) = (1-z)^{\gamma-\alpha-\beta} g_0(\gamma-\alpha, \gamma-\beta, \gamma; z), \tag{39}$$

$$g_0(\alpha, \beta, \gamma; z) = (1-z)^{\gamma-\alpha-\beta} g(\gamma-\alpha, \gamma-\beta, \gamma; z), \tag{40}$$

$$g_1(\alpha, \beta, \gamma; z) = (1-z)^{\gamma-\alpha-\beta} g_1(\gamma-\beta, \gamma-\alpha, \gamma; z).$$

§ 6. We have seen that if γ is a non-positive integer and the parameter β equals one of the numbers $0, -1, -2, \ldots \gamma$, then (1) has the solution (8). Consequently $(1-z)^{-\alpha} f\left(\alpha, \gamma-\beta, \gamma; \frac{z}{z-1}\right)$ is also a solution and furthermore (7) is a solution. There is thus a linear relation of the form

$$(1-z)^{-\alpha} f\left(\alpha, \gamma-\beta, \gamma; \frac{z}{z-1}\right) - f(\alpha, \beta, \gamma; z) = C z^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z), \tag{41}$$

C being a constant. If we expand in powers of z and equate the coefficients of $z^{1-\gamma}$, we obtain

$$C = \frac{(\alpha)_{1-\gamma}}{(1-\gamma)!} \sum_{\nu=0}^{\beta-\gamma} \frac{(\gamma-\beta)_\nu (\gamma-1)_\nu}{\nu!\,(\gamma)_\nu}.$$

By Vandermonde's theorem this reduces to

$$C = (-1)^{\beta-\gamma} \frac{\Gamma(\beta-\gamma+1)\,\Gamma(1-\beta)}{\Gamma(1-\gamma)\,\Gamma(2-\gamma)}\, \alpha(\alpha+1)(\alpha+2)\ldots(\alpha-\gamma). \tag{42}$$

In the same manner it is seen that

$$(1-z)^{-\beta} f\left(\gamma-\alpha,\ \beta,\ \gamma;\ \frac{z}{z-1}\right) = f(\alpha,\ \beta,\ \gamma;\ z), \tag{43}$$

where, as before, β equals one of the numbers $0, -1, -2, \ldots \gamma$ and α has any value. Combining (41) and (43) we get

$$(1-z)^{\gamma-\alpha-\beta} f(\gamma-\alpha, \gamma-\beta, \gamma; z) - f(\alpha, \beta, \gamma; z) = Cz^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z), \tag{44}$$

C being the constant (42). The gamma functions figuring in (42) are positive integers. C vanishes if, and only if, α equals one of the numbers $0, -1, -2, \ldots \gamma$. It follows that

$$f(\alpha, \beta, \gamma; z) = (1-z)^{-\alpha} f\left(\alpha,\ \gamma-\beta,\ \gamma;\ \frac{z}{z-1}\right),$$

$$f(\alpha, \beta, \gamma; z) = (1-z)^{\gamma-\alpha-\beta} f(\gamma-\alpha, \gamma-\beta, \gamma; z),$$

provided that both α and β are non-positive integers $\geq \gamma$.

§ 7. If γ is not an integer and $\alpha+\beta-\gamma$ is not a negative integer, (1) has the solutions (6), (7), and (16). These three solutions are connected by the well-known linear relation

$$\left.\begin{aligned}\Gamma(1-\gamma)\, F(\alpha, \beta, \gamma; z) + \frac{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)\,\Gamma(\gamma-1)}{\Gamma(\alpha)\,\Gamma(\beta)}\, z^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ \frac{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(\alpha+\beta-\gamma+1)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z).\end{aligned}\right\} \tag{45}$$

If γ tends to a positive integer and α or β are not integers $< \gamma$, the expression on the left tends to a limit, as shown by Gauss [11] in a similar case. Putting $\gamma = 1+p-\varepsilon$, where $p = 0, 1, 2, \ldots$, the left-hand side of (45) can be written

$$\frac{\Gamma(p-\varepsilon)}{\Gamma(\alpha)\,\Gamma(\beta)} \sum_{\nu=0}^{p-1} \frac{\Gamma(\alpha-p+\varepsilon+\nu)\,\Gamma(\beta-p+\varepsilon+\nu)}{\nu!\,(1-p+\varepsilon)_\nu}\, z^{\nu-p+\varepsilon} +$$

$$\frac{(-1)^p \pi}{\sin \pi\varepsilon} \frac{1}{\Gamma(\alpha)\,\Gamma(\beta)} \sum_{\nu=0}^{\infty} \left[\frac{\Gamma(\alpha+\nu)\,\Gamma(\beta+\nu)}{\nu!\,\Gamma(p-\varepsilon+\nu+1)} - \frac{\Gamma(\alpha+\varepsilon+\nu)\,\Gamma(\beta+\varepsilon+\nu)}{\Gamma(1+\varepsilon+\nu)\,\Gamma(p+\nu+1)}\, z^{\varepsilon}\right] z^{\nu},$$

where $\sum_{0}^{p-1}$ is to be interpreted as zero, when $p = 0$. If $|z| < 1$ the series converges uniformly with respect to ε, and it is easily seen that if $\varepsilon \to 0$, this expression tends to $\frac{(-1)^{p+1}}{p!}\, g(\alpha, \beta, p+1; z)$. It follows that if γ tends to a positive integer, the equation (45) takes the form

$$g(\alpha, \beta, \gamma; z) = (-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(\alpha+\beta-\gamma+1)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \tag{46}$$

where it is supposed that α and β are not integers $< \gamma$. The function $g(\alpha, \beta, \gamma; z)$ thus is regular at $z = 1$. The origin and infinity are the only singularities for the branch under consideration. If in (46) we replace α and β by $\gamma - \alpha$ and $\gamma - \beta$, we get from (40)

$$g_0(\alpha, \beta, \gamma; z) = (-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(1-\alpha)\,\Gamma(1-\beta)}{\Gamma(\gamma-\alpha-\beta+1)} (1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \tag{47}$$

provided that α and β are not positive integers. The function $g_0(\alpha, \beta, \gamma; z)$ thus has a branch-point at $z = 1$ unless $\gamma - \alpha - \beta$ is an integer. If it is positive, $z = 1$ is a zero for g_0, but if $\gamma - \alpha - \beta$ is a negative integer, the first terms in the series on the right vanish and the right-hand side of (47) reduces to the right-hand side of (46). Conversely, if $\gamma - \alpha - \beta$ is a positive integer, the first terms in (46) vanish, and (46) takes the form of (47). In the actual case α and β cannot be integers, but $\alpha + \beta$ is an integer and therefore $g = g_0$ by virtue of (23).

We now turn to the function g_1. From (33) and (46) we have

$$g_1(\alpha, \beta, \gamma; z) = (-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(1-\alpha)\,\Gamma(\beta-\gamma+1)}{\Gamma(\beta-\alpha+1)} (1-z)^{-\beta} F\left(\gamma-\alpha, \beta, \beta-\alpha+1; \frac{1}{1-z}\right).$$

Now, by (26)

$$F\left(\gamma-\alpha, \beta, \beta-\alpha+1; \frac{1}{1-z}\right) = \left(\frac{-z}{1-z}\right)^{-\beta} F\left(\beta-\gamma+1, \beta, \beta-\alpha+1; \frac{1}{z}\right).$$

We thus obtain

$$g_1(\alpha, \beta, \gamma; z) = (-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(1-\alpha)\,\Gamma(\beta-\gamma+1)}{\Gamma(\beta-\alpha+1)} (-z)^{-\beta} F\left(\beta-\gamma+1, \beta, \beta-\alpha+1; \frac{1}{z}\right), \tag{48}$$

provided that α and $\gamma - \beta$ are not positive integers. If $\alpha - \beta$ is a positive integer, the first terms in the series on the right vanish and we get

$$g_1(\alpha, \beta, \gamma; z) = (-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(1-\beta)\,\Gamma(\alpha-\gamma+1)}{\Gamma(\alpha-\beta+1)} (-z)^{-\alpha} F\left(\alpha-\gamma+1, \alpha, \alpha-\beta+1; \frac{1}{z}\right). \tag{49}$$

§ 8. We shall now consider the behavior of the logarithmic solutions as $z \to 1$. We have already seen that $g(z)$ is regular at $z = 1$. From (46) we get

$$g(\alpha, \beta, \gamma; 1) = (-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(\alpha+\beta-\gamma+1)}, \tag{50}$$

and from (47) it follows that

$$\lim_{z \to 1} (1-z)^{\alpha+\beta-\gamma} g_0(\alpha, \beta, \gamma; z) = (-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(1-\alpha)\,\Gamma(1-\beta)}{\Gamma(\gamma-\alpha-\beta+1)}. \tag{51}$$

Using Gauss's formula

$$F(\alpha, \beta, \gamma; 1) = \frac{\Gamma(\gamma)\,\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)}, \quad \Re(\gamma-\alpha-\beta) > 0 \tag{52}$$

we get from (48)

$$g_1(\alpha, \beta, \gamma; 1) = e^{\pm \pi i (\beta - \gamma)} \frac{\Gamma(\gamma)\,\Gamma(\beta - \gamma + 1)\,\Gamma(\gamma - \alpha - \beta)}{\Gamma(\gamma - \alpha)}, \tag{53}$$

provided that $\Re(\gamma - \alpha - \beta) > 0$. The upper or lower sign is taken according as z tends to a point on the upper or lower edge of the cut from 0 to ∞. From (21) we obtain

$$G(\alpha, \beta, \gamma; 1) = \frac{\Gamma(\gamma)\,\Gamma(\gamma - \alpha - \beta)}{\Gamma(\gamma - \alpha)\,\Gamma(\gamma - \beta)} [\Psi(\gamma) + \Psi(1) - \Psi(1 - \alpha) - \Psi(1 - \beta)], \tag{54}$$

provided that α and β are not positive integers and $\Re(\gamma - \alpha - \beta) > 0$. We next consider the equation (28). If we use (52), it follows that

$$\lim_{z \to 1} (1 - z)^{\alpha + \beta - \gamma} F(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)\,\Gamma(\alpha + \beta - \gamma)}{\Gamma(\alpha)\,\Gamma(\beta)}, \quad \Re(\alpha + \beta - \gamma) > 0. \tag{55}$$

In a similar way we get from (31) using (54) and (55)

$$\lim_{z \to 1} (1 - z)^{\alpha + \beta - \gamma} G(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)\,\Gamma(\alpha + \beta - \gamma)}{\Gamma(\alpha)\,\Gamma(\beta)} [\Psi(\gamma) + \Psi(1) - \Psi(\alpha) - \Psi(\beta)], \tag{56}$$

provided that $\Re(\alpha + \beta - \gamma) > 0$. Dealing with the case when $\gamma = \alpha + \beta$, we observe that putting $\gamma = 1$ in (46), we obtain

$$F(\alpha, \beta, \alpha + \beta; z) = \frac{-\Gamma(\alpha + \beta)}{\Gamma(\alpha)\,\Gamma(\beta)} g(\alpha, \beta, 1; 1 - z).$$

Dividing both sides by $\log(1 - z)$, we get

$$\lim_{z \to 1} \frac{F(\alpha, \beta, \alpha + \beta; z)}{\log(1 - z)} = \frac{-\Gamma(\alpha + \beta)}{\Gamma(\alpha)\,\Gamma(\beta)}. \tag{57}$$

Now from (20) it follows that

$$g(\alpha, \beta, \alpha + \beta; z) = G(\alpha, \beta, \alpha + \beta; z) +$$
$$[\Psi(\alpha) + \Psi(\beta) - \Psi(\alpha + \beta) - \Psi(1)]\, F(\alpha, \beta, \alpha + \beta; z).$$

The function on the left is regular at $z = 1$. Dividing both sides by $\log(1 - z)$ and using (57), we therefore obtain

$$\lim_{z \to 1} \frac{G(\alpha, \beta, \alpha + \beta; z)}{\log(1 - z)} = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\,\Gamma(\beta)} [\Psi(\alpha) + \Psi(\beta) - \Psi(\alpha + \beta) - \Psi(1)]. \tag{58}$$

For the existence of $G(\alpha, \beta, \gamma; z)$ it is necessary to assume that α and β are different from $1, 2, \ldots \gamma - 1$, but the formula (54) has been proved only when α and β are not positive integers. If α tends to an integer $\geq \gamma$, the first factor on the

right vanishes and the second factor tends to infinity, but the product remains finite. If $\alpha = \gamma + n$, where $n = 0, 1, 2, \ldots$, we have by Gauss's formula (52) that $\lim_{z \to 1} F(\gamma + n, \beta, \gamma; z) = 0$, provided that $\Re(\beta) < -n$. From (20) it now follows that

$$G(\gamma + n, \beta, \gamma; 1) = g(\gamma + n, \beta, \gamma; 1), \quad \Re(\beta) < -n.$$

and using (50) we obtain

$$G(\gamma + n, \beta, \gamma; 1) = \frac{(-1)^{\gamma}\,\Gamma(\gamma)\,n!}{(\beta + n)(\beta + n - 1)\ldots(\beta - \gamma + 1)}, \tag{59}$$

provided that $\Re(\beta + n) < 0$. It is easily seen that the right-hand side of (59) is the limit of the right-hand side of (54), as $\alpha \to \gamma + n$.

It may also be useful to observe that from (13) we obtain

$$\lim_{z \to 0} z^{\gamma - 1} g(\alpha, \beta, \gamma; z) = \frac{(-1)^{\gamma}\,\Gamma(\gamma)\,\Gamma(\gamma - 1)}{(1 - \alpha)_{\gamma - 1}\,(1 - \beta)_{\gamma - 1}}, \tag{60}$$

provided that $\gamma > 1$. But if $\gamma = 1$, we have

$$\lim_{z \to 0} \frac{g(\alpha, \beta, 1; z)}{\log z} = 1. \tag{61}$$

For the sake of completeness we shall add that for the function $f(z)$ defined by (8), we get by Vandermonde's theorem

$$f(\alpha, \beta, \gamma; 1) = \frac{\Gamma(\alpha - \gamma + 1)\,\Gamma(\beta - \gamma + 1)}{\Gamma(1 - \gamma)\,\Gamma(\alpha + \beta - \gamma + 1)}.$$

When α is a negative integer $-n$, the theorem becomes

$$f(-n, \beta, \gamma; 1) = \frac{(\gamma - \beta)_n}{(\gamma)_n}.$$

These special values for $z = 1$ are useful when we want to calculate the constants figuring in the linear relations between the solutions of (1).

For example, if γ is a positive integer and $\gamma - \alpha - \beta$ is not an integer, we have the relation

$$G(\alpha, \beta, \gamma; z) = C_1 F(\alpha, \beta, \alpha + \beta - \gamma + 1; 1 - z) + C_2 (1 - z)^{\gamma - \alpha - \beta} F(\gamma - \alpha, \gamma - \beta, \gamma - \alpha - \beta + 1; 1 - z),$$

provided that α and $\beta \neq 1, 2, \ldots \gamma - 1$. Using (28), (54) and (56), we get for the constants C_1 and C_2 the following values

$$C_1 = \frac{\Gamma(\gamma)\,\Gamma(\gamma - \alpha - \beta)}{\Gamma(\gamma - \alpha)\,\Gamma(\gamma - \beta)}\,[\Psi(\gamma) + \Psi(1) - \Psi(1 - \alpha) - \Psi(1 - \beta)],$$

$$C_2 = \frac{\Gamma(\gamma)\,\Gamma(\alpha + \beta - \gamma)}{\Gamma(\alpha)\,\Gamma(\beta)}\,[\Psi(\gamma) + \Psi(1) - \Psi(\alpha) - \Psi(\beta)].$$

Integral Representations

§ 9. The function $g(\alpha, \beta, \gamma; z)$ was defined when γ is a positive integer and α or β are not integers $< \gamma$. It is easily seen that this function in several ways may be represented by integrals of the Barnes type [4], e. g. we have

$$g(\alpha, \beta, \gamma; z) = \frac{(-1)^{\gamma}}{2\pi i} \frac{\Gamma(\gamma)}{\Gamma(\alpha)\,\Gamma(\beta)} \int_{-i\infty}^{+i\infty} z^{-t}\,\Gamma(t)\,\Gamma(t-\gamma+1)\,\Gamma(\alpha-t)\,\Gamma(\beta-t)\,dt, \quad (62)$$

where the path of integration is indented so that the poles of $\Gamma(t)\,\Gamma(t-\gamma+1)$ lie to the left and the poles of $\Gamma(\alpha-t)\,\Gamma(\beta-t)$ to the right of it. This integral converges for $|\arg z| < 2\pi$. Evaluating the integral as $2\pi i$ times the sum of the residues of the integrand at the simple poles $t = \gamma-1, \gamma-2, \ldots 1$ and the poles of the second order $t = 0, -1, -2, \ldots$, we get the series on the right of (13). Putting $z = 1$ in (62) and using Barnes' lemma [4, p. 155], we get the formula (50). Differentiating both sides of (62) with respect to z and putting $z = 1$, we obtain the formula (46). This formula is equivalent to the integral representation

$$\left.\begin{aligned} &g(\alpha, \beta, \gamma; z) = \\ &(-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(\alpha)\,\Gamma(\beta)\,2\pi i} \int_{-i\infty}^{+i\infty} (z-1)^{-t} \frac{\Gamma(t)\,\Gamma(\alpha-t)\,\Gamma(\beta-t)}{\Gamma(\alpha+\beta-\gamma+1-t)}\,dt, \end{aligned}\right\} \quad (63)$$

in which $|\arg(z-1)| < \pi$ and the contour passes between the poles of $\Gamma(t)$ and the poles of $\Gamma(\alpha-t)\,\Gamma(\beta-t)$. Furthermore we have

$$\left.\begin{aligned} &g(\alpha, \beta, \gamma; z) = \\ &\frac{(-1)^{\gamma}\,\Gamma(\gamma)}{2\pi i} z^{1-\gamma} \int_{-i\infty}^{+i\infty} (z-1)^{\gamma-1-t} \frac{\Gamma(t-\gamma+1)\,\Gamma(\alpha-t)\,\Gamma(\beta-t)}{\Gamma(\alpha+\beta-t)}\,dt, \end{aligned}\right\} \quad (64)$$

and the last integral is also convergent for $|\arg(z-1)| < \pi$.

For the function g_0 we obtain [28]

$$\begin{aligned} &g_0(\alpha, \beta, \gamma; z) = \\ &\frac{(-1)^{\gamma}}{2\pi i}\,\Gamma(\gamma)\,\Gamma(1-\alpha)\,\Gamma(1-\beta) \int_{\gamma-i\infty}^{\gamma+i\infty} z^{-t} \frac{\Gamma(t)\,\Gamma(t-\gamma+1)\,dt}{\Gamma(t-\alpha+1)\,\Gamma(t-\beta+1)} \end{aligned}$$

provided that[1] $0 < z < 1$ and $\Re(\gamma-\alpha-\beta) > -1$. The path of integration is a straight line parallel to the imaginary axis and intersecting the real axis at the point γ. Evaluating the latter integral as $2\pi i$ times the sum of the residues of the integrand at the poles $t = \gamma-1, \gamma-2, \gamma-3, \ldots$ we get the series on the right-hand side of (14).

[1] The integral is vanishing for $z > 1$. It is divergent for negative and for complex values of z.

Similarly, the function $g_1(z)$ can be represented by the following integral

$$g_1(\alpha, \beta, \gamma; z) = \frac{(-1)^\gamma}{2\pi i} \frac{\Gamma(\gamma)\,\Gamma(1-\alpha)}{\Gamma(\beta)} \int_{\gamma-i\infty}^{\gamma+i\infty} (-z)^{-t} \frac{\Gamma(t)\,\Gamma(t-\gamma+1)\,\Gamma(\beta-t)}{\Gamma(t-\alpha+1)}\, dt,$$

provided that $|\arg(-z)| < \pi$. The contour is a line parallel to the imaginary axis, except that it is curved, if necessary, so that the increasing sequence of poles β, $\beta+1$, $\beta+2$, ... lie to the right, and the decreasing sequence of poles $\gamma-1$, $\gamma-2$, $\gamma-3$, ... to the left of the path of integration. Evaluating the integral as $2\pi i$ times the sum of the residues at the poles $\gamma-1$, $\gamma-2$, $\gamma-3$, ... we get the series on the right-hand side of (15), provided that $|z|<1$, but if we assume $|z|>1$ and take minus $2\pi i$ times the sum of the residues at the poles β, $\beta+1$, $\beta+2$, ... we get the series on the right of (48).

Continuation Formulae

§ 10. In the following tables m, n, p, and q denote non-negative integers. In case of an ambigous sign the upper or lower sign is to be taken according as $I(z)$ is positive or negative.

We consider two independent solutions in the neighbourhood of a singular point, and we shall write down the formulae giving the analytic continuation of these solutions into the neighbourhood of another singular point. Thus, in the first case below, where $\alpha+\beta-\gamma$ is a non-negative integer q and γ not an integer, we get the formulae (1) and (4) from (46) and (47) by changing γ into $\alpha+\beta-\gamma+1$ and z into $1-z$. The four other formulae in this table are easily verified, being simple relations between rational functions after a factor eventually has been removed. If α and β are not integers, we use the formulae (1) and (4). If α or β is a non-positive integer, we have (2) and (4). If α or β is equal to $1, 2, \ldots q$, we take (3) and (6). Finally, if α or β is equal to $q+1$, $q+2$, $q+3$, ..., (1) and (5) are to be used. It follows that the solutions $F(\alpha, \beta, \gamma; z)$ and $z^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z)$ have a logarithmic singularity at $z = 1$, provided that α and β are not integers. But if α or β is a negative integer or an integer $> q$, one of these solutions is regular at $z = 1$, and the other is logarithmic. Finally, if α or β is equal to one of the numbers $1, 2, \ldots q$, both solutions have a pole of order q at $z = 1$.

Considering the sixth case, where γ and $\gamma-\alpha-\beta$ are positive integers, we see that the first formula is merely another form of (46), and the second is the same as (47). The third is a combination of the two first using (25). By permutation of α and β the fourth follows from the third. The three following formulae are obvious, being relations between rational functions.

In a similar way all formulae in the following tables can be proved.

1. $\alpha+\beta-\gamma=q$, γ not an integer.

$$F(\alpha,\beta,\gamma;z)=\frac{(-1)^{\alpha+\beta-\gamma+1}\Gamma(\gamma)}{\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)\,\Gamma(\alpha+\beta-\gamma+1)}\,g(\alpha,\beta,\alpha+\beta-\gamma+1;1-z), \tag{1}$$
$$|\arg(1-z)|<\pi, \quad \alpha \text{ and } \beta \neq q, q-1, q-2, \ldots$$

$$F(\alpha,\beta,\gamma;z)=\frac{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(1-\gamma)\,\Gamma(\alpha+\beta-\gamma+1)}\,F(\alpha,\beta,\alpha+\beta-\gamma+1;1-z), \tag{2}$$
$$\alpha \text{ or } \beta = 0, -1, -2, \ldots$$

$$F(\alpha,\beta,\gamma;z)=\frac{\Gamma(\gamma)\,\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha)\,\Gamma(\beta)}\,(1-z)^{\gamma-\alpha-\beta}\,f(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z), \tag{3}$$
$$\alpha \text{ or } \beta = 1, 2, \ldots q.$$

$$z^{1-\gamma}F(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;z)=$$
$$\frac{(-1)^{\alpha+\beta-\gamma+1}\Gamma(2-\gamma)}{\Gamma(1-\alpha)\,\Gamma(1-\beta)\,\Gamma(\alpha+\beta-\gamma+1)}\,g_0(\alpha,\beta,\alpha+\beta-\gamma+1;1-z), \tag{4}$$
$$|\arg z|<\pi, \quad |\arg(1-z)|<\pi, \quad \alpha \text{ and } \beta \neq 1, 2, 3, \ldots$$

$$z^{1-\gamma}F(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;z)=$$
$$\frac{\Gamma(\alpha)\,\Gamma(\beta)}{\Gamma(\gamma-1)\,\Gamma(\alpha+\beta-\gamma+1)}\,F(\alpha,\beta,\alpha+\beta-\gamma+1;1-z), \tag{5}$$
$$|\arg z|<\pi, \quad \alpha \text{ or } \beta = q+1, q+2, q+3, \ldots$$

$$z^{1-\gamma}F(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;z)=$$
$$\frac{\Gamma(2-\gamma)\,\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}\,z^{1-\gamma}(1-z)^{\gamma-\alpha-\beta}\,f(1-\alpha,1-\beta,\gamma-\alpha-\beta+1;1-z), \tag{6}$$
$$\alpha \text{ or } \beta = 1, 2, \ldots q.$$

2. $\gamma-\alpha-\beta=q$, γ not an integer.

$$F(\alpha,\beta,\gamma;z)=$$
$$\frac{(-1)^{\gamma-\alpha-\beta+1}\Gamma(\gamma)\,(1-z)^{\gamma-\alpha-\beta}}{\Gamma(\alpha)\,\Gamma(\beta)\,\Gamma(\gamma-\alpha-\beta+1)}\,g(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z), \tag{1}$$
$$|\arg(1-z)|<\pi, \quad \alpha \text{ and } \beta \neq 0, -1, -2, \ldots$$

$$F(\alpha,\beta,\gamma;z)=$$
$$\frac{\Gamma(1-\alpha)\,\Gamma(1-\beta)}{\Gamma(1-\gamma)\,\Gamma(\gamma-\alpha-\beta+1)}\,(1-z)^{\gamma-\alpha-\beta}\,F(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z), \tag{2}$$
$$\alpha \text{ or } \beta = -q, -q-1, -q-2, \ldots$$

$$\left.\begin{array}{c} F(\alpha,\beta,\gamma;z)=\dfrac{\Gamma(\gamma)\,\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)}f(\alpha,\beta,\alpha+\beta-\gamma+1;1-z), \\ \alpha \text{ or } \beta = 0,-1,-2,\ldots 1-q. \end{array}\right\} \quad (3)$$

$$\left.\begin{array}{c} z^{1-\gamma}F(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;z)= \\ \dfrac{(-1)^{\gamma-\alpha-\beta+1}\,\Gamma(2-\gamma)\,(1-z)^{\gamma-\alpha-\beta}}{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)\,\Gamma(\gamma-\alpha-\beta+1)}g_0(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z), \\ |\arg z|<\pi, \quad |\arg(1-z)|<\pi, \quad \alpha \text{ and } \beta \neq 1-q, 2-q, 3-q,\ldots \end{array}\right\} \quad (4)$$

$$\left.\begin{array}{c} z^{1-\gamma}F(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;z)= \\ \dfrac{\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)}{\Gamma(\gamma-1)\,\Gamma(\gamma-\alpha-\beta+1)}(1-z)^{\gamma-\alpha-\beta}F(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z), \\ |\arg z|<\pi, \quad \alpha \text{ or } \beta = 1,2,3,\ldots \end{array}\right\} \quad (5)$$

$$\left.\begin{array}{c} z^{1-\gamma}F(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;z)= \\ \dfrac{\Gamma(2-\gamma)\,\Gamma(\gamma-\alpha-\beta)}{\Gamma(1-\alpha)\,\Gamma(1-\beta)}z^{1-\gamma}f(\alpha-\gamma+1,\beta-\gamma+1,\alpha+\beta-\gamma+1;1-z), \\ \alpha \text{ or } \beta = 0,-1,\ldots 1-q. \end{array}\right\} \quad (6)$$

3. $\gamma = 1+p$, $\quad \gamma-\alpha-\beta$ not an integer.

$$\left.\begin{array}{c} F(\alpha,\beta,\gamma;z)=\dfrac{\Gamma(\gamma)\,\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)}F(\alpha,\beta,\alpha+\beta-\gamma+1;1-z)+ \\ \dfrac{\Gamma(\gamma)\,\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha)\,\Gamma(\beta)}(1-z)^{\gamma-\alpha-\beta}F(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z), \\ |\arg(1-z)|<\pi, \end{array}\right\} \quad (1)$$

$$\left.\begin{array}{c} g(\alpha,\beta,\gamma;z)= \\ (-1)^{\gamma}\dfrac{\Gamma(\gamma)\,\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(\alpha+\beta-\gamma+1)}F(\alpha,\beta,\alpha+\beta-\gamma+1;1-z), \\ |\arg z|<\pi, \quad \alpha \text{ and } \beta \neq p, p-1, p-2,\ldots \end{array}\right\} \quad (2)$$

$$\left.\begin{array}{c} g_0(\alpha,\beta,\gamma;z)= \\ (-1)^{\gamma}\dfrac{\Gamma(\gamma)\,\Gamma(1-\alpha)\,\Gamma(1-\beta)}{\Gamma(\gamma-\alpha-\beta+1)}(1-z)^{\gamma-\alpha-\beta}F(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z), \\ |\arg z|<\pi, \quad |\arg(1-z)|<\pi, \quad \alpha \text{ and } \beta \neq 1,2,3,\ldots \end{array}\right\} \quad (3)$$

$$F(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)\,\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad \alpha \text{ or } \beta = 0, -1, -2, \ldots \tag{4}$$

$$F(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)\,\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha)\,\Gamma(\beta)} (1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad |\arg(1-z)| < \pi, \quad \alpha \text{ or } \beta = p+1, p+2, p+3, \ldots \tag{5}$$

$$z^{1-\gamma} f(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \frac{\Gamma(\alpha)\,\Gamma(\beta)}{\Gamma(\gamma-1)\,\Gamma(\alpha+\beta-\gamma+1)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad \alpha \text{ or } \beta = 1, 2, \ldots p. \tag{6}$$

$$z^{1-\gamma}(1-z)^{\gamma-\alpha-\beta} f(1-\alpha, 1-\beta, 2-\gamma; z) = \frac{\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)\,(1-z)^{\gamma-\alpha-\beta}}{\Gamma(\gamma-1)\,\Gamma(\gamma-\alpha-\beta+1)} F(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad \alpha \text{ or } \beta = 1, 2, \ldots p. \tag{7}$$

4. $\gamma = 1-p, \quad \gamma-\alpha-\beta$ not an integer.

$$z^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \frac{\Gamma(2-\gamma)\,\Gamma(\gamma-\alpha-\beta)}{\Gamma(1-\alpha)\,\Gamma(1-\beta)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z) + \frac{\Gamma(2-\gamma)\,\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)} (1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad |\arg z| < \pi, \quad |\arg(1-z)| < \pi. \tag{1}$$

$$z^{1-\gamma} g(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = (-1)^{\gamma} \frac{\Gamma(2-\gamma)\,\Gamma(\alpha)\,\Gamma(\beta)}{\Gamma(\alpha+\beta-\gamma+1)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad |\arg z| < \pi, \quad \alpha \text{ and } \beta \neq 0, -1, -2, \ldots \tag{2}$$

$$z^{1-\gamma} g_0(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = (-1)^{\gamma} \frac{\Gamma(2-\gamma)\,\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)}{\Gamma(\gamma-\alpha-\beta+1)} (1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad |\arg z| < \pi, \quad |\arg(1-z)| < \pi, \quad \alpha \text{ and } \beta \neq 1-p, 2-p, 3-p, \ldots \tag{3}$$

$$z^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) =$$
$$\frac{\Gamma(2-\gamma)\,\Gamma(\gamma-\alpha-\beta)}{\Gamma(1-\alpha)\,\Gamma(1-\beta)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad (4)$$
$$|\arg z| < \pi, \quad \alpha \text{ or } \beta = -p, -p-1, -p-2, \ldots$$

$$z^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) =$$
$$\frac{\Gamma(2-\gamma)\,\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)} (1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad (5)$$
$$|\arg z| < \pi, \quad |\arg(1-z)| < \pi, \quad \alpha \text{ or } \beta = 1, 2, 3, \ldots$$

$$f(\alpha, \beta, \gamma; z) = \frac{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(1-\gamma)\,\Gamma(\alpha+\beta-\gamma+1)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad (6)$$
$$\alpha \text{ or } \beta = 0, -1, \ldots 1-p.$$

$$(1-z)^{\gamma-\alpha-\beta} f(\gamma-\alpha, \gamma-\beta, \gamma; z) =$$
$$\frac{\Gamma(1-\alpha)\,\Gamma(1-\beta)}{\Gamma(1-\gamma)\,\Gamma(\gamma-\alpha-\beta+1)} (1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad (7)$$
$$\alpha \text{ or } \beta = 0, -1, \ldots 1-p.$$

5. $\gamma = 1+p, \quad \alpha+\beta-\gamma = q.$

$$F(\alpha, \beta, \gamma; z) =$$
$$\frac{(-1)^{\alpha+\beta-\gamma+1}\,\Gamma(\gamma)}{\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)\,\Gamma(\alpha+\beta-\gamma+1)} g(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad (1)$$
$$|\arg(1-z)| < \pi, \quad \alpha \text{ and } \beta \neq q, q-1, q-2, \ldots$$

$$g(\alpha, \beta, \gamma; z) =$$
$$(-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(\alpha+\beta-\gamma+1)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad (2)$$
$$|\arg z| < \pi, \quad \alpha \text{ and } \beta \neq p, p-1, p-2, \ldots$$

$$g_1(\alpha, \beta, \gamma; z) = -e^{\mp \pi i \alpha} \frac{(1-\alpha)_q}{(1-\alpha)_p} \frac{p!}{q!} g_1(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad (3)$$
$$\alpha \neq 1, 2, 3, \ldots$$

$$g_1(\beta, \alpha, \gamma; z) = -e^{\mp \pi i \beta} \frac{(1-\beta)_q \, p!}{(1-\beta)_p \, q!} g_1(\beta, \alpha, \alpha+\beta-\gamma+1; 1-z), \quad \beta \neq 1, 2, 3, \ldots \tag{4}$$

$$F(\alpha, \beta, \gamma; z) = (-1)^n \frac{(q+1)_n}{(p+1)_n} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad \alpha \text{ or } \beta = -n, \quad n = 0, 1, 2, \ldots \tag{5}$$

$$F(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)\,\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha)\,\Gamma(\beta)} (1-z)^{\gamma-\alpha-\beta} f(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad \alpha \text{ or } \beta = 1, 2, \ldots q. \tag{6}$$

$$z^{1-\gamma} f(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \frac{\Gamma(\alpha)\,\Gamma(\beta)}{\Gamma(\gamma-1)\,\Gamma(\alpha+\beta-\gamma+1)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad \alpha \text{ or } \beta = 1, 2, \ldots p. \tag{7}$$

6. $\gamma = 1+p, \quad \gamma-\alpha-\beta = q.$

$$F(\alpha, \beta, \gamma; z) = \frac{(-1)^{\gamma-\alpha-\beta+1}\,\Gamma(\gamma)\,(1-z)^{\gamma-\alpha-\beta}}{\Gamma(\alpha)\,\Gamma(\beta)\,\Gamma(\gamma-\alpha-\beta+1)} g(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad |\arg(1-z)| < \pi, \quad \alpha \text{ and } \beta \neq 0, -1, -2, \ldots \tag{1}$$

$$g_0(\alpha, \beta, \gamma; z) = (-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(1-\alpha)\,\Gamma(1-\beta)}{\Gamma(\gamma-\alpha-\beta+1)} (1-z)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad |\arg z| < \pi, \quad \alpha \text{ and } \beta \neq 1, 2, 3, \ldots \tag{2}$$

$$g_1(\alpha, \beta, \gamma; z) = e^{\pm \pi i (\beta+q)} \frac{\Gamma(\gamma)\,\Gamma(1-\beta)}{\Gamma(\alpha)\,\Gamma(\gamma-\alpha-\beta+1)} (1-z)^{\gamma-\alpha-\beta} g_1(\gamma-\beta, \gamma-\alpha, \gamma-\alpha-\beta+1; 1-z), \quad \beta \neq p, p-1, p-2, \ldots \tag{3}$$

$$g_1(\beta, \alpha, \gamma; z) = e^{\pm \pi i (\alpha+q)} \frac{\Gamma(\gamma)\,\Gamma(1-\alpha)}{\Gamma(\beta)\,\Gamma(\gamma-\alpha-\beta+1)} (1-z)^{\gamma-\alpha-\beta} g_1(\gamma-\alpha, \gamma-\beta, \gamma-\alpha-\beta+1; 1-z), \quad \alpha \neq p, p-1, p-2, \ldots \tag{4}$$

$$F(\alpha,\beta,\gamma;z)=(-1)^n\frac{(1+q)_n}{(1+p)_n}(1-z)^{\gamma-\alpha-\beta}F(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z),$$
$$\alpha \text{ or } \beta=\gamma+n,\quad n=0,1,2,\ldots \tag{5}$$

$$F(\alpha,\beta,\gamma;z)=\frac{\Gamma(\gamma)\,\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)}f(\alpha,\beta,\alpha+\beta-\gamma+1;1-z),$$
$$\alpha \text{ or } \beta=0,-1,\ldots 1-q. \tag{6}$$

$$z^{1-\gamma}(1-z)^{\gamma-\alpha-\beta}f(1-\alpha,1-\beta,2-\gamma;z)=$$
$$\frac{\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)\,(1-z)^{\gamma-\alpha-\beta}}{\Gamma(\gamma-1)\,\Gamma(\gamma-\alpha-\beta+1)}F(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z),$$
$$\alpha \text{ or } \beta=1,2,\ldots p. \tag{7}$$

7. $\gamma=1-p,\quad \gamma-\alpha-\beta=q.$

$$z^{1-\gamma}F(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;z)=$$
$$\frac{(-1)^{q+1}\,\Gamma(2-\gamma)\,(1-z)^{\gamma-\alpha-\beta}}{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)\,\Gamma(\gamma-\alpha-\beta+1)}g_0(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z),$$
$$|\arg(1-z)|<\pi,\quad \alpha \text{ and } \beta\neq -p,-p-1,-p-2,\ldots \tag{1}$$

$$z^{1-\gamma}g_0(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;z)=$$
$$(-1)^{\gamma}\frac{\Gamma(2-\gamma)\,\Gamma(\gamma-\alpha)\,\Gamma(\gamma-\beta)}{\Gamma(\gamma-\alpha-\beta+1)}(1-z)^{\gamma-\alpha-\beta}F(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z),$$
$$|\arg z|<\pi,\quad \alpha \text{ and } \beta\neq -q,-q-1,-q-2,\ldots \tag{2}$$

$$z^{1-\gamma}g_1(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;z)=$$
$$e^{\mp\pi i(\alpha+1)}\frac{p!\,(\alpha)_q}{q!\,(\alpha)_p}(1-z)^{\gamma-\alpha-\beta}g_1(\gamma-\beta,\gamma-\alpha,\gamma-\alpha-\beta+1;1-z),$$
$$\beta\neq 0,-1,-2,\ldots \tag{3}$$

$$z^{1-\gamma}g_1(\beta-\gamma+1,\alpha-\gamma+1,2-\gamma;z)=$$
$$e^{\mp\pi i(\beta+1)}\frac{p!\,(\beta)_q}{q!\,(\beta)_p}(1-z)^{\gamma-\alpha-\beta}g_1(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z),$$
$$\alpha\neq 0,-1,-2,\ldots \tag{4}$$

$$z^{1-\gamma}F(\alpha-\gamma+1,\beta-\gamma+1,2-\gamma;z)=$$
$$(-1)^n\frac{(q+1)_n}{(p+1)_n}(1-z)^{\gamma-\alpha-\beta}F(\gamma-\alpha,\gamma-\beta,\gamma-\alpha-\beta+1;1-z),$$
$$\alpha \text{ or } \beta=n+1,\quad n=0,1,2,\ldots \tag{5}$$

$$\left.\begin{array}{c}(1-z)^{\gamma-\alpha-\beta}f(\gamma-\alpha,\ \gamma-\beta,\ \gamma;\ z)= \\ \dfrac{\Gamma(1-\alpha)\,\Gamma(1-\beta)\,(1-z)^{\gamma-\alpha-\beta}}{\Gamma(1-\gamma)\,\Gamma(\gamma-\alpha-\beta+1)}F(\gamma-\alpha,\ \gamma-\beta,\ \gamma-\alpha-\beta+1;\ 1-z), \\ \alpha\ \text{or}\ \beta=0,\ -1,\ \ldots\ 1-p.\end{array}\right\}\quad(6)$$

$$\left.\begin{array}{c}z^{1-\gamma}F(\alpha-\gamma+1,\ \beta-\gamma+1,\ 2-\gamma;\ z)= \\ \dfrac{\Gamma(2-\gamma)\,\Gamma(\gamma-\alpha-\beta)}{\Gamma(1-\alpha)\,\Gamma(1-\beta)}\,z^{1-\gamma}f(\alpha-\gamma+1,\ \beta-\gamma+1,\ \alpha+\beta-\gamma+1;\ 1-z), \\ \alpha\ \text{or}\ \beta=0,\ -1,\ \ldots\ 1-q.\end{array}\right\}\quad(7)$$

8. $\gamma=1-p,\quad \alpha+\beta-\gamma=q.$

$$\left.\begin{array}{c}z^{1-\gamma}F(\alpha-\gamma+1,\ \beta-\gamma+1,\ 2-\gamma;\ z)= \\ \dfrac{(-1)^{\alpha+\beta-\gamma+1}\,\Gamma(2-\gamma)}{\Gamma(1-\alpha)\,\Gamma(1-\beta)\,\Gamma(\alpha+\beta-\gamma+1)}\,g_0(\alpha,\ \beta,\ \alpha+\beta-\gamma+1;\ 1-z), \\ |\arg(1-z)|<\pi,\quad \alpha\ \text{and}\ \beta\neq 1,\ 2,\ 3,\ \ldots\end{array}\right\}\quad(1)$$

$$\left.\begin{array}{c}z^{1-\gamma}\,g\,(\alpha-\gamma+1,\ \beta-\gamma+1,\ 2-\gamma;\ z)= \\ (-1)^{\gamma}\dfrac{\Gamma(2-\gamma)\,\Gamma(\alpha)\,\Gamma(\beta)}{\Gamma(\alpha+\beta-\gamma+1)}F(\alpha,\ \beta,\ \alpha+\beta-\gamma+1;\ 1-z), \\ |\arg z|<\pi,\quad \alpha\ \text{and}\ \beta\neq 0,\ -1,\ -2,\ \ldots\end{array}\right\}\quad(2)$$

$$\left.\begin{array}{c}z^{1-\gamma}\,g_1(\alpha-\gamma+1,\ \beta-\gamma+1,\ 2-\gamma;\ z)= \\ -\dfrac{e^{\mp\pi i\,(\alpha+q)}\,\Gamma(\alpha)\,p!}{\Gamma(\alpha+p-q)\,q!}\,g_1(\alpha,\ \beta,\ \alpha+\beta-\gamma+1;\ 1-z), \\ \alpha\neq 1-p,\ 2-p,\ 3-p,\ \ldots\end{array}\right\}\quad(3)$$

$$\left.\begin{array}{c}z^{1-\gamma}\,g_1(\beta-\gamma+1,\ \alpha-\gamma+1,\ 2-\gamma;\ z)= \\ -\dfrac{e^{\mp\pi i\,(\beta+q)}\,\Gamma(\beta)\,p!}{\Gamma(\beta+p-q)\,q!}\,g_1(\beta,\ \alpha,\ \alpha+\beta-\gamma+1;\ 1-z), \\ \beta\neq 1-p,\ 2-p,\ 3-p,\ \ldots\end{array}\right\}\quad(4)$$

$$\left.\begin{array}{c}z^{1-\gamma}F(\alpha-\gamma+1,\ \beta-\gamma+1,\ 2-\gamma;\ z)= \\ (-1)^{n}\dfrac{(q+1)_n}{(p+1)_n}F(\alpha,\ \beta,\ \alpha+\beta-\gamma+1;\ 1-z), \\ \alpha\ \text{or}\ \beta=-p-n,\quad n=0,\ 1,\ 2,\ \ldots\end{array}\right\}\quad(5)$$

$$f(\alpha, \beta, \gamma; z) = \frac{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(1-\gamma)\,\Gamma(\alpha+\beta-\gamma+1)} F(\alpha, \beta, \alpha+\beta-\gamma+1; 1-z), \quad \alpha \text{ or } \beta = 0, -1, \ldots 1-p. \tag{6}$$

$$z^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \frac{\Gamma(2-\gamma)\,\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)} z^{1-\gamma}(1-z)^{\gamma-\alpha-\beta} f(1-\alpha, 1-\beta, \gamma-\alpha-\beta+1; 1-z), \quad \alpha \text{ or } \beta = 1, 2, \ldots q. \tag{7}$$

9. $\beta = \alpha + m$, γ not an integer.

$$F(\alpha, \beta, \gamma; z) = \frac{(-1)^{m-1}\,\Gamma(\gamma)\,(-z)^{-\beta}}{\Gamma(\alpha)\,\Gamma(\gamma-\beta)\,\Gamma(\beta-\alpha+1)} g_1\left(\beta-\gamma+1, \beta, \beta-\alpha+1; \frac{1}{z}\right), \quad |\arg(-z)| < \pi, \quad \alpha \text{ and } \gamma-\beta \neq 0, -1, -2, \ldots \tag{1}$$

$$F(\alpha, \beta, \gamma; z) = \frac{\Gamma(1-\alpha)\,\Gamma(\beta-\gamma+1)}{\Gamma(1-\gamma)\,\Gamma(\beta-\alpha+1)} (-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad \gamma-\alpha \text{ or } \beta = 0, -1, -2, \ldots \tag{2}$$

$$F(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(\beta)\,\Gamma(\gamma-\alpha)} (-z)^{-\alpha} f\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right), \quad \beta = 1, 2, \ldots m. \tag{3}$$

$$F(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(\beta)\,\Gamma(\gamma-\alpha)} (-z)^{-\alpha}\left(1-\frac{1}{z}\right)^{\gamma-\alpha-\beta} f\left(1-\beta, \gamma-\beta, \alpha-\beta+1; \frac{1}{z}\right), \quad \beta-\gamma = 0, 1, 2, \ldots m-1. \tag{4}$$

$$(-z)^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \frac{(-1)^{m-1}\,\Gamma(2-\gamma)\,(-z)^{-\beta}}{\Gamma(1-\beta)\,\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\alpha+1)} g_1\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad |\arg(-z)| < \pi, \quad \beta \text{ and } \gamma-\alpha \neq 1, 2, 3, \ldots \tag{5}$$

$$(-z)^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \frac{\Gamma(\beta)\,\Gamma(\gamma-\alpha)}{\Gamma(\gamma-1)\,\Gamma(\beta-\alpha+1)} (-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad \alpha \text{ or } \gamma-\beta = 1, 2, 3, \ldots \tag{6}$$

$$\left.\begin{array}{c}(-z)^{1-\gamma} F(\alpha-\gamma+1,\ \beta-\gamma+1,\ 2-\gamma;\ z) = \\ \dfrac{\Gamma(2-\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(\beta-\gamma+1)\,\Gamma(1-\alpha)}(-z)^{\alpha} f\left(\alpha,\ \alpha-\gamma+1,\ \alpha-\beta+1;\ \frac{1}{z}\right), \\ \beta-\gamma = 0,\ 1,\ \ldots\ m-1.\end{array}\right\} \quad (7)$$

$$\left.\begin{array}{c}(-z)^{1-\gamma} F(\alpha-\gamma+1,\ \beta-\gamma+1,\ 2-\gamma;\ z) = \\ \dfrac{\Gamma(2-\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(\beta-\gamma+1)\,\Gamma(1-\alpha)}(-z)^{-\alpha}\left(1-\frac{1}{z}\right)^{\gamma-\alpha-\beta} f\left(1-\beta,\ \gamma-\beta,\ \alpha-\beta+1;\ \frac{1}{z}\right), \\ \beta = 1,\ 2,\ \ldots\ m.\end{array}\right\} \quad (8)$$

10. $\gamma = 1+p$, $\quad \alpha-\beta$ non-integer.

$$\left.\begin{array}{c}F(\alpha,\ \beta,\ \gamma;\ z) = \dfrac{\Gamma(\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(\beta)\,\Gamma(\gamma-\alpha)}(-z)^{-\alpha} F\left(\alpha,\ \alpha-\gamma+1,\ \alpha-\beta+1;\ \frac{1}{z}\right) + \\ \dfrac{\Gamma(\gamma)\,\Gamma(\alpha-\beta)}{\Gamma(\alpha)\,\Gamma(\gamma-\beta)}(-z)^{-\beta} F\left(\beta,\ \beta-\gamma+1,\ \beta-\alpha+1;\ \frac{1}{z}\right), \\ |\arg(-z)| < \pi.\end{array}\right\} \quad (1)$$

$$\left.\begin{array}{c}g_1(\alpha,\ \beta,\ \gamma;\ z) = \\ (-1)^{\gamma}\dfrac{\Gamma(\gamma)\,\Gamma(1-\alpha)\,\Gamma(\beta-\gamma+1)}{\Gamma(\beta-\alpha+1)}(-z)^{-\beta} F\left(\beta,\ \beta-\gamma+1,\ \beta-\alpha+1;\ \frac{1}{z}\right), \\ |\arg(-z)| < \pi, \quad \alpha \text{ and } \gamma-\beta \neq 1,\ 2,\ 3,\ \ldots\end{array}\right\} \quad (2)$$

$$\left.\begin{array}{c}g_1(\beta,\ \alpha,\ \gamma;\ z) = \\ (-1)^{\gamma}\dfrac{\Gamma(\gamma)\,\Gamma(1-\beta)\,\Gamma(\alpha-\gamma+1)}{\Gamma(\alpha-\beta+1)}(-z)^{-\alpha} F\left(\alpha,\ \alpha-\gamma+1,\ \alpha-\beta+1;\ \frac{1}{z}\right), \\ |\arg(-z)| < \pi, \quad \beta \text{ and } \gamma-\alpha \neq 1,\ 2,\ 3,\ \ldots\end{array}\right\} \quad (3)$$

$$\left.\begin{array}{c}F(\alpha,\ \beta,\ \gamma;\ z) = \dfrac{\Gamma(\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(\beta)\,\Gamma(\gamma-\alpha)}(-z)^{-\alpha} F\left(\alpha,\ \alpha-\gamma+1,\ \alpha-\beta+1;\ \frac{1}{z}\right), \\ \alpha \text{ or } \gamma-\beta = 0,\ -1,\ -2,\ \ldots\end{array}\right\} \quad (4)$$

$$\left.\begin{array}{c}F(\alpha,\ \beta,\ \gamma;\ z) = \dfrac{\Gamma(\gamma)\,\Gamma(\alpha-\beta)}{\Gamma(\alpha)\,\Gamma(\gamma-\beta)}(-z)^{-\beta} F\left(\beta,\ \beta-\gamma+1,\ \beta-\alpha+1;\ \frac{1}{z}\right), \\ \beta \text{ or } \gamma-\alpha = 0,\ -1,\ -2,\ \ldots\end{array}\right\} \quad (5)$$

$$\left.\begin{gathered}(-z)^{1-\gamma} f(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ \frac{\Gamma(\alpha)\,\Gamma(\gamma-\beta)}{\Gamma(\gamma-1)\,\Gamma(\alpha-\beta+1)}(-z)^{-\alpha} F\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right), \\ \alpha = 1, 2, \ldots p.\end{gathered}\right\} \quad (6)$$

$$\left.\begin{gathered}(-z)^{1-\gamma} f(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ \frac{\Gamma(\beta)\,\Gamma(\gamma-\alpha)}{\Gamma(\gamma-1)\,\Gamma(\beta-\alpha+1)}(-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \\ \beta = 1, 2, \ldots p.\end{gathered}\right\} \quad (7)$$

$$\left.\begin{gathered}(-z)^{1-\gamma}(1-z)^{\gamma-\alpha-\beta} f(1-\alpha, 1-\beta, 2-\gamma; z) = \\ \frac{\Gamma(\beta)\,\Gamma(\gamma-\alpha)}{\Gamma(\gamma-1)\,\Gamma(\beta-\alpha+1)}(-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \\ \alpha = 1, 2, \ldots p.\end{gathered}\right\} \quad (8)$$

$$\left.\begin{gathered}(-z)^{1-\gamma}(1-z)^{\gamma-\alpha-\beta} f(1-\alpha, 1-\beta, 2-\gamma; z) = \\ \frac{\Gamma(\alpha)\,\Gamma(\gamma-\beta)}{\Gamma(\gamma-1)\,\Gamma(\alpha-\beta+1)}(-z)^{-\alpha} F\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right), \\ \beta = 1, 2, \ldots p.\end{gathered}\right\} \quad (9)$$

11. $\gamma = 1-p$, $\quad \alpha-\beta$ non-integer.

$$\left.\begin{gathered}(-z)^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ \frac{\Gamma(2-\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(1-\alpha)\,\Gamma(\beta-\gamma+1)}(-z)^{-\alpha} F\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right) + \\ \frac{\Gamma(2-\gamma)\,\Gamma(\alpha-\beta)}{\Gamma(1-\beta)\,\Gamma(\alpha-\gamma+1)}(-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \\ |\arg(-z)| < \pi.\end{gathered}\right\} \quad (1)$$

$$\left.\begin{gathered}(-z)^{1-\gamma} g_1(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ (-1)^{\gamma}\frac{\Gamma(2-\gamma)\,\Gamma(\gamma-\alpha)\,\Gamma(\beta)}{\Gamma(\beta-\alpha+1)}(-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \\ |\arg(-z)| < \pi, \quad \beta \text{ and } \gamma-\alpha \neq 0, -1, -2, \ldots\end{gathered}\right\} \quad (2)$$

$$\left.\begin{gathered}(-z)^{1-\gamma} g_1(\beta-\gamma+1, \alpha-\gamma+1, 2-\gamma; z) = \\ (-1)^{\gamma}\frac{\Gamma(2-\gamma)\,\Gamma(\gamma-\beta)\,\Gamma(\alpha)}{\Gamma(\alpha-\beta+1)}(-z)^{-\alpha} F\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right), \\ \alpha \text{ and } \gamma-\beta \neq 0, -1, -2, \ldots\end{gathered}\right\} \quad (3)$$

$$(-z)^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) =$$
$$\frac{\Gamma(2-\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(1-\alpha)\,\Gamma(\beta-\gamma+1)} (-z)^{-\alpha} F\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right), \quad (4)$$
$$\beta \text{ or } \gamma-\alpha = 1, 2, 3, \ldots$$

$$(-z)^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) =$$
$$\frac{\Gamma(2-\gamma)\,\Gamma(\alpha-\beta)}{\Gamma(1-\beta)\,\Gamma(\alpha-\gamma+1)} (-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad (5)$$
$$\alpha \text{ or } \gamma-\beta = 1, 2, 3, \ldots$$

$$f(\alpha, \beta, \gamma; z) = \frac{\Gamma(\alpha-\gamma+1)\,\Gamma(1-\beta)}{\Gamma(1-\gamma)\,\Gamma(\alpha-\beta+1)} (-z)^{-\alpha} F\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right), \quad (6)$$
$$\alpha = 0, -1, \ldots 1-p.$$

$$f(\alpha, \beta, \gamma; z) = \frac{\Gamma(\beta-\gamma+1)\,\Gamma(1-\alpha)}{\Gamma(1-\gamma)\,\Gamma(\beta-\alpha+1)} (-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad (7)$$
$$\beta = 0, -1, \ldots 1-p.$$

$$(1-z)^{\gamma-\alpha-\beta} f(\gamma-\alpha, \gamma-\beta, \gamma; z) =$$
$$\frac{\Gamma(\beta-\gamma+1)\,\Gamma(1-\alpha)}{\Gamma(1-\gamma)\,\Gamma(\beta-\alpha+1)} (-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad (8)$$
$$\alpha = 0, -1, \ldots 1-p.$$

$$(1-z)^{\gamma-\alpha-\beta} f(\gamma-\alpha, \gamma-\beta, \gamma; z) =$$
$$\frac{\Gamma(\alpha-\gamma+1)\,\Gamma(1-\beta)}{\Gamma(1-\gamma)\,\Gamma(\alpha-\beta+1)} (-z)^{-\alpha} F\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right), \quad (9)$$
$$\beta = 0, -1, \ldots 1-p.$$

12. $\gamma = 1+p, \quad \beta = \alpha+m.$

$$F(\alpha, \beta, \gamma; z) = \frac{(-1)^{m+1}\,\Gamma(\gamma)\,(-z)^{-\beta}}{\Gamma(\alpha)\,\Gamma(\gamma-\beta)\,\Gamma(\beta-\alpha+1)} g_1\left(\beta-\gamma+1, \beta, \beta-\alpha+1; \frac{1}{z}\right), \quad (1)$$
$$|\arg(-z)| < \pi, \quad \alpha \text{ and } \gamma-\beta \neq 0, -1, -2, \ldots$$

$$g_1(\alpha, \beta, \gamma; z) =$$
$$(-1)^{\gamma} \frac{\Gamma(\gamma)\,\Gamma(1-\alpha)\,\Gamma(\beta-\gamma+1)}{\Gamma(\beta-\alpha+1)} (-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad (2)$$
$$|\arg(-z)| < \pi, \quad \alpha \text{ and } \gamma-\beta \neq 1, 2, 3, \ldots$$

$$g(\alpha, \beta, \gamma; z) = (-1)^{m-p} \frac{\Gamma(\gamma)\,\Gamma(\beta-\gamma+1)}{\Gamma(\alpha)\,\Gamma(\beta-\alpha+1)} z^{-\beta}\, g\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad (3)$$
$$|\arg z| < \pi, \quad \gamma - \alpha \neq 1, 2, 3, \ldots$$

$$g_0(\alpha, \beta, \gamma; z) =$$
$$-e^{\pm \pi i \beta} \frac{\Gamma(\gamma)\,\Gamma(1-\alpha)}{\Gamma(\gamma-\beta)\,\Gamma(\beta-\alpha+1)} (-z)^{-\beta}\, g_0\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad (4)$$
$$\beta \neq 1, 2, 3, \ldots$$

$$F(\alpha, \beta, \gamma; z) = (-1)^{\varepsilon} \frac{p!\,(1-\beta)_m}{m!\,(1-\beta)_p} z^{-\beta}\, F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad (5)$$
$$\text{provided that} \quad \beta = 0, -1, -2, \ldots \quad \text{and} \quad \varepsilon = 0,$$
$$\text{or} \quad \beta = p+m+1, p+m+2, \ldots \quad \text{and} \quad \varepsilon = 1.$$

$$(-z)^{1-\gamma} f(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) =$$
$$\frac{\Gamma(\beta)\,\Gamma(\gamma-\alpha)}{\Gamma(\gamma-1)\,\Gamma(\beta-\alpha+1)} (-z)^{-\beta}\, F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \frac{1}{z}\right), \quad (6)$$
$$\beta = 1, 2, \ldots p.$$

$$F(\alpha, \beta, \gamma; z) =$$
$$\frac{\Gamma(\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(\gamma-\alpha)\,\Gamma(\beta)} (-z)^{-\alpha} f\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right), \quad (7)$$
$$\beta = 1, 2, \ldots m.$$

$$F(\alpha, \beta, \gamma; z) =$$
$$\frac{\Gamma(\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(\gamma-\alpha)\,\Gamma(\beta)} (-z)^{-\alpha} \left(1-\frac{1}{z}\right)^{\gamma-\alpha-\beta} f\left(1-\beta, \gamma-\beta, \alpha-\beta+1; \frac{1}{z}\right), \quad (8)$$
$$\beta = p+1, p+2, \ldots p+m.$$

$$z^{1-\gamma} f(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) =$$
$$\frac{\Gamma(\alpha)\,\Gamma(\beta-\alpha)}{\Gamma(\gamma-1)\,\Gamma(\beta-\gamma+1)} z^{-\alpha} f\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \frac{1}{z}\right), \quad (9)$$
$$\beta = p+1, \; p+2, \ldots p+m \quad \text{if} \quad p \geqq m,$$
$$\beta = m+1, m+2, \ldots m+p \quad \text{if} \quad p < m.$$

13. $\gamma = 1 - p, \quad \beta = \alpha + m.$

$$\left.\begin{array}{c} (-z)^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ \dfrac{(-1)^{m+1}\Gamma(2-\gamma)(-z)^{-\beta}}{\Gamma(\alpha-\gamma+1)\Gamma(1-\beta)\Gamma(\beta-\alpha+1)} g_1\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \dfrac{1}{z}\right), \\ |\arg(-z)| < \pi, \quad \beta \text{ and } \gamma-\alpha \neq 1, 2, 3, \ldots \end{array}\right\} \quad (1)$$

$$\left.\begin{array}{c} (-z)^{1-\gamma} g_1(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ (-1)^{\gamma} \dfrac{\Gamma(2-\gamma)\Gamma(\gamma-\alpha)\Gamma(\beta)}{\Gamma(\beta-\alpha+1)} (-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \dfrac{1}{z}\right), \\ |\arg(-z)| < \pi, \quad \beta \text{ and } \gamma-\alpha \neq 0, -1, -2, \ldots \end{array}\right\} \quad (2)$$

$$\left.\begin{array}{c} z^{1-\gamma} g(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ \dfrac{(-1)^{m-p}\Gamma(2-\gamma)\Gamma(\beta)}{\Gamma(\alpha-\gamma+1)\Gamma(\beta-\alpha+1)} z^{-\beta} g\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \dfrac{1}{z}\right), \\ |\arg z| < \pi, \quad \alpha \neq 0, -1, -2, \ldots \end{array}\right\} \quad (3)$$

$$\left.\begin{array}{c} z^{1-\gamma} g_0(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ -e^{\pm\pi i\beta} \dfrac{\Gamma(2-\gamma)\Gamma(\gamma-\alpha)}{\Gamma(1-\beta)\Gamma(\beta-\alpha+1)} (-z)^{-\beta} g_0\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \dfrac{1}{z}\right), \\ \gamma-\beta \neq 0, -1, -2, \ldots \end{array}\right\} \quad (4)$$

$$\left.\begin{array}{c} (-z)^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ \dfrac{(-1)^{m+\varepsilon} p!}{m!\,(\beta)_{p-m}} z^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \dfrac{1}{z}\right), \\ \text{provided that } \beta = -p, -p-1, -p-2, \ldots \text{ and } \varepsilon = 0, \\ \text{or } \beta = m+1, m+2, m+3, \ldots \text{ and } \varepsilon = 1. \end{array}\right\} \quad (5)$$

$$\left.\begin{array}{c} f(\alpha, \beta, \gamma; z) = \\ \dfrac{\Gamma(\beta-\gamma+1)\Gamma(1-\alpha)}{\Gamma(1-\gamma)\Gamma(\beta-\alpha+1)} (-z)^{-\beta} F\left(\beta, \beta-\gamma+1, \beta-\alpha+1; \dfrac{1}{z}\right), \\ \beta = 0, -1, -2, \ldots 1-p. \end{array}\right\} \quad (6)$$

$$\left.\begin{array}{c} (-z)^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ \dfrac{\Gamma(2-\gamma)\Gamma(\beta-\alpha)}{\Gamma(\beta-\gamma+1)\Gamma(1-\alpha)} (-z)^{-\alpha} f\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \dfrac{1}{z}\right), \\ \beta-\gamma = 0, 1, 2, \ldots m-1. \end{array}\right\} \quad (7)$$

$$\left.\begin{array}{c}(-z)^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; z) = \\ \dfrac{\Gamma(2-\gamma)\,\Gamma(\beta-\alpha)}{\Gamma(\beta-\gamma+1)\,\Gamma(1-\alpha)}(-z)^{-\alpha}\left(1-\dfrac{1}{z}\right)^{\gamma-\alpha-\beta} f\left(1-\beta, \gamma-\beta, \alpha-\beta+1; \dfrac{1}{z}\right), \\ \beta = 1, 2, 3, \ldots m.\end{array}\right\} \quad (8)$$

$$\left.\begin{array}{c}f(\alpha, \beta, \gamma; z) = \\ \dfrac{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\alpha)}{\Gamma(1-\gamma)\,\Gamma(\beta)} z^{-\alpha} f\left(\alpha, \alpha-\gamma+1, \alpha-\beta+1; \dfrac{1}{z}\right) \\ \beta = 1, 2, 3, \ldots m \qquad \text{if} \quad p \geqq m, \\ \beta = m-p+1, m-p+2, \ldots m \quad \text{if} \quad p < m.\end{array}\right\} \quad (9)$$

Chapter II

Quadratic Transformations

§ 11. Quadratic transformations of the hypergeometric function $F(\alpha, \beta, \gamma; z)$ have been investigated by GAUSS and in a more complete manner by KUMMER and GOURSAT. We shall now give some examples of such transformations of the logarithmic and other exceptional solutions. We take the cases considered by GAUSS. If we put

$$x = \frac{4z}{(1+z)^2}, \qquad Y = (1+z)^{2\alpha} y,$$

the equation

$$x(1-x)\frac{d^2Y}{dx^2} + [\gamma - (\alpha+\beta+1)x]\frac{dY}{dx} - \alpha\beta Y = 0 \quad (65)$$

is transformed into

$$\left.\begin{array}{c}z(1-z^2)\dfrac{d^2y}{dz^2} + [\gamma - (4\beta - 2\gamma)z + (\gamma - 4\alpha - 2)z^2]\dfrac{dy}{dz} \\ -2\alpha[2\beta - \gamma + (2\alpha - \gamma + 1)z]y = 0.\end{array}\right\} \quad (66)$$

If $\beta = \alpha + \frac{1}{2}$ this equation reduces to

$$z(1-z)\frac{d^2y}{dz^2} + [\gamma - (4\alpha - \gamma + 2)z]\frac{dy}{dz} - 2\alpha(2\alpha - \gamma + 1)y = 0. \quad (67)$$

It has the solution $F(2\alpha, 2\alpha - \gamma + 1, \gamma; z)$ and consequently

$$F\left(\alpha, \alpha + \frac{1}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = (1+z)^{2\alpha} F(2\alpha, 2\alpha - \gamma + 1, \gamma; z), \quad (68)$$

as shown by GAUSS. If γ is a positive integer, (65) has the solution $G\left(\alpha, \alpha+\frac{1}{2}, \gamma; x\right)$ and (67) has the second solution $G(2\alpha, 2\alpha-\gamma+1, \gamma; z)$, provided that neither α nor β is one of the numbers $1, 2, \ldots \gamma-1$. It follows that

$$\left.\begin{aligned} G\left(\alpha, \alpha+\frac{1}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = (1+z)^{2\alpha}\,[C_1\, G(2\alpha, 2\alpha-\gamma+1, \gamma; z) + \\ C\ F(2\alpha, 2\alpha-\gamma+1, \gamma; z)], \end{aligned}\right\} \tag{69}$$

where C and C_1 are constants. We divide both sides of (69) by $z^{1-\gamma}$ or by $\log z$, if $\gamma = 1$. Now let $z \to 0$, and using (60) or (61), we find that $C_1 = 1$. Next we let $z \to 1$, and using (54), we obtain, if $\Re(\gamma - 2\alpha) > \frac{1}{2}$,

$$C = \Psi(\gamma - 2\alpha) + \Psi(1-2\alpha) - \Psi(1-\alpha) - \Psi\left(\frac{1}{2}-\alpha\right). \tag{70}$$

If $\Re(\gamma - 2\alpha) < \frac{1}{2}$, we use (55) and (56) and we get in the same manner

$$C = \Psi(2\alpha-\gamma+1) + \Psi(2\alpha) - \Psi(\alpha) - \Psi\left(\frac{1}{2}+\alpha\right). \tag{71}$$

Now we have the relation

$$2\Psi(2\alpha) - \Psi(\alpha) - \Psi\left(\alpha+\frac{1}{2}\right) = \log 4.$$

(71) therefore reduces to

$$C = \Psi(2\alpha-\gamma+1) - \Psi(2\alpha) + \log 4 = \sum_{s=1}^{\gamma-1} \frac{1}{s-2\alpha} + \log 4. \tag{72}$$

In a similar manner we get from (70)

$$C = \Psi(\gamma-2\alpha) - \Psi(1-2\alpha) + \log 4 = \sum_{s=1}^{\gamma-1} \frac{1}{s-2\alpha} + \log 4.$$

The relation (69) can therefore be written

$$\left.\begin{aligned} G\left(\alpha, \alpha+\frac{1}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = (1+z)^{2\alpha}\, G(2\alpha, 2\alpha-\gamma+1, \gamma; z) \\ + C\, F\left(\alpha, \alpha+\frac{1}{2}, \gamma; \frac{4z}{(1+z)^2}\right), \end{aligned}\right\} \tag{73}$$

where C is defined by (72) and $\alpha \neq \frac{1}{2}, 1, \frac{3}{2}, \ldots \gamma-1$.

Using (20) or (21), we get from (73)

$$\left.\begin{aligned} g\left(\alpha, \alpha+\frac{1}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = (1+z)^{2\alpha}\, g(2\alpha, 2\alpha-\gamma+1, \gamma; z) \\ = \left(1+\frac{1}{z}\right)^{2\alpha} g\left(2\alpha, 2\alpha-\gamma+1, \gamma; \frac{1}{z}\right), \end{aligned}\right\} \tag{74}$$

provided that 2α is not an integer $< 2\gamma - 1$, and

$$g_0\left(\alpha, \alpha+\frac{1}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = (1+z)^{2\alpha} g_0(2\alpha, 2\alpha-\gamma+1, \gamma; z), \tag{75}$$

provided that 2α is not a positive integer. Furthermore using (24) and Table 12, we find that

$$\left.\begin{aligned} (1+z)^{-2\alpha} g_1\left(\alpha, \alpha+\frac{1}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = \\ g_1(2\alpha, 2\alpha-\gamma+1, \gamma; z) + \frac{\pi}{\sin 2\pi\alpha} F(2\alpha, 2\alpha-\gamma+1, \gamma; z) = \\ g_1(2\alpha, 2\alpha-\gamma+1, \gamma; z) - (-z)^{-2\alpha} g_1\left(2\alpha, 2\alpha-\gamma+1, \gamma; \frac{1}{z}\right) = \\ \left[F(2\alpha, 2\alpha-\gamma+1, \gamma; z) - (-z)^{-2\alpha} F\left(2\alpha, 2\alpha-\gamma+1, \gamma; \frac{1}{z}\right)\right] \frac{\pi}{\sin 2\pi\alpha}, \end{aligned}\right\} \tag{76}$$

provided that 2α is not an integer.

We now consider the rational solutions. The differential equation (65) has the solution $f(\alpha, \alpha+\frac{1}{2}, \gamma; x)$, and (67) has the solutions $f(2\alpha, 2\alpha-\gamma+1, \gamma; z)$ and $z^{1-\gamma} F(2\alpha-\gamma+1, 2\alpha-2\gamma+2, 2-\gamma; z)$, if γ is a non-positive integer, and α has one of the values $0, -\frac{1}{2}, -1, -\frac{3}{2}, \ldots \gamma-\frac{1}{2}$. Hence

$$\left.\begin{aligned} (1+z)^{-2\alpha} f\left(\alpha, \alpha+\frac{1}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = C_1 f(2\alpha, 2\alpha-\gamma+1, \gamma; z) \\ + C z^{1-\gamma} F(2\alpha-\gamma+1, 2\alpha-2\gamma+2, 2-\gamma; z). \end{aligned}\right\} \tag{77}$$

Now make $z \to 0$. It is readily seen that $C_1 = 1$. In order to determine the constant C we assume, first, that 2α is one of the numbers $0, -1, -2, \ldots \gamma$. The left side and the first term on the right side of (77) then are polynomials of z of degree -2α, but the second term contains higher powers of z. Therefore C is zero in this case and (77) reduces to

$$\left.\begin{aligned} (1+z)^{-2\alpha} f\left(\alpha, \alpha+\frac{1}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = f(2\alpha, 2\alpha-\gamma+1, \gamma; z) \\ = z^{-2\alpha} f\left(2\alpha, 2\alpha-\gamma+1, \gamma; \frac{1}{z}\right), \end{aligned}\right\} \tag{78}$$

provided that 2α has any of the values $0, -1, -2, \ldots \gamma$. The last expression is obtained by reversing the order of the terms.

Next, we assume that $2\alpha = \gamma-1, \gamma-2, \gamma-3, \ldots 2\gamma-1$. The first term on the right side of (77) now is a polynomial of a lower degree than -2α, and the second term is a polynomial which, by reversing the order of the terms, can be written

$$\left.\begin{aligned} & z^{1-\gamma} F(2\alpha-\gamma+1,\ 2\alpha-2\gamma+2,\ 2-\gamma;\ z) = \\ & \frac{(-1)^{\gamma-2\alpha-1}\,\Gamma(1-\gamma)\,\Gamma(2-\gamma)}{\Gamma(2\alpha-2\gamma+2)\,\Gamma(1-2\alpha)}\, z^{-2\alpha} f\left(2\alpha,\ 2\alpha-\gamma+1,\ \gamma;\ \frac{1}{z}\right). \end{aligned}\right\} \quad (79)$$

Now we multiply both sides of (77) by $z^{2\alpha}$ and let $z \to \infty$. We then obtain the relation

$$1 = C\,\frac{(-1)^{\gamma-2\alpha-1}\,\Gamma(1-\gamma)\,\Gamma(2-\gamma)}{\Gamma(2\alpha-2\gamma+2)\,\Gamma(1-2\alpha)},$$

which gives the value of C. Substituting this value in (77), we get

$$(1+z)^{-2\alpha} f\left(\alpha,\ \alpha+\frac{1}{2},\ \gamma;\ \frac{4z}{(1+z)^2}\right) = f(2\alpha,\ 2\alpha-\gamma+1,\ \gamma;\ z) +$$

$$(-1)^{\gamma-2\alpha-1}\,\frac{\Gamma(2\alpha-2\gamma+2)\,\Gamma(1-2\alpha)}{\Gamma(1-\gamma)\,\Gamma(2-\gamma)}\, z^{1-\gamma} F(2\alpha-\gamma+1, 2\alpha-2\gamma+2,\ 2-\gamma;\ z).$$

But using (79) we can also write this relation in the following manner:

$$\left.\begin{aligned} f\left(\alpha,\ \alpha+\frac{1}{2},\ \gamma;\ \frac{4z}{(1+z)^2}\right) &= (1+z)^{2\alpha} f(2\alpha,\ 2\alpha-\gamma+1,\ \gamma;\ z) + \\ &\left(1+\frac{1}{z}\right)^{2\alpha} f\left(2\alpha,\ 2\alpha-\gamma+1,\ \gamma;\ \frac{1}{z}\right), \end{aligned}\right\} \quad (80)$$

where it is supposed that 2α is an integer and $\gamma > 2\alpha \geq 2\gamma - 1$.

§ 12. If we apply the transformation (27) to the left-hand side of (68), we obtain the relation

$$F\left(\alpha,\ \gamma-\alpha-\frac{1}{2},\ \gamma;\ \frac{-4z}{(1-z)^2}\right) = (1-z)^{2\alpha} F(2\alpha,\ 2\alpha-\gamma+1,\ \gamma;\ z), \quad (81)$$

which was given by KUMMER.

If γ is a positive integer, it follows from (30) that

$$G\left(\alpha,\ \alpha+\frac{1}{2},\ \gamma;\ \frac{4z}{(1+z)^2}\right) = \left(\frac{1+z}{1-z}\right)^{2\alpha} G\left(\alpha,\ \gamma-\alpha-\frac{1}{2},\ \gamma;\ \frac{-4z}{(1-z)^2}\right) +$$

$$\left(\pm\pi i + \sum_{s=1}^{\gamma-1} \frac{1}{s-\alpha-\frac{1}{2}}\right) F\left(\alpha,\ \alpha+\frac{1}{2},\ \gamma;\ \frac{4z}{(1+z)^2}\right).$$

If we use this relation to transform the left-hand side of (73), we get the following relation

$$\left.\begin{aligned} G\left(\alpha,\ \gamma-\alpha-\frac{1}{2},\ \gamma;\ \frac{-4z}{(1-z)^2}\right) &= (1-z)^{2\alpha} G(2\alpha,\ 2\alpha-\gamma+1,\ \gamma;\ z) \\ &+ C_1 F\left(\alpha,\ \gamma-\alpha-\frac{1}{2},\ \gamma;\ \frac{-4z}{(1-z)^2}\right), \end{aligned}\right\} \quad (82)$$

provided that $\alpha \neq \frac{1}{2}, 1, \frac{3}{2}, \ldots \gamma - 1$. The constant C_1 figuring in this relation has the following value

$$C_1 = \log 4 \mp \pi i + \sum_{s=1}^{\gamma-1} \left(\frac{1}{s - 2\alpha} - \frac{1}{s - \alpha - \frac{1}{2}} \right),$$

where the upper or lower sign is to be taken according as $I(z) \gtrless 0$.

If we apply the transformation (37) to the left-hand side of (74), we obtain

$$g_1\left(\gamma - \alpha - \frac{1}{2}, \alpha, \gamma; \frac{-4z}{(1-z)^2}\right) = (1-z)^{2\alpha} g(2\alpha, 2\alpha - \gamma + 1, \gamma; z), \tag{83}$$

provided that 2α is not an integer $< 2\gamma - 1$. Similarly, if we apply the transformation (38) to the left-hand side of (75) we get

$$g_1\left(\alpha, \gamma - \alpha - \frac{1}{2}, \gamma; \frac{-4z}{(1-z)^2}\right) = (1-z)^{2\alpha} g_0(2\alpha, 2\alpha - \gamma + 1, \gamma; z), \tag{84}$$

provided that 2α is not a positive integer. If we use the transformation (35), it follows from (76) that

$$\left.\begin{aligned} g_0\left(\alpha, \gamma - \alpha - \frac{1}{2}, \gamma; \frac{-4z}{(1-z)^2}\right) &= (1-z)^{2\alpha} g_1(2\alpha, 2\alpha - \gamma + 1, \gamma; z) \\ &\quad - \left(1 - \frac{1}{z}\right)^{2\alpha} g_1\left(2\alpha, 2\alpha - \gamma + 1, \gamma; \frac{1}{z}\right) \end{aligned}\right\} \tag{85}$$

under the condition that 2α is not an integer.

If γ is zero or a negative integer, we employ the relation (41) and then from (78) and (80) get the following formulae

$$\left.\begin{aligned} f\left(\alpha, \gamma - \alpha - \frac{1}{2}, \gamma; \frac{-4z}{(1-z)^2}\right) &= (1-z)^{2\alpha} f(2\alpha, 2\alpha - \gamma + 1, \gamma; z) \\ &\quad + \left(1 - \frac{1}{z}\right)^{2\alpha} f\left(2\alpha, 2\alpha - \gamma + 1, \gamma; \frac{1}{z}\right), \end{aligned}\right\} \tag{86}$$

where α has any of the values $\frac{\gamma-1}{2}, \frac{\gamma-2}{2}, \frac{\gamma-3}{2}, \ldots \gamma - \frac{1}{2}$.

$$\left.\begin{aligned} f\left(\alpha, \gamma - \alpha - \frac{1}{2}, \gamma; \frac{-4z}{(1-z)^2}\right) &= (1-z)^{2\alpha} f(2\alpha, 2\alpha - \gamma + 1, \gamma; z) \\ &= \left(1 - \frac{1}{z}\right)^{2\alpha} f\left(2\alpha, 2\alpha - \gamma + 1, \gamma; \frac{1}{z}\right), \end{aligned}\right\} \tag{87}$$

provided that α is a non-positive integer $\geqq \frac{\gamma}{2}$,

$$\left.\begin{aligned} f\left(\alpha,\ \gamma-\alpha-\frac{1}{2},\ \gamma;\ \frac{-4z}{(1-z)^2}\right) &= (1-z)^{2\gamma-2\alpha-1} f(\gamma-2\alpha,\ 2\gamma-2\alpha-1,\ \gamma;\ z) \\ &\quad + \left(1-\frac{1}{z}\right)^{2\gamma-2\alpha-1} f\left(\gamma-2\alpha,\ 2\gamma-2\alpha-1,\ \gamma;\ \frac{1}{z}\right), \end{aligned}\right\} \tag{88}$$

provided that 2α is an odd integer and $0 > 2\alpha \geq \gamma$.

§ 13. We now assume that $\beta = \frac{1}{2}\gamma$ instead of $\beta = \alpha + \frac{1}{2}$. The differential equation (66) then reduces to

$$z(1-z^2)\frac{d^2y}{dz^2} + [\gamma - (4\alpha - \gamma + 2)z^2]\frac{dy}{dz} - 2\alpha(2\alpha + 1 - \gamma)zy = 0.$$

Put $z^2 = x$ and we obtain the hypergeometric equation

$$x(1-x)\frac{d^2y}{dx^2} + \left[\frac{\gamma+1}{2} - \left(2\alpha - \frac{\gamma}{2} + \frac{3}{2}\right)x\right]\frac{dy}{dx} - \alpha\left(\alpha + \frac{1-\gamma}{2}\right)y = 0 \tag{89}$$

with the parameters α, $\alpha + \frac{1-\gamma}{2}$ and $\frac{\gamma+1}{2}$. It has the solution $F\left(\alpha,\ \alpha + \frac{1-\gamma}{2},\ \frac{\gamma+1}{2};\ z^2\right)$ and (65) has the solution $F\left(\alpha, \frac{\gamma}{2}, \gamma; \frac{4z}{(1+z)^2}\right)$. Hence

$$F\left(\alpha, \frac{\gamma}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = (1+z)^{2\alpha} F\left(\alpha,\ \alpha + \frac{1-\gamma}{2},\ \frac{\gamma+1}{2};\ z^2\right). \tag{90}$$

This formula is due to Gauss.

If γ is an odd positive integer and if α is not an integer $< \gamma$, then (65) also has the solution $g\left(\alpha, \frac{\gamma}{2}, \gamma; \frac{4z}{(1+z)^2}\right)$ and (89) also has the solution $g\left(\alpha,\ \alpha + \frac{1-\gamma}{2},\ \frac{\gamma+1}{2};\ z^2\right)$. It follows that

$$\begin{aligned} g\left(\alpha, \frac{\gamma}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = (1+z)^{2\alpha} \Bigg[& C_1 g\left(\alpha,\ \alpha + \frac{1-\gamma}{2},\ \frac{\gamma+1}{2};\ z^2\right) \\ & + C F\left(\alpha,\ \alpha + \frac{1-\gamma}{2},\ \frac{\gamma+1}{2};\ z^2\right)\Bigg]. \end{aligned}$$

We divide both sides by $z^{1-\gamma}$ (or by $\log z$ if $\gamma = 1$). Let $z \to 0$ and using (60) or (61) we find in both cases that $C_1 = \frac{1}{2}$. Next, let $z \to 1$ and we get $C = 0$. Hence

$$g\left(\alpha, \frac{\gamma}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = \frac{1}{2}(1+z)^{2\alpha} g\left(\alpha,\ \alpha + \frac{1-\gamma}{2},\ \frac{\gamma+1}{2};\ z^2\right). \tag{91}$$

If γ is an odd negative integer and if α has any of the values $0, -1, -2, \ldots \gamma$, then (65) has the solution $f\left(\alpha, \frac{\gamma}{2}, \gamma; \frac{4z}{(1+z)^2}\right)$ and (89) has the solutions $f\left(\alpha, \alpha+\frac{1-\gamma}{2}, \frac{\gamma+1}{2}; z^2\right)$ and $z^{1-\gamma} F\left(\alpha+\frac{1-\gamma}{2}, \alpha-\gamma+1, \frac{3-\gamma}{2}; z^2\right)$. Hence

$$\left.\begin{aligned}(1+z)^{-2\alpha} f\left(\alpha, \frac{\gamma}{2}, \gamma; \frac{4z}{(1+z)^2}\right) &= f\left(\alpha, \alpha+\frac{1-\gamma}{2}, \frac{\gamma+1}{2}; z^2\right) \\ &+ C z^{1-\gamma} F\left(\alpha+\frac{1-\gamma}{2}, \alpha-\gamma+1, \frac{3-\gamma}{2}; z^2\right).\end{aligned}\right\} \quad (92)$$

In order to determine the constant C we assume, first, that α has one of the values $0, -1, -2, \ldots \frac{\gamma+1}{2}$. The left-hand side and the first term on the right-hand side of (92) then are polynomials of the degree -2α, but the second term contains higher powers of z. Therefore, C is zero in this case. Next, we assume that α has one of the values $\frac{\gamma-1}{2}, \frac{\gamma-3}{2}, \frac{\gamma-5}{2}, \ldots \gamma$. By reversing the order of the terms, we get

$$z^{1-\gamma} F\left(\alpha+\frac{1-\gamma}{2}, \alpha-\gamma+1, \frac{3-\gamma}{2}; z^2\right) =$$

$$(-1)^{\frac{\gamma-1}{2}-\alpha} \frac{\Gamma\left(\frac{3-\gamma}{2}\right)\Gamma\left(\frac{1-\gamma}{2}\right)}{\Gamma(1-\alpha)\,\Gamma(\alpha-\gamma+1)} z^{-2\alpha} f\left(\alpha, \alpha+\frac{1-\gamma}{2}, \frac{\gamma+1}{2}; \frac{1}{z^2}\right).$$

Now we multiply both sides of (92) by $z^{2\alpha}$ and let $z \to \infty$. We then obtain

$$C = (-1)^{\alpha+\frac{1-\gamma}{2}} \frac{\Gamma(1-\alpha)\,\Gamma(\alpha-\gamma+1)}{\Gamma\left(\frac{1-\gamma}{2}\right)\Gamma\left(\frac{3-\gamma}{2}\right)}.$$

It follows that

$$f\left(\alpha, \frac{\gamma}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = (1+z)^{2\alpha} f\left(\alpha, \alpha+\frac{1-\gamma}{2}, \frac{\gamma+1}{2}; z^2\right)$$
$$+\left(1+\frac{1}{z}\right)^{2\alpha} f\left(\alpha, \alpha+\frac{1-\gamma}{2}, \frac{\gamma+1}{2}; z^{-2}\right),$$

provided that $\alpha = \frac{\gamma-1}{2}, \frac{\gamma-3}{2}, \frac{\gamma-5}{2}, \ldots \gamma$, and

$$f\left(\alpha, \frac{\gamma}{2}, \gamma; \frac{4z}{(1+z)^2}\right) = (1+z)^{2\alpha} f\left(\alpha, \alpha+\frac{1-\gamma}{2}, \frac{\gamma+1}{2}; z^2\right)$$
$$= \left(1+\frac{1}{z}\right)^{2\alpha} f\left(\alpha, \alpha+\frac{1-\gamma}{2}, \frac{\gamma+1}{2}; z^{-2}\right),$$

provided that $\alpha = 0, -1, -2, \ldots \frac{\gamma+1}{2}$.

§ 14. If we put $z = \frac{1-\sqrt{1-x}}{2}$, the differential equation (65) is transformed to

$$z(1-z)\frac{d^2Y}{dz^2} + [\gamma - (4\alpha+4\beta+2)z + (4\alpha+4\beta+2)z^2]\frac{1}{1-2z}\frac{dY}{dz} - 4\alpha\beta Y = 0.$$

If $\gamma = \alpha+\beta+\frac{1}{2}$, this equation takes the form

$$z(1-z)\frac{d^2Y}{dz^2} + \left[\alpha+\beta+\frac{1}{2} - (2\alpha+2\beta+1)z\right]\frac{dY}{dz} - 4\alpha\beta Y = 0. \tag{93}$$

It has the solution $F\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1-\sqrt{1-x}}{2}\right)$. Hence, we have the relation

$$F\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1-\sqrt{1-x}}{2}\right) = F\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; x\right), \tag{94}$$

a result given by GAUSS.

If γ is a positive integer, and if 2α is not an integer, then (93) has the second solution $g\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1-\sqrt{1-x}}{2}\right)$, and $g\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; x\right)$ is a solution of (65). It follows that there exist constants C and C_1 such that

$$g\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1-\sqrt{1-x}}{2}\right) = C_1 g\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; x\right) + CF\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; x\right).$$

Now make $x \to 0$. It is readily seen that $C_1 = 1$. Next, we let $x \to 1$ and we obtain

$$\left.\begin{aligned} C\frac{\Gamma\left(\alpha+\beta+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\alpha+\frac{1}{2}\right)\Gamma\left(\beta+\frac{1}{2}\right)} &= g\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1}{2}\right) \\ &\quad - g\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; 1\right). \end{aligned}\right\} \tag{95}$$

Using (46) we see that

$$g\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; 1\right) = (-1)^{\alpha+\beta+\frac{1}{2}}\frac{\Gamma\left(\alpha+\beta+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}-\alpha\right)\Gamma\left(\frac{1}{2}-\beta\right)}{\Gamma\left(\frac{1}{2}\right)},$$

$$\left.\begin{aligned} & g\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1}{2}\right) \\ &= (-1)^{\alpha+\beta+\frac{1}{2}} \Gamma\left(\alpha-\beta+\frac{1}{2}\right) \Gamma\left(\beta-\alpha+\frac{1}{2}\right) F\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1}{2}\right) \\ &= (-1)^{\alpha+\beta+\frac{1}{2}} \frac{\Gamma\left(\alpha+\beta+\frac{1}{2}\right) \Gamma\left(\alpha-\beta+\frac{1}{2}\right) \Gamma\left(\beta-\alpha+\frac{1}{2}\right) \Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\alpha+\frac{1}{2}\right) \Gamma\left(\beta+\frac{1}{2}\right)}. \end{aligned}\right\} \quad (96)$$

Substituting these values in (95), we get

$$C = \frac{\pi}{\sin 2\pi\alpha}.$$

It follows that

$$\left.\begin{aligned} g\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1-\sqrt{1-x}}{2}\right) &= g\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; x\right) \\ &+ \frac{\pi}{\sin 2\pi\alpha} F\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; x\right), \end{aligned}\right\} \quad (97)$$

provided that 2α is not an integer. Using (20) we derive from this formula that

$$\left.\begin{aligned} G\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1-\sqrt{1-x}}{2}\right) &= G\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; x\right) \\ &+ K F\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; x\right), \end{aligned}\right\} \quad (98)$$

where the constant K has the value

$$K = \Psi(\alpha) + \Psi(\beta) - \Psi(2\alpha) - \Psi(2\beta) + \frac{\pi}{\sin 2\pi\alpha},$$

and it is easily seen that this expression reduces to

$$\begin{aligned} K &= \sum_{s=1}^{2\gamma-2} \frac{(-1)^s}{2\alpha - s} - \log 4 \\ &= \sum_{s=1}^{2\gamma-2} \frac{(-1)^s}{2\beta - s} - \log 4. \end{aligned}$$

The relation (98) is true if $2\alpha \neq 1, 2, 3, \ldots 2\gamma - 2$.
In a similar way it is seen that

$$g\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1+\sqrt{1-x}}{2}\right) = -\frac{\pi}{\sin 2\pi\alpha} F\left(\alpha, \beta, \alpha+\beta+\frac{1}{2}; x\right).$$

If $\gamma = \alpha+\beta+\frac{1}{2}$ is a negative integer, $f\left(2\alpha, 2\beta, \gamma; \frac{1-\sqrt{1-x}}{2}\right)$ is a solution of (93), again $f(\alpha, \beta, \gamma; x)$ and $x^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; x)$ are solutions of (65), provided that α has any of the values $0, -\frac{1}{2}, -1, -\frac{3}{2}, \ldots \gamma-\frac{1}{2}$. These solutions are connected by a linear relation

$$\left.\begin{aligned} f\left(2\alpha, 2\beta, \gamma; \frac{1-\sqrt{1-x}}{2}\right) = f(\alpha, \beta, \gamma; x) + \\ Cx^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; x), \end{aligned}\right\} \quad (99)$$

C being a constant. If $\alpha = 0, -1, -2, \ldots -\left[\frac{|\gamma|}{2}\right]$ we have $\beta < \alpha$. For large negative values of x the left-hand side and the first term on the right-hand side of (99) are $O(|x|^{-\alpha})$, while the second term on the right is $O(|x|^{-\beta})$. But if $\alpha = -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, \ldots \frac{1}{2}+\left[\frac{\gamma}{2}\right]$ the left side is again $O(|x|^{-\alpha})$, whereas both terms on the right side are $O(|x|^{-\beta})$. Multiply both sides of (99) by $(-x)^{\beta}$ and let $x \to -\infty$. In the first case we get $C = 0$. Using Table 11 Formulae (1) and (7), we get in the second case

$$C = -\frac{\Gamma\left(\frac{1}{2}-\alpha\right)\Gamma\left(\frac{1}{2}-\beta\right)\Gamma(1-\alpha)\Gamma(1-\beta)}{\pi\,\Gamma(1-\gamma)\Gamma(2-\gamma)}. \quad (100)$$

Now in the second case (99) can be reduced. If γ is a negative integer and if β has one of the values $0, -1, -2, \ldots \gamma$, it follows from (44) that

$$\begin{aligned} (1-x)^{\gamma-\alpha-\beta} f(\gamma-\alpha, \gamma-\beta, \gamma; x) = f(\alpha, \beta, \gamma; x) + \\ Cx^{1-\gamma} F(\alpha-\gamma+1, \beta-\gamma+1, 2-\gamma; x), \end{aligned}$$

where C has the value (100). As in the actual case $\gamma-\alpha-\beta = \frac{1}{2}$ Formula (99) reduces to

$$f\left(2\alpha, 2\beta, \gamma; \frac{1-\sqrt{1-x}}{2}\right) = \sqrt{1-x}\, f\left(\alpha+\frac{1}{2}, \beta+\frac{1}{2}, \gamma; x\right), \quad (101)$$

provided that α or β is equal to one of the numbers $-\frac{1}{2}, -\frac{3}{2}, \ldots \frac{1}{2}+\left[\frac{\gamma}{2}\right]$. Furthermore

$$f\left(2\alpha, 2\beta, \gamma; \frac{1-\sqrt{1-x}}{2}\right) = f(\alpha, \beta, \gamma; x), \quad (102)$$

provided that α or β is equal to one of the numbers $0, -1, -2, \ldots -\left[\frac{|\gamma|}{2}\right]$. Finally, we have two expansions proceeding in descending powers of x

$$f\left(2\alpha, 2\beta, \gamma; \frac{1-\sqrt{1-x}}{2}\right) = \frac{\Gamma\left(\frac{1}{2}-\beta\right)\Gamma(1-\beta)}{\Gamma(1-\gamma)\,\Gamma(\alpha-\beta+1)}(-x)^{-\alpha}F\left(\alpha, \frac{1}{2}-\beta, \alpha-\beta+1; \frac{1}{x}\right),$$

when $2\alpha = 0, -1, -2, \ldots \gamma$ and

$$f\left(2\alpha, 2\beta, \gamma; \frac{1-\sqrt{1-x}}{2}\right) = \frac{\Gamma\left(\frac{1}{2}-\alpha\right)\Gamma(1-\alpha)}{\Gamma(1-\gamma)\,\Gamma(\beta-\alpha+1)}(-x)^{-\beta}F\left(\frac{1}{2}-\alpha, \beta, \beta-\alpha+1; \frac{1}{x}\right),$$

when $2\beta = 0, -1, -2, \ldots \gamma$.

§ 15. Some special cases may be set down. Putting $x = 1$ in (94), we get

$$F\left(2\alpha, 2\beta, \alpha+\beta+\frac{1}{2}; \frac{1}{2}\right) = \frac{\Gamma\left(\alpha+\beta+\frac{1}{2}\right)\sqrt{\pi}}{\Gamma\left(\alpha+\frac{1}{2}\right)\Gamma\left(\beta+\frac{1}{2}\right)}. \tag{103}$$

Putting $z = -1$ in (81), we obtain

$$F(2\alpha, 2\alpha-\gamma+1, \gamma; -1) = \frac{2^{-2\alpha}\Gamma(\gamma)\sqrt{\pi}}{\Gamma\left(\alpha+\frac{1}{2}\right)\Gamma(\gamma-\alpha)}, \quad \gamma \neq 0, -1, -2, \ldots \tag{104}$$

The first of these formulae is due to GAUSS and the second is due to KUMMER. If we apply the transformation (28) on the left side of Gauss' formula we obtain

$$F\left(\alpha, 1-\alpha, \gamma; \frac{1}{2}\right) = \frac{2^{1-\gamma}\Gamma(\gamma)\sqrt{\pi}}{\Gamma\left(\frac{\alpha+\gamma}{2}\right)\Gamma\left(\frac{\gamma-\alpha+1}{2}\right)}, \quad \gamma \neq 0, -1, -2, \ldots \tag{105}$$

If γ is a negative integer and either α or β is equal to one of the numbers $0, -1, -2, \ldots \gamma$. we have for the rational solution as shown in § 8

$$f(\alpha, \beta, \gamma; 1) = \frac{\Gamma(\alpha-\gamma+1)\,\Gamma(\beta-\gamma+1)}{\Gamma(1-\gamma)\,\Gamma(\alpha+\beta-\gamma+1)}.$$

If $\gamma = \alpha+\beta+\frac{1}{2}$, we get from (102) and (101)

$$f\left(2\alpha, 2\beta, \gamma; \frac{1}{2}\right) = \frac{\Gamma\left(\frac{1}{2}-\alpha\right)\Gamma\left(\frac{1}{2}-\beta\right)}{\Gamma(1-\gamma)\,\Gamma\left(\frac{1}{2}\right)},$$

when α or $\beta = 0, -1, -2, \ldots -\left[\frac{|\gamma|}{2}\right]$, and

$$f\left(2\alpha, 2\beta, \gamma; \frac{1}{2}\right) = 0,$$

when α or $\beta = -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, \ldots \frac{1}{2} + \left[\frac{\gamma}{2}\right]$. Putting $z = -1$ in (87) and (86), we obtain

$$f(2\alpha, 2\alpha - \gamma + 1, \gamma; -1) = \frac{\Gamma(\alpha - \gamma + 1)\,\Gamma\left(\frac{1}{2} - \alpha\right)}{\Gamma(1-\gamma)\,\Gamma\left(\frac{1}{2}\right) 2^{2\alpha}},$$

when α is a non-positive integer $> \frac{\gamma}{2}$, and

$$f(2\alpha, 2\alpha - \gamma + 1, \gamma; -1) = \frac{\Gamma(\alpha - \gamma + 1)\,\Gamma\left(\frac{1}{2} - \alpha\right)}{\Gamma(1-\gamma)\,\Gamma\left(\frac{1}{2}\right) 2^{2\alpha+1}},$$

when α has any of the values $\frac{\gamma-1}{2}, \frac{\gamma-2}{2}, \frac{\gamma-3}{2}, \ldots \gamma - \frac{1}{2}$. Applying the transformation (43), we get from the last-mentioned formula

$$f\left(\alpha, 1-\alpha, \gamma; \frac{1}{2}\right) = \frac{\Gamma\left(1 - \frac{\alpha+\gamma}{2}\right)\Gamma\left(\frac{\alpha-\gamma+1}{2}\right)}{\Gamma(1-\gamma)\,\Gamma\left(\frac{1}{2}\right) 2^{\gamma}},$$

provided that α is an integer and $\gamma < \alpha < 1 - \gamma$, γ as before being a negative integer.

In the following formulae for the logarithmic solutions γ is a positive integer. If $\gamma = \alpha + \beta + \frac{1}{2}$, we get from (96)

$$g\left(2\alpha, 2\beta, \gamma; \frac{1}{2}\right) = \frac{(-1)^{\gamma}}{2\sqrt{\pi}}\,\Gamma(\gamma)\,\Gamma\left(\frac{1}{2} - \alpha\right)\Gamma\left(\frac{1}{2} - \beta\right),$$

provided that $2\alpha \neq 0, \pm 1, \pm 2, \ldots$ Putting $x = 1$ in (98), we obtain

$$G\left(2\alpha, 2\beta, \gamma; \frac{1}{2}\right) = \frac{\Gamma(\gamma)\sqrt{\pi}}{\Gamma\left(\alpha + \frac{1}{2}\right)\Gamma\left(\beta + \frac{1}{2}\right)}\left[\Psi(\gamma) + \Psi(1) - \Psi\left(\alpha + \frac{1}{2}\right) - \Psi\left(\beta + \frac{1}{2}\right) - \log 4 - \sum_{s=1}^{2\gamma-2} \frac{(-1)^s}{2\alpha - s}\right],$$

provided that $2\alpha \neq 1, 2, 3, \ldots 2\gamma - 2$.

If we let $z \to -1$ in (82), we get

$$2^{2\alpha} G(2\alpha, 2\alpha-\gamma+1, \gamma; -1 \pm io) = G\left(\alpha, \gamma-\alpha-\frac{1}{2}, \gamma; 1\right) - C_1 F\left(\alpha, \gamma-\alpha-\frac{1}{2}, \gamma; 1\right).$$

Using (54) we find that

$$\left.\begin{aligned} G(2\alpha, 2\alpha-\gamma+1, \gamma; -1 \pm io) = \frac{\Gamma(\gamma)\sqrt{\pi}\, 2^{-2\alpha}}{\Gamma\left(\alpha+\frac{1}{2}\right)\Gamma(\gamma-\alpha)} \Bigg[\Psi(\gamma)+\Psi(1)-\Psi\left(\alpha+\frac{1}{2}\right) \\ -\Psi(1-\alpha)-\log 4 \pm \pi i + \sum_{s=1}^{\gamma-1} \frac{1}{2\alpha-s} \Bigg], \end{aligned}\right\} \quad (106)$$

if $2\alpha \neq 1, 2, 3, \ldots 2\gamma-2$. Substituting this value in (20) and using (104), we obtain, after some manipulations

$$g(2\alpha, 2\alpha-\gamma+1, \gamma; -1 \pm io) = (-1)^{\gamma} \frac{\Gamma(\gamma)\Gamma(\alpha-\gamma+1)\sqrt{\pi}}{\Gamma\left(\alpha+\frac{1}{2}\right)2^{2\alpha}} e^{\pm \pi i \alpha},$$

provided that 2α is not an integer $< 2\gamma-1$. This result could also be obtained from (83). At the point -1 the difference of the values on the opposite edges of the cross-cut from 0 to $-\infty$ is thus

$$G(2\alpha, 2\alpha-\gamma+1, \gamma; -1+io) - G(2\alpha, 2\alpha-\gamma+1, \gamma; -1-io) = g(2\alpha, 2\alpha-\gamma+1, \gamma; -1+io) - g(2\alpha, 2\alpha-\gamma+1, \gamma; -1-io) - \frac{\Gamma(\gamma)\sqrt{\pi}\, 2^{-2\alpha} 2\pi i}{\Gamma\left(\alpha+\frac{1}{2}\right)\Gamma(\gamma-\alpha)}.$$

Using (30), (104), and (106) we find that

$$G\left(\alpha, 1-\alpha, \gamma; \frac{1}{2}\right) = \frac{\Gamma(\gamma)\sqrt{\pi}\, 2^{1-\gamma}}{\Gamma\left(\frac{\alpha+\gamma}{2}\right)\Gamma\left(\frac{\gamma-\alpha+1}{2}\right)} \left[\Psi(\gamma)+\Psi(1)-2\Psi(\alpha)+\pi \operatorname{tg} \pi\left(\frac{\alpha+\gamma}{2}\right)\right],$$

provided that $\alpha \neq 0, \pm 1, \pm 2, \ldots \pm(\gamma-2), \gamma-1$. From this formula we get, using (20),

$$g\left(\alpha, 1-\alpha, \gamma; \frac{1}{2}\right) = \frac{(-1)^{\gamma}}{\sqrt{\pi}} \Gamma(\gamma)\Gamma\left(1-\frac{\alpha+\gamma}{2}\right)\Gamma\left(\frac{\alpha-\gamma+1}{2}\right)2^{-\gamma},$$

where α is not an integer. Again from (24), using (105), we obtain

$$g_1\left(\alpha,\ 1-\alpha,\ \gamma;\ \frac{1}{2}\pm io\right)=\frac{\Gamma(\gamma)\sqrt{\pi}\,\Gamma\left(1-\frac{\alpha+\gamma}{2}\right)}{2^{\gamma-1}\,\Gamma\left(\frac{\gamma-\alpha+1}{2}\right)}\,e^{\mp\frac{\pi i\,(\alpha+\gamma)}{2}},$$

under the condition that $\alpha+\gamma-1$ is not a positive integer. It follows that

$$g_1\left(\alpha,\ 1-\alpha,\ \gamma;\ \frac{1}{2}+io\right)-g_1\left(\alpha,\ 1-\alpha,\ \gamma;\ \frac{1}{2}-io\right)=-\frac{\Gamma(\gamma)\sqrt{\pi}\,2^{1-\gamma}\,2\pi i}{\Gamma\left(\frac{\alpha+\gamma}{2}\right)\Gamma\left(\frac{\gamma-\alpha+1}{2}\right)}.$$

Chapter III

Riemann's Differential Equation

§ 16. We now consider the exceptional solutions of the differential equation for Riemann's P-function

$$\frac{d^2y}{dz^2}+\left(\frac{1-\alpha-\alpha'}{z}-\frac{1-\gamma-\gamma'}{1-z}\right)\frac{dy}{dz}+\left(\frac{\alpha\alpha'}{z}+\frac{\gamma\gamma'}{1-z}-\beta\beta'\right)\frac{y}{z(1-z)}=0, \tag{1}$$

where $\alpha+\alpha'+\beta+\beta'+\gamma+\gamma'=1$. The interrelations of the fundamental solutions can of course in this case be written in a shorter form. If $\alpha-\alpha'$ is not an integer, (1) admits near $z=0$ the linearly independent solutions

$$P^{\alpha}=z^{\alpha}\,(1-z)^{\gamma}\,F(\alpha+\beta+\gamma,\ \alpha+\beta'+\gamma,\ \alpha-\alpha'+1;\ z),$$
$$P^{\alpha'}=z^{\alpha'}(1-z)^{\gamma}\,F(\alpha'+\beta+\gamma,\ \alpha'+\beta'+\gamma,\ \alpha'-\alpha+1;\ z).$$

If $\gamma-\gamma'$ is not an integer, we have in the vicinity of $z=1$ the solutions

$$P^{\gamma}=(1-z)^{\gamma}\,z^{\alpha}\,F(\alpha+\beta+\gamma,\ \alpha+\beta'+\gamma,\ \gamma-\gamma'+1;\ 1-z),$$
$$P^{\gamma'}=(1-z)^{\gamma'}\,z^{\alpha}\,F(\alpha+\beta+\gamma',\ \alpha+\beta'+\gamma',\ \gamma'-\gamma+1;\ 1-z).$$

If $\beta-\beta'$ is non-integer, (1) has for $|z|>1$ the solutions

$$P^{\beta}=z^{-\beta}\left(1-\frac{1}{z}\right)^{\gamma}F\left(\alpha+\beta+\gamma,\ \alpha'+\beta+\gamma,\ \beta-\beta'+1;\ \frac{1}{z}\right),$$
$$P^{\beta'}=z^{-\beta'}\left(1-\frac{1}{z}\right)^{\gamma}F\left(\alpha+\beta'+\gamma,\ \alpha'+\beta'+\gamma,\ \beta'-\beta+1;\ \frac{1}{z}\right).$$

We now put

$$Q_{\gamma}^{\alpha}=z^{\alpha}(1-z)^{\gamma}\,g(\alpha+\beta+\gamma,\ \alpha+\beta'+\gamma,\ \alpha-\alpha'+1;\ z), \tag{2}$$

$$p_{\gamma}^{\alpha}=z^{\alpha}(1-z)^{\gamma}\,f(\alpha+\beta+\gamma,\ \alpha+\beta'+\gamma,\ \alpha-\alpha'+1;\ z). \tag{3}$$

If we interchange γ and γ' in (2) and (3), we get $Q^{\alpha}_{\gamma'}$ and $p^{\alpha}_{\gamma'}$. If we interchange in (2) and (3) α and γ, z and $1-z$, we get Q^{γ}_{α} and p^{γ}_{α}. Finally, interchanging α and β, z and $\frac{1}{z}$ in (2) and (3), we get Q^{β}_{γ} and p^{β}_{γ}.

In a similar way we put

$$R^{\alpha}_{\beta} = z^{\alpha}(1-z)^{\gamma} g_1(\alpha+\beta+\gamma,\ \alpha+\beta'+\gamma,\ \alpha-\alpha'+1;\ z). \tag{4}$$

If we interchange β and β' in (4), we get $R^{\alpha}_{\beta'}$. If we interchange in (4) α and γ, z and $1-z$, we get R^{γ}_{β}. Finally, interchanging α and β, z and $\frac{1}{z}$ in (4) we get R^{β}_{α}. For brevity's sake we shall write

$$\alpha_{\gamma} = \frac{\Gamma(\alpha-\alpha'+1)\,\Gamma(\gamma'-\gamma)}{\Gamma(\alpha+\beta+\gamma')\,\Gamma(\alpha+\beta'+\gamma')},$$

$$\dot{\alpha}_{\gamma} = (-1)^{\alpha-\alpha'+1}\frac{\Gamma(\alpha'+\beta+\gamma)\,\Gamma(\alpha'+\beta'+\gamma)\,\Gamma(\alpha-\alpha'+1)}{\Gamma(\gamma-\gamma'+1)}.$$

The other constants follow from these by interchange of letters, for example

$$\gamma_{\alpha} = \frac{\Gamma(\gamma-\gamma'+1)\,\Gamma(\alpha'-\alpha)}{\Gamma(\alpha'+\beta+\gamma)\,\Gamma(\alpha'+\beta'+\gamma)},$$

$$\dot{\gamma}_{\alpha} = (-1)^{\gamma-\gamma'+1}\frac{\Gamma(\alpha+\beta+\gamma')\,\Gamma(\alpha+\beta'+\gamma')\,\Gamma(\gamma-\gamma'+1)}{\Gamma(\alpha-\alpha'+1)}.$$

If $\alpha-\alpha'$ equals a positive integer p, (1) admits the solutions P^{α} and Q^{α}_{γ}, provided that $\alpha+\beta+\gamma$ and $\alpha+\beta'+\gamma \neq p,\ p-1,\ p-2,\ \ldots$ But if $\alpha+\beta+\gamma$ or $\alpha+\beta'+\gamma = 1, 2, \ldots p$, we have the linearly independent solutions P^{α} and $p^{\alpha'}_{\gamma}$. Similarly for the other cases.

The continuation formulae now take the following form

1. $\gamma-\gamma' = q$, $\quad \alpha-\alpha'$ not an integer.

$$\dot{\gamma}_{\alpha}\,P^{\alpha} = Q^{\gamma}_{\alpha}, \qquad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta'+\gamma \neq q,\ q-1,\ q-2,\ \ldots \tag{1}$$

$$\dot{\gamma}_{\alpha'}\,P^{\alpha'} = Q^{\gamma}_{\alpha'}, \qquad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta'+\gamma \neq 1, 2, 3, \ldots \tag{2}$$

$$\gamma_{\alpha}\,P^{\alpha} = P^{\gamma}, \qquad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = 0, -1, -2, \ldots \tag{3}$$

$$\gamma_{\alpha'}\,P^{\alpha'} = P^{\gamma}, \qquad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = q+1, q+2, q+3, \ldots \tag{4}$$

$$P^{\alpha} = \alpha_{\gamma'}\,p^{\gamma'}_{\alpha}, \qquad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = 1, 2, \ldots q \tag{5}$$

$$P^{\alpha'} = \alpha'_{\gamma'}\,p^{\gamma'}_{\alpha'}, \qquad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = 1, 2, \ldots q. \tag{6}$$

2. $\alpha - \alpha' = p, \quad \gamma - \gamma'$ not an integer.

$$P^{\alpha} = \alpha_{\gamma} P^{\gamma} + \alpha_{\gamma'} P^{\gamma'}, \tag{1}$$

$$Q^{\alpha}_{\gamma} = \dot{\alpha}_{\gamma} P^{\gamma}, \quad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta'+\gamma \neq p, p-1, p-2, \ldots \tag{2}$$

$$Q^{\alpha}_{\gamma'} = \dot{\alpha}_{\gamma'} P^{\gamma'}, \quad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta'+\gamma \neq 1, 2, 3, \ldots \tag{3}$$

$$P^{\alpha} = \alpha_{\gamma} P^{\gamma}, \quad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = 0, -1, -2, \ldots \tag{4}$$

$$P^{\alpha} = \alpha_{\gamma'} P^{\gamma'}, \quad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = p+1, p+2, p+3, \ldots \tag{5}$$

$$\gamma_{\alpha'} p^{\alpha'}_{\gamma} = P^{\gamma}, \quad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = 1, 2, \ldots p \tag{6}$$

$$\gamma'_{\alpha'} p^{\alpha'}_{\gamma'} = P^{\gamma'}, \quad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = 1, 2, \ldots p. \tag{7}$$

3. $\alpha - \alpha' = p, \quad \gamma - \gamma' = q.$

$$\dot{\gamma}_{\alpha} P^{\alpha} = Q^{\gamma}_{\alpha}, \quad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta'+\gamma \neq q, q-1, q-2, \ldots \tag{1}$$

$$Q^{\alpha}_{\gamma} = \dot{\alpha}_{\gamma} P^{\gamma}, \quad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta'+\gamma \neq p, p-1, p-2, \ldots \tag{2}$$

$$R^{\alpha}_{\beta} = e^{\mp \pi i (\alpha+\beta+\gamma)} \frac{\sin \pi (\alpha+\beta+\gamma)}{\pi} \dot{\alpha}_{\gamma} R^{\gamma}_{\beta}, \quad \alpha+\beta+\gamma \neq 1, 2, 3, \ldots \tag{3}$$

$$R^{\alpha}_{\beta'} = e^{\mp \pi i (\alpha+\beta'+\gamma)} \frac{\sin \pi (\alpha+\beta'+\gamma)}{\pi} \dot{\alpha}_{\gamma} R^{\gamma}_{\beta'}, \quad \alpha+\beta'+\gamma \neq 1, 2, 3, \ldots \tag{4}$$

$$P^{\alpha} = (-1)^n \frac{(q+1)_n}{(p+1)_n} P^{\gamma}, \quad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = -n, \; n = 0, 1, 2, \ldots \tag{5}$$

$$P^{\alpha} = \alpha_{\gamma'} p^{\gamma'}_{\alpha} \quad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = 1, 2, \ldots q \tag{6}$$

$$\gamma_{\alpha'} p^{\alpha'}_{\gamma} = P^{\gamma}, \quad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta'+\gamma = 1, 2, \ldots p. \tag{7}$$

4. $\beta - \beta' = m, \quad \alpha - \alpha'$ not an integer.

$$\dot{\beta}_{\alpha} P^{\alpha} = e^{\pm \pi i (\alpha+\beta)} R^{\beta}_{\alpha'}, \quad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta+\gamma' \neq m, m-1, m-2, \ldots \tag{1}$$

$$\dot{\beta}_{\alpha'} P^{\alpha'} = e^{\pm \pi i (\alpha'+\beta)} R^{\beta}_{\alpha}, \quad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta+\gamma' \neq 1, 2, 3, \ldots \tag{2}$$

$$\beta_{\alpha} P^{\alpha} = e^{\pm \pi i (\alpha+\beta)} P^{\beta}, \quad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta+\gamma' = 0, -1, -2, \ldots \tag{3}$$

$$\beta_{\alpha'} P^{\alpha'} = e^{\pm \pi i (\alpha'+\beta)} P^{\beta}, \quad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta+\gamma' = m+1, m+2, m+3, \ldots \tag{4}$$

$$P^{\alpha} = e^{\pm \pi i (\alpha+\beta')}\ \alpha_{\beta'}\ p^{\beta'}_{\gamma}, \qquad \alpha+\beta+\gamma = 1, 2, \ldots m \tag{5}$$

$$P^{\alpha} = e^{\pm \pi i (\alpha+\beta')}\ \alpha_{\beta'}\ p^{\beta'}_{\gamma'}, \qquad \alpha+\beta+\gamma' = 1, 2, \ldots m \tag{6}$$

$$P^{\alpha'} = e^{\pm \pi i (\alpha'+\beta')}\ \alpha'_{\beta'}\ p^{\beta'}_{\gamma}, \qquad \alpha+\beta+\gamma' = 1, 2, \ldots m \tag{7}$$

$$P^{\alpha'} = e^{\pm \pi i (\alpha'+\beta')}\ \alpha'_{\beta'}\ p^{\beta'}_{\gamma'}, \qquad \alpha+\beta+\gamma = 1, 2, \ldots m. \tag{8}$$

5. $\alpha - \alpha' = p, \quad \beta - \beta'$ not an integer.

$$P^{\alpha} = e^{\pm \pi i (\alpha+\beta)}\ \alpha_{\beta}\ P^{\beta} + e^{\pm \pi i (\alpha+\beta')}\ \alpha_{\beta'}\ P^{\beta'}, \tag{1}$$

$$R^{\alpha}_{\beta} = e^{\pm \pi i (\alpha+\beta')}\ \dot{\alpha}_{\beta'}\ P^{\beta'}, \qquad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta+\gamma' \neq 1, 2, 3, \ldots \tag{2}$$

$$R^{\alpha}_{\beta'} = e^{\pm \pi i (\alpha+\beta)}\ \dot{\alpha}_{\beta}\ P^{\beta}, \qquad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta+\gamma' \neq p, p-1, p-2, \ldots \tag{3}$$

$$P^{\alpha} = e^{\pm \pi i (\alpha+\beta)}\ \alpha_{\beta}\ P^{\beta}, \qquad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta+\gamma' = 0, -1, -2, \ldots \tag{4}$$

$$P^{\alpha} = e^{\pm \pi i (\alpha+\beta')}\ \alpha_{\beta'}\ P^{\beta'}, \qquad \alpha+\beta+\gamma \quad \text{or} \quad \alpha+\beta+\gamma' = p+1, p+2, p+3, \ldots \tag{5}$$

$$\beta_{\alpha'}\ p^{\alpha'}_{\gamma} = e^{\pm \pi i (\alpha'+\beta)}\ P^{\beta}, \qquad \alpha+\beta+\gamma = 1, 2, \ldots p \tag{6}$$

$$\beta'_{\alpha'}\ p^{\alpha'}_{\gamma} = e^{\pm \pi i (\alpha'+\beta')}\ P^{\beta'}, \qquad \alpha+\beta+\gamma' = 1, 2, \ldots p \tag{7}$$

$$\beta'_{\alpha'}\ p^{\alpha'}_{\gamma'} = e^{\pm \pi i (\alpha'+\beta')}\ P^{\beta'}, \qquad \alpha+\beta+\gamma = 1, 2, \ldots p \tag{8}$$

$$\beta_{\alpha'}\ p^{\alpha'}_{\gamma'} = e^{\pm \pi i (\alpha'+\beta)}\ P^{\beta}, \qquad \alpha+\beta+\gamma' = 1, 2, \ldots p. \tag{9}$$

6. $\alpha - \alpha' = p, \quad \beta - \beta' = m.$

$$\beta_{\alpha}\ P^{\alpha} = e^{\pm \pi i (\alpha+\beta)}\ R^{\beta}_{\alpha'}, \qquad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta+\gamma' \neq m, m-1, m-2, \ldots \tag{1}$$

$$R^{\alpha}_{\beta'} = e^{\pm \pi i (\alpha+\beta)}\ \dot{\alpha}_{\beta}\ P^{\beta}, \qquad \alpha+\beta+\gamma \quad \text{and} \quad \alpha+\beta+\gamma' \neq p, \ p-1, \ p-2, \ldots \tag{2}$$

$$Q^{\alpha}_{\gamma} = -\frac{e^{\mp \pi i \gamma}}{\pi}\ \sin \pi (\alpha+\beta+\gamma)\ \dot{\alpha}_{\beta}\ Q^{\beta}_{\gamma}, \qquad \alpha+\beta+\gamma' \neq 1, 2, 3, \ldots \tag{3}$$

$$Q^{\alpha}_{\gamma'} = -\frac{e^{\mp \pi i \gamma'}}{\pi} \sin \pi (\alpha'+\beta'+\gamma')\ \dot{\alpha}_{\beta}\ Q^{\beta}_{\gamma'}, \qquad \alpha+\beta+\gamma \neq 1, 2, 3, \ldots \tag{4}$$

$$P^{\alpha} = e^{\mp \pi i \gamma}\ \frac{(m+1)_n}{(p+1)_n}\ P^{\beta}, \qquad \alpha'+\beta'+\gamma' = 1+n, \ n = 0, 1, 2, \ldots \tag{5}$$

$$P^{\alpha} = e^{\mp \pi i \gamma'}\ \frac{(m+1)_n}{(p+1)_n}\ P^{\beta}, \qquad \alpha'+\beta'+\gamma = 1+n, \ n = 0, 1, 2, \ldots \tag{6}$$

$$\beta_{\alpha'}\, p_{\gamma}^{\alpha'} = e^{\pm \pi i\,(\alpha'+\beta)}\, P^{\beta}, \qquad \alpha+\beta+\gamma = 1, 2, \ldots p \tag{7}$$

$$P^{\alpha} = e^{\pm \pi i\,(\alpha+\beta')}\, \alpha_{\beta'}\, p_{\gamma}^{\beta'}, \qquad \alpha+\beta+\gamma = 1, 2, \ldots m \tag{8}$$

$$P^{\alpha} = e^{\pm \pi i\,(\alpha+\beta')}\, \alpha_{\beta'}\, p_{\gamma'}^{\beta'}, \qquad \alpha+\beta+\gamma' = 1, 2, \ldots m \tag{9}$$

$$\left.\begin{aligned} p_{\gamma}^{\alpha'} &= e^{\mp \pi i \gamma}\, \frac{\Gamma(\alpha+\beta'+\gamma)}{\Gamma(\alpha'+\beta+\gamma)}\, \frac{\Gamma(m)}{\Gamma(p)}\, p_{\gamma}^{\beta'}, \\ &\text{provided that} \quad \alpha+\beta+\gamma = p+1,\ p+2, \ldots p+m \quad \text{if} \quad p \geq m \\ &\qquad\qquad\quad \alpha+\beta+\gamma = m+1,\ m+2, \ldots m+p \quad \text{if} \quad p < m. \end{aligned}\right\} \tag{10}$$

Chapter IV

Confluent Hypergeometric Functions

§ 17. The solutions of KUMMER's differential equation

$$z\,\frac{d^2y}{dz^2} + (\gamma - z)\,\frac{dy}{dz} - \alpha y = 0 \tag{1}$$

have been considered in recent papers by F. G. TRICOMI [38–40] and L. J. SLATER [33], to which we may refer the reader.

Using the familiar method of FROBENIUS we put

$$y = \sum_{s=0}^{\infty} c_s(\varrho)\, z^{\varrho+s}. \tag{2}$$

Substitution into the equation (1) yields the identity

$$\varrho\,(\varrho+\gamma-1)\,c_0(\varrho)\,z^{\varrho-1} + \sum_{s=0}^{\infty} [(\varrho+s+1)\,(\varrho+\gamma+s)\,c_{s+1}(\varrho) - (\varrho+\alpha+s)\,c_s(\varrho)]\,z^{\varrho+s} = 0.$$

If we determine the $c_s(\varrho)$'^{s} such that

$$(\varrho+1+s)\,(\varrho+\gamma+s)\,c_{s+1}(\varrho) = (\varrho+\alpha+s)\,c_s(\varrho), \qquad s = 0, 1, 2, \ldots, \tag{3}$$

the series (2) will be a solution of the non-homogeneous equation

$$z\,\frac{d^2y}{dz^2} + (\gamma - z)\,\frac{dy}{dz} - \alpha y = \varrho\,(\varrho+\gamma-1)\,c_0(\varrho)\,z^{\varrho-1}. \tag{4}$$

From (3) we get

$$c_s(\varrho) = \frac{(\varrho+\alpha)_s}{(\varrho+1)_s\,(\varrho+\gamma)_s}\, c_0(\varrho), \qquad s = 1, 2, 3, \ldots \tag{5}$$

By setting $\varrho = 0$ or $\varrho = 1 - \gamma$ and taking $c_0 = 1$ we see that (1) has the solutions

$$\sum_{s=0}^{\infty} \frac{(\alpha)_s z^s}{s!\,(\gamma)_s} = \Phi(\alpha, \gamma; z) \tag{6}$$

and

$$z^{1-\gamma}\,\Phi(\alpha - \gamma + 1, 2 - \gamma; z), \tag{7}$$

where $\Phi(\alpha, \gamma; z)$ is KUMMER's function. If γ is nonintegral, both of these solutions are applicable, and they are linearly independent. If $\gamma = 1$, the two solutions become identical, and if γ tends to an integer different from 1, one of them becomes meaningless.

1°. We suppose, first, that γ is an integer < 1 and that α is equal to one of the numbers $0, -1, -2, \ldots \gamma$. Setting $\varrho = 0$ the equations (3) leave c_0 and $c_{1-\gamma}$ indeterminate and (1) has the solution

$$c_0 \sum_{s=0}^{-\alpha} \frac{(\alpha)_s z^s}{s!\,(\gamma)_s} + c_{1-\gamma} z^{1-\gamma} \sum_{s=0}^{\infty} \frac{(\alpha - \gamma + 1)_s z^s}{s!\,(2 - \gamma)_s},$$

where c_0 and $c_{1-\gamma}$ are arbitrary constants. For brevity's sake we put

$$\varphi(\alpha, \gamma; z) = \sum_{s=0}^{-\alpha} \frac{(\alpha)_s z^s}{s!\,(\gamma)_s}. \tag{8}$$

Besides (7) we then have the rational solution $\varphi(\alpha, \gamma; z)$.

2°. Next, we suppose that γ is an integer > 1, and that α is a positive integer $< \gamma$. Taking $\varrho = 1 - \gamma$ the equations (3) leave c_0 and $c_{\gamma-1}$ indeterminate. It follows that (1) has the solution

$$c_0 z^{1-\gamma} \sum_{s=0}^{\gamma-\alpha-1} \frac{(\alpha - \gamma + 1)_s z^s}{s!\,(2 - \gamma)_s} + c_{\gamma-1} \sum_{s=0}^{\infty} \frac{(\alpha)_s z^s}{s!\,(\gamma)_s},$$

containing the arbitrary constants c_0 and $c_{\gamma-1}$. Besides KUMMER's function (6) we then have the rational solution $z^{1-\gamma}\varphi(\alpha - \gamma + 1, 2 - \gamma; z)$.

3°. Now it is assumed that γ is a positive integer, and that $\alpha \neq 1, 2, 3, \ldots \gamma - 1$. Putting $\varrho = 1 - \gamma$, we can give $c_{\gamma-1}$ any value and we get again the solution (6). The two roots of the indicial equation then give the same solution. To get a second solution we observe that, if we take $c_{\gamma-1} = 1$, it follows from (3) that

$$c_{s+\gamma-1}(\varrho) = \frac{(\varrho + \alpha + \gamma - 1)_s}{(\varrho + \gamma)_s (\varrho + 2\gamma - 1)_s}, \quad s \geq 1 - \gamma.$$

These functions are all regular at the point $\varrho = 1 - \gamma$. Particularly putting $s = 1 - \gamma$ we obtain

$$c_0(\varrho) = \frac{(\varrho + 1)(\varrho + 2) \ldots (\varrho + 2\gamma - 2)}{(\varrho + \alpha)(\varrho + \alpha + 1) \ldots (\varrho + \alpha + \gamma - 2)}.$$

It follows that $c_0(\varrho)$ has a zero of the first order at the point $\varrho = 1-\gamma$, and the right-hand side of (4) has consequently a zero of the second order at $\varrho = 1-\gamma$. The differential quotient of (2) is therefore a solution of (1), when $\varrho = 1-\gamma$. Hence, (1) has the solution

$$\left.\begin{aligned} G(\alpha, \gamma; z) = &\sum_{s=1}^{\gamma-1} (-1)^{s-1} (s-1)! \frac{(\alpha)_{-s}}{(\gamma)_{-s}} z^{-s} \\ &+ \sum_{s=0}^{\infty} \frac{(\alpha)_s z^s}{s!\,(\gamma)_s} ([\alpha, \gamma; s] + \log z), \end{aligned}\right\} \tag{9}$$

where for $s = 1, 2, 3, \ldots$

$$[\alpha, \gamma; s] = \sum_{r=0}^{s-1} \left(\frac{1}{\alpha+r} - \frac{1}{\gamma+r} - \frac{1}{1+r} \right),$$

and

$$[\alpha, \gamma; 0] = 0.$$

Here the first term on the right-hand side of (9) should be replaced by zero if $\gamma = 1$. The series on the right of (9) converges for all finite values of z different from zero.

Another solution is obtained if c_0 is chosen in the following manner:

$$c_0(\varrho) = \frac{\Gamma(\varrho+\alpha)}{\Gamma(\varrho+1)\,\Gamma(\varrho+\gamma)}.$$

From (5) it now follows that

$$c_s(\varrho) = \frac{\Gamma(\varrho+\alpha+s)}{\Gamma(\varrho+1+s)\,\Gamma(\varrho+\gamma+s)},$$

and consequently (1) has the solution

$$\left.\begin{aligned} g(\alpha, \gamma; z) = &\sum_{s=1}^{\gamma-1} (-1)^{s-1} (s-1)! \frac{(\alpha)_{-s}}{(\gamma)_{-s}} z^{-s} + \\ &\sum_{s=0}^{\infty} \frac{(\alpha)_s z^s}{s!\,(\gamma)_s} [\Psi(\alpha+s) - \Psi(\gamma+s) - \Psi(1+s) + \log z]. \end{aligned}\right\} \tag{10}$$

If α tends to a non-positive integer, (10) becomes meaningless as $\Psi(\alpha)$ has poles at $\alpha = 0, -1, -2, \ldots$ To remedy this inconvenience we also consider the case

$$c_0(\varrho) = \frac{1}{\Gamma(1-\varrho-\alpha)\,\Gamma(\varrho+1)\,\Gamma(\varrho+\gamma)}$$

and thus get a solution denoted $g_1(\alpha, \gamma; z)$ and defined by

$$\left.\begin{aligned} g_1(\alpha, \gamma; z) = &\sum_{s=1}^{\gamma-1} (-1)^{s-1} (s-1)! \frac{(\alpha)_{-s}}{(\gamma)_{-s}} z^{-s} + \\ &\sum_{s=0}^{\infty} \frac{(\alpha)_s z^s}{s!\,(\gamma)_s} [\Psi(1-\alpha-s) - \Psi(\gamma+s) - \Psi(1+s) + \log(-z)], \end{aligned}\right\} \tag{11}$$

where α is not a positive integer. The series (10) and (11) converge for all finite values of z different from zero.

4°. If γ is a non-positive integer and α is different from $0, -1, -2, \ldots \gamma$, it is seen in the same manner that (1) has the solutions (7) and $z^{1-\gamma} G(\alpha-\gamma+1, 2-\gamma; z)$.

§ 18. From the expansions in powers of z it follows immediately that the solutions defined in § 17 are connected by the following linear relations

$$g(\alpha, \gamma; z) = G(\alpha, \gamma; z) + [\Psi(\alpha) - \Psi(\gamma) - \Psi(1)]\, \Phi(\alpha, \gamma; z), \tag{12}$$

$$g_1(\alpha, \gamma; z) = G(\alpha, \gamma; z) + [\Psi(1-\alpha) - \Psi(\gamma) - \Psi(1) \mp \pi i]\, \Phi(\alpha, \gamma; z), \tag{13}$$

$$g_1(\alpha, \gamma; z) = g(\alpha, \gamma; z) + \frac{\pi e^{\mp \pi i \alpha}}{\sin \pi\alpha}\, \Phi(\alpha, \gamma; z). \tag{14}$$

For KUMMER's function we have

$$\frac{d^n}{dz^n}\, \Phi(\alpha, \gamma; z) = \frac{(\alpha)_n}{(\gamma)_n}\, \Phi(\alpha+n, \gamma+n; z).$$

Also

$$\frac{d^n}{dz^n}\, g(\alpha, \gamma; z) = \frac{(\alpha)_n}{(\gamma)_n}\, g(\alpha+n, \gamma+n; z),$$

$$\frac{d^n}{dz^n}\, [z^{\gamma-1} g(\alpha, \gamma; z)] = (-1)^n (1-\gamma)_n\, z^{\gamma-n-1} g(\alpha, \gamma-n; z),$$

as is obvious by differentiation of the power series.

In KUMMER's equation (1) let $y = e^z y_1$ and $z = -z_1$. This transformation carries (1) into

$$z_1 \frac{d^2 y_1}{dz_1^2} + (\gamma - z_1) \frac{dy_1}{dz_1} - (\gamma - \alpha)\, y_1 = 0.$$

It is of the same form as (1). It follows that (1) has the solutions $\Phi(\alpha, \gamma; z)$ and $e^z \Phi(\gamma-\alpha, \gamma; -z)$ if $\gamma \neq 0, -1, -2, \ldots$, and it is easily seen that these two solutions are connected by KUMMER's relation

$$\Phi(\alpha, \gamma; z) = e^z \Phi(\gamma-\alpha, \gamma; -z), \tag{15}$$

a limiting case of EULER's relation

$$F(\alpha, \beta, \gamma; z) = (1-z)^{-\beta} F\left(\gamma-\alpha, \beta, \gamma; \frac{z}{z-1}\right)$$

for the Gaussian hypergeometric function. Furthermore, if γ is an integer >1 and α is different from $1, 2, \ldots \gamma-1$, it follows that (1) has the solutions $\Phi(\alpha, \gamma; z)$, $G(\alpha, \gamma; z)$ and $e^z G(\gamma-\alpha, \gamma; -z)$. Among these three solutions there is a linear relation of the form

$$G(\alpha, \gamma; z) = C_1 e^z G(\gamma-\alpha, \gamma; -z) + C \Phi(\alpha, \gamma; z). \tag{16}$$

Multiply both sides by $z^{\gamma-1}$ and let $z \to 0$. We obtain $C_1 = 1$. Next, we expand e^z in powers of z and carry out the multiplication by G. If we equate the constant terms on both sides of (16), we obtain

$$C = \pm \pi i + \sum_{s=1}^{\gamma-1} \frac{1}{s} \frac{(1-\gamma)_s}{(1+\alpha-\gamma)_s},$$

which reduces to

$$C = \pm \pi i + \Psi(\alpha - \gamma + 1) - \Psi(\alpha)$$
$$= \pm \pi i + \sum_{s=1}^{\gamma-1} \frac{1}{s-\alpha}.$$

Thus (16) may be written

$$G(\alpha, \gamma; z) = e^z G(\gamma - \alpha, \gamma; -z) + \left(\pm \pi i + \sum_{s=1}^{\gamma-1} \frac{1}{s-\alpha} \right) \Phi(\alpha, \gamma; z), \tag{17}$$

the ambiguous sign being the same as the sign of $I(z)$. If $\gamma = 1$, (17) reduces to

$$G(\alpha, 1; z) = e^z G(1-\alpha, 1; -z) \pm \pi i \Phi(\alpha, 1; z). \tag{18}$$

If we equate the coefficients of z^n on both sides of (17), we obtain

$$\sum_{\nu=1}^{n} \frac{(-n)_\nu (\alpha)_\nu}{\nu! (\gamma)_\nu} [\alpha, \gamma; \nu] = n! \sum_{\nu=1}^{\gamma-1} \frac{(1-\gamma)_\nu}{(1-\alpha)_\nu (\nu)_{n+1}} +$$
$$\frac{(\gamma-\alpha)_n}{(\gamma)_n} \left([\gamma-\alpha, \gamma; n] + \sum_{s=1}^{\gamma-1} \frac{1}{\gamma-\alpha-s} \right).$$

If $\gamma = 1$, this formula reduces to

$$\sum_{\nu=1}^{n} \frac{(-n)_\nu (\alpha)_\nu}{(\nu!)^2} [\alpha, 1; \nu] = \frac{(1-\alpha)_n}{n!} [1-\alpha, 1; n].$$

Eliminating G between the equations (12), (13), and (17), we find that

$$g(\alpha, \gamma; z) = e^z g_1(\gamma - \alpha, \gamma; -z), \tag{19}$$

where γ is a positive integer and α is not an integer $< \gamma$.
Similarly we derive the formula

$$g_1(\alpha, \gamma; z) = e^z g(\gamma - \alpha, \gamma; -z), \tag{20}$$

provided that γ is a positive integer and $\alpha \neq 1, 2, 3, \ldots$ Using KUMMER's relation (15) we can also write (19) and (20) in the following manner:

$$g(\alpha, \gamma; z) = e^z g(\gamma - \alpha, \gamma; -z) - \frac{\pi e^{\mp \pi i \alpha}}{\sin \pi \alpha} \Phi(\alpha, \gamma; z), \tag{21}$$

$$g_1(\alpha, \gamma; z) = e^z g_1(\gamma - \alpha, \gamma; -z) + \frac{\pi e^{\mp \pi i \alpha}}{\sin \pi \alpha} \Phi(\alpha, \gamma; z), \tag{22}$$

provided that α is not an integer. For the logarithmic solution $g(\alpha, \gamma; z)$ (19) is the analogue of KUMMER's relation (15).

In the same manner we finally for the rational solution $\varphi(\alpha, \gamma; z)$ get the following relation[1]

$$\left.\begin{aligned} \varphi(\alpha, \gamma; z) &= e^z \varphi(\gamma - \alpha, \gamma; -z) \\ -(-1)^{\alpha-\gamma} \frac{\Gamma(\alpha-\gamma+1)\,\Gamma(1-\alpha)}{\Gamma(2-\gamma)\,\Gamma(1-\gamma)} z^{1-\gamma} &\Phi(\alpha-\gamma+1, 2-\gamma; z), \end{aligned}\right\} \quad (23)$$

if $\gamma = 0, -1, -2, \ldots$ and α is any of the numbers $0, -1, -2, \ldots \gamma$. When we replace γ by $2-\gamma$ and α by $\alpha-\gamma+1$, we obtain

$$\left.\begin{aligned} z^{1-\gamma} \varphi(\alpha-\gamma+1, 2-\gamma; z) &= e^z \varphi(1-\alpha, 2-\gamma; -z) \\ +(-1)^{\alpha} \frac{\Gamma(\alpha)\,\Gamma(\gamma-\alpha)}{\Gamma(\gamma)\,\Gamma(\gamma-1)} &\Phi(\alpha, \gamma; z), \end{aligned}\right\} \quad (24)$$

provided that γ is an integer >1 and α is one of the numbers $1, 2, \ldots \gamma-1$.

§ 19. For KUMMER's function we have the integral representation

$$\Phi(\alpha, \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\,\Gamma(\gamma-\alpha)} \int_0^1 e^{zt}\, t^{\alpha-1} (1-t)^{\gamma-\alpha-1}\, dt,$$

provided that $\Re(\gamma) > \Re(\alpha) > 0$. This follows at once by expanding e^{zt} in powers of zt and integrating term by term. A further solution is TRICOMI's function $\Psi(\alpha, \gamma; z)$ as defined by the Laplace integral

$$\Psi(\alpha, \gamma; z) = \frac{1}{\Gamma(\alpha)} \int_0^\infty e^{-zt}\, t^{\alpha-1} (1+t)^{\gamma-\alpha-1}\, dt, \quad (25)$$

if $\Re(\alpha) > 0$ and $\Re(z) > 0$. If we expand $(1+t)^{\gamma-\alpha-1}$ in powers of t, it is seen that this function admits the single asymptotic expansion[2]

$$\Psi(\alpha, \gamma; z) = \frac{1}{z^\alpha} \left[\sum_{\nu=0}^{n} \frac{(\alpha)_\nu (\alpha-\gamma+1)_\nu}{\nu!\,(-z)^\nu} + O(|z|^{-n-1}) \right] \quad (26)$$

valid in the sector $\frac{3\pi}{2} > \arg z > -\frac{3\pi}{2}$. From the Laplace-integral (25) we can easily deduce the Mellin-Barnes integral[3]

$$\Psi(\alpha, \gamma; z) = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} z^{-t} \frac{\Gamma(t)\,\Gamma(t-\gamma+1)\,\Gamma(\alpha-t)}{\Gamma(\alpha)\,\Gamma(\alpha-\gamma+1)}\, dt, \quad (27)$$

[1] Cf. WATSON, *Theory of Bessel Functions*, p. 103.
[2] See Erdélyi [7, p. 278].
[3] Cf. Erdélyi [7, p. 256].

provided that $\alpha \neq 0, -1, -2, \ldots$; $\alpha - \gamma \neq -1, -2, -3, \ldots$ and $|\arg z| < \frac{3\pi}{2}$. The path of integration is a line parallel to the imaginary axis, except that it is curved, if necessary, so that the decreasing sequences of poles lie to the left, and the increasing sequences of poles to the right of it. Let now $\Re(z) > 0$. Put $ze^{\pm \pi i}$ for z in (27) and multiply both sides by $e^{\pm \pi i \alpha}$. From the two equations thus obtained we get by subtraction

$$\Psi(\alpha, \gamma; z) = \frac{e^z}{2\pi i} \int_{\lambda - i\infty}^{\lambda + i\infty} z^{-t} \frac{\Gamma(t)\,\Gamma(t - \gamma + 1)}{\Gamma(t + \alpha - \gamma + 1)}\, dt, \tag{28}$$

where the poles lie to the left of the contour. The formula (28) has the advantage that there is no restriction upon the parameters. For the solution $e^z \Psi(\gamma - \alpha, \gamma; -z)$ we get from (28)

$$e^z \Psi(\gamma - \alpha, \gamma; -z) = \frac{1}{2\pi i} \int_{\lambda - i\infty}^{\lambda + i\infty} (-z)^{-t} \frac{\Gamma(t)\,\Gamma(t - \gamma + 1)}{\Gamma(t - \alpha + 1)}\, dt. \tag{29}$$

Evaluating the integrals on the right of (28) and (29) as $2\pi i$ times the sum of the residues at the poles, the following linear relations between the solutions are obtained (see Erdélyi [7, p. 259]):

$$\left.\begin{aligned} \Psi(\alpha, \gamma; z) &= \frac{\Gamma(1 - \gamma)}{\Gamma(\alpha - \gamma + 1)} \Phi(\alpha, \gamma; z) \\ &+ \frac{\Gamma(\gamma - 1)}{\Gamma(\alpha)} z^{1-\gamma} \Phi(\alpha - \gamma + 1, 2 - \gamma; z), \quad \gamma \neq 0, \pm 1, \pm 2, \ldots \end{aligned}\right\} \tag{30}$$

$$\left.\begin{aligned} \Phi(\alpha, \gamma; z) &= e^{\pm \pi i \alpha} \frac{\Gamma(\gamma)}{\Gamma(\gamma - \alpha)} \Psi(\alpha, \gamma; z) \\ &+ e^{\pm \pi i (\alpha - \gamma)} \frac{\Gamma(\gamma)}{\Gamma(\alpha)} e^z \Psi(\gamma - \alpha, \gamma; -z), \quad \gamma \neq 0, -1, -2, \ldots \end{aligned}\right\} \tag{31}$$

$$\left.\begin{aligned} z^{1-\gamma} \Phi(\alpha - \gamma + 1, 2 - \gamma; z) &= -e^{\pm \pi i (\alpha - \gamma)} \frac{\Gamma(2 - \gamma)}{\Gamma(1 - \alpha)} \Psi(\alpha, \gamma; z) \\ &+ e^{\pm \pi i (\alpha - \gamma)} \frac{\Gamma(2 - \gamma)}{\Gamma(\alpha - \gamma + 1)} e^z \Psi(\gamma - \alpha, \gamma; -z), \quad \gamma \neq 2, 3, 4, \ldots \end{aligned}\right\} \tag{32}$$

$$\left.\begin{aligned} g(\alpha, \gamma; z) &= (-1)^\gamma \Gamma(\gamma)\,\Gamma(\alpha - \gamma + 1)\,\Psi(\alpha, \gamma; z), \\ \gamma &= 1, 2, 3, \ldots \quad \alpha \neq \gamma - 1, \gamma - 2, \gamma - 3, \ldots \end{aligned}\right\} \tag{33}$$

$$\left.\begin{aligned} g_1(\alpha, \gamma; z) &= (-1)^\gamma \Gamma(\gamma)\,\Gamma(1 - \alpha)\, e^z \Psi(\gamma - \alpha, \gamma; -z), \\ \gamma &= 1, 2, 3, \ldots \quad \alpha \neq 1, 2, 3, \ldots \end{aligned}\right\} \tag{34}$$

$$\left.\begin{aligned} z^{1-\gamma} g(\alpha - \gamma + 1, 2 - \gamma; z) &= (-1)^\gamma \Gamma(\alpha)\,\Gamma(2 - \gamma)\,\Psi(\alpha, \gamma; z), \\ \gamma &= 1, 0, -1, -2, \ldots \quad \alpha \neq 0, -1, -2, \ldots \end{aligned}\right\} \tag{35}$$

$$\left.\begin{array}{c} z^{1-\gamma}\, g_1(\alpha-\gamma+1,\, 2-\gamma;\, z) = -\,\Gamma(\gamma-\alpha)\,\Gamma(2-\gamma)\, e^z\, \Psi(\gamma-\alpha,\, \gamma;\, -z), \\ \gamma = 1,\, 0,\, -1,\, -2,\, \ldots \quad \alpha \neq \gamma,\, \gamma+1,\, \gamma+2,\, \ldots \end{array}\right\} \tag{36}$$

To these seven relations we shall add the following two

$$\left.\begin{array}{c} (-1)^{\alpha}\,(\gamma)_{\alpha}\, \varphi(\alpha,\, \gamma;\, z) = \Psi(\alpha,\, \gamma;\, z), \\ \gamma = 0,\, -1,\, -2,\, \ldots \quad \alpha = 0,\, -1,\, -2,\, \ldots \gamma, \end{array}\right\} \tag{37}$$

$$\left.\begin{array}{c} (\alpha)_{\gamma-\alpha-1}\, z^{1-\gamma}\, \varphi(\alpha-\gamma+1,\, 2-\gamma;\, z) = \Psi(\alpha,\, \gamma;\, z), \\ \gamma = 2,\, 3,\, 4,\, \ldots \quad \alpha = 1,\, 2,\, 3,\, \ldots \gamma-1. \end{array}\right\} \tag{38}$$

Substituting (26) in (33), we get the asymptotic expansion

$$g(\alpha,\, \gamma;\, z) \sim (-1)^{\gamma}\, \frac{\Gamma(\gamma)\,\Gamma(\alpha-\gamma+1)}{z^{\alpha}} \sum_{\nu=0}^{\infty} \frac{(\alpha)_{\nu}\,(\alpha-\gamma+1)_{\nu}}{\nu!\,(-z)^{\nu}}, \tag{39}$$

valid in the sector $\frac{3\pi}{2} > \arg z > -\frac{3\pi}{2}$. From (20) and (39) it now follows that

$$g_1(\alpha,\, \gamma;\, z) \sim (-1)^{\gamma}\, \frac{\Gamma(\gamma)\,\Gamma(1-\alpha)}{(-z)^{\gamma-\alpha}}\, e^z \sum_{\nu=0}^{\infty} \frac{(\gamma-\alpha)_{\nu}\,(1-\alpha)_{\nu}}{\nu!\, z^{\nu}}, \tag{40}$$

provided that $|\arg(-z)| < \frac{3\pi}{2}$. The asymptotic behavior of $g_1(\alpha,\, \gamma;\, z)$ is thus quite different from that of $g(\alpha,\, \gamma;\, z)$. From (31) we obtain for KUMMER's function the well-known asymptotic expansion

$$\left.\begin{array}{l} \Phi(\alpha,\, \gamma;\, z) \sim \dfrac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)} \displaystyle\sum_{\nu=0}^{\infty} \frac{(\alpha)_{\nu}\,(\alpha-\gamma+1)_{\nu}}{\nu!\,(-z)^{\alpha+\nu}} \\ \qquad\qquad + \dfrac{\Gamma(\gamma)}{\Gamma(\alpha)}\, e^z \displaystyle\sum_{\nu=0}^{\infty} \frac{(\gamma-\alpha)_{\nu}\,(1-\alpha)_{\nu}}{\nu!\, z^{\gamma-\alpha+\nu}}. \end{array}\right\} \tag{41}$$

Now use this result on the right of (12) and we get

$$G(\alpha,\, \gamma;\, z) \sim \frac{\Gamma(\gamma)}{\Gamma(\alpha)}\,(\Psi(\gamma) - \Psi(\alpha) + \Psi(1))\, e^z \sum_{\nu=0}^{\infty} \frac{(\gamma-\alpha)_{\nu}\,(1-\alpha)_{\nu}}{\nu!\, z^{\gamma-\alpha+\nu}}, \tag{42}$$

provided that $|\arg z| < \frac{\pi}{2}$. But if $\Re(z) \to -\infty$, so that $|\arg(-z)| < \frac{\pi}{2}$, we obtain the asymptotic expansion

$$G(\alpha,\, \gamma;\, z) \sim C \sum_{\nu=0}^{\infty} \frac{(\alpha)_{\nu}\,(\alpha-\gamma+1)_{\nu}}{\nu!\,(-z)^{\alpha+\nu}}, \tag{43}$$

where the constant C has the value

$$C = (-1)^{\gamma}\,\Gamma(\gamma)\,\Gamma(\alpha-\gamma+1)\left[e^{\mp\pi i\alpha} - \frac{\sin\pi\alpha}{\pi}\,(\Psi(\gamma)-\Psi(\alpha)+\Psi(1))\right],$$

that is

$$C = \frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)}\,[\Psi(\gamma)+\Psi(1)-\Psi(1-\alpha)\pm\pi i].$$

If $\alpha = \gamma$, (9) reduces to

$$G(\gamma,\gamma;z) = e^{z}\log z - \sum_{\nu=0}^{\infty}\frac{z^{\nu}}{\nu!}\left(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{\nu}\right) - \sum_{\nu=1}^{\gamma-1}\frac{\Gamma(\nu)}{(-z)^{\nu}},$$

and for this solution we get from (42) and (43) the asymptotic expansion

$$G(\gamma,\gamma;z) \sim \Psi(1)\,e^{z} + \sum_{\nu=\gamma}^{\infty}\frac{\Gamma(\nu)}{(-z)^{\nu}}, \qquad |\arg z| \leq \pi.$$

If γ is an integer >1 and α is one of the numbers $1, 2, \ldots \gamma-1$, the two series in (41) terminate and the asymptotic expansion (41) reduces to the relation (24), where the series are written in the reverse order.

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COULOMB EXCITATION IN DEFORMED NUCLEI

BY

HANS LÜTKEN AND AAGE WINTHER

København 1964

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Errata:

In Table 2 (p. 20) replace the three table headings by

$$\chi^{(1)}(\vartheta, \xi)/\chi^{(1)}$$

$$\chi^{(2)}(\vartheta, \xi)/\chi^{(2)}$$

$$\chi^{(3)}(\vartheta, \xi)/\chi^{(3)}$$

as indicated in the figure caption.

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CONTENTS

Synopsis

In multiple Coulomb excitations of deformed nuclei one may observe also a weaker excitation of rotational bands which are associated with states of different intrinsic structure. In the present work, the excitation amplitudes of such states have been computed in the approximation where one neglects the energy differences between the states of a rotational band. For the case of dipole, quadrupole and octupole excitations the results are given in the form of tables. They show that the relative population of the states within a band depends strongly on the spin and K quantum numbers as well as on admixtures in the wave function of components from the ground-state band. A detailed investigation of the dependence of the cross sections on scattering angle is presented. One finds here appreciable deviations from the so-called $\chi(\vartheta)$-approximation, especially concerning the excitation of the unnatural parity states.

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I. Introduction

In recent years it has been possible by means of accelerated heavy ions to perform multiple Coulomb excitation in deformed nuclei to high lying rotational states[1, 2]. In these nuclei one may also excite states which differ from the ground state by having a different intrinsic structure[3]. The excitation probabilities of these states are in general so small that one is justified in describing the mechanism of their excitation by a perturbation treatment[4]. Such a treatment is complicated by the fact that many states in the ground-state band as well as in the rotational band associated with the final state are involved in the excitation process. Even though we consider the transition between the two intrinsic structures only to first order, we must take into account that this transition may take place between a number of different rotational members of the two bands; the virtual excitation preceding as well as the virtual excitation or de-excitation succeeding the transition between the bands must be treated as multiple Coulomb excitations.

It was shown earlier[4] how one may compute the excitation amplitudes of such states in the impact approximation, neglecting the energy differences between the nuclear states. Computations were made for backward scattering, and the results were generalized to other deflection angles by means of the so-called $\chi(\vartheta)$-approximation.

In the present work we generalize these calculations in three respects. Firstly, we include the possibility of Coulomb excitations of multipolarities other than quadrupole. Secondly, we discuss the effect of impurities in the rotational bands. Finally, we include in the calculations the effects of a finite energy difference between the intrinsic nuclear states. While in the sudden approximation the two first generalizations are quite trivial, the last generalization introduces a number of complications in the theory. It is thus necessary to consider the deviations from the $\chi(\vartheta)$ approximation as revealed e.g. in the non-negligible excitation of "unnatural" parity states. More serious complications are associated with the computation of the excitation of impure rotational bands, and it has here proved quite convenient to formulate the deviations from the pure rotational model in terms of a modification of the nuclear multipole moments[7].

In Chapter II we give a formulation of the theory of Coulomb excitation in deformed nuclei, together with a summary of the theory of small deviations from the pure rotational model.

The application of the theory to the excitation of pure rotational states is discussed in Chapter III. One finds here that the total excitation probability of a given rotational band is identical to the result of the ordinary first order perturbation theory. The relative excitation probabilities are determined by simple functions of the intrinsic quadrupole moment, which functions are tabulated in Appendix 2. These functions also depend strongly on the spin and K-quantum numbers of the states, and a measurement of the relative probabilities thus offers a convenient method of determining these quantities.

Finally, in Chapter IV, we consider the effect of weak band mixing. We evaluate explicitly the correction to be applied to the results of Chapter III for the important case of quadrupole excitations of bands which show admixture with the ground-state band.

II. General Theory

In the semi-classical approximation the Coulomb excitation amplitude of a state $|f\rangle$ from the state $|i\rangle$ is given by the expression[4]

$$a_f = \langle f | T e^{-\frac{i}{\hbar}\int_{-\infty}^{\infty} \tilde{\mathcal{H}}(t)\, dt} | i \rangle . \tag{1}$$

In this formula T stands for the time ordering operator. The operator $\tilde{\mathcal{H}}(t)$ is given by

$$\tilde{\mathcal{H}}(t) = e^{\frac{i}{\hbar} H_0 t}\, \mathcal{H}(t)\, e^{-\frac{i}{\hbar} H_0 t} \tag{2}$$

in terms of the time dependent Coulomb interaction $\mathcal{H}(t)$ between the nucleus and the projectile and the Hamiltonian H_0 of the free nucleus.

In the present investigation we study the excitation of nuclei with a non-spherical equilibrium shape. For such nuclei the Hamiltonian H_0 is conveniently written in the form[5]

$$H_0 = H_{\text{int}} + H_{\text{rot}} + H_c . \tag{3}$$

The first term is the intrinsic Hamiltonian which describes the motion of the nucleons in the intrinsic coordinate system defined by the shape of the nucleus. In the intrinsic motion are included vibrations of the nucleus around the equilibrium shape. The second term represents the energy associated with the rotation of the intrinsic system and is an operator that only depends on the Eulerian angles which specify the orientation of the intrinsic coordinate system. The last term represents the coupling between the intrinsic motion and the rotation.

The nuclear states $|i\rangle$ and $|f\rangle$ are eigenstates of H_0. In the pure rotational model one neglects the term H_c and the eigenstates may then be written as the product of eigenstates of H_{int} and of H_{rot}. For an axially symmetric nuclear shape this product wave function is given by

$$| IKM \rangle | nK \rangle = \sqrt{\frac{2I+1}{4\pi}} D^I_{MK}(\alpha, \beta, 0) | nK \rangle. \tag{4}$$

These wave functions represent the rigid rotation with total angular momentum I and magnetic quantum number M of a system described by the intrinsic wave function $| nK \rangle$. The quantum number K denotes the component of the intrinsic angular momentum along the symmetry axis, while α and β are the Eulerian angles specifying the orientation of this axis.

The actual wave functions for the states in pure rotational bands differ from (4) only through a symmetrization with respect to the sign of K. The correct rotational wave functions are found to be[5)]

$$| IKMn \rangle = \left\{ \begin{array}{ll} | I\,0\,M \rangle\, n\,0 \rangle & \text{for} \quad K = 0 \\ \frac{1}{\sqrt{2}} \left\{ | IKM \rangle | nK \rangle + (-1)^{I+K} | I-KM \rangle | n-K \rangle \right\}; & \text{for} \quad K > 0 \end{array} \right\} \tag{5}$$

where the intrinsic wave function $| nK \rangle$ determines the parity of the states. For $K = 0$ only states of even I or only states of odd I occur.

It is well known from nuclear spectroscopy that even in strongly deformed nuclei there are deviations from the pure rotational model. These deviations must be ascribed to the presence of the coupling term H_c. While the explicit form of the Hamiltonian H_c depends on the details of the nuclear model, one may argue that the most important parts of H_c can be obtained from a series expansion in powers of the rotational angular momentum[7)]. Utilizing the invariance and symmetry principles appropriate for an axial symmetric nuclear shape one obtains to second order

$$H_c = h_1 I_- + h_{-1} I_+ + h_2 I_-^2 + h_{-2} I_+^2 + h_0 I^2. \tag{6}$$

In (6) h_i denotes an operator in the intrinsic degrees of freedom which changes the K-quantum number by i units. The operator I denotes the total angular momentum while I_+ and I_- refer to the components of this quantity in the intrinsic coordinate system.

The effect of the interaction (6) may be taken into account by a perturbation treatment. One finds then that the perturbed states may be written in the form

$$| nIKM \rangle_m = e^{iS} | nIKM \rangle. \tag{7}$$

The intrinsic matrix elements of the hermitian operator S are here given by

$$\left. \begin{array}{l} \langle n' \pm (K+1) | S | n \pm K \rangle = \pm i \varepsilon_1 I_\pm \\ \langle n' \pm (K+2) | S | n \pm K \rangle = i \varepsilon_2 I_\pm^2 \\ \langle n' \pm K | S | n \pm K \rangle = i \varepsilon_0 I^2, \end{array} \right\} \tag{8}$$

where ε_i is the matrix element of h_i divided by the energy difference between the intrinsic states $|n'\rangle$ and $|n\rangle$[7].

In the computation of Coulomb excitation amplitudes we neglect the energy differences associated with H_{rot} and H_c. The operator $\tilde{\mathfrak{H}}(t)$ is thus given by

$$\tilde{\mathfrak{H}}(t) = e^{\frac{i}{\hbar} H_{\mathrm{int}} t}\, \mathfrak{H}(t)\, e^{-\frac{i}{\hbar} H_{\mathrm{int}} t}. \tag{9}$$

In the present investigation we deal with a situation in which the interaction $\mathfrak{H}(t)$ may be written as a sum of two terms: A large term $\mathfrak{H}_0(t)$ which represents the interaction with the intrinsic quadrupole moment and a small term $\mathfrak{H}_1(t)$ which represents a residual interaction which may cause transitions to other intrinsic states. Under these circumstances one may perform a series expansion of the exponential function of (1) in powers of the quantity $\mathfrak{H}_1(t)$. To first order in $\mathfrak{H}_1(t)$ one finds

$$\left.\begin{aligned} a_f = {} & \langle f | e^{-\frac{i}{\hbar}\int_{\infty}^{\infty} \mathfrak{H}_0(t)\, dt} | i \rangle \\ & -\frac{i}{\hbar} \langle f | \int_{-\infty}^{\infty} dt\, e^{-\frac{i}{\hbar}\int_{t}^{\infty} \mathfrak{H}_0(t')\, dt'}\, \tilde{\mathfrak{H}}_1(t)\, e^{-\frac{i}{\hbar}\int_{-\infty}^{t} \mathfrak{H}_0(t')\, dt'} | i \rangle . \end{aligned}\right\} \tag{10}$$

We have here left out the time ordering in the exponential functions since $\mathfrak{H}_0(t)$ only gives rise to transitions within rotational bands and therefore, according to the assumption (9), $\tilde{\mathfrak{H}}_0(t)$ is equal to $\mathfrak{H}_0(t)$.

The Coulomb interaction, $\mathfrak{H}_0(t)$, with the quadrupole moment of the deformed nucleus may be written in the form

$$\mathfrak{H}_0(t) = Z_1 e \sqrt{\frac{\pi}{5}}\, Q_0 \sum_{\mu} r_p^{-3}\, Y_{2\mu}(\vartheta_p, \varphi_p)\, D^{2*}_{\mu 0}(\alpha, \beta, 0), \tag{11}$$

where $Z_1 e$ is the charge and r_p, ϑ_p and φ_p are the coordinates of the projectile, while Q_0 is the intrinsic quadrupole moment of the ground state.

The residual interaction $\mathfrak{H}_1(t)$ is then given by

$$\mathfrak{H}_1(t) = \mathfrak{H}(t) - \mathfrak{H}_0(t) \tag{12}$$

with

$$\mathfrak{H}(t) = 4\pi Z_1 e \sum_{\lambda\mu} (2\lambda+1)^{-1}\, r_p^{-\lambda-1}\, Y_{\lambda\mu}(\vartheta_p, \varphi_p)\, \mathfrak{M}^*(E\lambda, \mu), \tag{13}$$

where $\mathfrak{M}(E\lambda, \mu)$ is the nuclear electric multipole monent of order λ. It is noted that the operator $\mathfrak{H}_1(t)$, besides causing transitions between different intrinsic states, also may describe effects from a small variation of the intrinsic quadrupole moment through the bands or from one band to another.

III. The Excitation of Pure Bands

In this chapter we consider the Coulomb excitation in the pure rotational model. The nuclear wave functions are here given by (5). We first compute the excitation amplitude with the product wave functions (4) and only in the end of the chapter consider the effects of the symmetrization.

For the computation of the excitation amplitudes (10) it is convenient to express the multipole moments in (13) in the form

$$\mathfrak{M}(E\lambda, \mu) = \sum_{\nu} D^{\lambda}_{\mu\nu}(\alpha, \beta, 0)\, \mathfrak{M}_{\mathrm{int}}(E\lambda, \nu) \tag{14}$$

in terms of the corresponding multipole moments $\mathfrak{M}_{\mathrm{int}}(E\lambda, \nu)$ in the intrinsic coordinate system. In the pure rotational model these moments are independent of the Eulerian angles.

The excitation amplitude of a state in the ground-state band is then determined solely by the first term of (10). Similarly, the second term in (10) determines the excitation of states where the intrinsic wave functions differ from that of the ground state. Since the operators $\mathfrak{H}_0(t)$ and $\mathfrak{H}_1(t)$ commute according to (11)–(14), the excitation amplitude from the state $|\, I_i K_0 M_i \rangle |\, n_0 K_0 \rangle$ to the state $|\, I_f K_1 M_f \rangle |\, n_1 K_1 \rangle$ may be written

$$b_{I_f M_f K_1 K_0} = -i \sum_{\lambda} \langle\, I_f K_1 M_f \,|\, k_\lambda\, e^{-ik_0} \,|\, I_i K_0 M_i \,\rangle \tag{15}$$

with

$$\left.\begin{aligned} k_0 &= \frac{1}{\hbar}\int_{-\infty}^{+\infty} \tilde{\mathfrak{H}}_0(t)\, dt \\ &= \frac{Z_1 e}{\hbar}\sqrt{\frac{\pi}{5}}\, Q_0 \sum_{\mu} S_{2\mu}(\vartheta, 0)\, D^{2*}_{\mu 0}(\alpha, \beta, 0) \end{aligned}\right\} \tag{16}$$

and

$$\left.\begin{aligned} k_\lambda &= \frac{1}{\hbar}\langle\, n_1 K_1 \,|\int_{-\infty}^{+\infty} \tilde{\mathfrak{H}}_1(t)\, dt \,|\, n_0 K_0 \,\rangle \\ &= \frac{4\pi Z_1 e}{(2\lambda+1)\hbar}\langle n_1 K_1 \,|\, \mathfrak{M}^{*}_{\mathrm{int}}(E\lambda, -K) \,|\, n_0 K_0 \,\rangle \\ &\quad \times \sum_{\mu} S_{\lambda\mu}(\vartheta, \xi)\, D^{\lambda *}_{\mu -K}(\alpha, \beta, 0). \end{aligned}\right\} \tag{17}$$

We have here introduced the notation $K = K_1 - K_0$ and

$$\xi = \frac{E_1 - E_0}{\hbar}\frac{a}{v}, \tag{18}$$

where a is half the distance of closest approach in a head-on collision, v is the relative velocity at large distances, and $E_1 - E_0$ is the energy difference between the intrinsic states $|\, n_1 K_1 \rangle$ and $|\, n_0 K_0 \rangle$. We shall evaluate the orbital integrals $S_{\lambda\mu}(\vartheta, \xi)$ in the coordinate system[4] where the z-axis is chosen along the symmetry axis of the hyperbolic orbit. In this coordinate system we introduce the functions $R_{\lambda\mu}(\vartheta, \xi)$ defined by the equation

$$R_{\lambda\mu}(\vartheta, \xi) = \frac{S_{\lambda\mu}(\vartheta, \xi)}{S_{\lambda 0}(\pi, 0)}. \tag{19}$$

With this notation, (16)–(17) may be written

$$k_0 = \frac{4}{3} q \sum_{\mu} R_{2\mu}(\vartheta, 0)\, D^{2*}_{\mu 0}(\alpha, \beta, 0) \tag{20}$$

$$k_\lambda = \chi^{(\lambda)} \sqrt{2\lambda + 1} \sum_{\mu} R_{\lambda\mu}(\vartheta, \xi)\, D^{\lambda *}_{\mu - K}(\alpha, \beta, 0) \tag{21}$$

in terms of the parameters q and $\chi^{(\lambda)}$ defined by[4]

$$\left.\begin{aligned} q &= \frac{Z_1 e\, Q_0}{4 \hbar v a^2} \\ \chi^{(\lambda)} &= \frac{\sqrt{16\pi}\, Z_1 e\, (\lambda - 1)!}{\hbar v a^\lambda (2\lambda + 1)!!} \langle\, n_0 K_0 \,|\, \mathfrak{M}_{\mathrm{int}}(E\lambda, -K) \,|\, n_1 K_1 \,\rangle. \end{aligned}\right\} \tag{22}$$

The functions $R_{\lambda,\mu}(\vartheta, \xi)$, which directly determine the relative magnitude of the terms in (20)–(21), are defined in Appendix 1 in terms of the integrals $I_{\lambda,\mu}(\vartheta, \xi)$ (see ref. 6). For the case of $\lambda = 2$ and $\xi = 0$ they are tabulated in ref. 4. It is seen there that in the matrix element (20), where we have assumed $\xi = 0$, the $\mu = 0$ term dominates strongly over the $\mu \neq 0$ terms for all angles. In the following we therefore neglect these terms, i.e. we use

$$k_0 = \frac{4}{3} q\, R_{20}(\vartheta, 0)\, D^2_{00}(\alpha, \beta, 0) = \frac{4}{3} q_0(\vartheta)\, D^2_{00}(\alpha, \beta, 0). \tag{23}$$

For the second matrix element (21) we may use a similar approximation if ξ is small or if the scattering angle is close to 180 degrees. If the value of ξ is of the order of 0.1 or larger, the terms with $\mu \neq 0$ in (21) may contribute significantly, especially for forward scattering angles. We therefore include these terms in the computation of the excitation amplitude. Including also the possibility of mixed multipole excitation we find by expanding the product of D-functions on D-functions the following expression for the excitation amplitude (15)

$$b_{I_f M_f K_1 K_0} = -i \sum_{\lambda\mu} \chi^{(\lambda)} R_{\lambda\mu}(\vartheta, \xi) \langle\, I_f K_1 M_f \,|\, C_{\lambda\mu}(q_0(\vartheta)) \,|\, I_i K_0 M_i \,\rangle \tag{24}$$

where

$$\left.\begin{aligned}&\langle I_f K_1 M_f \mid C_{\lambda\mu}(x) \mid I_i K_0 M_i \rangle \\ &= (-1)^{M_i - K_0} \sqrt{(2I_f+1)(2I_i+1)} \sum_I \sqrt{2I+1} \begin{pmatrix} I_f & I_i & I \\ -M_f & M_i & \mu \end{pmatrix} \begin{pmatrix} I_f & I_i & I \\ -K_1 & K_0 & K \end{pmatrix} B^{\lambda\mu}_{IK}(x).\end{aligned}\right\} \quad (25)$$

The functions $B^{\lambda\mu}_{IK}(x)$ are given by

$$B^{\lambda\mu}_{IK}(x) = (-1)^{K-\mu} \sqrt{(2\lambda+1)(2I+1)} \sum_J (2J+1) \begin{pmatrix} I & \lambda & J \\ -\mu & \mu & 0 \end{pmatrix} \begin{pmatrix} I & \lambda & J \\ -K & K & 0 \end{pmatrix} A_J(x) \quad (26)$$

in terms of the functions

$$A_J(x) = \frac{1}{2} \int_{-1}^{+1} P_J(y)\, e^{-i\frac{4}{3}x P_2(y)}\, dy \quad (27)$$

which are tabulated in refs. 4 and 8.

It is seen from eq. (25) that the dependence of the excitation amplitude on the quadrupole moment Q_0 is contained in the functions $B^{\lambda\mu}_{IK}$. Explicit formulae for these functions are given in Appendix 2 for $\lambda = 1$, 2 and 3, together with tables for the lowest values of I.

It is noted that even in the pure rotational model the intrinsic quadrupole moment may be different for different rotational bands. The series expansion (10) with $\mathfrak{H}_0$ given by (11) is, however, valid only for states where the quadrupole moments are nearly equal to Q_0. A possible small deviation is contained in our expansion, and it is seen that to first order it gives no contribution to the excitation of the coupled band. To minimize the error one should, however, choose Q_0 to be the average quadrupole moment of the two bands.

The physical significance of the functions $B^{\lambda\mu}_{IK}(q)$ is illustrated by the special case of the excitation of an even-even nucleus with $I_i = K_0 = 0$. In this case one finds from (25)

$$\langle I_f K_1 M_f \mid C_{\lambda\mu}(q) \mid 000 \rangle = B^{\lambda\mu}_{I_f K_1}(q)\, \delta_{M_f \mu} (-1)^{\mu + K_1} \quad (28)$$

and therefore

$$b_{I_f M_f K_1 0} = -i \sum_\lambda \chi^{(\lambda)} R_{\lambda M_f}(\vartheta, \xi) (-1)^{M_f + K_1} B^{\lambda M_f}_{I_f K_1}. \quad (29)$$

Eq. (29) shows that the functions $B^{\lambda\mu}_{IK_1}$ for fixed λ, μ and K_1 are the relative excitation amplitudes for $E\lambda$ excitations of the states of spin I and magnetic quantum number $M_f = \mu$ in a band with $K = K_1$.

A comparison with Eq. 5.8 of ref. 4 shows that the function $B^{\lambda\mu}_{IK_1}$ is identical to the multiple quadrupole excitation amplitude $a_{I\mu}$ from a ground state $\mid \lambda K_1 \mu \rangle \mid K_1 \rangle$ of spin λ and magnetic quantum number μ to a state $\mid I K_1 \mu \rangle \mid K_1 \rangle$ in the ground state band which has $K = K_1$. From this identity follows immediately the relation

$$\sum_I \mid B^{\lambda\mu}_{IK}(q) \mid^2 = 1, \quad (30)$$

which simply expresses the fact that the nucleus in this model must stay in the ground state rotational band. By choosing the initial state to be a superposition of the states $|\lambda K_1 \mu\rangle |K_1\rangle$ and $|\lambda' K_1 \mu\rangle |K_1\rangle$ one may in a similar way show the more general relation

$$\sum_I (B_{IK}^{\lambda' \mu}(q))^* B_{IK}^{\lambda \mu}(q) = \delta_{\lambda \lambda'}. \tag{31}$$

From the excitation amplitude (24)–(27) one may compute the excitation probability $P_{I_f K_1}$ of the state with spin I_f in the $K = K_1$ band. One finds

$$\left.\begin{aligned} P_{I_f K_1} &= \frac{1}{2 I_i + 1} \sum_{M_i M_f} |b_{I_f M_f K_1 K_0}|^2 \\ &= \sum_{\lambda \lambda' \mu} \chi^{(\lambda')} \chi^{(\lambda)} R_{\lambda' \mu}(\vartheta, \xi) R_{\lambda \mu}(\vartheta, \xi)(2 I_f + 1) \\ &\quad \times \sum_I \begin{pmatrix} I_f & I_i & I \\ -K_1 & K_0 & K \end{pmatrix}^2 (B_{IK}^{\lambda' \mu}(q_0(\vartheta)))^* B_{IK}^{\lambda \mu}(q_0(\vartheta)). \end{aligned}\right\} \tag{32}$$

It is interesting also to compute the total excitation probability P_{K_1} of the $K = K_1$ band. From (32) one finds

$$P_{K_1} = \sum_{I_f} P_{I_f K_1} = \sum_{\lambda} (\chi^{(\lambda)})^2 \sum_{\mu} (R_{\lambda \mu}(\vartheta, \xi))^2. \tag{33}$$

We have here used the completeness relation for the 3-j symbols and the orthogonality property (31) for the functions $B_{IK}^{\lambda \mu}(q)$. This result shows that the total excitation probability of the K_1 band is exactly the same as that one would find in the ordinary first order perturbation treatment. The effect of the multiple excitation that takes place is merely a redistribution of this probability on the various members of the band.

In the following we neglect the complications associated with the possibility of mixed multipole transitions between the two bands. For pure $E\lambda$ transitions the excitation probability (32) takes the simpler form

$$P_{I_f K_1} = (\chi^{(\lambda)})^2 \sum_{\mu} |R_{\lambda \mu}(\vartheta, \xi)|^2 (2 I_f + 1) \sum_I \begin{pmatrix} I_f & I_i & I \\ -K_1 & K_0 & K \end{pmatrix}^2 |B_{IK}^{\lambda \mu}(q_0(\vartheta))|^2. \tag{34}$$

The functions $|B_{IK}^{\lambda \mu}|^2$ which determine the excitation probabilities are illustrated on Figs. 1 and 2 for the case of $\lambda = 2$. For $\lambda = 1, 2, 3$ and $\mu = 0$ they are given in Table 4, while for $\lambda = 2$ and $\mu \neq 0$ they are given in Table 5.

A further simplification in (34) is achieved for backward scatterings since $R_{\lambda \mu}(\pi, \xi)$ vanishes for $\mu \neq 0$. Also for other scattering angles one may, to a first approximation, neglect the terms in (34) with $\mu \neq 0$. In general, this $\mu = 0$ approximation is only accurate for large scattering angles. However, for small values of ξ the accuracy is quite good even for intermediate angles.

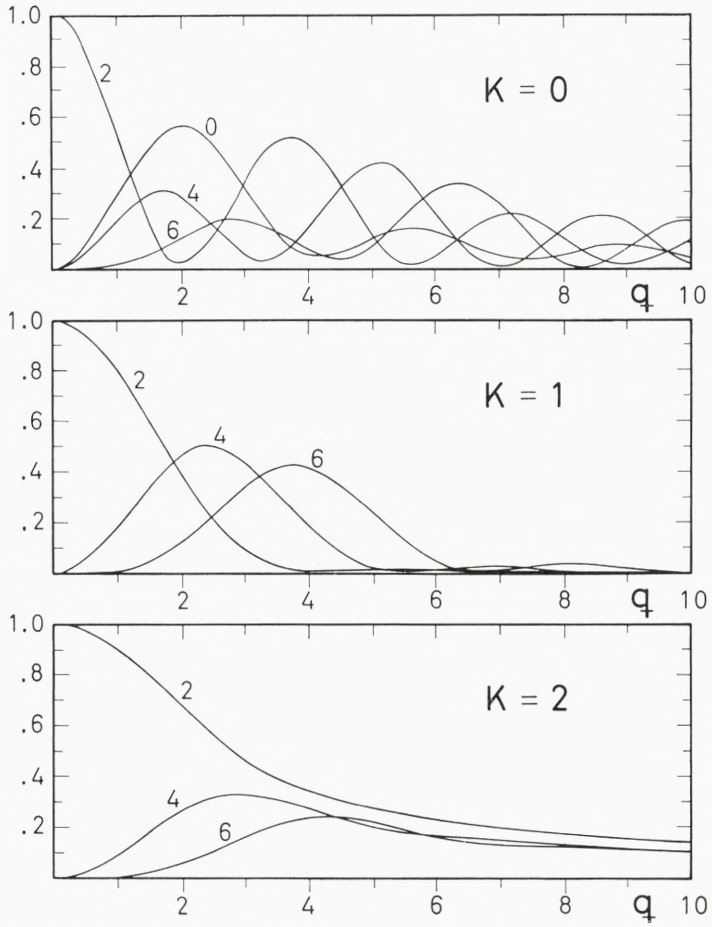

Fig. 1. The quantity $|B^{\lambda}_{IK}(q)|^2$ for $\lambda = 2$ and $I \leq 6$ as a function of q. For backward scattering, these quantities give the relative quadrupole excitation probabilities in an even-even nucleus of the various rotational states in a band with $K = 0{,}1$ or 2. For other deflection angles they give the relative excitation probabilities of the magnetic substates with $M_f = 0$. The functions are given separately for the three values of $|K|$ while the spins I are indicated on the curves.

In the $\mu = 0$ approximation the excitation is determined by the quantities $B^{\lambda 0}_{IK} = B^{\lambda}_{IK}$. As can be seen from the definition (26), these functions vanish when $\lambda + I$ is odd. This is a reflection of the general selection rule that only natural parity states can be excited in even-even nuclei by backward scattering. The functions B^{λ}_{IK} are given in Table 3 for $\lambda = 1$, 2 and 3.

As an example of the application of the results of this chapter we consider the quadrupole excitation of a band with $K = 2$ in an even-even nucleus. In this case, the excitation probability (34) takes the simple form

$$P_{I_f 2} = |\chi^{(2)}|^2 \sum_{\mu} |R_{2\mu}(\vartheta, \xi)|^2 \, |B^{2\mu}_{I_f 2}(q_0(\vartheta))|^2. \tag{35}$$

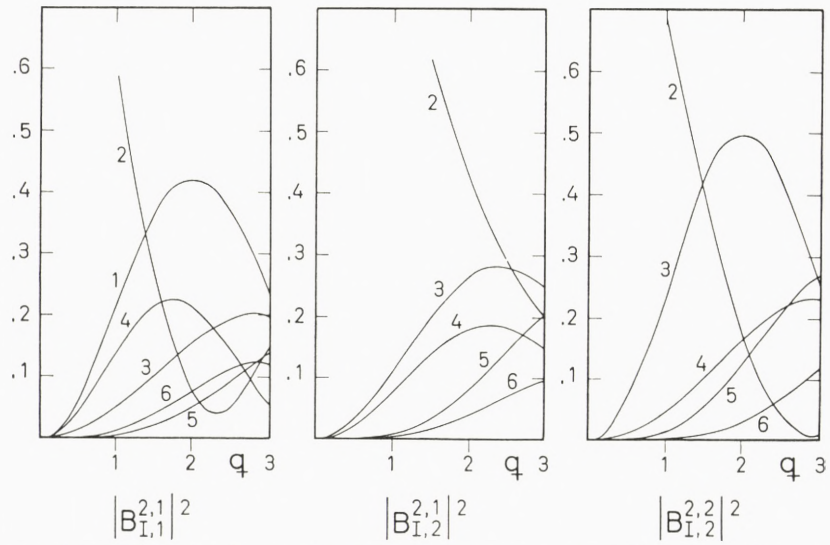

Fig. 2. The quantities $|B^{\lambda\mu}_{IK}(q)|^2$ for $\lambda = 2$ and $I \leq 6$ as functions of q. These quantities give the relative quadrupole excitation probabilities in an even-even nucleus of the various rotational substates with spin I and fixed magnetic quantum number $M = \mu$ in a band with a definite value of K. The functions are given separately for different values of K and μ. Others may be obtained by means of the relations (67)–(68). The spin I is indicated on the curves.

The differential cross section which is given by

$$\left(\frac{d\sigma}{d\Omega}\right)_{I_f} = \frac{1}{4}\, a^2 \sin^{-4}\vartheta/2\; P_{I_f\,2} \tag{36}$$

is illustrated in Fig. 3 as a function of ϑ for a special choice of parameters ξ, q and $\chi^{(2)}$ described in the figure caption. The figure also shows (by dashed curves) the result of the above mentioned $\mu = 0$ approximation where all terms in (35) with $\mu \neq 0$ are neglected. It is seen that this approximation is accurate only for rather large deflection angles.

For the excitation probabilities a considerable improvement over the $\mu = 0$ approximation can be achieved by assuming that the coefficients $B^{\lambda\mu}_{IK}$ in (34) are independent of μ and equal to B^{λ}_{IK}. The constribution from the terms with $\mu \neq 0$ is then correct for forward scattering where $q_0(\vartheta) \ll 1$, since $B^{\lambda\mu}_{IK}(0) = B^{\lambda}_{IK} = \delta_{I\lambda}$. In this approximation the excitation probabilities are given by

$$P_{I_f K_1} = [\chi^{(\lambda)}(\vartheta, \xi)]^2 (2I_f + 1) \sum_I \begin{pmatrix} I_f & I_i & I \\ -K_1 & K_0 & K \end{pmatrix}^2 |B^{\lambda}_{IK}(q_0(\vartheta))|^2 \tag{37}$$

with (cf. ref. 4)

$$\chi^{(\lambda)}(\vartheta, \xi) = \chi^{(\lambda)} \Big(\sum_{\mu} [R_{\lambda\mu}(\vartheta, \xi)]^2 \Big)^{1/2}. \tag{38}$$

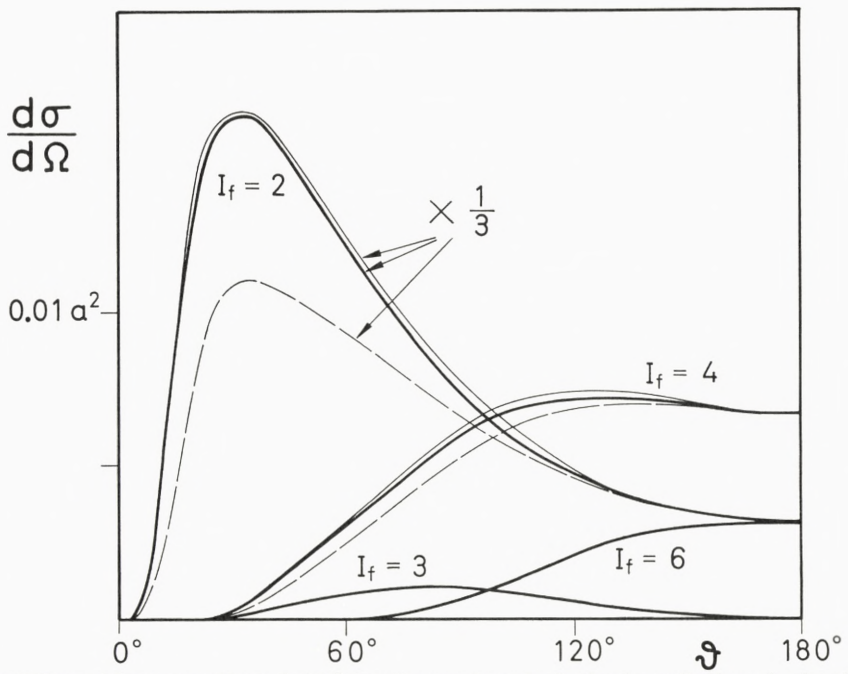

Fig. 3. The differential cross sections $d\sigma/d\Omega$ for the quadrupole Coulomb excitation of a band with $K = 2$ in an even-even nucleus. We have assumed that $q = 3$, $\chi^{(2)} = 0.4$ and $\xi = 0.3$, and the cross section is given in units of a^2. The broad full-drawn curves show the result of applying Eqs. (35)–(36). The dashed curves and the thin full-drawn curves show the results of the $\mu = 0$ approximation and of the $\chi^{(\lambda)}(\vartheta, \xi)$ approximation, respectively. For the state with $I_f = 2$, which can be reached directly from the ground state the curves have been scaled down by a factor of 3. For the $I_f = 6$ state the three curves coincide within the accuracy of the drawing. For the $I_f = 3$ state no excitation takes place in the $\mu = 0$ and in the $\chi^{(2)}(\vartheta, \xi)$ approximations.

The approximation (37) is thus a modification of the $\mu = 0$ approximation where one applies the parameter $\chi^{(\lambda)}(\vartheta, \xi)$ instead of $\chi^{(\lambda)} R_{\lambda 0}(\vartheta, \xi)$. For backward scattering angles the two approximations coincide since $\chi^{(\lambda)}(\pi, \xi) = \chi^{(\lambda)} R_{\lambda 0}(\pi, \xi)$. For forward scattering angles, however, the expression (37) agrees with the result of the perturbation treatment, which applies in the limit of small ϑ. Finally, one obtains with (37) for all angles the correct result (33) for the total excitation probability of the K_1-band.

The $\chi^{(\lambda)}(\vartheta, \xi)$ approximation is analogous to the $q(\vartheta)$ approximation of ref. 4; however, the systematic substitution of $q_0(\vartheta) = q_{\text{eff}}(\vartheta)$ with $q(\vartheta)$ is not expected to improve the approximation further in the present case.

For the special case which is illustrated in Fig. 3 the results of the $\chi^{(\lambda)}(\vartheta, \xi)$ approximation are indicated by thin full-drawn curves. A considerable improvement over the $\mu = 0$ approximation is noted for forward scatterings. For intermediate angles the expression (37) offers no significant improvement and in both approximations the excitation of the states of odd spins is neglected.

The accuracy of the $\chi^{(\lambda)}(\vartheta, \xi)$ approximation is expected to be inferior for larger values of q and ξ. This is connected with the fact that the terms with $\mu = 1$ in (34)

can be of importance already for angles where $q_0(\vartheta)$ is still so large that the coefficient $B^{\lambda 1}_{IK}$ is essentially different from B^{λ}_{IK}.

The functions $\chi^{(\lambda)}(\vartheta, \xi)$ are given for $\lambda = 1$, 2 and 3 in Table 2.

We conclude the present chapter by considering the effects which are associated with the fact that the nuclear wave functions are given by the symmetrized expressions (5) instead of the simple product (4).

For $K_0 = K_1 = 0$, where both the initial and final states are described by product wave functions, the Coulomb excitation amplitude of the state $| I_f K_1 M_f n_1 \rangle$ is given by (24)

$$a_{I_f M} = b_{I_f M_f 00}. \tag{39}$$

It is noticed that the excitation amplitude $b_{I_f M_f 00}$, as seen from (25) and (26), vanishes unless $I_f + I_i + \lambda$ is even. Since on the other hand the symmetrization implies that in the K_1-band only states of even spin or only states of odd spin occur, we obtain the following selection rule for the $K_0 = K_1 = 0$ case:

$$(-1)^{I_i + I_f} = \Delta\pi \tag{40}$$

where $\Delta\pi$ is the relative parity of the two bands.

If $K_0 = 0$ and $K_1 > 0$ (or $K_0 > 0$ and $K_1 = 0$) we find that the excitation amplitude of the state $| I_f K_1 M_f n_1 \rangle$ is given by

$$a_{I_f M_f} = \frac{1}{\sqrt{2}} [b_{I_f M_f K_1 0} + (-1)^{I_f + K_1} b_{I_f M_f - K_1 0}]. \tag{41}$$

However, due to symmetry relations between matrix elements of the multipole moments the two terms of (41) are equal, and we get the result

$$a_{I_f M_f} = \sqrt{2}\, b_{I_f M_f K_1 0}. \tag{42}$$

This factor $\sqrt{2}$ will appear also in the ordinary perturbation treatment, and we thus still have the rule that the total excitation probability of the coupled band is given by the result of the perturbation calculation.

For the case where both $K_0 > 0$ and $K_1 > 0$ the excitation amplitude contains four terms. Due to symmetry relations the expression reduces to

$$a_{I_f M_f} = b_{I_f M_f K_1 K_0} + (-1)^{I_i + K_0} b_{I_f M_f K_1 - K_0}. \tag{43}$$

The two terms are here essentially different. The first term is proportional to the matrix element connecting the intrinsic states $| K_1 \rangle$ and $| K_0 \rangle$ while the second is proportional to the matrix element between $| K_1 \rangle$ and $| -K_0 \rangle$. If $K_0 + K_1 \leq \lambda$ both terms may contribute to the same transition.

IV. The Excitation of Mixed Bands

While, in the preceding chapter, we considered the Coulomb excitation of pure rotational bands, we shall now investigate the effect of deviations from the pure rotational model. These deviations are caused by the presence of the coupling term (6) in the nuclear Hamiltonian, which gives rise to admixtures in the pure rotational wave functions of states with different intrinsic structure.

We assume that the admixture is so small that it may be evaluated in a perturbation treatment (7)–(8). Even small mixings may, however, in some cases have an important effect on the Coulomb excitation amplitude. This is, e.g., the case if the excited band contains an admixture of the intrinsic wave function of the ground-state band. The contribution to the Coulomb excitation amplitude from the admixture is proportional to the large matrix elements between identical intrinsic states, and even when the admixture is small this contribution may be comparable to the contribution from the main part of the wave functions.[7] [11]

Also mixing in the ground-state band or in the excited band of states with K values between K_0 and K_1 may be of importance. As an example one may consider the excitation of a band with $K_1 = K_0 + 3$, and with the same parity as the ground state. In this case, the direct transition is of $E4$ type. The mixing between the bands occurs only through a third-order term in H_c, and it may be expected that the admixture in the ground state band of states with $K = K_0 + 1$ as well as admixtures in the excited band with $K = K_0 + 2$ may lead to $E2$ transitions of comparable magnitude

In the following we limit ourselves to the case where the $E2$ transition between the bands is allowed. In this case the main correction to the results of Chapter III arises from the mixing between the two bands.

In Chapter II, the effect of the mixing was expressed through a modification (7)–(8) of the wave functions. An equivalent formulation of the mixing, which is more convenient for our purpose, is to maintain the pure rotational wave functions and instead modify the multipole operators.

When, in this representation, we expand the expression (1) for the Coulomb excitation amplitude, the only contribution to the excitation arises from the second term in (10). In this matrix element the operator $\mathfrak{H}_1(t)$ is given by the expressions (9), (12), and (13).

The multipole moment is, however, no longer given by the simple form (14) but may instead be expressed as

$$\left.\begin{aligned} \mathfrak{M}(E2\,\mu) &= e^{-iS} \sum_{\nu} D^2_{\mu\nu}(\alpha, \beta, 0)\, \mathfrak{M}_{\text{int}}(E2\,\nu)\, e^{iS} \\ &\approx \sum_{\nu} D^2_{\mu\nu}\, \mathfrak{M}_{\text{int}}(E2\,,\nu) - i\Big[S, \sum_{\nu} D^2_{\mu\nu}\, \mathfrak{M}_{\text{int}}(E2\,\nu)\Big] \end{aligned}\right\} \quad (44)$$

to first order in S, where S is given by (8).

For the evaluation of the excitation amplitude we distinguish between the three cases where $|K_0 - K_1| = \Delta K = 1$, 2 and 0.

For $\Delta K = 1$ we find from (44), utilizing (8), that the intrinsic matrix elements of $\mathfrak{M}(E2\mu)$ are given by

$$\left.\begin{aligned} &\langle n' \pm (K+1) \,|\, \mathfrak{M}(E2,\mu) \,|\, n \pm K \rangle \\ &= \langle n' \pm (K+1) \,|\, \mathfrak{M}_{\text{int}}(E2 \pm 1) \,|\, n \pm K \rangle D^2_{\mu \pm 1} \\ &\quad \pm \varepsilon_1 \sqrt{\frac{5}{16\pi}}\, Q_0 \sqrt{6}\, D^2_{\mu \pm 1}. \end{aligned}\right\} \tag{45}$$

We have here neglected the terms with $\nu \neq 0$ in the commutator in (44) and only included the matrix elements proportional to the intrinsic quadrupole moment which again is assumed to be the same in the two bands.

As is seen from the result (45), the effect of the mixing is merely a change of the intrinsic matrix element of the quadrupole moment, and the change in the Coulomb excitation amplitude can therefore be described by a renormalization of χ.

For $\Delta K = 0$ one finds similarly from (44) and (8) the modified matrix element

$$\left.\begin{aligned} \langle n' \pm K \,|\, \mathfrak{M}(E2,\mu) \,|\, n \pm K \rangle &= \langle n' \pm K \,|\, \mathfrak{M}_{\text{int}}(E20) \,|\, n \pm K \rangle D^2_{\mu 0} \\ &\quad + \varepsilon_0 \sqrt{\frac{5}{16\pi}}\, Q_0 [I^2, D^2_{\mu 0}]. \end{aligned}\right\} \tag{46}$$

Inserting (46) in (10) one finds that the correction due to the mixing is a matrix element of similar structure to that encountered in the computation of multiple Coulomb excitation for finite ξ (cf. ref. 4). The result may be expressed as the following correction to the excitation amplitude (15) (or (24)–(26)):

$$\left.\begin{aligned} \delta b_{I_f M_f K_0 K_0} &= -i\frac{4}{3} q \varepsilon_0 \sum_\mu R_{2\mu}(\vartheta,\xi) \langle I_f K_0 M_f \,|\, e^{-ik_0} 6\, D^{2*}_{\mu 0} \,|\, I_i K_0 M_i \rangle \\ &\quad + i\frac{4}{3} q \varepsilon_0 \sum_\mu R_{2\mu}(\vartheta,\xi) \langle I_f K_0 M_f \,|\, e^{-ik_0} \sqrt{6}\,(D^{2*}_{\mu 1} I_- + D^{2*}_{\mu -1} I_+) \,|\, I_i K_0 M_i \rangle \\ &\quad - \left(\frac{4}{3} q\right)^2 \varepsilon_0 \sum_{\mu_1 \mu_2} \frac{1}{2} (R_{2\mu_1}(\vartheta,0) R_{2\mu_2}(\vartheta,\xi) + i G_{\mu_1\mu_2}(\vartheta,0,\xi)) \\ &\quad \times \langle I_f K_0 M_f \,|\, e^{-ik_0} 6\,(D^{2*}_{\mu_1 1} D^{2*}_{\mu_2 -1} + D^{2*}_{\mu_1 -1} D^{2*}_{\mu_2 1}) \,|\, I_i K_0 M_i \rangle \end{aligned}\right\} \tag{47}$$

where k_0 is given by (16). The last matrix element is multiplied by a second order orbital integral which we have separated in real and imaginary parts[6] according to the definition

$$G_{\mu_1\mu_2}(\vartheta,\xi_1,\xi_2) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{d\xi'}{\xi'} R_{2\mu_1}(\vartheta,\xi_1+\xi') R_{2\mu_2}(\vartheta,\xi_2-\xi') \tag{48}$$

where P denotes the principal part. The function $G_{\mu_1 \mu_2}(\vartheta, \xi_1, \xi_2)$ has been tabulated[10] for a wide range of ξ_1 and ξ_2 values. Values for $\xi_1 = 0$ and $\mu_1 = \mu_2 = 0$ are given in Table 1.

In the expression (47) the first term represents a renormalization of the χ for the transition between the bands by an amount

$$\delta\chi = \frac{8}{\sqrt{5}} q \varepsilon_0 .$$

The second term in (47) vanishes for even even nuclei. In other cases it may easily be expressed in terms of the functions $B^{2\mu}_{I1}$. In the third term it is convenient to expand the product of the two D-functions on D-functions. In this way the matrix element can be expressed in terms of the functions $B^{J\mu}_{I0}$ with $J = 0, 2, 4$.

We shall here only consider the $\mu = 0$ approximation. In this approximation one may write the expression (47) in the form

$$\left.\begin{aligned}
\delta b_{I_f M_f K_0 K_0} &= \frac{R_{20}(\vartheta, \xi)}{R_{20}(\vartheta, 0)} \varepsilon_0 \langle I_f K_0 M_f | [I^2, e^{-ik_0}] | I_i K_0 M_i \rangle \\
&\quad - i\, 6 \left(\frac{4}{3} q\right)^2 \varepsilon_0 G_{00}(\vartheta, 0, \xi) \times \langle I_f K_0 M_f | e^{-ik_0} D^2_{01} D^2_{0-1} | I_i K_0 M_i \rangle \\
&= \frac{R_{20}(\vartheta, \xi)}{R_{20}(\vartheta, 0)} \varepsilon_0 [I_f(I_f+1) - I_i(I_i+1)] B^{I_i M_i}_{I_f K_0}(q_0(\vartheta)) \\
&\quad - i\, 6 \left(\frac{4}{3} q\right)^2 \varepsilon_0 G_{00}(\vartheta, 0, \xi) \\
&\quad \times \sum_J \sqrt{2J+1} \begin{pmatrix} 2\,2\,J \\ 0\,0\,0 \end{pmatrix} \begin{pmatrix} 2\,2\,J \\ -1\,1\,0 \end{pmatrix} \langle I_f K_0 M_f | C_{J0}(q_0(\vartheta)) | I_i K_0 M_i \rangle
\end{aligned}\right\} \quad (49)$$

where the matrix elements of $C_{J0}(q)$ are given by (25).

For $\xi = 0$ the last term in (49) vanishes since $G_{00}(\vartheta, 0, 0) = 0$. The resultant simple expression for δb can in this case be obtained more directly inserting the mixed wave functions (7) in the expression (10). The correction term δb then arises from the first term in (10).

For small values of ξ one may still neglect the second term in (49). The order of magnitude of the error may be estimated by the number $q^2 \varepsilon_0 G_{00}(\vartheta, 0, \xi)$.

It is noted that the symmetrization of the rotational wave functions has no effect on the result (49) except for $K_0 = \frac{1}{2}$, where additional corrections with $\Delta K = 1$ may appear, and for $K_0 = 1$, where one obtains additional terms with $\Delta K = 2$.

TABLE 1.

The quantity $G_{00}(\vartheta, 0, \xi)$. This function which is defined by Eq. (48) may be used for the computation of quadrupole Coulomb excitation of impure bands for finite ξ. The entries are given in the form of a number followed by the power of ten, by which it should be multiplied.

$\vartheta \backslash \xi$	0.1	0.2	0.4	0.6	0.8	1.2	2.0
180°	1.530 (−1)	2.459 (−1)	3.031 (−1)	2.711 (−1)	2.114 (−1)	1.048 (−1)	1.729 (−2)
160°	1.442 (−1)	2.321 (−1)	2.870 (−1)	2.574 (−1)	2.013 (−1)	1.003 (−1)	1.668 (−2)
140°	1.203 (−1)	1.946 (−1)	2.430 (−1)	2.198 (−1)	1.732 (−1)	8.737 (−2)	1.485 (−2)
120°	8.776 (−2)	1.435 (−1)	1.820 (−1)	1.668 (−1)	1.329 (−1)	6.817 (−2)	1.183 (−2)
100°	5.479 (−2)	9.106 (−2)	1.184 (−1)	1.102 (−1)	8.871 (−2)	4.600 (−2)	7.972 (−3)
80°	2.812 (−2)	4.801 (−2)	6.434 (−2)	6.070 (−2)	4.900 (−2)	2.509 (−2)	4.090 (−3)
60°	1.101 (−2)	1.965 (−2)	2.714 (−2)	2.546 (−2)	2.008 (−2)	9.534 (−3)	1.272 (−3)
40°	2.831 (−3)	5.386 (−3)	7.354 (−3)	6.373 (−3)	4.514 (−3)	1.665 (−3)	1.261 (−4)
20°	3.153 (−4)	5.861 (−4)	5.722 (−4)	3.206 (−4)	1.416 (−4)	1.934 (−5)	1.855 (−7)

For $\Delta K = 2$ mixing the evaluation of the corrections to the excitation amplitude is completely analogous to the case of $\Delta K = 0$. We shall here only quote the result for the $\mu = 0$ approximation. One finds

$$
\left.
\begin{aligned}
\delta b_{I_f M_f K_0 \pm 2 K_0} &= \frac{R_{20}(\vartheta, \xi)}{R_{20}(\vartheta, 0)} \varepsilon_{\pm 2} \langle I_f K_0 \pm 2 M_f | [I_{\mp}^2, e^{-ik_0}] | I_i K_0 M_i \rangle \\
&\quad - i \left(\frac{4}{3} q\right)^2 G_{00}(\vartheta, 0, \xi) \varepsilon_{\pm 2} \times \langle I_f K_0 \pm 2 M_f | e^{-ik_0} (D^2_{0 \pm 1})_i | I_0 K_0 M_i \rangle \\
&= \frac{R_{20}(\vartheta, \xi)}{R_{20}(\vartheta, 0)} \varepsilon_{\pm 2} \Big[\sqrt{(I_f \pm K_0 + 2)(I_f \pm K_0 + 1)(I_f \mp K_0)(I_f \mp K_0 - 1)}\, B^{I_i M_i}_{I_f K_0}(q_0(\vartheta)) \\
&\quad - \sqrt{(I_i \pm K_0 + 2)(I_i \pm K_0 + 1)(I_i \mp K_0)(I_i \mp K_0 - 1)}\, B^{I_i M_i}_{I_f K_0 \pm 2}(q_0(\vartheta)) \Big] \\
&\quad - i\, 6 \left(\frac{4}{3} q\right)^2 \varepsilon_{\pm 2} G_{00}(\vartheta, 0, \xi) \sum_J (2J+1)^{1/2} \begin{pmatrix} 2 & 2 & J \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 2 & J \\ 1 & 1 & -2 \end{pmatrix} \\
&\quad \times \langle I_f K_0 \pm 2 M_f | C_{J0}(q_0(\vartheta)) | I_i K_0 M_i \rangle .
\end{aligned}
\right\} \tag{50}
$$

Again the simple result for $\xi = 0$ can be obtained directly inserting the mixed wave functions (7) in (10). For $K_0 = 0$ the symmetrization gives rise to an additional factor $\sqrt{2}$.

Acknowledgement

The authors are indebted to Professors AAGE BOHR and BEN MOTTELSON for valuable discussions.

Appendix 1

In the present work the orbital integrals $S_{\lambda\mu}(\vartheta, \xi)$ are to be evaluated in the coordinate system, where the z axis is chosen in the plane of the orbit in such a way that it bisects the angle between $-\vec{v}_i$ and $\vec{v}_f$, where $\vec{v}_i$ and $\vec{v}_f$ are the initial and final velocities of the projectile. We shall here express the integrals $S_{\lambda\mu}(\vartheta, \xi)$ by functions $R_{\lambda\mu}(\vartheta, \xi)$ which are normalized in such a way that they attain the value 1 for $\mu = 0$, $\vartheta = \pi$ and $\xi = 0$, i.e.

$$S_{\lambda\mu}(\vartheta, \xi) = \frac{1}{v a^{\lambda}} \sqrt{\frac{2\lambda + 1}{\pi}} \frac{(\lambda - 1)!}{(2\lambda - 1)!!} R_{\lambda\mu}(\vartheta, \xi). \tag{51}$$

Since the orbital integrals transform like spherical tensors under rotations of the coordinate system, the functions $R_{\lambda\mu}(\vartheta, \xi)$ are related to the integrals $I_{\lambda\mu}(\vartheta, \xi)$ in the focal system (cf. refs. 5 and 8) by the relation

$$R_{\lambda\mu}(\vartheta, \xi) = \frac{(2\lambda - 1)!!}{2(\lambda - 1)!} \sum_{\nu} D^{\lambda}_{\mu\nu}\left(0, \frac{\pi}{2}, 0\right) D^{\lambda}_{0\nu}\left(0, \frac{\pi}{2}, 0\right) I_{\lambda\nu}(\vartheta, \xi), \tag{52}$$

where we have utilized the following explicit formula for $I_{\lambda\mu}(\pi, 0)$:

$$I_{\lambda\mu}(\pi, 0) = 2 \frac{(\lambda - 1)!}{(2\lambda - 1)!!}. \tag{53}$$

The functions $R_{\lambda\mu}(\vartheta, \xi)$ satisfy the following symmetry relation

$$R_{\lambda-\mu}(\vartheta, \xi) = R_{\lambda\mu}(\vartheta, \xi). \tag{54}$$

Furthermore one finds

$$R_{\lambda\mu}(\vartheta, -\xi) = (-1)^{\mu} R_{\lambda\mu}(\vartheta, \xi), \tag{55}$$

which implies that $R_{\lambda\mu}(\vartheta, 0)$ vanishes for odd values of μ. Finally we note the following property:

$$R_{\lambda\mu}(\pi, \xi) = 0 \quad \text{for} \quad \mu \neq 0. \tag{56}$$

A tabulation of the functions $R_{\lambda\mu}(\vartheta, \xi)$ will be published separately[10]. For $\xi = 0$ the functions $R_{\lambda\mu}(\vartheta, 0)$ are proportional to the functions $J_{\lambda\mu}(\vartheta)$ which for $\lambda = 2$ are tabulated in ref. 4. The relations are

$$\left.\begin{aligned} R_{2,0}(\vartheta, 0) &= \frac{3}{4} \; J_{2,0}(\vartheta) \\ R_{2,2}(\vartheta, 0) &= -\frac{3\sqrt{3}}{4\sqrt{2}} J_{2,2}(\vartheta). \end{aligned}\right\} \tag{57}$$

TABLE 2.

The quantity $\chi^{(\lambda)}(\vartheta, \xi)/\chi^{(\lambda)}$ for $\lambda = 1, 2$ and 3 as a function of ϑ and ξ. The square of this function gives the variation of the total excitation probabilty of the intrinsic state with particle energy and deflection angle, relative to the case of $\vartheta = \pi$ and $\xi = 0$. It is noted that $\chi^{(\lambda)}(\pi, \xi)/\chi^{(\lambda)} = R_{\lambda 0}(\pi, \xi)$. Furthermore, $\chi^{(\lambda)}(\vartheta, 0)/\chi^{(\lambda)} \approx R_{\lambda 0}(\vartheta, 0)$ which implies that $q_0(\vartheta)/q \approx \chi^{(2)}(\vartheta, 0)/\chi^{(2)}$.

$\chi^{(1)}(\vartheta, \xi)$

$\vartheta \backslash \xi$	0.0	0.2	0.4	0.6	0.8	1.0	2.0
180°	1.0000	0.6344	0.3734	0.2140	0.1209	0.06766	0.003449
160°	0.9848	0.6261	0.3695	0.2123	0.1202	0.06740	0.003467
140°	0.9397	0.6014	0.3573	0.2065	0.1175	0.06618	0.003455
120°	0.8660	0.5601	0.3356	0.1950	0.1114	0.06283	0.003261
100°	0.7660	0.5017	0.3022	0.1755	0.0997	0.05582	0.002736
80°	0.6428	0.4261	0.2547	0.1453	0.0807	0.04398	0.001847
60°	0.5000	0.3320	0.1908	0.1030	0.0537	0.02745	0.000815
40°	0.3420	0.2179	0.1100	0.0511	0.0228	0.00990	0.000128
20°	0.1736	0.0828	0.0252	0.0069	0.0018	0.00045	0.000000

$\chi^{(2)}(\vartheta, \xi)$

$\vartheta \backslash \xi$	0.0	0.2	0.4	0.6	0.8	1.0	2.0
180°	1.0000	0.8342	0.5929	0.3924	0.2488	0.1536	0.01100
160°	0.9728	0.8148	0.5828	0.3882	0.2479	0.1539	0.01133
140°	0.8943	0.7579	0.5519	0.3742	0.2428	0.1530	0.01191
120°	0.7729	0.6679	0.4992	0.3461	0.2288	0.1462	0.01182
100°	0.6216	0.5513	0.4243	0.3000	0.2006	0.1290	0.01026
80°	0.4561	0.4175	0.3294	0.2345	0.1560	0.0991	0.00704
60°	0.2932	0.2779	0.2204	0.1531	0.0978	0.0591	0.00310
40°	0.1498	0.1462	0.1095	0.0682	0.0382	0.0200	0.00048
20°	0.0438	0.0407	0.0209	0.0081	0.0027	0.0008	0.00000

$\chi^{(3)}(\vartheta, \xi)$

$\vartheta \backslash \xi$	0.0	0.2	0.4	0.6	0.8	1.0	2.0
180°	1.0000	0.9077	0.7201	0.5268	0.3653	0.2439	0.02345
160°	0.9624	0.8761	0.7008	0.5176	0.3626	0.2445	0.02461
140°	0.8528	0.7862	0.6436	0.4878	0.3503	0.2419	0.02671
120°	0.6935	0.6513	0.5518	0.4327	0.3203	0.2268	0.02707
100°	0.5102	0.4908	0.4327	0.3512	0.2667	0.1923	0.02353
80°	0.3307	0.3269	0.2998	0.2497	0.1920	0.1387	0.01584
60°	0.1778	0.1813	0.1715	0.1434	0.1083	0.0758	0.00672
40°	0.0692	0.0725	0.0687	0.0539	0.0370	0.0230	0.00099
20°	0.0118	0.0128	0.0098	0.0052	0.0009	0.0009	0.00000

It was shown in Chapter III that in many cases it will be sufficient to know the following combination of the functions $R_{\lambda\mu}(\vartheta, \xi)$:

$$\chi^{(\lambda)}(\vartheta, \xi)/\chi^{(\lambda)} = \Big[\sum_{\mu} (R_{\lambda\mu}(\vartheta, \xi))^2\Big]^{1/2}. \tag{58}$$

This function is related to the differential excitation function $df_{E\lambda}(\vartheta, \xi)$ in the first order perturbation theory (cf. refs. 5 and 8) by the formula

$$\chi^{(\lambda)}(\vartheta, \xi)/\chi^{(\lambda)} = [df_{E\lambda}(\vartheta, \xi)/df_{E\lambda}(\pi, 0)]^{1/2} \sin^2 \vartheta/2. \tag{59}$$

These functions are given in Table 2 for $\lambda = 1, 2$ and 3.

Appendix 2

The excitation amplitudes of states in deformed nuclei are all expressed through the functions $B_{IK}^{\lambda\mu}$ which may be written in the form

$$B_{IK}^{\lambda\mu}(q) = \langle IK\mu \,|\, \sqrt{2\lambda+1}\, D_{\mu K}^{\lambda} e^{-i\frac{4}{3} q D_{00}^{2}} \,|\, 000 \rangle. \tag{60}$$

In the $\chi^{(\lambda)}(\vartheta, \xi)$ approximation and in the $\mu = 0$ approximation one needs only the functions (60) with $\mu = 0$. For these quantities we use the notation B_{IK}^{λ}, i.e.

$$B_{IK}^{\lambda 0} = B_{IK}^{\lambda}. \tag{61}$$

From Eq. (26) one finds for $\lambda = 1, 2$ and 3 the following explicit expressions for B_{IK}^{λ} in terms of the functions A_I defined by (27):

$$\left.\begin{aligned} B_{I,0}^{1} &= \sqrt{\frac{3}{2I+1}}\,[IA_{I-1} + (I+1)\,A_{I+1}] \\ B_{I,1}^{1} &= \sqrt{\frac{3\,I(I+1)}{2\,(2I+1)}}\,[A_{I-1} - A_{I+1}] \end{aligned}\right\} \tag{62}$$

$$\left.\begin{aligned} B_{I,0}^{2} &= \sqrt{\frac{5\,(2I+1)}{4}}\left[\frac{3\,(I-1)\,I}{(2I-1)\,(2I+1)} A_{I-2} + \frac{2\,I(I+1)}{(2I-1)\,(2I+3)} A_I \right. \\ &\qquad \left. + \frac{3\,(I+1)\,(I+2)}{(2I+1)\,(2I+3)} A_{I+2}\right] \\ B_{I,1}^{2} &= \sqrt{\frac{15\,I(I+1)\,(2I+1)}{2}}\left[\frac{I-1}{(2I-1)\,(2I+1)} A_{I-2}\right. \\ &\qquad \left. + \frac{1}{(2I-1)\,(2I+3)} A_I - \frac{I+2}{(2I+1)\,(2I+3)} A_{I+2}\right] \\ B_{I,2}^{2} &= \sqrt{\frac{15\,(I-1)\,I(I+1)\,(I+2)\,(2I+1)}{8}}\left[\frac{1}{(2I-1)\,(2I+1)} A_{I-2}\right. \\ &\qquad \left. - \frac{2}{(2I-1)\,(2I+3)} A_I + \frac{1}{(2I+1)\,(2I+3)} A_{I+2}\right] \end{aligned}\right\} \tag{63}$$

$$
\begin{aligned}
B^3_{I,0} &= \sqrt{\frac{7}{4\,(2\,I+1)}}\left[\frac{5\,(I-2)\,(I-1)\,I}{(2\,I-3)\,(2\,I-1)}A_{I-3}+\frac{3\,(I-1)\,I\,(I+1)}{(2\,I-3)\,(2\,I+3)}A_{I-1}\right.\\
&\quad\left.+\frac{3\,I\,(I+1)\,(I+2)}{(2\,I-1)\,(2\,I+5)}A_{I+1}+\frac{5\,(I+1)\,(I+2)\,(I+3)}{(2\,I+3)\,(2\,I+5)}A_{I+3}\right]\\
B^3_{I,1} &= \sqrt{\frac{21\,I\,(I+1)}{16\,(2\,I+1)}}\left[\frac{5\,(I-2)\,(I-1)}{(2\,I-3)\,(2\,I-1)}A_{I-3}+\frac{(I-1)\,(I+6)}{(2\,I-3)\,(2\,I+3)}A_{I-1}\right.\\
&\quad\left.-\frac{(I-5)\,(I+2)}{(2\,I-1)\,(2\,I+5)}A_{I+1}-\frac{5\,(I+2)\,(I+3)}{(2\,I+3)\,(2\,I+5)}A_{I+3}\right]\\
B^3_{I,2} &= \sqrt{\frac{105\,(I-1)\,I\,(I+1)\,(I+2)}{8\,(2\,I+1)}}\left[\frac{I-2}{(2\,I-3)\,(2\,I-1)}A_{I-3}\right.\\
&\quad\left.-\frac{I-3}{(2\,I-3)\,(2\,I+3)}A_{I-1}-\frac{I+4}{(2\,I-1)\,(2\,I+5)}A_{I+1}+\frac{I+3}{(2\,I+3)\,(2\,I+5)}A_{I+3}\right]\\
B^3_{I,3} &= \sqrt{\frac{35\,(I-2)\,(I-1)\,I\,(I+1)\,(I+2)\,(I+3)}{16\,(2\,I+1)}}\left[\frac{1}{(2\,I-3)\,(2\,I-1)}A_{I-3}\right.\\
&\quad\left.-\frac{3}{(2\,I-3)\,(2\,I+3)}A_{I-1}+\frac{3}{(2\,I-1)\,(2\,I+5)}A_{I+1}-\frac{1}{(2\,I+3)\,(2\,I+5)}A_{I+3}\right].
\end{aligned}
\tag{64}
$$

TABLE 3.

The quantities $B^{\lambda}_{IK}(q)$. The table lists the real and imaginary part of this quantity for $\lambda = 1, 2$ and 3, and $I < \lambda + 4$ as a function of q. In the use of the tables the symmetry relations (65) should be employed. The quantity B^2_{00} has been omitted because of its simple relation (66) to the function $A_2(q)$. The tables have been computed by means of the relations (62)–(64) from the functions $A_I(q)$ as they are tabulated in ref. 4.

q	Re $B^1_{1.0}$	Im $B^1_{1.0}$	Re $B^1_{3.0}$	Im $B^1_{3.0}$	Re $B^1_{5.0}$	Im $B^1_{5.0}$
0.0	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.5	0.93169	−0.25556	−0.05647	−0.24974	−0.03190	0.00664
1.0	0.74457	−0.44841	−0.20654	−0.43136	−0.11374	0.04960
1.5	0.48634	−0.53440	−0.39849	−0.49869	−0.20901	0.14865
2.0	0.22007	−0.50052	−0.56619	−0.44190	−0.27331	0.29737
2.5	0.00530	−0.36721	−0.65117	−0.28935	−0.27188	0.46337
3.0	−0.11902	−0.10851	−0.62214	−0.09682	−0.19400	0.59947
3.5	−0.14402	0.00361	−0.48453	0.07219	−0.05789	0.66093
4.0	−0.09039	0.13687	−0.27727	0.16768	0.09494	0.62240
4.5	0.00148	0.19262	−0.05866	0.16881	0.21476	0.48819
5.0	0.02204	0.17150	0.11394	0.08861	0.26156	0.29196
5.5	0.13098	0.08816	0.20260	−0.04283	0.21978	0.08571
6.0	0.12080	0.00854	0.19958	−0.14671	0.10398	−0.07774
6.5	0.06502	−0.06088	0.12711	−0.20908	−0.04646	−0.16222
7.0	−0.01110	−0.08843	0.02663	−0.20029	−0.18163	−0.15950
7.5	−0.07736	−0.07127	−0.05772	−0.12758	−0.25860	−0.09024
8.0	−0.11025	−0.02414	−0.09487	−0.02083	−0.25622	0.00527
8.5	−0.10116	0.02851	−0.07653	0.08404	−0.18124	0.08288
9.0	−0.04457	0.06324	−0.01760	0.14214	−0.06440	0.11078
9.5	−0.00080	0.06650	0.05204	0.14786	0.05192	0.07997
10.0	0.04761	0.03906	0.10086	0.10309	0.12973	0.00597

(continued)

TABLE 3 (continued).

q	Re $B^1_{1.1}$	Im $B^1_{1.1}$	Re $B^1_{3.1}$	Im $B^1_{3.1}$	Re $B^1_{5.1}$	Im $B^1_{5.1}$
0.0	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.5	0.96853	0.13192	0.00013	−0.20952	−0.02524	0.00127
1.0	0.87738	0.25542	0.00224	−0.39422	−0.09593	0.00963
1.5	0.73585	0.36224	0.01063	−0.53335	−0.19807	0.02908
2.0	0.55838	0.44466	0.03060	−0.61352	−0.31205	0.05849
2.5	0.36086	0.49598	0.06616	−0.63025	−0.41698	0.09136
3.0	0.16208	0.51135	0.11804	−0.58788	−0.49517	0.11731
3.5	−0.02177	0.48850	0.18236	−0.49778	−0.53542	0.12510
4.0	−0.17709	0.42853	0.25089	−0.37551	−0.53429	0.10606
4.5	−0.29408	0.33620	0.31239	−0.23768	−0.49568	0.05702
5.0	−0.36728	0.21883	0.35487	−0.09947	−0.42833	−0.01818
5.5	−0.39549	0.09542	0.36840	0.01944	−0.34303	−0.10924
6.0	−0.38122	−0.03880	0.34738	0.13412	−0.24989	−0.20145
6.5	−0.32911	−0.15550	0.29177	0.21654	−0.15631	−0.27909
7.0	−0.25014	−0.24824	0.20729	0.27214	−0.06664	−0.32881
7.5	−0.15095	−0.30866	0.10418	0.30019	0.01697	−0.34249
8.0	−0.04305	−0.33224	−0.00476	0.30096	0.09334	−0.31852
8.5	0.06282	−0.31871	−0.10652	0.27556	0.16063	−0.26152
9.0	0.15659	−0.27180	−0.19001	0.22636	0.21563	−0.18082
9.5	0.22951	−0.19852	−0.24730	0.15737	0.25367	−0.08792
10.0	0.27507	−0.10821	−0.27453	0.07463	0.26994	0.00560

q	Re $B^2_{2.0}$	Im $B^2_{2.0}$	Re $B^2_{4.0}$	Im $B^2_{4.0}$	Re $B^2_{6.0}$	Im $B^2_{6.0}$
0.0	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.5	0.90692	−0.17790	−0.04471	−0.24229	−0.03080	0.00548
1.0	0.65243	−0.28547	−0.15906	−0.41037	−0.10932	0.04098
1.5	0.30295	−0.27690	−0.29108	−0.45511	−0.19916	0.12000
2.0	−0.05430	−0.14681	−0.37667	−0.36841	−0.25659	0.23110
2.5	−0.33783	0.06798	−0.36414	−0.18469	−0.24903	0.33959
3.0	−0.49570	0.30096	−0.23477	0.03274	−0.16932	0.39971
3.5	−0.51794	0.47857	−0.01108	0.21456	−0.03934	0.37311
4.0	−0.43492	0.54458	0.24965	0.30997	0.09738	0.24576
4.5	−0.30242	0.47804	0.47471	0.30320	0.19253	0.03431
5.0	−0.17974	0.29879	0.60044	0.21656	0.21204	−0.20721
5.5	−0.10880	0.05215	0.59355	0.09038	0.15002	−0.42244
6.0	−0.10157	−0.17497	0.46128	0.00879	0.03191	−0.55300
6.5	−0.13943	−0.34505	0.24735	−0.01475	−0.09414	−0.56771
7.0	−0.18415	−0.41829	0.01557	0.03987	−0.17543	−0.47049
7.5	−0.19537	−0.39438	−0.17234	0.15016	−0.17438	−0.29825
8.0	−0.14741	−0.30135	−0.27675	0.26984	−0.08308	−0.10701
8.5	−0.03966	−0.18188	−0.29053	0.34728	0.07334	0.04828
9.0	0.10353	−0.07638	−0.23729	0.34539	0.24548	0.13222
9.5	0.24223	−0.00915	−0.15846	0.25495	0.37809	0.13952
10.0	0.33620	0.01757	−0.09524	0.09786	0.42535	0.09404

(continued)

TABLE 3 (continued).

q	Re $B^2_{2.1}$	Im $B^2_{2.1}$	Re $B^2_{4.1}$	Im $B^2_{4.1}$	Re $B^2_{6.1}$	Im $B^2_{6.1}$
0.0	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.5	0.96867	−0.09207	−0.02765	−0.22720	−0.02777	0.00377
1.0	0.87978	−0.16602	−0.10317	−0.41953	−0.10344	0.02816
1.5	0.74722	−0.20793	−0.20647	−0.54991	−0.20628	0.08670
2.0	0.59073	−0.21122	−0.31017	−0.60501	−0.30889	0.18043
2.5	0.43159	−0.17778	−0.38689	−0.58708	−0.38478	0.29681
3.0	0.28827	−0.11712	−0.41638	−0.51228	−0.41591	0.41334
3.5	0.17318	−0.04365	−0.39051	−0.40540	−0.39740	0.50391
4.0	0.09113	0.02710	−0.31448	−0.29294	−0.33800	0.54634
4.5	0.03988	0.08211	−0.20488	−0.19656	−0.25656	0.52891
5.0	0.01209	0.11349	−0.08438	−0.12855	−0.17570	0.45365
5.5	−0.00165	0.11620	0.02430	−0.09906	−0.11482	0.33554
6.0	−0.00986	0.10458	0.10385	−0.07545	−0.08464	0.19801
6.5	−0.01820	0.07600	0.14626	−0.07098	−0.08486	0.06656
7.0	−0.02854	0.04269	0.15280	−0.06508	−0.10541	−0.03802
7.5	−0.03957	0.01225	0.13236	−0.04953	−0.13066	−0.10416
8.0	−0.04814	−0.01050	0.09757	−0.02230	−0.14499	−0.13112
8.5	−0.05106	−0.02413	0.06062	0.01273	−0.13778	−0.12732
9.0	−0.04654	−0.02981	0.03008	0.04790	−0.10651	−0.10607
9.5	−0.03487	−0.03030	0.00946	0.07489	−0.05673	−0.08078
10.0	−0.01841	−0.02843	−0.00235	0.08760	0.00034	−0.06093

q	Re $B^2_{2.2}$	Im $B^2_{2.2}$	Re $B^2_{4.2}$	Im $B^2_{4.2}$	Re $B^2_{6.2}$	Im $B^2_{6.2}$
0.0	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.5	0.96849	0.18792	0.00992	−0.16214	−0.01772	−0.00004
1.0	0.87678	0.36078	0.03907	−0.30790	−0.06818	−0.00019
1.5	0.73301	0.50478	0.08530	−0.42281	−0.14366	−0.00120
2.0	0.54984	0.60862	0.14507	−0.49610	−0.23268	−0.00482
2.5	0.34317	0.66442	0.21336	−0.52180	−0.32198	−0.01345
3.0	0.13054	0.66846	0.28381	−0.49922	−0.39857	−0.03001
3.5	−0.07052	0.62154	0.34912	−0.43275	−0.45165	−0.05696
4.0	−0.24415	0.52888	0.40155	−0.33099	−0.47384	−0.09537
4.5	−0.37757	0.39972	0.43395	−0.20557	−0.46214	−0.14425
5.0	−0.46213	0.24642	0.44050	−0.06967	−0.41752	−0.19999
5.5	−0.49395	0.08331	0.41776	0.05752	−0.34462	−0.25683
6.0	−0.47406	−0.07464	0.36528	0.18190	−0.25066	−0.30731
6.5	−0.40809	−0.21337	0.28595	0.27569	−0.14417	−0.34360
7.0	−0.30555	−0.32097	0.18588	0.33794	−0.03410	−0.35881
7.5	−0.17879	−0.38889	0.07378	0.36492	0.07094	−0.34821
8.0	−0.04178	−0.41268	−0.04000	0.35618	0.16344	−0.31030
8.5	0.09130	−0.39236	−0.14472	0.31441	0.23709	−0.24700
9.0	0.20736	−0.33228	−0.23051	0.24501	0.28726	−0.16365
9.5	0.29560	−0.24056	−0.28954	0.15562	0.31083	−0.06803
10.0	0.34843	−0.12816	−0.31686	0.05539	0.30675	0.03046

(continued)

TABLE 3 (continued).

q	Re $B^3_{3.0}$	Im $B^3_{3.0}$	Re $B^3_{5.0}$	Im $B^3_{5.0}$	Re $B^3_{7.0}$	Im $B^3_{7.0}$
0.0	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.5	0.92002	−0.16436	−0.04240	−0.24144	−0.03065	0.00530
1.0	0.70468	−0.25402	−0.15033	−0.41653	−0.10975	0.03966
1.5	0.41948	−0.22136	−0.27340	−0.48338	−0.20401	0.11547
2.0	0.14795	−0.06293	−0.34988	−0.43871	−0.27459	0.22299
2.5	−0.03650	0.17913	−0.33166	−0.31801	−0.29269	0.32940
3.0	−0.09545	0.43210	−0.20395	−0.18144	−0.25409	0.39269
3.5	−0.03553	0.61829	0.00782	−0.08956	−0.18074	0.37852
4.0	0.09555	0.68187	0.24605	−0.08238	−0.11229	0.27631
4.5	0.22908	0.60745	0.44146	−0.15995	−0.08957	0.10550
5.0	0.30095	0.42378	0.53791	−0.28737	−0.13657	−0.08861
5.5	0.27476	0.18559	0.51238	−0.41581	−0.24866	−0.25072
6.0	0.15361	−0.01684	0.38241	−0.45984	−0.39192	−0.33508
6.5	−0.02306	−0.14678	0.19888	−0.41197	−0.51432	−0.32258
7.0	−0.19579	−0.17469	0.02641	−0.26452	−0.56498	−0.22795
7.5	−0.30786	−0.11523	−0.08031	−0.05527	−0.51357	−0.09405
8.0	−0.32584	−0.01197	−0.09569	0.15547	−0.36295	0.02404
8.5	−0.25046	0.08137	−0.03069	0.30708	−0.14934	0.08025
9.0	−0.11437	0.12212	0.07369	0.36005	0.06985	0.05437
9.5	0.03175	0.09365	0.16384	0.30917	0.23581	−0.04032
10.0	0.13884	0.00984	0.19512	0.18396	0.30896	−0.16299

q	Re $B^3_{3.1}$	Im $B^3_{3.1}$	Re $B^3_{5.1}$	Im $B^3_{5.1}$	Re $B^3_{7.1}$	Im $B^3_{7.1}$
0.0	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.5	0.94033	−0.12797	−0.03360	−0.23128	−0.02860	0.00429
1.0	0.77238	−0.22544	−0.12356	−0.41192	−0.10454	0.03208
1.5	0.52654	−0.27028	−0.24081	−0.50381	−0.20110	0.09777
2.0	0.24554	−0.25481	−0.34718	−0.49108	−0.28325	0.19830
2.5	−0.02517	−0.18742	−0.40656	−0.39107	−0.32010	0.31468
3.0	−0.25071	−0.09005	−0.39599	−0.20959	−0.29359	0.41627
3.5	−0.39597	0.00823	−0.31256	−0.01307	−0.20468	0.47095
4.0	−0.46452	0.07937	−0.17385	0.16445	−0.07290	0.45556
4.5	−0.46144	0.10383	−0.01282	0.29156	0.07030	0.36442
5.0	−0.40596	0.07534	0.13195	0.35406	0.19162	0.21190
5.5	−0.32146	−0.00309	0.22708	0.34778	0.26608	0.02920
6.0	−0.22876	−0.09788	0.25318	0.31564	0.28406	−0.14438
6.5	−0.14185	−0.19901	0.20902	0.25683	0.25325	−0.27225
7.0	−0.06649	−0.27830	0.11062	0.20120	0.19460	−0.33033
7.5	−0.00194	−0.31910	−0.01477	0.16157	0.13446	−0.31286
8.0	0.05590	−0.31479	−0.13686	0.13929	0.09548	−0.23241
8.5	0.11046	−0.26889	−0.23042	0.12599	0.08934	−0.11486
9.0	0.16190	−0.19266	−0.28093	0.10871	0.11365	0.00926
9.5	0.20612	−0.10106	−0.28625	0.07578	0.15373	0.11336
10.0	0.23599	−0.00884	−0.25453	0.02192	0.18874	0.18145

(continued)

TABLE 3 (continued).

q	Re $B^3_{3.2}$	Im $B^3_{3.2}$	Re $B^3_{5.2}$	Im $B^3_{5.2}$	Re $B^3_{7.2}$	Im $B^3_{7.2}$
0.0	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.5	0.97996	0.00069	−0.01009	−0.19764	−0.02250	0.00181
1.0	0.92190	0.00525	−0.03772	−0.37542	−0.08577	0.01340
1.5	0.83151	0.01657	−0.07585	−0.51672	−0.17810	0.04193
2.0	0.71735	0.03577	−0.11444	−0.61057	−0.28337	0.08894
2.5	0.58954	0.06189	−0.14299	−0.65269	−0.38351	0.14992
3.0	0.45825	0.09201	−0.15300	−0.64589	−0.46302	0.21533
3.5	0.33260	0.12185	−0.13987	−0.59860	−0.51158	0.27275
4.0	0.21952	0.14669	−0.10375	−0.52270	−0.52537	0.30990
4.5	0.12352	0.16235	−0.04960	−0.43103	−0.50708	0.31758
5.0	0.04654	0.16597	0.01422	−0.33520	−0.46416	0.29206
5.5	−0.01157	0.15664	0.07774	−0.25136	−0.40647	0.23574
6.0	−0.05227	0.13538	0.13140	−0.16297	−0.34359	0.15659
6.5	−0.07790	0.10498	0.16800	−0.09409	−0.28281	0.06636
7.0	−0.09092	0.06926	0.18381	−0.03726	−0.22792	−0.02219
7.5	−0.09361	0.03248	0.17868	0.00885	−0.17942	−0.09760
8.0	−0.08797	−0.00140	0.15580	0.04565	−0.13546	−0.15198
8.5	−0.07581	−0.02932	0.12040	0.07396	−0.09336	−0.18180
9.0	−0.05882	−0.04937	0.07861	0.09375	−0.05114	−0.18780
9.5	−0.03873	−0.06087	0.03621	0.10449	−0.00850	−0.17394
10.0	−0.01746	−0.06419	−0.00221	0.10562	0.03290	−0.14610

q	Re $B^3_{3.3}$	Im $B^3_{3.3}$	Re $B^3_{5.3}$	Im $B^3_{5.3}$	Re $B^3_{7.3}$	Im $B^3_{7.3}$
0.0	1.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.5	0.96658	0.21912	0.01361	−0.13171	−0.01301	−0.00057
1.0	0.86926	0.42004	0.05307	−0.25006	−0.05028	−0.00411
1.5	0.71659	0.58615	0.11424	−0.34310	−0.10671	−0.01343
2.0	0.52192	0.70411	0.19065	−0.40152	−0.17430	−0.03098
2.5	0.30212	0.76484	0.27407	−0.41969	−0.24369	−0.05808
3.0	0.07591	0.76454	0.35527	−0.39616	−0.30505	−0.09519
3.5	−0.13769	0.70482	0.42492	−0.33372	−0.34945	−0.14143
4.0	−0.32142	0.59259	0.47446	−0.23905	−0.36990	−0.19443
4.5	−0.46108	0.43928	0.49713	−0.12186	−0.36229	−0.25045
5.0	−0.54690	0.25982	0.48850	0.00598	−0.32558	−0.30444
5.5	−0.57435	0.07916	0.44720	0.12708	−0.26198	−0.35075
6.0	−0.54386	−0.10965	0.37517	0.24392	−0.17671	−0.38345
6.5	−0.46312	−0.26643	0.27740	0.33148	−0.07704	−0.39736
7.0	−0.34131	−0.38601	0.16166	0.38681	0.02826	−0.38854
7.5	−0.19299	−0.45912	0.03773	0.40539	0.12988	−0.35510
8.0	−0.03408	−0.48122	−0.08364	0.38644	0.21900	−0.29768
8.5	0.11914	−0.45286	−0.19174	0.33269	0.28792	−0.21940
9.0	0.25174	−0.37945	−0.27715	0.25025	0.33095	−0.12592
9.5	0.35133	−0.27053	−0.33247	0.14771	0.34459	−0.02467
10.0	0.40942	−0.13882	−0.35340	0.03547	0.32814	0.07570

These functions have been computed for $I = \lambda,\ \lambda+2,\ \lambda+4$, and $q \leq 10$ and the result is given in Table 3. For odd values of $\lambda+I$ the functions B^{λ}_{IK} vanish, while for $I<\lambda$ and $K<0$ they can be found from the symmetry relations

$$\left.\begin{aligned} B^{\lambda}_{IK} &= B^{I}_{\lambda K} \\ \text{and} \qquad B^{\lambda}_{IK} &= B^{\lambda}_{I-K}. \end{aligned}\right\} \tag{65}$$

For $I = 0$ the functions B^{λ}_{IK} are proportional to the functions A_λ which are tabulated in refs. 4 and 8.

$$B^{\lambda}_{00}(q) = \sqrt{2\lambda+1}\, A_\lambda(q) \tag{66}$$

and we have therefore omitted the table of B^{2}_{00}.

For convenience we have computed also the functions $|B^{\lambda}_{IK}|^2$ which determine the relative excitation probabilities. They are given for $\lambda = 1,\ 2$ and 3 and $I \leq \lambda+4$ in Table 4.

TABLE 4.

The quantities $|B^{\lambda}_{IK}(q)|^2$ for $\lambda = 1,\ 2$ and 3 and $I \leq \lambda+4$ as functions of q. These quantities determine in the $\chi(\vartheta, \xi)$ approximation, Eq. (37), the relative excitation probability of the rotational states in the coupled band.

	$\lvert B^{1}_{I,0}\rvert^2$			$\lvert B^{1}_{I,1}\rvert^2$		
q	$I=1$	$I=3$	$I=5$	$I=1$	$I=3$	$I=5$
0.0	1.0000	0.0000	0.0000	1.0000	0.0000	0.0000
0.5	0.9334	0.0656	0.0010	0.9555	0.0439	0.0006
1.0	0.7555	0.2287	0.0154	0.8350	0.1554	0.0093
1.5	0.5221	0.4075	0.0658	0.6727	0.2846	0.0401
2.0	0.2990	0.5158	0.1631	0.5095	0.3773	0.1008
2.5	0.1349	0.5078	0.2887	0.3762	0.4016	0.1822
3.0	0.0468	0.3964	0.3970	0.2878	0.3596	0.2590
3.5	0.0208	0.2400	0.4402	0.2391	0.2810	0.3023
4.0	0.0269	0.1050	0.3964	0.2150	0.2040	0.2967
4.5	0.0371	0.0319	0.2844	0.1995	0.1541	0.2490
5.0	0.0299	0.0208	0.1536	0.1832	0.1358	0.1838
5.5	0.0249	0.0429	0.0556	0.1655	0.1361	0.1296
6.0	0.0147	0.0614	0.0168	0.1468	0.1387	0.1030
6.5	0.0079	0.0599	0.0285	0.1325	0.1320	0.1023
7.0	0.0091	0.0408	0.0584	0.1242	0.1170	0.1126
7.5	0.0111	0.0196	0.0750	0.1181	0.1010	0.1176
8.0	0.0114	0.0094	0.0657	0.1122	0.0906	0.1102
8.5	0.0110	0.0129	0.0397	0.1055	0.0873	0.0942
9.0	0.0070	0.0205	0.0164	0.0984	0.0874	0.0792
9.5	0.0044	0.0246	0.0091	0.0921	0.0859	0.0721
10.0	0.0062	0.0208	0.0169	0.0874	0.0809	0.0729

(continued)

TABLE 4 (continued).

	$\lvert B^2_{I,0}\rvert^2$				$\lvert B^2_{I,1}\rvert^2$		
q	$I=0$	$I=2$	$I=4$	$I=6$	$I=2$	$I=4$	$I=6$
0.0	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000	0.0000
0.5	0.0841	0.8542	0.0607	0.0010	0.9468	0.0524	0.0008
1.0	0.2850	0.5072	0.1937	0.0136	0.8016	0.1866	0.0115
1.5	0.4812	0.1684	0.2919	0.0541	0.6016	0.3450	0.0501
2.0	0.5597	0.0245	0.2776	0.1192	0.3936	0.4622	0.1280
2.5	0.4842	0.1188	0.1667	0.1773	0.2179	0.4944	0.2362
3.0	0.3098	0.3363	0.0562	0.1884	0.0968	0.4358	0.3438
3.5	0.1389	0.4973	0.0462	0.1408	0.0319	0.3168	0.4118
4.0	0.0514	0.4857	0.1584	0.0699	0.0090	0.1847	0.4127
4.5	0.0600	0.3200	0.3173	0.0382	0.0083	0.0806	0.3456
5.0	0.1158	0.1216	0.4073	0.0879	0.0130	0.0236	0.2367
5.5	0.1540	0.0146	0.3605	0.2010	0.0135	0.0104	0.1258
6.0	0.1412	0.0409	0.2129	0.3068	0.0110	0.0165	0.0464
6.5	0.0917	0.1385	0.0614	0.3312	0.0061	0.0264	0.0116
7.0	0.0459	0.2089	0.0018	0.2521	0.0026	0.0276	0.0126
7.5	0.0343	0.1937	0.0522	0.1194	0.0017	0.0200	0.0279
8.0	0.0552	0.1125	0.1494	0.0184	0.0024	0.0100	0.0382
8.5	0.0819	0.0347	0.2050	0.0077	0.0032	0.0038	0.0352
9.0	0.0879	0.0166	0.1756	0.0777	0.0030	0.0032	0.0226
9.5	0.0685	0.0588	0.0901	0.1624	0.0021	0.0057	0.0097
10.0	0.0408	0.1133	0.0186	0.1898	0.0012	0.0077	0.0037

	$\lvert B^2_{I,2}\rvert^2$			$\lvert B^3_{I,0}\rvert^2$			
q	$I=2$	$I=4$	$I=6$	$I=1$	$I=3$	$I=5$	$I=7$
0.0	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
0.5	0.9733	0.0264	0.0003	0.0656	0.8734	0.0601	0.0009
1.0	0.8989	0.0963	0.0046	0.2287	0.5611	0.1961	0.0136
1.5	0.7921	0.1860	0.0206	0.4075	0.2250	0.3084	0.0550
2.0	0.6728	0.2672	0.0542	0.5158	0.0258	0.3149	0.1251
2.5	0.5592	0.3178	0.1038	0.5078	0.0334	0.2111	0.1942
3.0	0.4639	0.3298	0.1598	0.3964	0.1958	0.0745	0.2188
3.5	0.3913	0.3092	0.2072	0.2400	0.3835	0.0081	0.1760
4.0	0.3393	0.2708	0.2336	0.1050	0.4741	0.0673	0.0890
4.5	0.3023	0.2306	0.2344	0.0319	0.4215	0.2205	0.0192
5.0	0.2743	0.1989	0.2143	0.0208	0.2702	0.3719	0.0265
5.5	0.2509	0.1778	0.1847	0.0429	0.1099	0.4354	0.1247
6.0	0.2303	0.1665	0.1573	0.0614	0.0239	0.3577	0.2659
6.5	0.2121	0.1578	0.1388	0.0599	0.0221	0.2093	0.3686
7.0	0.1964	0.1488	0.1299	0.0408	0.0688	0.0707	0.3711
7.5	0.1832	0.1386	0.1263	0.0196	0.1080	0.0095	0.2726
8.0	0.1720	0.1285	0.1230	0.0094	0.1063	0.0333	0.1323
8.5	0.1623	0.1198	0.1172	0.0129	0.0694	0.0952	0.0287
9.0	0.1534	0.1132	0.1093	0.0205	0.0280	0.1351	0.0078
9.5	0.1452	0.1080	0.1012	0.0246	0.0098	0.1224	0.0572
10.0	0.1378	0.1035	0.0950	0.0208	0.0194	0.0719	0.1220

(continued)

TABLE 4 (continued).

	$\lvert B^3_{I,1} \rvert^2$			
q	$I = 1$	$I = 3$	$I = 5$	$I = 7$
0.0	0.0000	1.0000	0.0000	0.0000
0.5	0.0439	0.9006	0.0546	0.0009
1.0	0.1554	0.6474	0.1849	0.0120
1.5	0.2846	0.3503	0.3118	0.0500
2.0	0.3773	0.1252	0.3617	0.1196
2.5	0.4016	0.0358	0.3182	0.2015
3.0	0.3596	0.0710	0.2007	0.2595
3.5	0.2810	0.1569	0.0979	0.2637
4.0	0.2040	0.2221	0.0573	0.2128
4.5	0.1541	0.2237	0.0852	0.1377
5.0	0.1358	0.1705	0.1428	0.0816
5.5	0.1361	0.1034	0.1725	0.0716
6.0	0.1387	0.0619	0.1637	0.0807
6.5	0.1320	0.0597	0.1096	0.1383
7.0	0.1170	0.0819	0.0527	0.1470
7.5	0.1010	0.1018	0.0263	0.1160
8.0	0.0906	0.1022	0.0381	0.0631
8.5	0.0873	0.0845	0.0690	0.0212
9.0	0.0874	0.0633	0.0907	0.0130
9.5	0.0859	0.0527	0.0877	0.0365
10.0	0.0809	0.0558	0.0652	0.0686

	$\lvert B^3_{I,2} \rvert^2$			$\lvert B^3_{I,3} \rvert^2$		
q	$I = 3$	$I = 5$	$I = 7$	$I = 3$	$I = 5$	$I = 7$
0.0	1.0000	0.0000	0.0000	1.0000	0.0000	0.0000
0.5	0.9603	0.0392	0.0005	0.9823	0.0175	0.0002
1.0	0.8499	0.1424	0.0075	0.9320	0.0654	0.0025
1.5	0.6917	0.2728	0.0335	0.8571	0.1308	0.0116
2.0	0.5159	0.3859	0.0882	0.7682	0.1976	0.0313
2.5	0.3514	0.4464	0.1696	0.6763	0.2512	0.0628
3.0	0.2185	0.4406	0.2608	0.5903	0.2832	0.1021
3.5	0.1255	0.3779	0.3361	0.5157	0.2919	0.1421
4.0	0.0697	0.2840	0.3720	0.4545	0.2823	0.1746
4.5	0.0416	0.1882	0.3580	0.4056	0.2620	0.1940
5.0	0.0297	0.1126	0.3007	0.3666	0.2387	0.1987
5.5	0.0247	0.0692	0.2208	0.3361	0.2161	0.1917
6.0	0.0211	0.0438	0.1426	0.3078	0.2002	0.1783
6.5	0.0171	0.0371	0.0844	0.2855	0.1868	0.1638
7.0	0.0131	0.0352	0.0524	0.2655	0.1758	0.1518
7.5	0.0098	0.0320	0.0417	0.2480	0.1658	0.1430
8.0	0.0077	0.0264	0.0414	0.2327	0.1563	0.1366
8.5	0.0066	0.0200	0.0418	0.2193	0.1474	0.1310
9.0	0.0059	0.0150	0.0379	0.2074	0.1394	0.1254
9.5	0.0052	0.0122	0.0303	0.1966	0.1324	0.1194
10.0	0.0044	0.0112	0.0224	0.1869	0.1262	0.1134

For a more accurate description of the dependence of the excitation amplitudes on the deflection angle one needs the functions $B_{IK}^{\lambda\mu}$ with $\mu \neq 0$. These functions satisfy a number of symmetry relations which are consequences of symmetry properties of the 3-j symbols and of the fact that A_J vanishes for odd values of J. These relations are

$$B_{IK}^{\lambda\mu} = B_{I\mu}^{\lambda K} = B_{\lambda K}^{I\mu} \tag{67}$$

and

$$B_{IK}^{\lambda\mu} = (-1)^{I-\lambda} B_{IK}^{\lambda-\mu} = B_{I-K}^{\lambda-\mu}. \tag{68}$$

For $\lambda = 1$ and 2 Eq. (26) reads explicitly

$$B_{I,1}^{1,1} = \begin{cases} \sqrt{\dfrac{3}{4(2I+1)}}\,[(I+1)A_{I-1} + IA_{I+1}] & I \text{ odd} \\ \sqrt{\dfrac{3(2I+1)}{4}}\,A_I & I \text{ even} \end{cases} \tag{69}$$

$$B_{I,1}^{2,1} = \begin{cases} \sqrt{\dfrac{5(2I+1)}{4}}\left[\dfrac{2(I-1)(I+1)}{(2I-1)(2I+1)}A_{I-2}\right. & \\ \quad \left. + \dfrac{3}{(2I-1)(2I+3)}A_I + \dfrac{2I(I+2)}{(2I+1)(2I+3)}A_{I+2}\right] & I \text{ even} \\ \sqrt{\dfrac{5}{4(2I+1)}}\,[(I-1)A_{I-1} + (I+2)A_{I+1}] & I \text{ odd} \end{cases}$$

$$B_{I,2}^{2,1} = \begin{cases} \sqrt{\dfrac{5(I-1)(I+2)(2I+1)}{4}}\left[\dfrac{I+1}{(2I-1)(2I+1)}A_{I-2}\right. & \\ \quad \left. - \dfrac{3}{(2I-1)(2I+3)}A_I - \dfrac{I}{(2I+1)(2I+3)}A_{I+2}\right] & I \text{ even} \\ \sqrt{\dfrac{5(I-1)(I+2)}{4(2I+1)}}\,[A_{I-1} - A_{I+1}] & I \text{ odd} \end{cases} \tag{70}$$

$$B_{I,2}^{2,2} = \begin{cases} \sqrt{\dfrac{5(2I+1)}{16}}\left[\dfrac{(I+1)(I+2)}{(2I-1)(2I+1)}A_{I-2}\right. & \\ \quad \left. + \dfrac{6(I-1)(I+2)}{(2I-1)(2I+3)}A_I + \dfrac{(I-1)I}{(2I+1)(2I+3)}A_{I+2}\right] & I \text{ even} \\ \sqrt{\dfrac{5}{4(2I+1)}}\,[(I+2)A_{I-1} + (I-1)A_{I+1}]. & I \text{ odd} \end{cases}$$

The absolute squares of the functions $B_{IK}^{2\mu}$ have been computed numerically and the result is given in Table 5.

We note finally that the functions $B_{IK}^{\lambda\mu}$ satisfy the relations

$$B_{IK}^{\lambda\mu}(0) = \delta_{I,\lambda} \tag{71}$$

and (cf. Eq. (31))

$$\sum_I B_{IK}^{\lambda'\mu*}(q)\, B_{IK}^{\lambda\mu}(q) = \delta_{\lambda',\lambda}. \tag{72}$$

TABLE 5.

The quantities $|B_{IK}^{\lambda\mu}(q)|^2$ for $\lambda = 2$, $\mu \neq 0$, $K \neq 0$, and $I \leq 6$ as functions of q. From these quantities the relative quadrupole excitation probabilities can be determined by means of Eq. (34). In the application of the table one should employ the symmetry relations (67)–(68). For $K = 0$ or $\mu = 0$ the functions reduce to the quantities $|B_{IK}^{\lambda}|^2$ given in Table 4.

$|B_{I,1}^{2,1}|^2$

q	$I = 1$	$I = 2$	$I = 3$	$I = 4$	$I = 5$	$I = 6$
0.0	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000
0.5	0.0631	0.8811	0.0126	0.0423	0.0003	0.0006
1.0	0.2138	0.5879	0.0484	0.1370	0.0042	0.0083
1.5	0.3609	0.2708	0.1005	0.2122	0.0187	0.0332
2.0	0.4198	0.0737	0.1548	0.2120	0.0487	0.0738
2.5	0.3632	0.0513	0.1921	0.1393	0.0918	0.1108
3.0	0.2324	0.1496	0.1958	0.0521	0.1368	0.1191

$|B_{I,2}^{2,1}|^2$

q	$I = 2$	$I = 3$	$I = 4$	$I = 5$	$I = 6$
0.0	1.0000	0.0000	0.0000	0.0000	0.0000
0.5	0.9470	0.0305	0.0217	0.0005	0.0002
1.0	0.8048	0.1079	0.0762	0.0072	0.0035
1.5	0.6157	0.1976	0.1373	0.0312	0.0152
2.0	0.4300	0.2620	0.1771	0.0784	0.0380
2.5	0.2861	0.2789	0.1798	0.1417	0.0682
3.0	0.1988	0.2497	0.1482	0.2014	0.0955

$|B_{I,2}^{2,2}|^2$

q	$I = 2$	$I = 3$	$I = 4$	$I = 5$	$I = 6$
0.0	1.0000	0.0000	0.0000	0.0000	0.0000
0.5	0.9125	0.0751	0.0114	0.0009	0.0001
1.0	0.6860	0.2539	0.0458	0.0124	0.0017
1.5	0.4087	0.4269	0.1003	0.0515	0.0090
2.0	0.1753	0.4924	0.1634	0.1234	0.0284
2.5	0.0419	0.4179	0.2135	0.2075	0.0658
3.0	0.0075	0.2538	0.2278	0.2658	0.1175

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THE RESTRICTED PROBLEM OF THREE BODIES

BY

JAMES H. BARTLETT

København 1964
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Synopsis

The case of two equal finite masses has been studied extensively, using Thiele(9) variables, a modified Runge-Kutta method, and an electronic computer. The main classes of Strömgren(4) have been traced continuously from beginning to end, and seven new classes are reported. For convenience, a class is represented by an eigensurface in (E, F, K) space, where K is the Jacobi integral. General methods of locating periodic solutions, in particular asymmetric ones, are discussed. Initial and final conditions, in the form of tables and curves, are given for more than 800 periodic orbits.

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The restricted problem of three bodies, which consists in the determination of the motion of a body of infinitesimal mass under the gravitational action of two other bodies of finite mass, has been investigated by many theoreticians and computers. POINCARÉ [1] and BIRKHOFF [2] obtained valuable general results; DARWIN [3], STRÖMGREN and his school [4], SHEARING [5], and GOUDAS [6] have made extensive computations, have shown in detail how some of the periodic solutions look, and have made limited studies of their stability.

A comprehensive picture of the simpler periodic solutions is perhaps best attained by means of the concept of a *class* of periodic orbits, which concept was introduced and employed effectively by STRÖMGREN for the case of equal finite masses. If one periodic orbit is known, then one may vary either the first integral (Jacobi constant) or the mass ratio, or both, and then adjust the initial conditions continuously to give another periodic orbit; the family of orbits so obtained is said to constitute a class. A good understanding should then be reached if one can describe and explain the internal structure of the simpler classes, and to show how and why various classes are interrelated. It is in this sense that the present program has been undertaken, rather than for the purpose of calculating orbits with extreme exactness.

In the present article, which is restricted to the case of equal finite masses, there are presented curves and tables which show how most of the main classes of STRÖMGREN develop continuously. (STRÖMGREN was, in most cases, only able to give a few typical members of the class, because his work was done before the advent of the modern electronic computer). Class (g), which was started by BURRAU and STRÖMGREN [7], and carried through about one-half of its development by the late P. PEDERSEN, is given completely. Seven new classes: (λ), (μ), (ν), (α), (β), (γ), and (δ), the the latter three of which are just as important as class (g), are reported for the first time.* We also indicate how to determine several classes of asymmetric orbits, and we show how one may use a suitable mapping to find all the periodic solutions. Inspection reveals that continuation to the case of unequal masses is straightforward, and work is proceeding along these lines. Definite statements about ultimate stability are, however, very difficult to make, because they require a very precise knowledge

* Presumably our (β) class is the same figure-of-eight class (C'; C'') predicted by Darwin, for the case $m_1 = 10\, m_2$, in part V of his second paper (3).

of the mapping near a fixed point (elliptic). MOSER [8] has shown that stability can occur for certain special mappings, but it remains to be seen whether our mappings fall into this category.

Equations of Motion

Suppose we have two bodies S and J with masses m_1 and m_2 respectively, which execute circular motions about their common center of gravity, and that the distance SJ between them has magnitude 2 units. Let us study the motion of a third body P which has vanishingly small mass and moves in the same plane as S and J do.

Let there be a coordinate system (x, y) fixed in the plane, with origin O at the center of gravity. Set $SO = r_1$, $OJ = r_2$, $SP = r$, $PJ = \varrho$. P, S, and J have as coordinates (x, y), (x_1, y_1) and (x_2, y_2). The equations of motion for P are

$$\left.\begin{aligned} \ddot{x} &= k^2 m_1 (x_1 - x)/r^3 + k^2 m_2 (x_2 - x)/\varrho^3 \\ \ddot{y} &= k^2 m_1 (y_1 - y)/r^3 + k^2 m_2 (y_2 - y)/\varrho^3 \end{aligned}\right\} \quad (1)$$

Now let us refer the motion to a rotating coordinate system (ξ, η), where the ξ-axis lies along SJ. The angular velocity is

$$\omega = (k/2)\left[(m_1 + m_2)/2\right]^{1/2} = k\,(M/8)^{1/2}$$

The equations of motion in this system are

$$\left.\begin{aligned} \ddot{\xi} - 2\,\omega\,\dot{\eta} - \omega^2 \xi + k^2 m_1 (\xi + r_1)/r^3 + k^2 m_2 (\xi - r_2)/\varrho^3 &= 0 \\ \ddot{\eta} + 2\,\omega\,\dot{\xi} - \omega^2 \eta + k^2 m_1\, \eta/r^3 + k^2 m_2\, \eta/\varrho^3 &= 0. \end{aligned}\right\} \quad (2)$$

If we set $\omega = 1$, then $k^2 M = 8$, and equations (2) may be written as

$$\ddot{\xi} - 2\,\dot{\eta} = \partial U/\partial \xi,\ \ddot{\eta} + 2\,\dot{\xi} = \partial U/\partial \eta \quad (3)$$

where

$$2\,U = \xi^2 + \eta^2 + 8(1 + \gamma)/r + 8(1 - \gamma)/\varrho \quad (4)$$

with

$$\gamma = (m_1 - m_2)/(m_1 + m_2),\ \text{and}\ (m_2/M) = \frac{1}{2}(1 - \gamma).$$

Equations (3) have the first integral

$$\dot{\xi}^2 + \dot{\eta}^2 = 2\,U - K \quad (5)$$

where K is the Jacobi constant (Strömgren's notation).

Equations (2) are singular at $r = 0$ and $\varrho = 0$, so that one cannot treat collision orbits on a par with other orbits. To overcome this difficulty, THIELE [9] introduced a transformation which allows one to vary parameters of a family (class) of orbits smoothly, paying no special heed to collision orbits. This transformation is

$$\left.\begin{aligned} \xi &= \cosh F \cos E + \gamma \\ \eta &= -\sinh F \sin E \\ d\psi &= (\omega/r\varrho)\, dt \end{aligned}\right\} \quad (6)$$

We have the further equations

$$r_1 = 1-\gamma, \quad r_2 = 1+\gamma$$

$$r = \cosh F + \cos E, \quad \varrho = \cosh F - \cos E$$

and

$$r\varrho = (1/2)\,(\cosh 2F - \cos 2E).$$

When $F = 0$, then $\xi = \cos E + \gamma$, $\eta = 0$, which corresponds to the ξ-axis between the 2 masses. When $E = 0$, $\xi = \cosh F - 1 + r_2$, $\eta = 0$, which represents the ξ-axis between m_2 and $+\infty$. Similarly, when $E = \pm\pi$, $\xi = 1 - \cosh F - r_1$, $\eta = 0$, describing the ξ-axis between m_1 and $-\infty$. The line $E = \pi/2$ has coordinates $\xi = \gamma$, $\eta = -\sinh F$, and is the locus of points equidistant from the 2 masses.

In what follows, a dot will denote differentiation re ψ rather than re t.

The equation for the first integral, namely (5), now transforms into

$$\left.\begin{aligned} \dot{E}^2 + \dot{F}^2 = (1/8)\,(\cosh 4F - \cos 4E) - (T/2)\,(\cosh 2F - \cos 2E) + 16\cosh F \\ + (\gamma/2)\,(\cos E \cosh 3F - \cos 3E \cosh F - 32\cos E) = 2H \end{aligned}\right\} \quad (7)$$

where $T = K - \gamma^2$.

The differential equations (3) themselves become

$$\left.\begin{aligned} \ddot{E} &= (\cosh 2F - \cos 2E)\,\dot{F} + \partial H/\partial E \\ \ddot{F} &= -(\cosh 2F - \cos 2E)\,\dot{E} + \partial H/\partial F. \end{aligned}\right\} \quad (8)$$

In the case of equal masses, $\gamma = 0$, $T = K$, and

$$\left.\begin{aligned} \ddot{E} &= (\cosh 2F - \cos 2E)\,\dot{F} + (1/4)\sin 4E - (T/2)\sin 2E \\ \ddot{F} &= -(\cosh 2F - \cos 2E)\,\dot{E} + (1/4)\sinh 4F - (T/2)\sinh 2F + 8\sinh F \end{aligned}\right\} \quad (9)$$

When $\gamma \neq 0$, the right hand sides of (9) have additional terms

$$\left.\begin{aligned} \Delta\ddot{E} &= -(\gamma/4)\,(\sin E \cosh 3F - 3\sin 3E \cosh F - 32\sin E) \\ \Delta\ddot{F} &= -(\gamma/4)\,(-3\cos E \sinh 3F + \cos 3E \sinh F). \end{aligned}\right\} \quad (10)$$

The present article will deal with equal masses ($\gamma = 0$), and so equations (7) and (9) will be applicable. Let us first make some general remarks about the invariance properties of equation (9).

This equation is still the same if E is replaced by $E + \pi$, which amounts, if $\gamma = 0$, to replacing ξ by $-\xi$ and η by $-\eta$. In other words, for equal masses the physical system remains invariant under a rotation of 180°.

The reversed motion is obtained either by replacing ψ with $-\psi$ or by changing F to $-F$. The latter is equivalent to the transformation $\xi' = \xi$, $\eta' = -\eta$, or reflection about the ξ-axis, and also, from the preceding, to reflection about the η-axis, i.e. $\xi' = -\xi$, $\eta' = \eta$. The equations (9) are thus invariant under $E' = \pi - E$, $F' = -F$.

Periodic Solutions

The periodic solutions occupy an important place in the theory of the equations, because some of them are quite stable and the system stays together for a long time. Therefore our first task will be to locate where the periodic solutions are, in general. We need only determine the simpler periodic solutions, because BIRKHOFF has proved the existence of solutions which have periods that are multiples of the basic period. A revision of this proof of Birkhoff's Fixed Point Theorem has been given by SIEGEL[10].

If the motion of a dynamical system is to be periodic, this means that after a period τ the dynamical variables return to their original values. Alternatively stated, one must in general solve a system of non-linear ordinary differential equations, subject to the boundary conditions that the final positions and velocities must have the same values as the initial ones.

Let us first consider motion in one dimension subject to a force which is not explicitly dependent on the time. The equation of motion $\ddot{u} + f(u) = 0$ has a first integral $\frac{1}{2}\dot{u}^2 = h - V(u)$, where h is constant and V is the potential energy. If V has a minimum, then librations will occur in the valley of V, and the period may be determined by a quadrature. Given h and u, one can determine the velocity $\dot{u}$ except for sign. The periodic motions may be easily visualized by drawing the trajectories in the phase plane $(u, \dot{u})$.

It is somewhat more difficult but still feasible to characterize periodic motion in 2 dimensions, such as is the case for the restricted 3-body problem. Let the JACOBI constant T have a definite value, and consider the totality of periodic motions belonging to this value. They will be closed curves in the (E, F) plane, which we shall call *eigencurves*. These curves can be symmetric with respect to (1) the ξ-axis (2) the η-axis (3) both the ξ-axis and the η-axis or (4) neither the ξ-axis nor the η-axis.

[The symmetry properties of the equations do not by any means exclude asymmetric solutions, but such solutions have hitherto been largely ignored because they are somewhat more complicated and also less easy to locate. However, STRÖMGREN [4] (see Tableau V, fig. 8) gives one example and RABE [11] some others]. When T is varied continuously, the eigencurves also change continuously, and generate *eigensurfaces* in (E, F, T) space. The totality of these surfaces is thus a representation of periodic motion for our problem. More generally, one can let γ, the mass-ratio parameter, vary and see how the eigensurfaces change. Each distinct surface is said to represent a *class* of periodic solutions.

Location of Periodic Solutions

For a given T, assume that the eigencurve is cut by some line such as E = const. Then we may take this value as our initial and final value of E, and consider the transformation S which carries the initial value of E over into its final value. This transformation will simultaneously take the initial values of F and $\dot{E}$ into new ones, i.e. $S(F_i, \dot{E}_i) = (F_f, \dot{E}_f)$. This may be regarded as mapping the $(F, \dot{E})$ plane into itself. Now, for any a, the equation $S(a, \dot{E}_i) = (a, \dot{E}_f)$ gives the intersection of the map of $F = a$ with the line $F = a$ itself, and if a be allowed to vary, we obtain the locus of "a" intersections. Likewise, from $S(F_i, b) = (F_f, b)$, we obtain the locus of "b" intersections, and the intersections of the two loci will be the fixed points $S(\alpha, \beta) = (\alpha, \beta)$. These fixed points characterize the periodic solutions which intersect the given line E = const.

Such a method of obtaining periodic solutions for a given T is systematic and thorough, and it guarantees that important periodic solutions will not be overlooked. In practice, it can involve excessive labor of computation, so that it is often better to use other methods based upon the physical nature of the problem. These will now be discussed.

The simplest type of periodic solution is that where the particle is at rest in the rotating system, which may occur at the libration points. These are five in number, namely $L_1: E = \pm\pi/2$, $F = 0$; $L_2: E = 0$, $F = \pm 1.5206$; $L_3: E = \pi$, $F = \pm 1.5206$; L_4: $E = \mp\pi/2$, $F = \pm 1.316958$; and $L_5: E = \pm\pi/2$, $F = \pm 1.316958$. Also, one might expect relatively simple periodic solutions near one of the masses, since the influence of the other mass would be relatively small there.

According to Strömgren, each class has a natural beginning and a natural end, and these can coincide. Furthermore, the beginning and end will, if not infinite, be related to the positions of the masses or of the libration points. (This will be made more explicit below). This principle enables one to discover at least one periodic orbit belonging to a class. It is then a simple matter to vary an appropriate initial condition, either E or F, and to determine how T must vary to preserve periodicity. Thus the whole class may be traced out.

Strömgren confined his attention mainly to orbits which were symmetrical either with respect to the E-axis, or to the F-axis, or perhaps both. This makes the location of a periodic orbit rather easy for a given T, because one knows that the initial inclination is perpendicular to one of these axes. Then it is only necessary to vary the distance along the axis until the final boundary conditions are fulfilled, provided of course that a periodic orbit of the desired type does exist for the value of T in question.

For many classes, a natural termination is an asymptotic orbit spiraling out from L_4 (or L_5). This can be symmetric with respect to the ξ-axis and spiral into L_5, or symmetric with respect to the η-axis and spiral into L_4, or completely asymmetric and spiral into L_4. Examples of all these orbits are given by Strömgren [4]

(see Fig. 15 and Tableau V, loc. cit). If one knows these limiting orbits, then a technique must be devised for finding the other members of the class. One feasible method is to make use of the coiling property of the eigensurface, which will now be explained and then applied.

Class (k) is a rather simple one and is well-suited for the demonstration of the coiling. If one considers the profile of the eigensurface corresponding to the plane $E = 0$, this is a curve which begins with a spiral about a point $F = F_i$, $K = 11$ and ends with a spiral about another point $F = F_j$, $K = 11$. The points F_i and F_j are the F-intercepts of Strömgren's asymptotic orbits I and II. Since this coiling does occur for all classes (for $\gamma = 0$) which terminate in asymptotic orbits, we are assured that there will be an orbit of the class at a finite distance from F_i (or F_j) and with $K = 11$. This simple observation enables us to find such an orbit readily, provided one knows what the limiting orbit of the class is. And it does not matter greatly if the orbit is an asymmetric one.

Some limiting orbits for asymmetric classes can be found in a simple and systematic manner. These are the orbits which begin and end at L_4. An orbit which ends at L_4 will be the mirror image in the η-axis of one which begins at L_4. Now all the asymptotic orbits calculated by STRÖMGREN cross the η-axis at points with ordinates η_o, not far from L_4, and at an angle of $57°42.25'$ with the η-axis. If we plot the slope $d\eta/d\xi$ at a subsequent crossing versus η_c, the value of η at the crossing, the resulting curve C may be regarded as consisting of two parts, C^+ if $d\eta/d\xi > 0$ and C^- if $d\eta/d\xi < 0$. Now replace all ordinates of C^- by their negatives, thereby obtaining the mirror image $(\overline{C^-})$, and intersect this image with C^+. The intersections will give us curves which begin and end at L_4, and these need not be symmetric either to the ξ-axis or to the η-axis. If not, we have a limiting orbit for an asymmetric class.

Structure of the Main Classes

In order to demonstrate how the principal simple symmetric classes develop, we show two profiles of the eigensurfaces, together with enlarged drawings where necessary. Figure 1 a is a plot of K vs. E_i for $F_i = 0$ and $\dot{F}_i > 0$, Figure 1 b an enlargement of part of Figure 1 a. Figure 2 a is a plot of K vs. F_i for $E_i = 0$ and $\dot{E}_i > 0$, and Figures 2 b and 2 c are corresponding enlargements. (The restrictions $\dot{F}_i > 0$ and $\dot{E}_i > 0$ are introduced for purposes of clarity in representation).

If two profiles intersect, the point of intersection corresponds to an orbit which is common to the two classes. For instance, in Figure 1 a, the initial values E_i are then the same, $F_i = 0$, K has the same value, and $\dot{F}_i$ is positive in both cases. The orbit is uniquely determined by these initial conditions and the differential equations, and so must be a common one. However, if $\dot{F}_i$ had been negative in one case and positive in the other, the conclusion would not be correct, and this is the reason for our convention that $\dot{F}_i$ shall be positive for the profile.

If two profiles are close to each other, the orbits of the two classes will be close initially, and usually close over an appreciable interval of time. Eventually they will diverge because, belonging to different classes, they will satisfy different final boundary conditions, in general. However, since both orbits are periodic, this divergence is later compensated for by a corresponding convergence, so that no immediate conclusion about stability can be drawn.

In Figure 1 a, an intersection of a profile with the K-axis marks the point $E_i = 0$, $F_i = 0$, so that we have a "periodic" ejection orbit with $\dot{E}_i = 0$. For Figure 2 a, similar intersections give "periodic" ejection orbits with $\dot{F}_i = 0$. (The word "periodic" is used here in a loose sense. These orbits are not actually periodic physically, but the nearby orbits of the class are, and there is a perfectly smooth transition through the ejection orbit). If a class does have an ejection orbit, it becomes very easy to locate the class. Accordingly, we show in Figures 3 a and 3 b ejection orbits for $\dot{E}_i = 0$, in Figures 4 a and 4 b ejection orbits for $\dot{F}_i = 0$, and in Figures 5 a, 5 b, and 5 c ejection orbits for $K = 10$ as a function of angle of ejection.

According to STRÖMGREN, a class is either closed or has a natural beginning and a natural end. In practice, this means that the eigensurface is either closed, becomes infinite at one of the masses, stretches to infinity, or is bounded by a limiting curve (asymptotic orbit). Combinations of these latter possibilities occur, as the general rule.

A class is a continuous family of periodic orbits with certain symmetry properties (including complete asymmetry). In some cases, one may integrate over one half period or even one quarter period, specifying certain initial and final boundary conditions. These conditions remain the same throughout the class, while other properties, such as whether the motion is retrograde or direct, or simply- or multiply- periodic, may not. STRÖMGREN did not confine himself to classes with simply-periodic orbits throughout, and he did omit classes which are as simple as the ones he included.

Three fairly simple "open" classes are (c), (f), and (m). Class (c) is defined by $F_i = 0$, $\dot{E}_i = 0$, $E_f = \pi/2$, and $\dot{F}_f = 0$. It starts with the libration point L_1, $K = 16$, $E_i = \pi/2$. The orbits in the neighborhood are simply-periodic and retrograde, and all are symmetric with respect to $E = \pi/2$ and $F = 0$. Class (f) is defined by $F_i = 0$, $E_i < 0$, $\dot{E}_i = 0$, $\dot{F}_i > 0$, $E_f = 0$, $\dot{F}_f = 0$. It starts at mass m_2, $K = \infty$, $E_i = 0$. The nearby orbits are simply-periodic and retrograde, and all are symmetric with respect to $E = 0$ and $F = 0$. For both classes, K falls rapidly at the start and goes through a series of damped oscillations as E_i decreases (or as F_f increases). The (c) profile stays below the (f) profile, running more or less parallel to it; the two profiles cannot intersect because of the different symmetries. The theory of this behavior at large distances has been given by J. P. MØLLER [12].

The class (m) has been included in the tables for completeness, but not in the figures (because the maximum value of K is only about $K = -2.47$. This class of retrograde periodic orbits around the two finite masses also has retrograde motion in the fixed coordinate frame (due to the high velocities at all points of the orbits).

The class begins with circles of infinite radius but zero period (in the limit, of course, as K goes to $-\infty$ and F_i goes to $+\infty$). As the class develops by closing in on the masses, the orbits become ellipses of increasing eccentricity. In the limit (as K again goes to $-\infty$, but F_i now goes to zero) the orbits become rectilinear orbits between the two masses, with zero period (i.e. an ellipse of eccentricity one).

Class (n) is defined to be symmetric with respect to just the E-axis, and retrograde. Its profile for $F_i = 0$ is periodic in E, with period π, as are the differential equations themselves for $\mu = 1/2$ $(\gamma = 0)$. This class is therefore closed in the (ξ, η) system, the one with immediate physical meaning. Between the minimum value of K and the value at $E_i = 0$ the orbits are doubly-periodic about one of the masses in the (ξ, η) system, but from the collision value of K to its maximum they are simply-periodic librations between the masses. At the minimum value of K there is a common orbit with class (f), since there is then symmetry also with respect to the F-axis. At the maximum value of K there is an orbit in common with class (c), and in this case symmetry with respect to the η-axis $(E = \pi/2)$.

Class (a) is defined to be symmetric about the F-axis only, and retrograde. Its simplest member is the stationary libration point L_2. The class is a closed one, so has no beginning or end, but it is convenient to start with L_2 and follow the development. Here the value of K is a maximum, corresponding to the fact that the velocity is zero. But this value falls rapidly as F_i is increased. The orbits at first are simply-periodic librations about L_2, and remain so until the ejection orbit is reached. The value of K goes through a minimum somewhat before this. After the ejection orbit, the motion is doubly-periodic about the mass m_2 in the (ξ, η) system. The value of K increases from that at ejection to a maximum and then drops to another minimum, after which the orbits are retraced in reverse sequence to L_2. At this minimum for K, there is an orbit in common with class (f), so that for this point only there is symmetry about both the E-axis and the F-axis. (The above development can be followed by referring to Figure 2a, and observing that the full line is a semi-profile of the eigen-surface. Each orbit has two intercepts on the F-axis, of the same sign for librations and of opposite sign for motion around the mass). From Figure 2a, it is evident that there is a maximum value of K just after ejection and that the maximum value of F_i occurs soon after this, i.e. is not coincident with ejection. It should be noted that the data of STRÖMGREN were extremely scanty for class (a), so that it was impossible to construct an accurate profile, such as is here presented.

As a third and final example of a closed class, let us consider class (δ), the profile of which is shown in Figures 2a and 2c. This class, which was unknown to STRÖMGREN is about as simple as class (a). It is a class which is generally symmetric only about the F-axis, and is partly retrograde and partly direct. At its maximum K it has an orbit in common with class (g), as also at its minimum K. The first is direct and the second retrograde, and both are symmetric with respect to both the E- and F-axes. At the maximum K, the motion is doubly-periodic, and direct about the mass. It remains so until the ejection orbit is reached, when it changes to a direct, simply-

periodic libration. This behavior persists until an intermediate minimum for K, where the orbit has but one intercept on the F-axis. The libration then changes to a retrograde one until the second ejection orbit, when the motion becomes doubly-periodic and retrograde around the mass. After K reaches the second minimum, where the orbit is in common with the (g) class, the development of the class proceeds in reverse sequence back to the maximum value for K. The general behavior of class (δ) is in some respects similar to that of class (a), even though the latter has only retrograde motions.

The remaining classes in this paper are all ones which terminate on asymptotic-periodic orbits from L_4 and L_5. We have completed class (g), made class (k) more precise and complete, and have discovered and traced out 6 other new classes, which we designate by (α), (β), (γ), (λ), (μ), and (ν). Class (α) was the first to be discovered, and is shown on Figures 2a and 2b and also tabulated. It is complicated and of minor importance, so that it will only be defined, as consisting of orbits which start out with $E = 0$, $\dot{F} = 0$, $\dot{E} > 0$ and after exactly one-half period satisfy these same conditions (but F has assumed a value different from the initial one). The other classes in this group are only a small fraction of the possible ones associated with L_4 and L_5, as is easily seen from the systematic method of generation. STRÖMGREN listed 5 simple periodic-asymptotic orbits and mentioned that one could combine these half-orbits together. As a matter of fact, any such combination can be regarded as the limiting orbit of a class, and we may trace out the class by the method described previously. The classes presented in this paper are simple ones which have been easy to locate, and it is hoped that their study will furnish a good picture of the general behavior.

Figure 1b shows the profile of class (g) in the neighborhood of our 2 new classes (β) and (γ), together with the profiles of the latter two classes. Class (β) consists of trajectories which are symmetric with respect to both the E- and F-axes. One quarter of each trajectory is a curve which starts up normal from the E-axis and ends normal to the F-axis and with $\dot{E} > 0$. Let us denote by VII that periodic-asymptotic orbit which proceeds from L_4, crosses the F-axis once and then strikes the F-axis normally at about $F = 1.75$. Then one-half of one limiting orbit for the (β)-class is composed of half-orbits III and VII, while the other half-orbit consists of IV and VII. The motion is for most of the class direct around the mass, but there is a small portion where $E_i < 0$ and the motion is retrograde. Class (γ) is symmetric in general only about the E-axis, as is class (n), but it is, for the most part, direct. For each permissible value for K, there is at least one pair of intercepts on the E-axis. When K is maximum, one intercept is the negative of the other. The two limiting orbits are each composed of 2 half-orbits (combined in opposite ways at the two spiral ends), one of which is Strömgren's III, while the other (XII) comes from $\eta_i = 1.719051$ and intercepts the E-axis normally at -0.037282.

The interrelations of the above classes are interesting. Class (β) has as a quarter-trajectory a curve ending with $\dot{E} > 0$, while class (g) has for its similar curve one ending with $\dot{E} < 0$, so that the profiles cannot possibly intersect. Class (γ) has a tra-

jectory symmetric about the F-axis at its maximum K, so that class (g) can and does intersect class (γ) there. The (g)-profile runs very close to the (β)-profile over a considerable range, indicating that only a small change in slope near the end of the quarter-trajectory will cause a change from class (g) to class (β). Class (β) can perhaps be regarded as a sort of combination of class (g) with class (a), and as corresponding to Darwin's figure-of-eight class (C', C'') for $\mu = 10/11$ $(\gamma = -9/11)$. In Figure 2b, we see that its F-profile is between those for (a) and (g).

Figure 2b shows partial profiles of classes (α), (g), (ν), (β), and (a). All these classes except (a) have limiting orbits consisting in part of semi-orbit VII. If the profiles were drawn to completion, they would all spiral around the limiting F-intercept of VII at $K = 11$. This happens for one end of (α), one end of (g), and both ends of (β) and (ν). Class (ν) starts out normal to the F-axis with $\dot{E} > 0$ and strikes the η-axis $(E = -\pi/2)$ normally. Since these boundary conditions are not compatible with those for (g) and (β), the profiles for these two classes will not be intersected by that for class (ν). Class (ν) has a maximum at about $K = 13.72$ near L_2, and a minimum at $K = 9.08$. At one spiral end it has as limiting half-orbit the Limiting Orbit VII. The other end has a double-spiral combination of Limiting Orbit VII plus half of another orbit due to STRÖMGREN (loc. cit., Tableau V, Figure 2) as its half-orbit. As the limiting orbits of (α), (g), (ν), and (β) are approached, the profiles come very close together, which reflects the fact that the limiting orbits all have semi-orbit VII in common.

Figure 2c shows in detail the relation between classes (g), (δ), (α), (k), and (μ). For $F_i > 0$, classes (g), (δ), (α), and (k) run close together, because there is a large loop in the trajectory and only a small variation in F_i is necessary to change the orientation of this loop, and hence to change from the satisfaction of one final boundary condition (say $\dot{F} = 0$ at $E = \pi/2$) to another (say $\dot{E} = 0$ at $F = 0$). Class (k), which is symmetric about the F- and η-axes, runs between the 2 limiting half-orbits I and II, with large variation in K. Class (μ), which is just symmetric about the F-axis, runs between a limiting orbit I + V at one end and II + V at the other, with only small variation in K. This may be due to the fact that orbit V corresponds to a large F_i, and that only a small change in the velocity there can lead to a large change of slope at the other end of the trajectory (at small F_i). The orbits of (μ) loop around both L_4 and L_5, but remain outside the mass m_2 for most of the class (i.e. except for that part which approaches Limiting Orbit II, with $F_i > 0$). They differ from the orbits of the (k) class because of the outer portion associated with Limiting Orbit V.

Figure 2a shows class (l) and how it spirals around the F_i of V. Another new class, (λ), spirals about a point with F_i slightly less than that for V, and corresponding to an asymptotic orbit (XIII) starting from L_5, looping near L_4, and then hitting the F-axis normally. The K for this class falls off with increasing F_i. One orbit of this class was erroneously assigned by STRÖMGREN to class (l).

To give a general idea of how the trajectories vary with F_i and E_i, we have chosen a convenient value of $K = 12.5$ and plotted the corresponding trajectories.

Figure 6a covers the range from $F_i = -1.25$ to $F_i = -0.5$, Figure 6b shows $F_i = -0.7$ to $F_i = 1.75$, and Figures 6c and 6d show how the trajectories depend on E_i (from $E_i = -1.8$ to $E_i = 0$, and $E_i = 0$ to $E_i = 1.6$). By referring to these diagrams, it is easy to see when the various boundary conditions, for periodic orbits, will be satisfied.

Figure 7 shows the different periodic orbits themselves for $K = 12.5$. It is particularly interesting to note how, when the profiles are close, the orbits themselves are close over a good portion of their paths. For example, the (δ) class is a sort of combination class, which is possible because the initial E for one (g) class orbit (with $E_i \cong 1.35$ and $F_f = -0.15$) is not too different from final E for another (g) class orbit (with $F_i \cong -0.8$ and $E_f \cong 1.2$). All that is needed is a small change of slope from the vertical to effect the transition to the (δ) class orbit. If we look at Figure 1a, the two "branches" of the (g) class run parallel and not too far apart in this region, for a wide variation in K.

Figures 8a, 8b, and 8c show, for the first time, the detailed and complete development of class (g). STRÖMGREN wrote "It is certain that in one way or another this class is "associated" with the points L_4 and L_5". But this statement lacked effective content, since the manner of association was completely unknown. P. PEDERSEN, in unpublished calculations made just before his death in 1958, followed class (g) to $K = 7.6$. We obtained more points on the profiles to this stage, and traced the class to its limiting orbit. The interpretation of its behavior is rather impossible unless one knows of the existence of classes (δ), (γ), (β), and (ν), which were discovered by us.

Class (g) begins with direct motion around mass m_2. The amplitude in both E and F directions increases until a cusp develops, followed by a loop. Now the F-profile becomes close to that of the (δ) class, with which there are 2 intersections, one at maximum K and the other at minimum K. The E-profile is at the same time close to that for class (c), as is easily possible when the loop is tight, and small changes in slope are all that are necessary to meet a desired boundary condition. Since there can be an intersection of the E-profiles of classes (g) and (γ), this will have to occur at the maximum K for class (γ), and so the (g) profile swings up to do this. Actually, the (g) profile can follow that of the (β) class for a longer stretch of development than for class (γ), and does so, as is seen in Figure 1b. However, the lower intercept of (β)-trajectories with the F-axis (where the slope is not horizontal) must remain positive. At the same time, the value of F_f for class (g) can vary smoothly and change sign. This is what happens, and at the F-ejection orbit (about $K = 10.2$) the two E-profiles part company, that for the (g) class suffering a sharp reversal of direction. The value of E_i now becomes negative, the motion retrograde, and the E- and F-amplitudes increase steadily. The loop has disappeared and the motion is now triply-periodic, although the class does have a common orbit with the simply-periodic retrograde class (f), at about the minimum K for class (g). From here on, the general development is that of slow changes in E and F, and rapid ones in K. The middle part of the quarter trajectory, which is at first in the fourth quadrant ($E>0$, $F<0$),

moves to the left and up, across a skew-angle ejection orbit ($E = 0$, $F = 0$), and then develops first a cusp and then a loop. The final (limiting) half-orbit is a double spiral around L_4 consisting of asymptotic orbits VII and VIII. The first neighboring class to be reached is (ν), with trajectories normal to $E = -\pi/2$. Then the trajectories become close to those of class (β) and remain so half-way around L_4, because this part of the limiting orbit (VII) is common. Since class (ν) has a maximum $K = 13.72$, and since class (g) cannot intersect it, the profile of class (g) must go around that of class (ν), which it does, to become asymptotic to the class (β) profile. This accounts completely for the F-profile of class (g), and the remainder of the E-profile does not seem to offer anything of interest.

Figure 9 shows the development of the closed (δ) class, which is rather complicated, from maximum K to minimum K. The development from minimum K to maximum K is obtained by taking the mirror images (about the E-axis) of the orbits shown in the figure.

Finally, Figure 10 shows the periodic-asymptotic orbits of STRÖMGREN, as well as nine others which we have found. These latter are necessary for an understanding of how various classes, in particular (g), terminate.

In order that the work be truly quantitative, it is imperative to give initial conditions for the periodic solutions which we have obtained. With these and an electronic computer, one can reproduce any orbit desired. In our calculations, the main work has consisted in varying the initial conditions so that the final ones would be satisfied, and the actual solutions (orbits) have been printed out only for cases which seemed particularly interesting, such as the (g) class. Our initial and final conditions, as well as the elapsed "time" $x = \Delta\psi$, are given in the tables. Also, the last table gives the initial and final conditions for all the asymptotic-periodic half-orbits shown in Figure 10.

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Class (a)

Initial Conditions: $E_i = 0$; $\dot{F}_i = 0$; $\dot{E}_i > 0$.

Final Conditions: $E_f = 0$; $\dot{F}_f = 0$; $\dot{E}_f < 0$.

Note: To obtain the remainder of the class take the mirror images, i.e. the values

$$F_i' = -F_f;\ F_f' = -F_i$$

K	F_i	F_f	x
13.81871	−1.500491	−1.540000	0.4985
13.80732	−1.489491	−1.550000	0.4989
13.79078	−1.478037	−1.560000	0.4994
13.76877	−1.466099	−1.570000	0.5001
13.74096	−1.453646	−1.580000	0.5009
13.70697	−1.440643	−1.590000	0.5020
13.66642	−1.427047	−1.600000	0.5032
13.64355	−1.420013	−1.605000	0.5040
13.61888	−1.412817	−1.610000	0.5047
13.57192	−1.400000	−1.618617	0.5062
13.40306	−1.360000	−1.643399	0.5117
13.20556	−1.320000	−1.665695	0.5180
13.09854	−1.300000	−1.675304	0.5219
12.98614	−1.280000	−1.684904	0.5258
12.50000	−1.200282	−1.718210	0.5433
12.49823	−1.200000	−1.718287	0.5434
11.97114	−1.120000	−1.744926	0.5645
11.49330	−1.050000	−1.765665	0.5849
11.00000	−0.977948	−1.783724	0.6084
10.47530	−0.900000	−1.800846	0.6364
9.829703	−0.800000	−1.821464	0.6761
9.234006	−0.700000	−1.841319	0.7206
8.706927	−0.600000	−1.862726	0.7703
8.274730	−0.500000	−1.887448	0.8259
7.976367	−0.400000	−1.917682	0.8889
7.873906	−0.300000	−1.954912	0.9616
8.048263	−0.200000	−1.998023	1.0467
8.512360	−0.100000	−2.039212	1.1426
8.929865	−0.020000	−2.061301	1.2145
9.009506	0	−2.065817	1.2291
9.079741	0.020000	−2.068127	1.2427
9.152730	0.050000	−2.072029	1.2592
9.200000	0.126497	−2.074709	1.2861
9.000000	0.231699	−2.076561	1.2938
8.500000	0.368000	−2.069787	1.2819
8.000000	0.478326	−2.053335	1.2662
7.398739	0.600000	−2.030726	1.2459
6.896330	0.700000	−2.005726	1.2291
6.404044	0.800000	−1.975115	1.2127
5.935352	0.900000	−1.938862	1.1970
5.502325	1.000000	−1.896388	1.1823
5.115463	1.100000	−1.847226	1.1689
4.784783	1.200000	−1.790620	1.1572
4.335157	1.400000	−1.650040	1.1407
4.243615	1.500000	−1.562275	1.1373

Class (c)

Initial Conditions: $F_i = 0$; $\dot{E}_i = 0$; $F_i > 0$.

Final Conditions: $E_f = \pi/2$; $F_f = 0$; $\dot{E}_f > 0$.

K	E_i	F_f	x
15.85000	1.538030	0.142749	0.5453
15.81000	1.533797	0.16084	0.5455
15.79000	1.531834	0.169227	0.5456
15.77051	1.530000	0.177017	0.5457
15.35576	1.500000	0.300644	0.5473
14.41663	1.450000	0.487065	0.5511
13.41040	1.400000	0.647834	0.5554
12.50000	1.350854	0.784318	0.5597
11.69009	1.300000	0.907716	0.5640
11.00000	1.247388	1.020574	0.5686
10.49915	1.200000	1.112129	0.5729
9.776064	1.100000	1.281767	0.5831
9.456517	1.000000	1.427175	0.5967
9.505903	0.900000	1.551850	0.6158
9.862181	0.800000	1.652969	0.6413
10.34752	0.700000	1.721674	0.6692
10.58818	0.600000	1.762157	0.6765
10.49841	0.500000	1.794275	0.6592
10.25000	0.400000	1.823555	0.6370

K	E_i	F_f	x
9.932907	0.300000	1.848083	0.6180
9.568509	0.200000	1.868300	0.6028
9.165277	0.100000	1.885035	0.5911
8.732000	0	1.898509	0.5825
8.273998	−0.100000	1.909331	0.5764
7.798774	−0.200000	1.917602	0.5727
7.313147	−0.300000	1.923475	0.5710
6.819865	−0.400000	1.927939	0.5709
6.324000	−0.500000	1.931505	0.5720
5.838000	−0.600000	1.932889	0.5746
5.360000	−0.700000	1.934013	0.5779
4.896639	−0.800000	1.934778	0.5820
4.449041	−0.900000	1.936347	0.5863
4.021914	−1.000000	1.938919	0.5906
3.616000	−1.100000	1.943636	0.5946
3.240000	−1.200000	1.949489	0.5984
2.890556	−1.300000	1.958641	0.6012
1.865209	−1.700000	2.029859	0.6029
1.722888	−2.000000	2.126496	0.5957
2.731019	−2.300000	2.256825	0.5932
6.000000	−2.684600	2.401692	0.6202
6.536376	−2.800000	2.423280	0.6253
6.708485	−2.900000	2.436111	0.6261
6.686781	−3.000000	2.445025	0.6252
6.000000	−3.280418	2.469526	0.6184
5.000000	−3.534626	2.489712	0.6147

Class (f)

Initial Conditions: $F_i = 0;\ E_i < 0;\ \dot{E}_i = 0;\ \dot{F}_i > 0.$

Final Conditions: $E_f = 0;\ F_f > 0;\ \dot{F}_f = 0;\ \dot{E}_f > 0.$

Note: This class is also represented by the conditions:

$$\begin{cases} E_i' = 0;\ F_i' > 0;\ \dot{F}_i' = 0;\ \dot{E}_i' > 0. \\ F_f' = 0;\ E_f' > 0;\ \dot{E}_f' = 0;\ \dot{F}_f' < 0. \end{cases}$$

To obtain this representation take $F_i' = F_f;\ E_f' = -E_i.$

K	E_i	F_f	x
12.50000	−0.922300	+0.870369	0.4462
11.25000	−0.981329	0.920610	0.4646
11.00000	−0.994345	0.931672	0.4684
10.00000	−1.051386	0.979800	0.4843
9.000000	−1.118210	1.035030	0.5008
8.000000	−1.196873	1.100000	0.5176
6.750000	−1.319917	1.198307	0.5381
4.844872	−1.600000	1.417370	0.5636
4.406971	−1.700000	1.494434	0.5673
4.087715	−1.800000	1.570804	0.5694
3.822524	−2.000000	1.724154	0.5711
5.000000	−2.347730	1.986894	0.5844
7.000000	−2.596185	2.124250	0.6123
7.500000	−2.694021	2.153503	0.6192
7.694946	−2.769554	2.170000	0.6209
4.145615	−3.860885	2.250000	0.6066
2.957395	−4.141600	2.252358	0.6135
2.210961	−4.341600	2.253806	0.6180
1.295156	−4.641600	2.271379	0.6193

Class (g)

Initial Conditions: $F_i = 0;\ \dot{E}_i = 0;\ \dot{F}_i > 0.$

Final Conditions: $E_f = 0;\ \dot{F}_f = 0;\ \dot{E}_f < 0.$

Note: This class is also represented by the conditions

$$\begin{cases} E_i' = 0;\ \dot{F}_i' = 0;\ \dot{E}_i' > 0. \\ F_f' = 0;\ \dot{E}_f' = 0;\ F_f' > 0. \end{cases}$$

To obtain this representation take $F_i' = -F_f;\ E_f = E_i.$

* These values are due to P. Pedersen (unpublished).

K	E_i	F_f	x
15.77000	1.067147	+0.933589	0.7117
15.455	1.100	0.944	*
15.08612	1.150000	+0.944618	0.8057
15.02927	1.161819	+0.940000	0.8180
14.97895	1.177672	+0.930000	0.8326
14.96060	1.189305	+0.920000	0.8421
14.956	1.200	0.910	*
15.02675	1.250000	+0.843970	0.8820
15.153	1.300	0.766	*
15.28072	1.350000	+0.680867	0.9686
15.38760	1.400000	+0.582305	1.0455
15.40455	1.410000	+0.559673	1.0664
15.41905	1.420000	+0.535307	1.0902
15.43004	1.430000	+0.508454	1.1179
15.43234	1.432914	+0.500000	1.1269
15.43562	1.440000	+0.477743	1.1511
15.43073	1.450000	+0.440012	1.1936
15.42537	1.453000	+0.426212	.2094
15.35624	1.463190	+0.350000	1.2955
15.26969	1.464367	+0.300000	1.3479
15.00000	1.456591	+0.203998	1.4332
14.54460	1.436592	+0.100000	1.5038
14.000	1.4104	0.009	*
13.000	1.3578	−0.125	*
12.50000	1.328125	−0.178220	1.6355

K	E_i	F_f	x	K	E_i	F_f	x
12.000	1.2949	− 0.230	*	9.4	− 0.2392	0.570	*
11.000	1.2109	− 0.317	*	9.02773	− 0.200	0.273	*
10.196	1.100	− 0.363	*	9.32	− 0.100	0.190	*
9.915	1.000	− 0.344	*	9.65813	0.000	0.125	*
10.0384	0.900	− 0.258	*	9.99803	0.100	0.057	*
10.55390	0.810757	− 0.062000	2.0179	10.15088	0.146658	0	1.8695
10.62750	0.804448	− 0.005000	2.0298	10.16324	0.152940	− 0.050000	1.8868
10.62932	0.804447	− 0.001000	2.0294	10.08924	0.134355	− 0.100000	1.8859
10.62969	0.804456	− 0.000002	2.0293	9.959187	0.100271	− 0.150000	1.8752
10.6056	0.810	0.046	*	9.958141	0.100000	− 0.150372	1.8751
10.2228	0.900	0.202	*	9.792165	0.056413	− 0.200000	1.8598
10.238	1.000	0.330	*	9.575164	0	− 0.255922	1.8407
10.738	1.100	0.483	*	9.18392	− 0.100	− 0.345	*
11.00000	1.129777	+ 0.537869	1.4421	8.928545	− 0.164434	− 0.400000	1.7926
11.9487	1.200	0.707	*	8.787	− 0.200	− 0.429	*
12.50000	1.223290	+ 0.793292	1.2261	8.390	− 0.300	− 0.511	*
13.00000	1.233426	+ 0.866735	1.1513	7.98	− 0.400	− 0.589	*
13.25000	1.233491	+ 0.900887	1.1106	7.622153	− 0.50000	− 0.666524	1.7232
13.50000	1.229108	+ 0.932627	1.0668	7.463546	− 0.543551	− 0.700000	1.7165
13.75000	1.218899	+ 0.961383	1.0195	6.935505	− 0.700000	− 0.817336	1.6954
14.00000	1.200304	+ 0.987776	0.9681	6.391237	− 0.900000	− 0.960491	1.6752
14.06565	1.193213	+ 0.995000	0.9536	6.192090	− 1.000000	− 1.028066	1.6675
14.12277	1.185710	+ 1.002000	0.9404	5.979706	− 1.200000	− 1.152400	1.6557
14.17037	1.177904	+ 1.009000	0.9286	6.072945	− 1.400000	− 1.262175	1.6452
14.20704	1.170115	+ 1.016000	0.9186	6.575256	− 1.600000	− 1.375607	1.6300
14.23303	1.162559	+ 1.023000	0.9104	7.142005	− 1.700000	− 1.453193	1.6194
14.25198	1.154299	+ 1.031000	0.9030	7.600000	− 1.744131	− 1.500910	1.6148
14.26518	1.140740	+ 1.045000	0.8937	7.800000	− 1.757026	− 1.518362	1.6138
14.24737	1.114031	+ 1.075000	0.8828	8.000000	− 1.767032	− 1.533985	1.6132
14.24022	1.109755	+ 1.080000	0.8819	8.400000	− 1.780311	− 1.560347	1.6134
14.21033	1.092749	+ 1.100000	0.8789	9.000000	− 1.788456	− 1.589560	1.6166
14.17500	1.075786	+ 1.120000	0.8776	9.500000	− 1.788293	− 1.606238	1.6218
14.16475	1.071504	+ 1.125000	0.8776	9.800000	− 1.786173	− 1.613439	1.6261
14.11490	1.049827	+ 1.150000	0.8784	10.00000	− 1.784111	− 1.617194	1.6294
14.09440	1.040952	+ 1.160000	0.8793	10.20000	− 1.781566	− 1.620155	1.6332
14.06313	1.027324	+ 1.175000	0.8812	10.40000	− 1.778874	− 1.622381	1.6377
14.01000	1.003453	+ 1.200000	0.8859	10.80000	− 1.772310	− 1.624650	1.6480
13.96863	0.983186	+ 1.220000	0.8909	11.00000	− 1.768701	− 1.624735	1.6541
13.90000	0.946090	+ 1.252383	0.9027	11.50000	− 1.758884	− 1.621895	1.6731
13.80000	0.877673	+ 1.296307	0.9291	11.80000	− 1.752580	− 1.618016	1.6876
13.708	0.800	1.319	*	12.00000	− 1.748238	− 1.614457	1.6989
13.60000	0.716260	+ 1.317022	0.9824	12.25000	− 1.742629	− 1.608811	1.7154
13.392	0.600	1.285	*	12.50000	− 1.737042	− 1.601685	1.7356
12.8324	0.400	1.186	*	12.75000	− 1.731457	− 1.592836	1.7608
12.50000	0.310989	+ 1.131696	1.0428	13.25000	− 1.719765	− 1.568305	1.8367
12.0187	0.200	1.053	*	13.50000	− 1.714453	− 1.551347	1.9093
11.00000	0.003349	+ 0.887609	1.1314	13.50063	− 1.714650	− 1.551300	1.9095
10.3818	− 0.100	0.779	*	13.54684	− 1.713568	− 1.547800	1.9298
9.70866	− 0.200	0.644	*	13.59292	− 1.713051	− 1.544300	1.9546

K	E_i	F_f	x
13.60000	−1.712944	−1.543770	1.9590
13.64183	−1.712487	−1.540800	1.9895
13.65289	−1.712239	−1.540100	1.9994
13.66530	−1.712168	−1.539400	2.0120
13.68146	−1.712225	−1.538700	2.0313
13.70000	−1.712301	−1.538452	2.0605
13.72000	−1.712617	−1.540099	2.1126
13.72342	−1.712354	−1.541000	2.1279
13.72577	−1.713018	−1.542000	2.1419
13.72730	−1.713303	−1.543000	2.1544
13.72876	−1.713988	−1.545000	2.1765
13.72888	−1.714065	−1.547000	2.1961
13.72737	−1.714736	−1.550000	2.2222
13.72443	−1.715077	−1.553000	2.2458
13.72037	−1.715650	−1.556000	2.2674
13.70953	−1.713700	−1.562000	2.3071
13.70735	−1.716483	−1.563000	2.3124
13.70512	−1.716791	−1.564000	2.3182
13.70041	−1.717565	−1.566000	2.3296
13.69270	−1.720058	−1.569000	2.3455
13.68433	−1.717709	−1.572000	2.3619
13.67517	−1.721161	−1.575000	2.3820
13.66536	−1.719597	−1.578000	2.3885
13.65480	−1.722859	−1.581000	2.4109
13.64360	−1.719845	−1.584000	2.4113
13.63163	−1.723527	−1.587000	2.4339
13.56120	−1.725874	−1.602000	2.4855
13.52785	−1.727897	−1.608000	2.5072
13.49140	−1.731437	−1.614000	2.5330
13.45177	−1.731662	−1.620000	2.5465
13.36236	−1.736543	−1.632000	2.5857
13.13871	−1.746565	−1.656000	2.6692
13.00145	−1.757562	−1.668000	2.7080
12.84481	−1.766647	−1.680000	2.7488
12.66654	−1.772116	−1.692000	2.7926
12.50000	−1.786034	−1.701971	2.8295
12.23370	−1.802228	−1.716000	2.8870
11.97202	−1.809285	−1.728000	2.9438
11.67361	−1.837315	−1.740000	3.0051
11.33152	−1.862229	−1.752000	3.0801
10.93205	−1.893103	−1.764000	3.1795
10.69688	−1.913555	−1.770000	3.2524
10.65300	−1.916950	−1.771000	3.2688
10.49309	−1.932305	−1.774000	3.3476
10.84943	−1.893065	−1.757006	3.7724
10.89800	−1.888436	−1.755483	3.8141
10.93000	−1.885906	−1.754506	3.8454
10.96000	−1.883661	−1.753614	3.8790
10.99000	−1.881730	−1.752751	3.9205

Class (k)

Initial Conditions: $E_i = 0$; $\dot{F}_i = 0$; $\dot{E}_i > 0$.

Final Conditions: $E_f = \pi/2$; $\dot{F}_f = 0$.

Note: The degenerate case of a cusp, with $\dot{E}_f = 0$ and $F_f < 0$, is included.

K	F_i	F_f	x
11.01000	−0.178326	−1.350059	1.7815
11.02000	−0.177874	−1.366491	1.7383
11.03000	−0.176305	−1.382065	1.7015
11.03523	−0.175000	−1.390245	1.6834
11.04000	−0.173452	−1.397921	1.6669
11.04766	−0.170000	−1.411146	1.6395
11.05464	−0.165000	−1.425549	1.6108
11.05800	−0.161067	−1.434723	1.5929
11.05880	−0.159755	−1.437497	1.5875
11.05960	−0.158120	−1.440787	1.5811
11.06004	−0.157000	−1.442979	1.5769
11.06058	−0.155000	−1.446626	1.5698
11.06081	−0.150000	−1.455016	1.5535
11.05708	−0.140000	−1.469248	1.5254
11.04821	−0.130000	−1.481162	1.5006
11.03368	−0.120000	−1.491592	1.4770
11.00000	−0.106920	−1.504330	1.4421
10.90000	−0.104286	−1.514648	1.3748
10.80000	−0.123978	−1.508639	1.3196
10.70000	−0.153306	−1.490708	1.2647
10.57793	−0.250000	−1.394416	1.1308
10.64305	−0.300000	−1.331032	1.0750
10.79181	−0.350000	−1.261394	1.0242
10.90000	−0.375688	−1.223068	0.9995
11.00000	−0.395883	−1.191575	0.9803
11.40000	−0.457584	−1.083667	0.9215
12.00000	−0.514266	−0.942706	0.8580
12.50000	−0.531857	−0.830932	0.8185
14.08304	−0.400000	−0.519540	0.7970
14.47934	−0.300000	−0.468345	0.8485
14.53573	−0.250000	−0.468594	0.8803
14.50197	−0.200000	−0.483197	0.9120
14.38918	−0.150000	−0.509465	0.9419
14.11919	−0.080000	−0.561559	0.9796
14.02093	−0.060000	−0.579180	0.9894
13.67570	0	−0.638425	1.0171
12.94616	0.100000	−0.757791	1.0588
12.50000	0.151334	−0.830558	1.0795
12.02800	0.200000	−0.909943	1.1001
11.50000	0.248068	−1.005200	1.1233
11.00000	0.285817	−1.108344	1.1481
10.70000	0.302165	−1.183163	1.1666

K	F_i	F_f	x
10.40000	0.304584	−1.287343	1.1955
10.30000	0.289585	−1.354040	1.2177
10.28540	0.270000	−1.397403	1.2351
10.30476	0.250000	−1.427747	1.2495
10.35053	0.225000	−1.455818	1.2657
10.40867	0.200000	−1.477184	1.2809
10.54233	0.150000	−1.506776	1.3110
10.80000	0.060258	−1.529486	1.3744
10.90000	0.028902	−1.527984	1.4099
10.95000	0.017594	−1.524041	1.4341
11.00000	0.013423	−1.516528	1.4672
11.04445	0.020000	−1.502849	1.5127
11.06615	0.030000	−1.488197	1.5523
11.07498	0.040000	−1.472621	1.5886
11.07517	0.050000	−1.454774	1.6289
11.06716	0.060000	−1.433368	1.6705

Class (l)

Initial Conditions: Same as class (k)

Final Conditions: „ „ „ „

Note: Same as class (k)

K	F_i	F_f	x
15.00000	2.420000	2.432235	0.0623
14.43600	2.292000	2.306153	0.0854
14.00000	2.198500	2.209775	0.1090
13.62360	2.108000	2.111160	0.1409
13.40000	2.055000	2.046758	0.1665
13.18580	2.010000	1.982502	0.1955
13.00000	1.979181	1.926679	0.2227
12.80000	1.956629	1.869102	0.2515
12.60800	1.944000	1.817073	0.2771
12.50000	1.939506	1.788699	0.2911
12.20000	1.935192	1.713904	0.3265
12.00000	1.936491	1.665592	0.3486
11.76700	1.940707	1.609391	0.3740
11.60000	1.945092	1.568347	0.3926
11.44620	1.950000	1.529342	0.4110
11.19308	1.960000	1.460643	0.4433
11.00000	1.969582	1.401354	0.4735
10.99311	1.970000	1.399026	0.4748
10.85900	1.978400	1.350371	0.5020
10.70000	1.993045	1.270456	0.5547
10.66017	2.000000	1.233761	0.5837
10.65713	2.010000	1.181805	0.6363
10.69481	2.015000	1.155900	0.6747
10.75000	2.018090	1.139731	0.7119
10.83617	2.020000	1.128450	0.7645
11.00000	2.016864	1.149267	0.8957
11.02655	2.015000	1.165802	0.9409
11.04097	2.013000	1.189138	0.9967
11.04222	2.012000	1.205102	1.0330

Class (m)

Initial Conditions: $E_i = 0$; $\dot{F}_i = 0$; $\dot{E}_i > 0$.

Final Conditions: $E_f = \pi/2$; $\dot{F}_f = 0$; $\dot{E}_f > 0$.

K	F_i	F_f	x
−385.9430	0.010000	0.051217	0.1504
−68.99444	0.050000	0.123359	0.2462
−30.33587	0.100000	0.188305	0.3301
−11.87477	0.200000	0.301149	0.3301
−6.340919	0.300000	0.406675	0.3433
−4.009862	0.400000	0.509140	0.3448
−3.376365	0.450000	0.559638	0.3429
−2.955235	0.500000	0.609748	0.3395
−2.535816	0.600000	0.708947	0.3293
−2.475000	0.700000	0.806923	0.3155
−2.471274	0.650000	0.758080	0.3228
−2.633037	0.800000	0.903772	0.2990
−2.931662	0.900000	0.999577	0.2805
−3.324117	1.000000	1.094444	0.2605
−3.781301	1.100000	1.188251	0.2398
−4.284452	1.200000	1.281980	0.2187
−5.385719	1.400000	1.467879	0.1775
−6.576374	1.600000	1.653771	0.1397
−7.838336	1.800000	1.840946	0.1069
−9.169998	2.000000	2.030153	0.0798

Class (n)

Initial Conditions: $F_i = 0$; $\dot{E}_i = 0$; $\dot{F}_i > 0$.

Final Conditions: $F_f = 0$; $\dot{E}_f = 0$; $\dot{F}_f < 0$.

Note: To obtain the remainder of the class take the mirror images, i.e. the values $E_i' = -E_f$; $E_f' = -E_i$.

K	E_i	E_f	x
4.870000	−1.594500	1.595414	1.1268
4.873414	−1.540000	1.649716	1.1266
4.886110	−1.500000	1.686880	1.1262
4.944520	−1.400000	1.774663	1.1244
4.988954	−1.350000	1.815711	1.1233
5.043931	−1.300000	1.854939	1.1220
5.109578	−1.250000	1.892482	1.1207

K	E_i	E_f	x
5.184459	−1.200000	1.929580	1.1200
5.600000	−1.000000	2.057225	1.1158
6.510801	−0.700000	2.209606	1.1193
6.872378	−0.600000	2.252829	1.1239
7.646494	−0.400000	2.333213	1.2292
8.449144	−0.200000	2.398000	1.1649
10.37	0.44627	2.69532	1.2931
6.038574	1.000000	3.984834	1.1159

Class (α)

Initial Conditions: $E_i = 0;\ \dot{F}_i = 0;\ \dot{E}_i > 0.$

Final Conditions: $E_f = 0;\ \dot{F}_f = 0;\ \dot{E}_f > 0.$

Note: To obtain the remainder of the class take the mirror images, i.e. the values

$$F_i' = F_f;\quad F_f' = F_i$$

K	F_i	F_f	x
10.41790	0.363000	1.774431	4.0088
10.45000	0.360288	1.773643	3.9572
10.50000	0.356883	1.773962	3.9182
10.74655	0.340000	1.769071	3.8058
11.00000	0.320953	1.762218	3.7233
11.01214	0.320000	1.762063	3.7196
11.25806	0.300000	1.754475	3.6509
11.49058	0.280000	1.746746	3.5907
11.71296	0.260000	1.738651	3.5356
11.92706	0.240000	1.730072	3.4835
12.13401	0.220000	1.720825	3.4334
12.33456	0.200000	1.711073	3.3841
12.50000	0.183040	1.702062	3.3423
12.71843	0.160000	1.688806	3.2847
12.90255	0.140000	1.675898	3.2326
13.08205	0.120000	1.661562	3.1767
13.25767	0.100000	1.644305	3.1147
13.34444	0.090000	1.634060	3.0799
13.43100	0.080000	1.623298	3.0398
13.51803	0.070000	1.609943	2.9925
13.61000	0.059724	1.592900	2.9263
13.66490	0.054000	1.579334	2.8702
13.71001	0.050000	1.564487	2.7979
13.74582	0.050000	1.540588	2.6370
13.74000	0.053543	1.533913	2.5627
13.72000	0.059071	1.531315	2.5028
13.70000	0.063587	1.531491	2.4709
13.65000	0.073612	1.534261	2.4228
13.60000	0.082780	1.538146	2.3920
13.50000	0.099944	1.545679	2.3510
13.00000	0.175591	1.574852	2.2570
12.50000	0.243316	1.592654	2.2138
12.00000	0.307075	1.602831	2.1872
11.00000	0.429593	1.605159	2.1556
10.00000	0.553587	1.582818	2.1369
9.500000	0.619567	1.559595	2.1297
9.000000	0.691425	1.524161	2.1231
8.750000	0.730731	1.500746	2.1199
8.500000	0.773761	1.471369	2.1168
8.000000	0.876841	1.390572	2.1109
7.500000	1.072182	1.205712	2.1062
7.450000	1.140000	1.140444	2.1070

Class (β)

Initial Conditions: $F_i = 0;\ \dot{E}_i = 0;\ \dot{F}_i > 0.$

Final Conditions: $E_f = 0;\ \dot{F}_f = 0;\ \dot{E}_f > 0.$

Note: This class is also represented by the conditions

$$\begin{cases} E_i' = 0;\ \dot{F}_i' = 0;\ \dot{E}_i' > 0. \\ F_f' = 0;\ \dot{E}_f' = 0;\ \dot{F}_f' < 0. \end{cases}$$

To obtain this representation take

$$F_i' = F_f;\quad E_f' = -E_i$$

K	E_i	F_f	x
11.00000	0.296314	1.753452	4.2909
10.99843	0.296000	1.753703	4.2207
10.99454	0.295000	1.753816	4.0978
10.99134	0.294000	1.753643	4.0165
10.98855	0.293000	1.753767	3.9496
10.98615	0.292000	1.754083	3.8894
10.98418	0.291000	1.754138	3.8314
10.98276	0.290000	1.754080	3.7715
10.98238	0.289000	1.754105	3.7009
10.98500	0.288304	1.754146	3.6085
11.00000	0.289930	1.753872	3.4587
11.00041	0.290000	1.753428	3.4563
11.01519	0.293000	1.753391	3.3766
11.01952	0.294000	1.753135	3.3573
11.02765	0.296000	1.752992	3.3238
11.05588	0.304000	1.752073	3.2249
11.07956	0.312000	1.751032	3.1511
11.09961	0.320000	1.752280	3.0873
11.11615	0.328000	1.749572	3.0311
11.12700	0.334737	1.749202	2.9844

K	E_i	F_f	x	K	E_i	F_f	x
11.13306	0.340000	1.748841	2.9476	13.62502	0.840000	1.602303	1.4603
11.13630	0.348000	1.748476	2.8871	13.62763	0.860000	1.601339	1.4549
11.13000	0.353563	1.748602	2.8342	13.62680	0.880000	1.601025	1.4501
11.11000	0.356919	1.749002	2.7756	13.62238	0.900000	1.601416	1.4461
11.08351	0.356500	1.749249	2.7313	13.61434	0.920000	1.601888	1.4439
11.06585	0.355000	1.749670	2.7089	13.60206	0.940000	1.604200	1.4419
11.04161	0.352000	1.750291	2.6832	13.56433	0.980000	1.609806	1.4445
11.00000	0.345162	1.751438	2.6472	13.53800	1.000000	1.612681	1.4497
10.96849	0.339000	1.752424	2.6244	13.50500	1.020000	1.617975	1.4559
10.90983	0.326000	1.754746	2.5881	13.46470	1.040000	1.623569	1.4651
10.85652	0.313000	1.755470	2.5609	13.41529	1.060000	1.629622	1.4777
10.80620	0.300000	1.756991	2.5379	13.35379	1.080000	1.636688	1.4940
10.73217	0.280000	1.759193	2.5082	13.27528	1.100000	1.645197	1.5148
10.48665	0.210000	1.766784	2.4314	13.17072	1.120000	1.655222	1.5423
10.24729	0.140000	1.774544	2.3749	13.01799	1.140000	1.668439	1.5807
10.00932	0.070000	1.782501	2.3283	12.90000	1.150327	1.677341	1.6091
9.774416	0.000002	1.791323	2.2863	12.80000	1.156523	1.684432	1.6322
9.675929	− 0.030000	1.794698	2.2691	12.60000	1.163673	1.697989	1.6759
9.548671	− 0.070000	1.800360	2.2451	12.50000	1.165269	1.702867	1.6977
9.428878	− 0.110000	1.805064	2.2198	12.20000	1.163870	1.719483	1.7587
9.323869	− 0.150000	1.812061	2.1880	11.80000	1.151349	1.735593	1.8390
9.281781	− 0.170000	1.815022	2.1684	11.60000	1.141187	1.743291	1.8790
9.254982	− 0.190000	1.818156	2.1421	11.40000	1.128500	1.748700	1.9208
9.270000	− 0.207453	1.821542	2.1016	11.30000	1.121059	1.753599	1.9412
9.290000	− 0.210817	1.820845	2.0869	11.20000	1.112896	1.756690	1.9629
9.340000	− 0.212568	1.820671	2.0611	11.00000	1.093879	1.762680	2.0088
9.440000	− 0.208197	1.819397	2.0242	10.80000	1.070102	1.768068	2.0598
9.640000	− 0.189526	1.815530	1.9692	10.70018	1.055600	1.770559	2.0886
9.840000	− 0.165474	1.810431	1.9250	10.65000	1.047400	1.770046	2.1052
10.02943	− 0.140000	1.805746	1.8882	10.60000	1.038270	1.772908	2.1212
10.56000	− 0.060000	1.798043	1.8025	10.50000	1.016265	1.774855	2.1607
10.92429	0	1.780024	1.7515	10.43580	0.997071	1.775997	2.1936
11.00000	0.013034	1.777580	1.7418	10.43562	0.997000	1.776002	2.1937
11.04000	0.020000	1.776537	1.7367	10.38694	0.975000	1.776447	2.2306
11.47957	0.100000	1.761059	1.6852	10.36263	0.950000	1.776051	2.2722
11.88240	0.180000	1.747610	1.6420	10.36970	0.926000	1.774716	2.3129
12.24890	0.260000	1.728032	1.6088	10.41139	0.900000	1.772659	2.3594
12.50000	0.320434	1.714170	1.5873	10.50676	0.870000	1.768379	2.4212
12.57639	0.340000	1.709719	1.5809	10.60514	0.850000	1.764910	2.4730
12.86304	0.420000	1.690604	1.5581	10.75450	0.830000	1.759856	2.5516
13.10698	0.500000	1.668635	1.5407	10.81456	0.825000	1.757207	2.5872
13.21189	0.540000	1.661300	1.5307	10.83000	0.824008	1.755278	2.5976
13.38780	0.620000	1.642144	1.5144	10.84942	0.823000	1.756707	2.6092
13.45820	0.660000	1.633121	1.5059	10.87000	0.822133	1.752688	2.6250
13.51687	0.700000	1.623098	1.4980	10.89800	0.821500	1.755133	2.6438
13.56333	0.740000	1.615229	1.4883	10.90000	0.821500	1.757126	2.6443
13.58190	0.760000	1.612215	1.4825	10.93000	0.821504	1.754201	2.6697
13.61000	0.800000	1.605204	1.4725	10.96000	0.822397	1.753314	2.6971
13.61910	0.820000	1.603748	1.4661	10.99000	0.824393	1.752569	2.7291

K	E_i	F_f	x
11.00000	0.825361	1.752191	2.7413
11.02000	0.827909	1.741727	2.7686
11.03243	0.830000	1.751292	2.7885
11.04216	0.832000	1.751064	2.8061
11.05033	0.834000	1.750917	2.8230
11.05725	0.836000	1.750610	2.8396
11.06314	0.838000	1.750551	2.8557
11.06575	0.839000	1.750455	2.8637
11.07236	0.842000	1.750232	2.8878
11.07736	0.845000	1.750350	2.9118
11.08257	0.850000	1.749694	2.9537
11.08410	0.855000	1.750051	2.9982
11.08193	0.860000	1.750648	3.0478
11.06314	0.870000	1.751375	3.1831
11.05300	0.872566	1.752803	3.2367
11.02500	0.876159	1.752910	3.3877
11.00000	0.875772	1.753818	3.5791

Class (γ)

Initial Conditions: same as class (n)
Final Conditions: „ „ „ „
Note: „ „ „ „

K	E_i	E_f	x
10.90000	0.817971	0.056915	3.1730
10.85000	0.819273	0.065338	3.1405
10.83200	0.820131	0.068339	3.1298
10.80000	0.822103	0.073621	3.1119
10.78772	0.823000	0.075635	3.1053
10.70404	0.831000	0.089144	3.0638
10.58929	0.847000	0.107084	3.0121
10.43938	0.879000	0.129144	2.9425
10.35416	0.911000	0.140549	2.8873
10.32287	0.943000	0.143254	2.8361
10.34358	0.975000	0.137866	2.7847
10.41720	1.007000	0.124167	2.7306
10.54691	1.039000	0.101503	2.6721
10.73882	1.071000	0.068107	2.6073
10.86153	1.087000	0.046619	2.5718
10.93053	1.095000	0.034432	2.5531
11.00000	1.102467	0.022067	2.5349
11.00516	1.103000	0.021146	2.5336
11.04475	1.107000	0.014054	2.5236
11.08597	1.111000	0.006639	2.5133
11.10721	1.113000	0.002798	2.5081
11.12890	1.115000	−0.001127	2.5028
11.15102	1.117000	−0.005164	2.4975
11.17365	1.119000	−0.009274	2.4920
11.19675	1.121000	−0.013496	2.4865
11.24449	1.125000	−0.022262	2.4753
11.29442	1.129000	−0.031492	2.4637
11.32026	1.131000	−0.036297	2.4578
11.34674	1.133000	−0.041236	2.4518
11.36021	1.134000	−0.043759	2.4487
11.37386	1.135000	−0.046318	2.4456
11.38768	1.136000	−0.048917	2.4425
11.41586	1.138000	−0.054227	2.4362
11.45000	1.140354	−0.060694	2.4286
11.50000	1.143670	−0.070231	2.4176
11.75000	0.119148	−1.158031	2.3638
12.00000	0.170468	−1.168722	2.3115
12.25000	1.175636	−0.224769	2.2595
12.50000	1.178148	−0.282896	2.2068
12.75000	1.174909	−0.346100	2.1521
13.00000	1.163301	−0.416443	2.0941
13.23527	1.140000	−0.492650	2.0347
13.25000	1.137959	−0.497871	2.0307
13.35851	1.120000	−0.538639	2.0010
13.44913	1.100000	−0.576578	1.9749
13.60106	1.050000	−0.653522	1.9286
13.69351	1.000000	−0.717404	1.8988
13.74940	0.950000	−0.774683	1.8803
13.77771	0.900000	−0.828037	1.8708
13.77800	0.860000	−0.859803	1.8725

Class (δ)

Initial Conditions: same as class (a)
Final Conditions: „ „ „ „
Note: „ „ „ „

K	F_i	F_f	x
15.42751	−0.431093	0.431164	2.4075
15.42472	−0.450000	0.411502	2.4087
15.39431	−0.500000	0.363021	2.4110
15.38426	−0.510000	0.353558	2.4117
15.33127	−0.550000	0.316085	2.4158
15.23746	−0.600000	0.270549	2.4232
15.11434	−0.650000	0.226170	2.4336
14.96243	−0.700000	0.182592	2.4477
14.77992	−0.750000	0.139089	2.4665
14.55881	−0.800000	0.094146	2.4928
14.26612	−0.850000	0.042882	2.5347
13.98826	−0.878648	0	2.5824
13.50000	−0.882014	−0.066433	2.6786
13.00000	−0.840666	−0.126677	2.7782
12.50000	−0.777582	−0.181433	2.8719

K	F_i	F_f	x
12.25000	−0.741723	−0.207122	2.9171
12.00000	−0.703796	−0.231782	2.9620
11.75000	−0.663960	−0.255441	3.0072
11.50000	−0.622102	−0.278051	3.0534
11.25000	−0.577804	−0.299544	3.1018
11.00000	−0.530173	−0.319742	3.1541
10.75000	−0.477313	−0.338323	3.2131
10.50000	−0.414263	−0.354717	3.2860
10.37803	−0.375000	−0.361671	3.3329
10.34761	−0.363293	−0.363293	3.3471
10.31673	−0.350000	−0.364907	3.3634
10.23915	−0.300000	−0.369171	3.4254
10.23082	−0.250000	−0.371252	3.4891
10.29758	−0.200000	−0.370589	3.5571
10.43171	−0.150000	−0.365520	3.6335
10.53000	−0.120716	−0.360430	3.6825
10.63000	−0.091068	−0.354481	3.7334
10.73000	−0.052594	−0.347941	3.7897
10.75000	−0.038431	−0.346567	3.8034
10.75878	−0.024200	−0.345972	3.8116
10.74980	0	−0.346634	3.8138
10.70000	0.034528	−0.350059	3.8002
10.60000	0.079294	−0.356577	3.7715
10.50000	0.116703	−0.362488	3.7457
10.40000	0.151271	−0.367676	3.7228
10.30000	0.184561	−0.371880	3.7021
10.20000	0.217621	−0.374714	3.6833
10.10000	0.251672	−0.375306	3.6660
10.05000	0.269742	−0.374176	3.6579
10.00000	0.289358	−0.371286	3.6500
9.950000	0.312682	−0.364455	3.6425
9.917145	0.338570	−0.349332	3.6376
9.915198	0.343950	−0.343877	3.6381

Class (λ)

Initial Conditions: same as class (k)
Final Conditions: „ „ „ „
Note: „ „ „ „

K	F_i	F_f	x
8.100000	2.249498	−1.822197	1.1933
8.500000	2.236850	−1.810056	1.2068
8.678465	2.230000	−1.802585	1.2146
8.900000	2.220000	−1.789342	1.2268
9.071346	2.210000	−1.774346	1.2389
9.193476	2.200000	−1.756117	1.2502
9.258044	2.190000	−1.733862	1.2592
9.228497	2.175000	−1.687927	1.2652
9.126486	2.165000	−1.643750	1.2622
9.060156	2.160000	−1.615732	1.2587
8.993231	2.155000	−1.582152	1.2545
8.936470	2.150000	−1.540651	1.2499
8.920393	2.148000	−1.520819	1.2481
8.911194	2.146000	−1.498221	1.2464
8.880000	2.145000	−1.494412	1.2430
8.900000	2.143993	−1.475326	1.2439
8.918614	2.143000	−1.456629	1.2444
8.930000	2.142000	−1.439750	1.2440
8.950259	2.141000	−1.420101	1.2439
8.982443	2.140000	−1.396882	1.2442
9.000000	2.138922	−1.376527	1.2428
9.200000	2.137409	−1.301869	1.2504
9.400000	2.136243	−1.240093	1.2579
9.600000	2.135506	−1.194433	1.2691
9.800000	2.134132	−1.149678	1.2812
10.20000	2.129964	−1.077203	1.3098
10.40000	2.126529	−1.043404	1.3272
10.56250	2.122914	−1.017429	1.3433
10.70000	2.119155	−0.996408	1.3587
10.80000	2.115905	−0.980988	1.3706
11.00000	2.107948	−0.952129	1.3987
11.20000	2.097267	−0.924341	1.4335
11.40000	2.082315	−0.898337	1.4808
11.58879	2.060000	−0.876191	1.5527
11.67662	2.040000	−0.868060	1.6239
11.68967	2.020000	−0.870892	1.7115
11.57100	2.000000	−0.894286	1.8526
11.46985	1.995000	−0.911587	1.9266
11.40000	1.993425	−0.923328	1.9736
11.30000	1.992877	−0.939657	2.0396
11.29000	1.992919	−0.940412	2.0462
11.28500	1.992937	−0.942038	2.0497

Class (μ)

Initial Conditions: same as class (a)
Final Conditions: „ „ „ „
Note: „ „ „ „

K	F_i	F_f	x
11.00000	0.072157	−2.012387	3.2029
10.96670	0.080000	−2.012861	2.8931
10.94752	0.090000	−2.011901	2.7397
10.94207	0.097000	−2.010610	2.6460
10.95000	0.104343	−2.008244	2.5314
11.00000	0.106976	−2.004080	2.3792
11.10000	0.095038	−2.000261	2.2332
11.20000	0.072707	−1.998959	2.1256
11.26799	0.050000	−1.999451	2.0562

K	F_i	F_f	x
11.35156	0	−2.002502	1.9589
11.37887	−0.050000	−2.005166	1.9070
11.37226	−0.100000	−2.005713	1.8912
11.33441	−0.150000	−2.003950	1.9137
11.28554	−0.180000	−2.002158	1.9550
11.22624	−0.200000	−2.001050	2.0098
11.17276	−0.210000	−2.000880	2.0633
11.06205	−0.215000	−2.002684	2.1991
11.00000	−0.208417	−2.005272	2.3131
10.98000	−0.203751	−2.006554	2.3679
10.96000	−0.195771	−2.008424	2.4532
10.95155	−0.180000	−2.011315	2.6320
10.96000	−0.172754	−2.012284	2.7424
11.00000	−0.166372	−2.012276	3.1527

Class (v)

Initial Conditions: $E_i = 0$; $\dot{F}_i = 0$; $\dot{E}_i > 0$.

Final Conditions: $E_f = -\pi/2$; $\dot{F}_f = 0$.

K	F_i	F_f	x
11.00000	1.752480	−0.982134	3.3688
10.75806	1.760000	−1.022996	3.1371
10.61518	1.765000	−1.049386	3.0433
10.49074	1.770000	−1.075521	2.9534
10.45183	1.772000	−1.084942	2.9103
10.45000	1.774192	−1.090898	2.8192
10.50000	1.773844	−1.084276	2.7731
10.59500	1.772193	−1.069324	2.7226
10.60000	1.772092	−1.068514	2.7204
10.70000	1.769894	−1.052050	2.6817
10.80000	1.767457	−1.035581	2.6492
10.90000	1.764844	−1.019031	2.6201
11.00000	1.762084	−1.002808	2.5935
11.20000	1.756160	−0.970468	2.5446
11.40000	1.749712	−0.938799	2.4996
11.60000	1.742710	−0.907601	2.4569
11.80000	1.735091	−0.876836	2.4155
12.00000	1.726767	−0.846368	2.3746
12.40000	1.707465	−0.785985	2.2919
12.50000	1.701947	−0.770908	2.2705
12.60000	1.696085	−0.755790	2.2485
12.80000	1.683133	−0.725442	2.2023
13.00000	1.668078	−0.694761	2.1517
13.20000	1.650008	−0.663420	2.0932
13.40000	1.627072	−0.630860	2.0195
13.57045	1.600000	−0.600929	1.9259
13.65645	1.580000	−0.583595	1.8430
13.68727	1.570000	−0.576119	1.7924
13.70920	1.560000	−0.569200	1.7312
13.71604	1.555000	−0.565825	1.6942
13.71863	1.550000	−0.562346	1.6495
13.71761	1.548000	−0.560850	1.6277
13.71500	1.546337	−0.559489	1.6063
13.71000	1.544887	−0.558120	1.5825
13.70000	1.543742	−0.556625	1.5527
13.60000	1.548590	−0.554514	1.4400
13.40000	1.564793	−0.559820	1.3573
13.20000	1.579213	−0.566901	1.3124
13.00000	1.591743	−0.573990	1.2818
12.80000	1.602777	−0.580631	1.2590
12.60000	1.612627	−0.586659	1.2413
12.50000	1.617182	−0.589415	1.2339
12.40000	1.621523	−0.591987	1.2272
12.20000	1.629641	−0.596568	1.2159
12.00000	1.637116	−0.600359	1.2068
11.80000	1.644059	−0.603328	1.1995
11.40000	1.656704	−0.606629	1.1892
11.00000	1.668206	−0.605944	1.1834
10.60000	1.679115	−0.600476	1.1815
10.20000	1.690028	−0.588675	1.1827
9.800000	1.701749	−0.567314	1.1867
9.600000	1.708336	−0.550703	1.1896
9.400000	1.715865	−0.526995	1.1930
9.200000	1.725406	−0.487529	1.1966
9.130168	1.730000	−0.463103	1.1975
9.081897	1.735000	−0.429781	1.1972
9.081479	1.740000	−0.383136	1.1945
9.122139	1.742500	−0.347436	1.1908
9.200000	1.744162	−0.307684	1.1853
9.300000	1.744806	−0.269995	1.1790
9.400000	1.744753	−0.238443	1.1732
9.600000	1.743611	−0.184157	1.1625
10.00000	1.739266	−0.091486	1.1435
10.40000	1.733379	−0.006948	1.1276
10.80000	1.726334	0.076240	1.1150
11.20000	1.718187	0.162890	1.1065
11.60000	1.708926	0.259121	1.1041
12.00000	1.698768	0.378954	1.1138
12.20000	1.693883	0.463593	1.1300
12.30000	1.692130	0.527666	1.1477
12.35000	1.692281	0.585255	1.1673
12.35000	1.696160	0.677680	1.2055
12.30000	1.700787	0.736167	1.2334
12.20000	1.707652	0.802294	1.2678
12.10000	1.713502	0.850924	1.2949
12.00000	1.718794	0.892170	1.3190

K	F_i	F_f	x	K	F_i	F_f	x
11.80000	1.728260	0.963810	1.3631	10.79000	1.761676	1.354741	1.6705
11.60000	1.736633	1.028624	1.4056	10.78500	1.761644	1.364331	1.6814
11.40000	1.744152	1.091488	1.4493	10.78500	1.761034	1.394146	1.7194
11.20000	1.750925	1.156344	1.4969	10.80000	1.760178	1.412335	1.7479
11.00000	1.756943	1.229411	1.5544	10.90000	1.756287	1.446734	1.8477
10.80000	1.761610	1.341783	1.6566	11.00000	1.753122	1.439686	1.9729

Simple asymptotic-periodic (limiting) half-orbits
symmetric with respect to the E- or F-axis.

$K = 11.0 \qquad E_i = -\pi/2.$

$\dot{F}_i$ has the same sign as $\dot{E}_i$ for a given orbit.

i = that intercept of the line $E = E_f$ at which $\dot{F}_f = 0$ is satisfied.

j = that intercept of the line $F = F_f$ at which $\dot{E}_f = 0$ is satisfied.

Orbit	F_i	$\dot{E}_i$	E_f	i	F_f	j	Simple classes involved
I	1.307735	−0.046274	$-\pi$	1	0.17150		k, μ
II	1.306357	−0.053104	$-\pi$	1	−0.07653		k, μ
III	1.319335	0.012090	−0.87056		0	1	β, γ
IV	1.321045	0.020829	−0.29566		0	1	β
V	1.324681	0.039521	0	1	2.0115		l, μ
VI	1.323609	0.033997	0	2	1.0030		
VII	1.310836	−0.030828	0	2	1.7538		g, α, β, ν
VIII	1.301025	−0.079346	−1.883		0	2	g
IX	1.328004	0.056745	π	1	2.4646		
X	1.311214	−0.028938	0	1	2.3122		
XI	1.322852	0.030100	0	3	0.4065		α
XII	1.310439	−0.032815	−3.10431		0	2	γ
XIII	1.321178	0.021508	$-\pi$	1	−1.9901		λ
XIV	1.322044	0.025964	0	3	−0.81235		

The values of η_i are, respectively:

I, 1.713681; II, 1.710949; III, 1.736810; IV, 1.740240; V, 1.747549; VI, 1.745392; VII, 1.719839; VIII, 1.700403; IX, 1.754245; X, 1.720592; XI, 1.743870; XII, 1.719051; XIII, 1.740506; XIV, 1.742247.

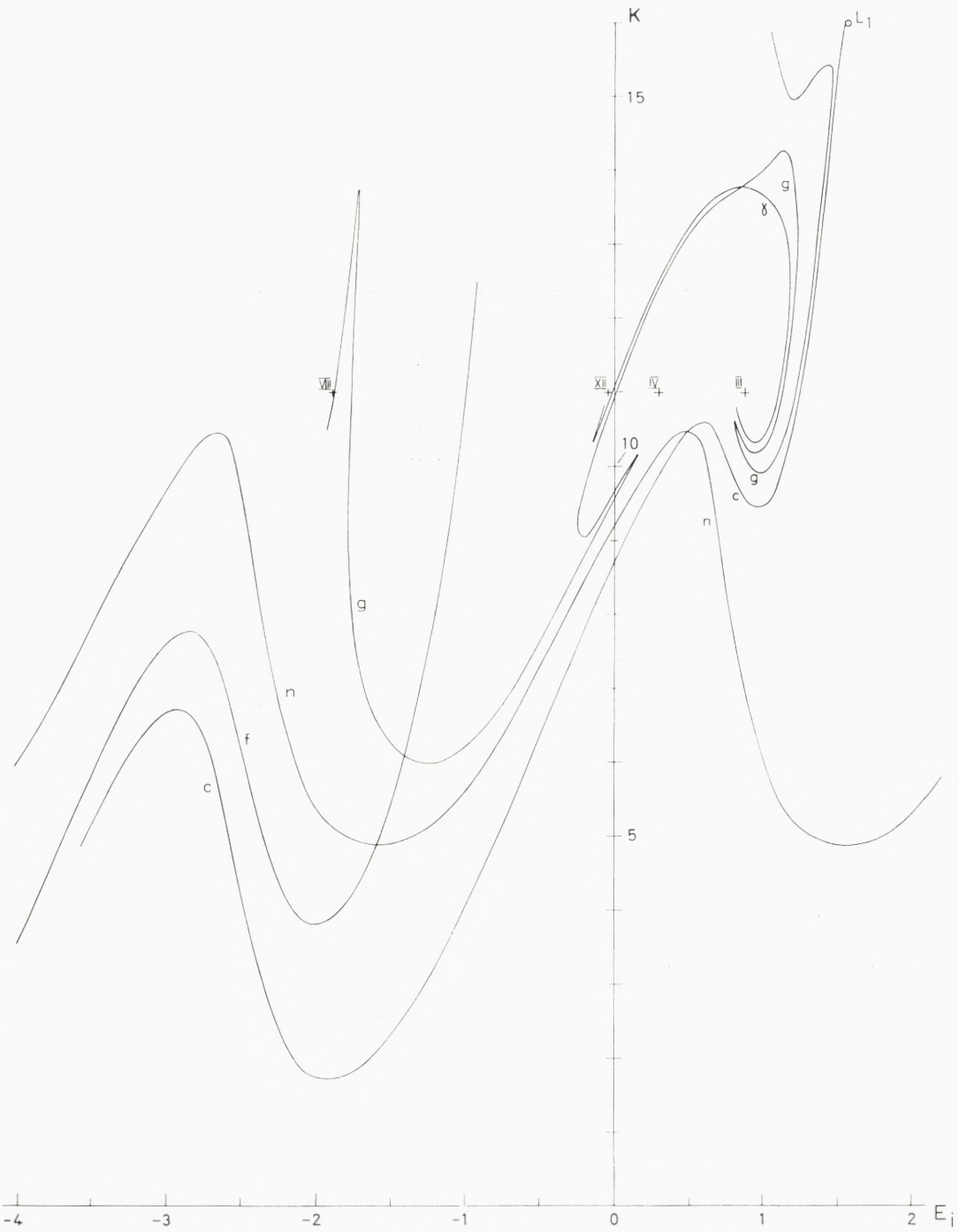

Figure 1 a: General Profile of Eigensurfaces, K vs E_i.
A cross (+) with a Roman numeral, at $K = 11.0$, represents a limiting orbit, shown in detail in Figure 10.

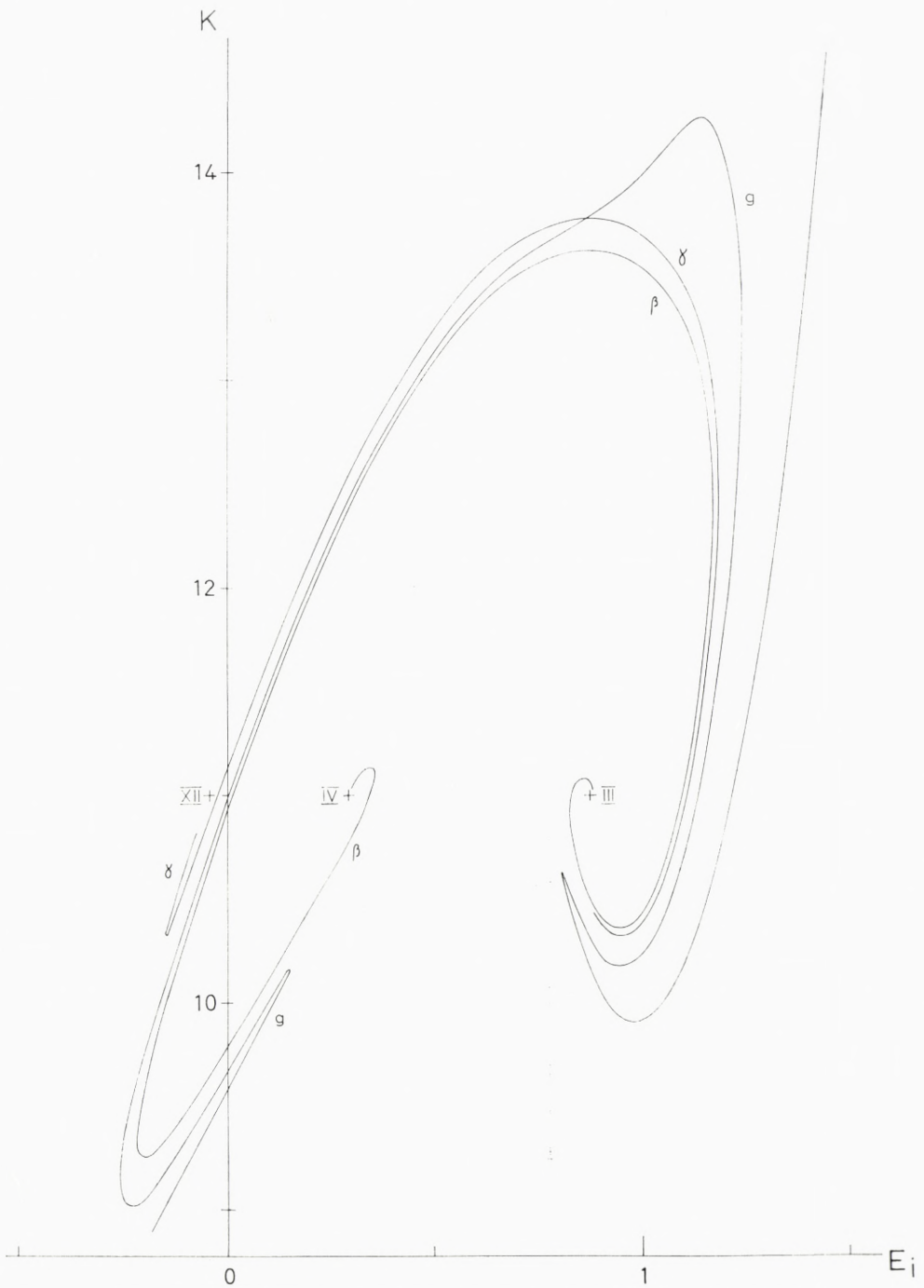

Figure 1 b: Detailed Profile, K vs E_i, showing the (β), (γ) and (g) classes. The crosses (+) at $K = 11.0$ represent limiting orbits.

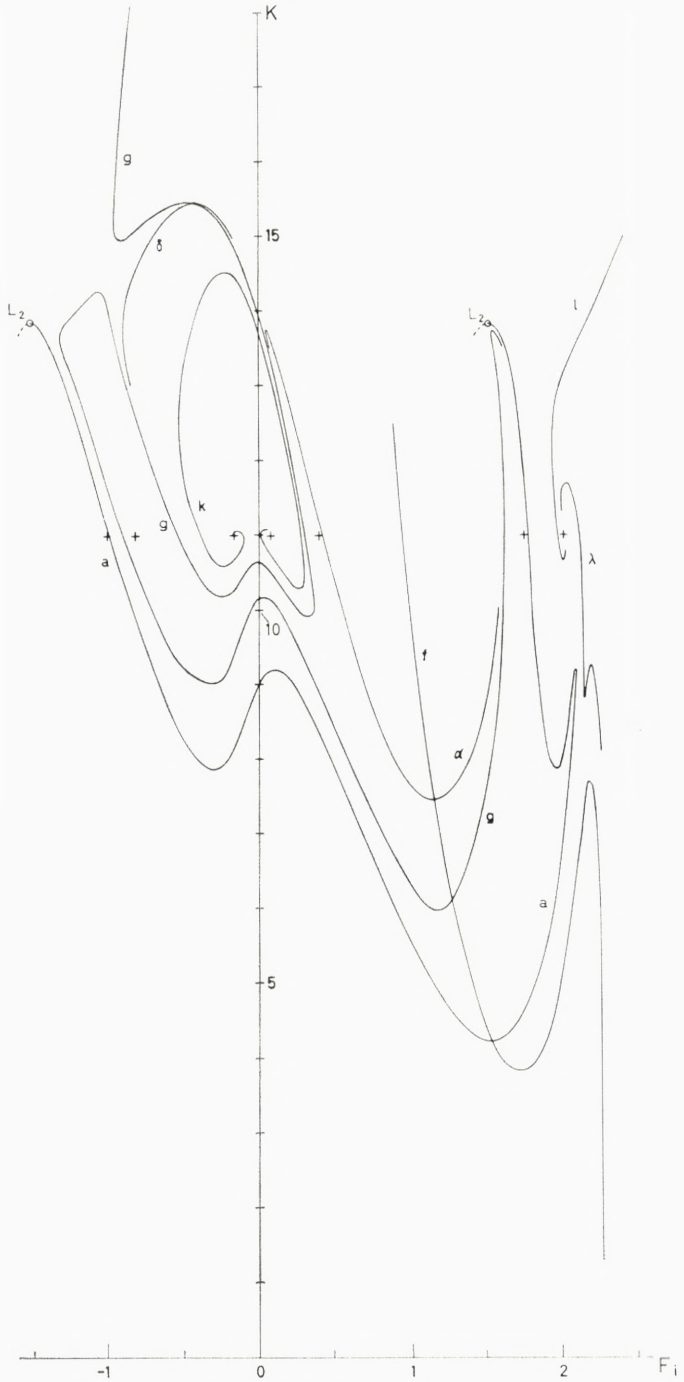

Figure 2 a: General Profile of Eigensurfaces, K vs F_i.
The crosses (+) at $K = 11.0$ represent limiting orbits. (Mr. C. Wagner first noticed the difference between classes λ and l).

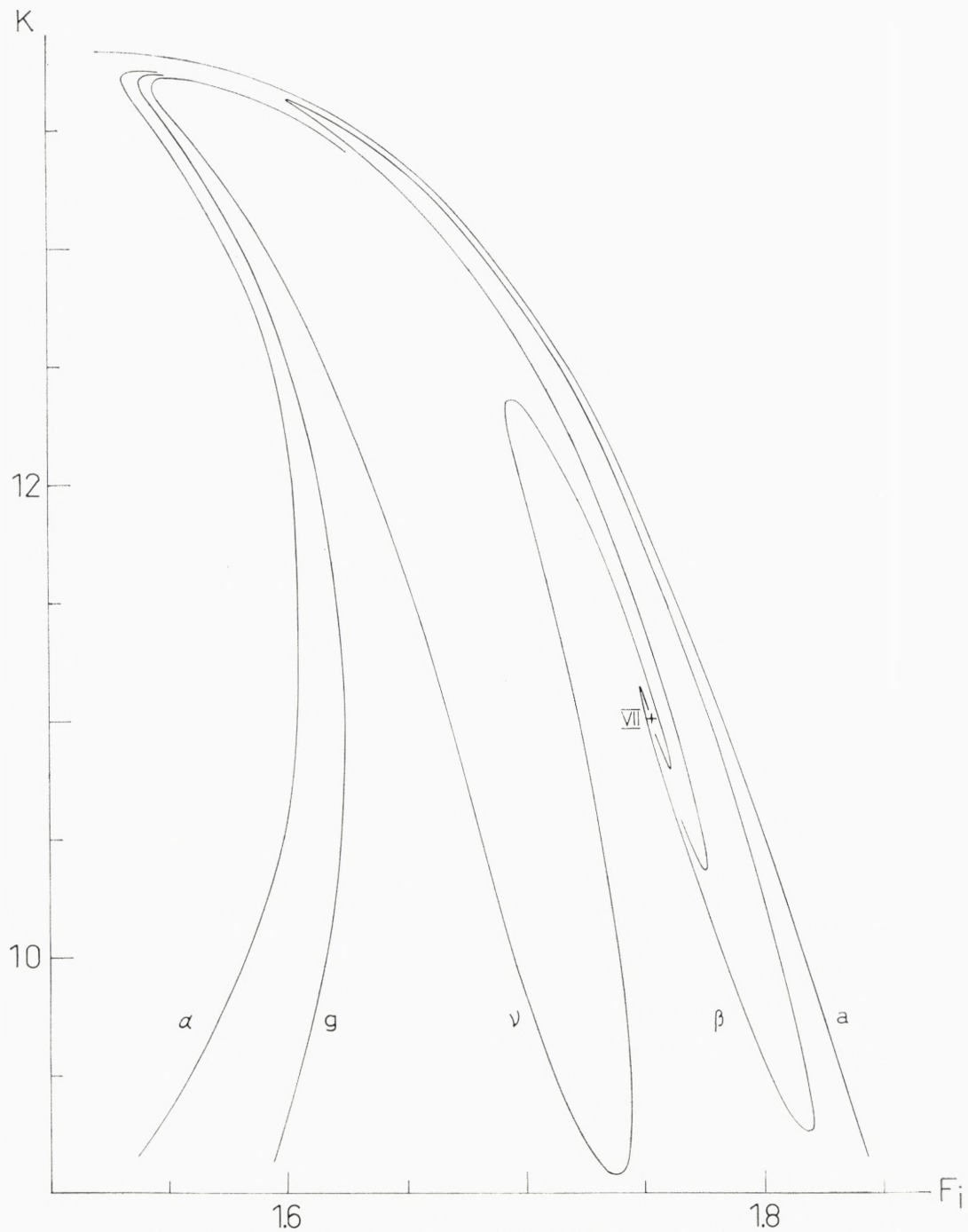

Figure 2 b: Detailed Profile, K vs F_i, showing the (α), (g), (ν), (β) and (a) classes.

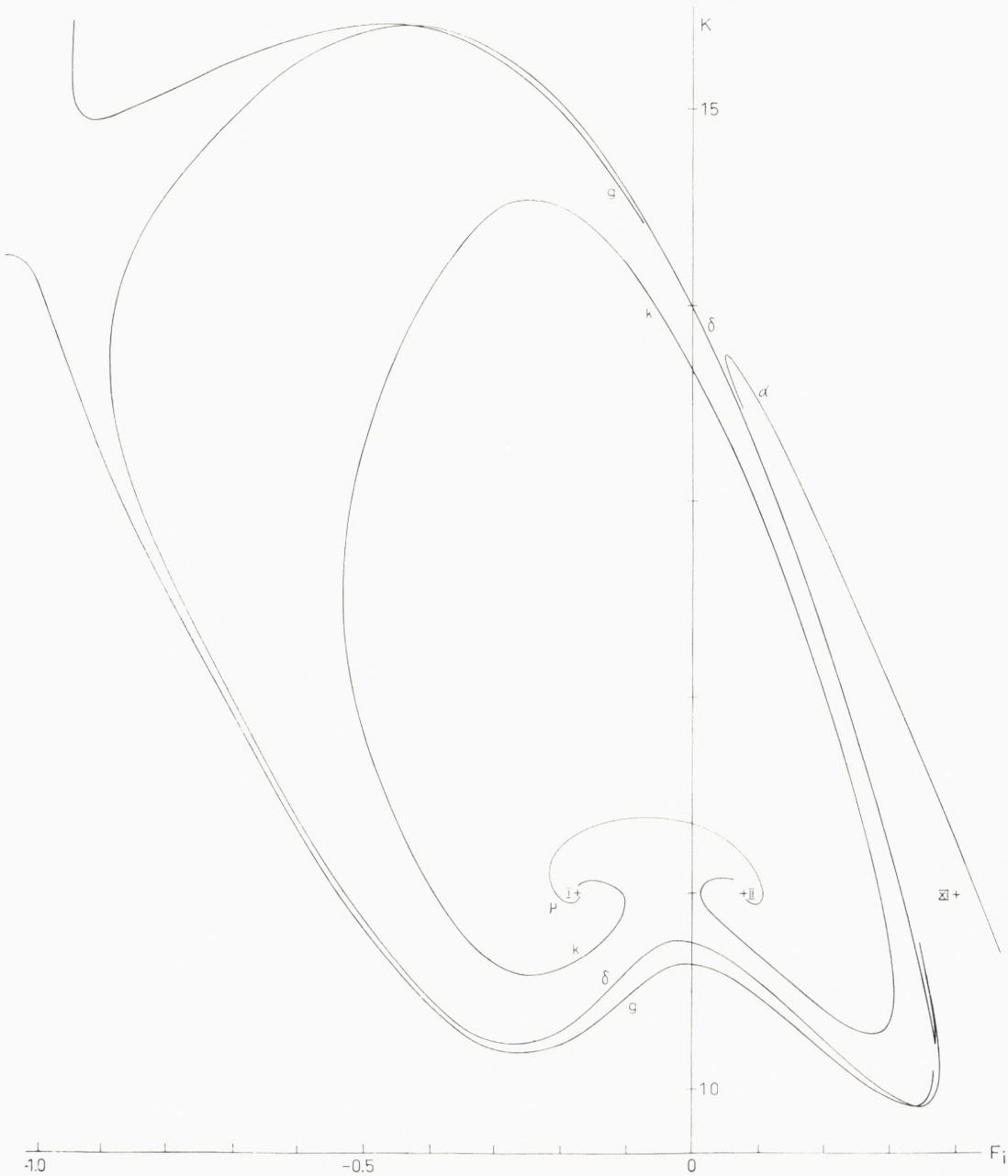

Figure 2 c: Detailed Profile, K vs F_i, showing the (g), (δ), (k), (μ), and (α) classes. The crosses (+) at $K = 11.0$ represent limiting orbits.

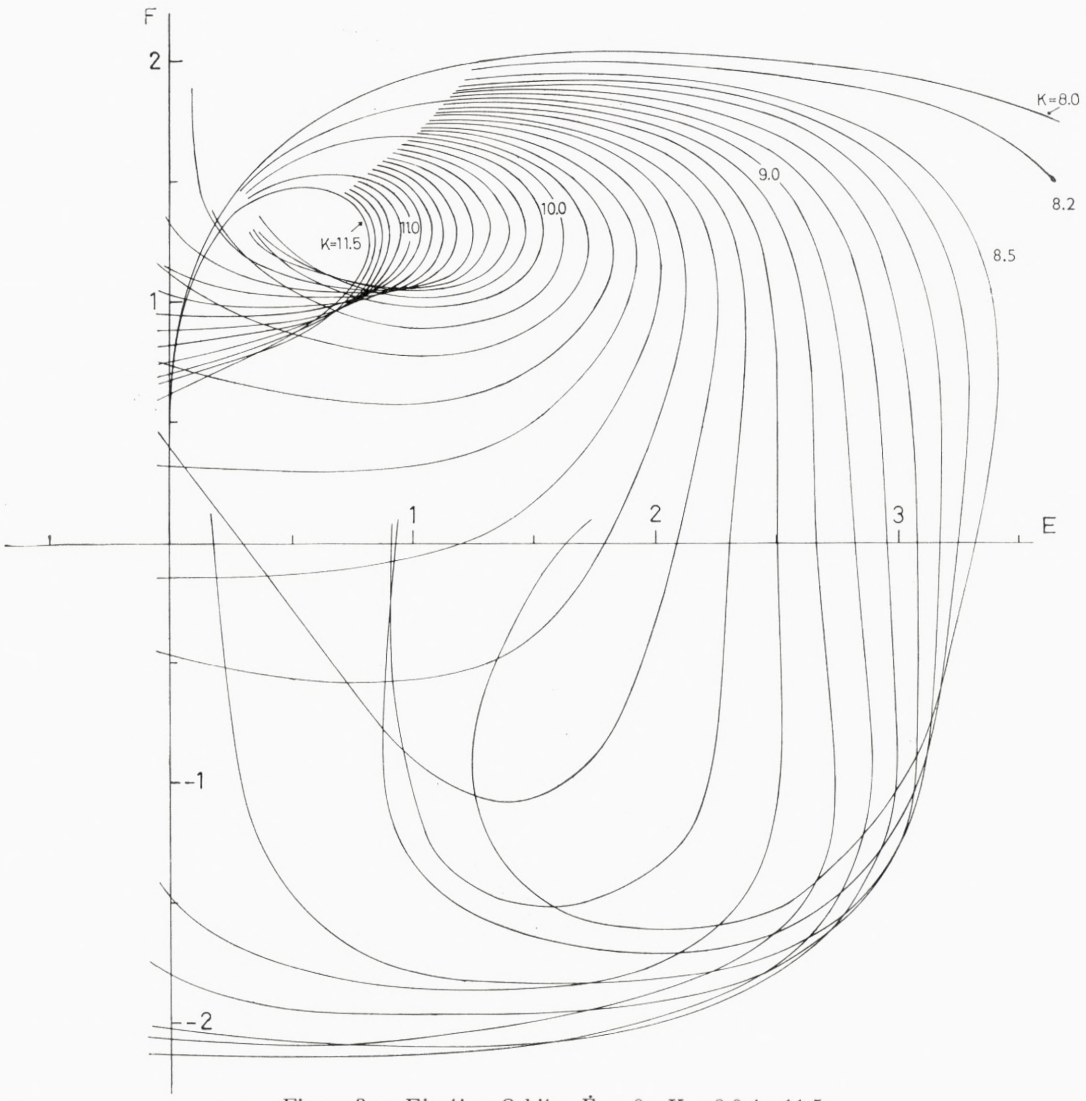

Figure 3 a: Ejection Orbits, $\dot{E}_i = 0$, $K = 8.0$ to 11.5.
Where the values of the Jacobi integral are not explicitly given, the increment from one curve to the next is constant. This remark holds for the subsequent figures, also.

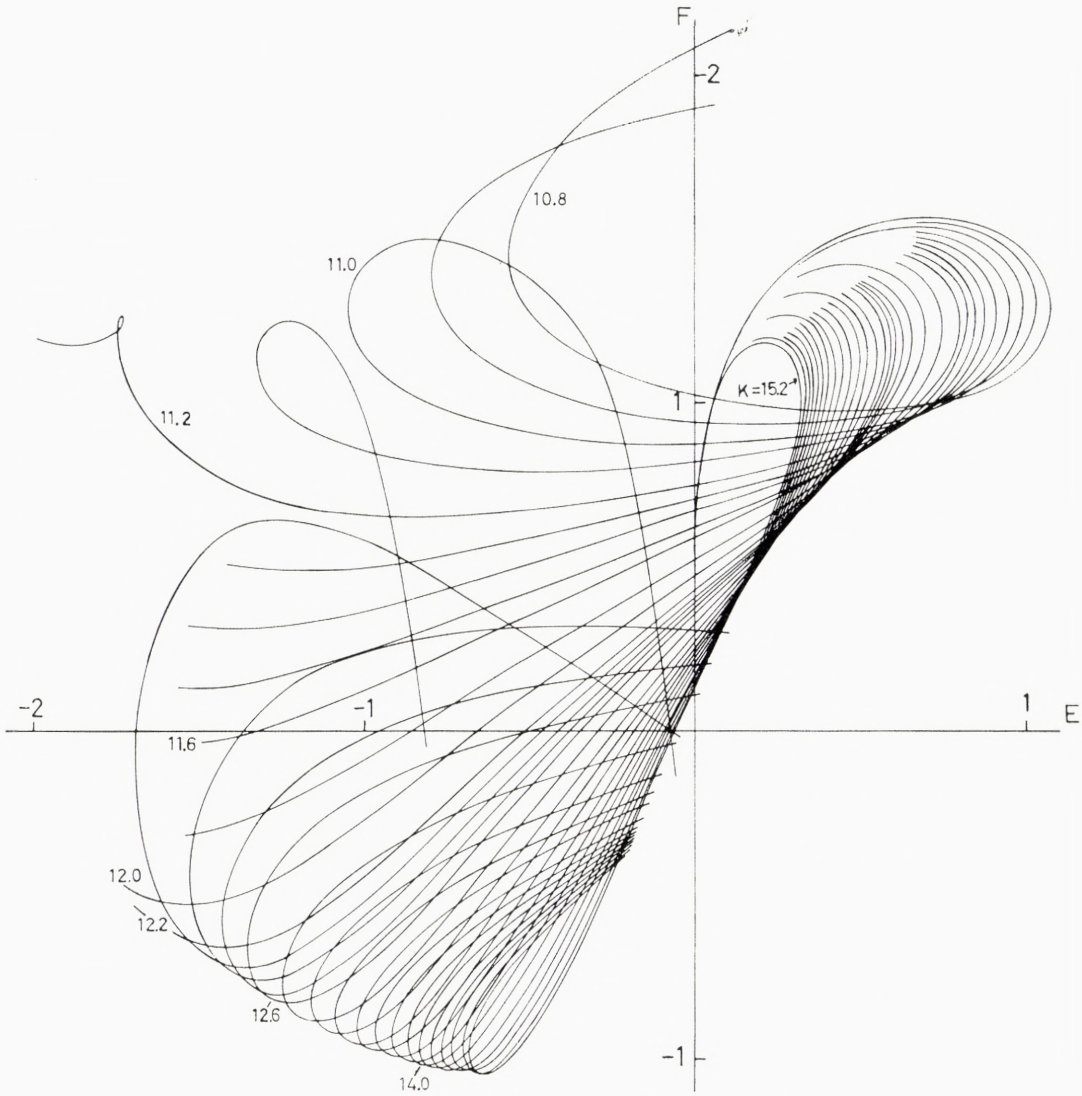

Figure 3 b: Ejection Orbits, $\dot{E}_i = 0$, $K = 10.8$ to 15.2.

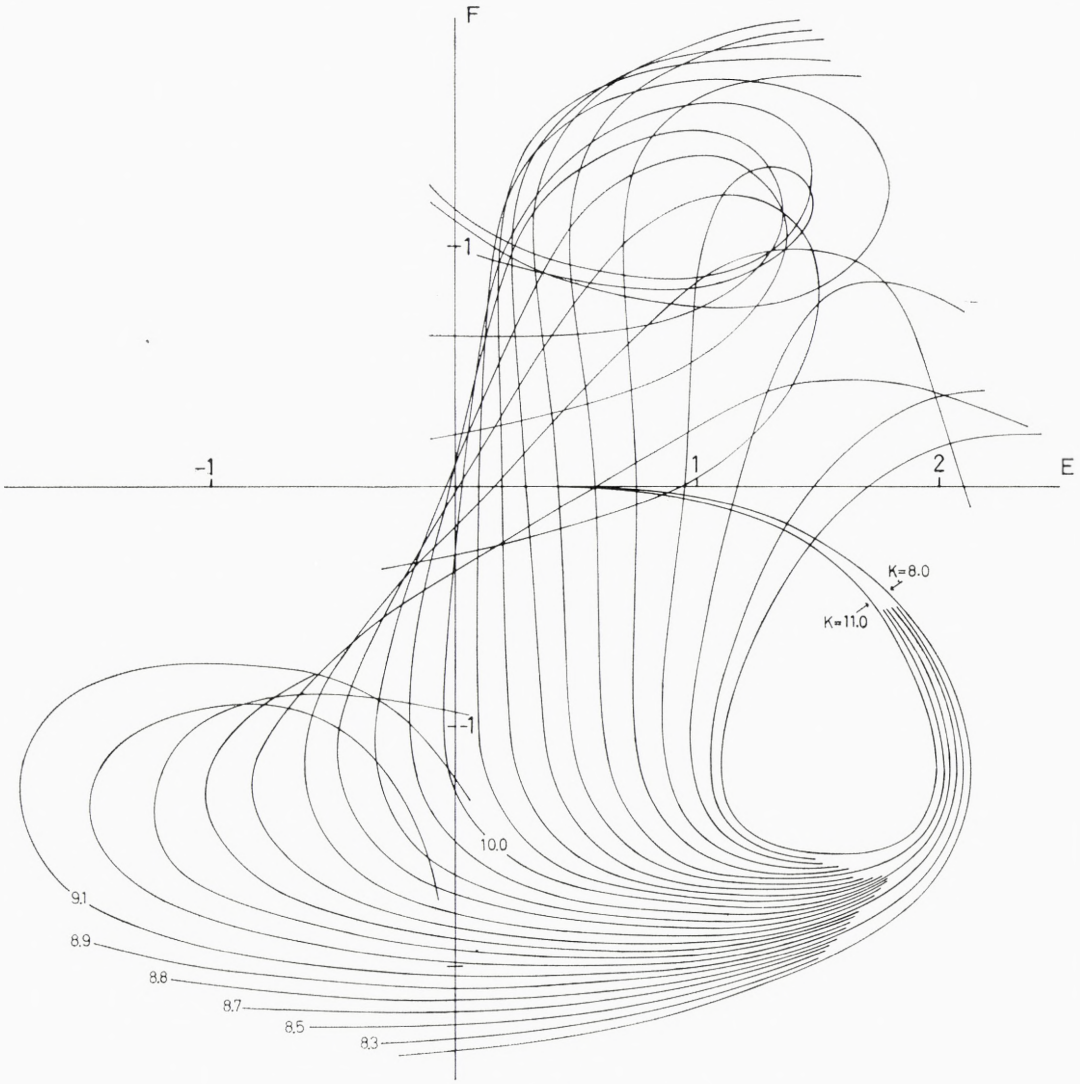

Figure 4 a: Ejection Orbits, $\dot{F}_i = 0$, $K = 8.0$ to 11.0.

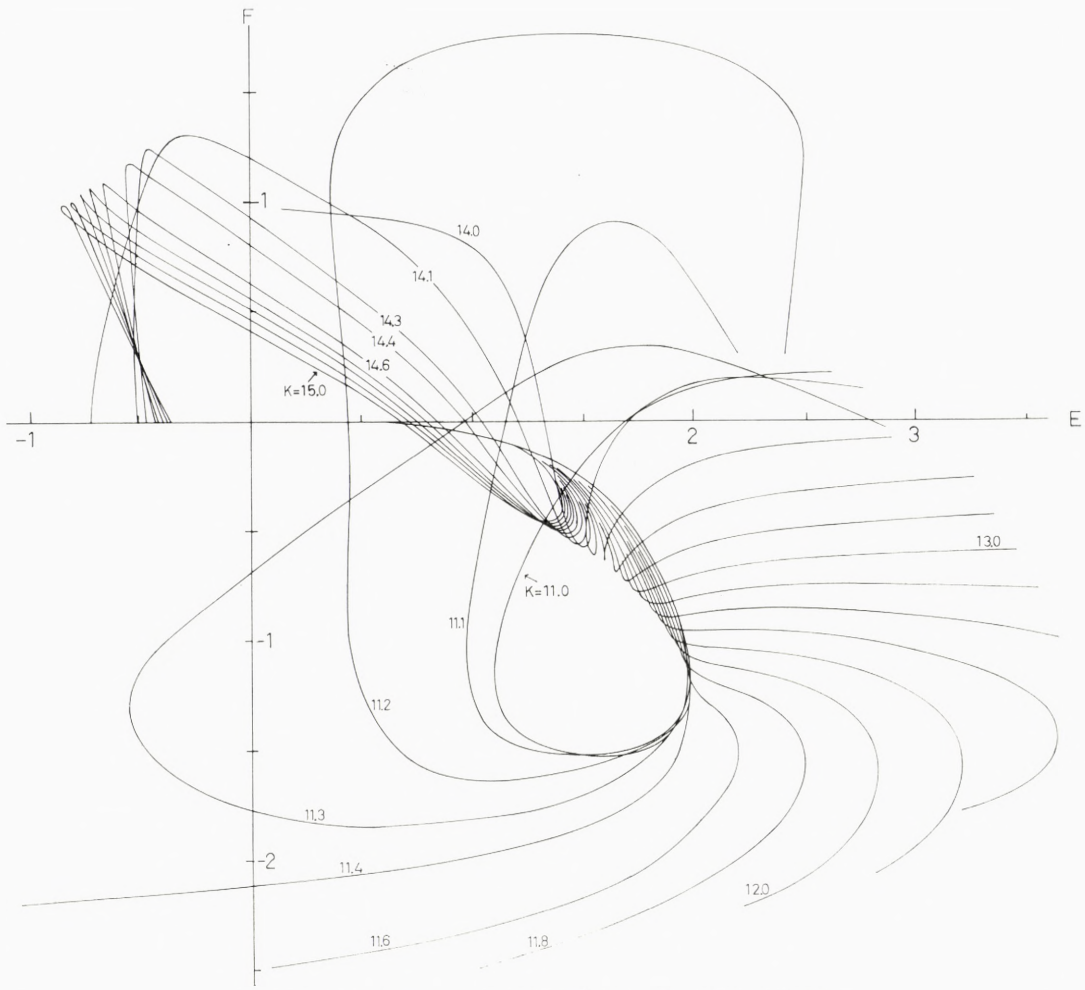

Figure 4 b: Ejection Orbits, $\dot{F}_i = 0$, $K = 11.0$ to 15.0.

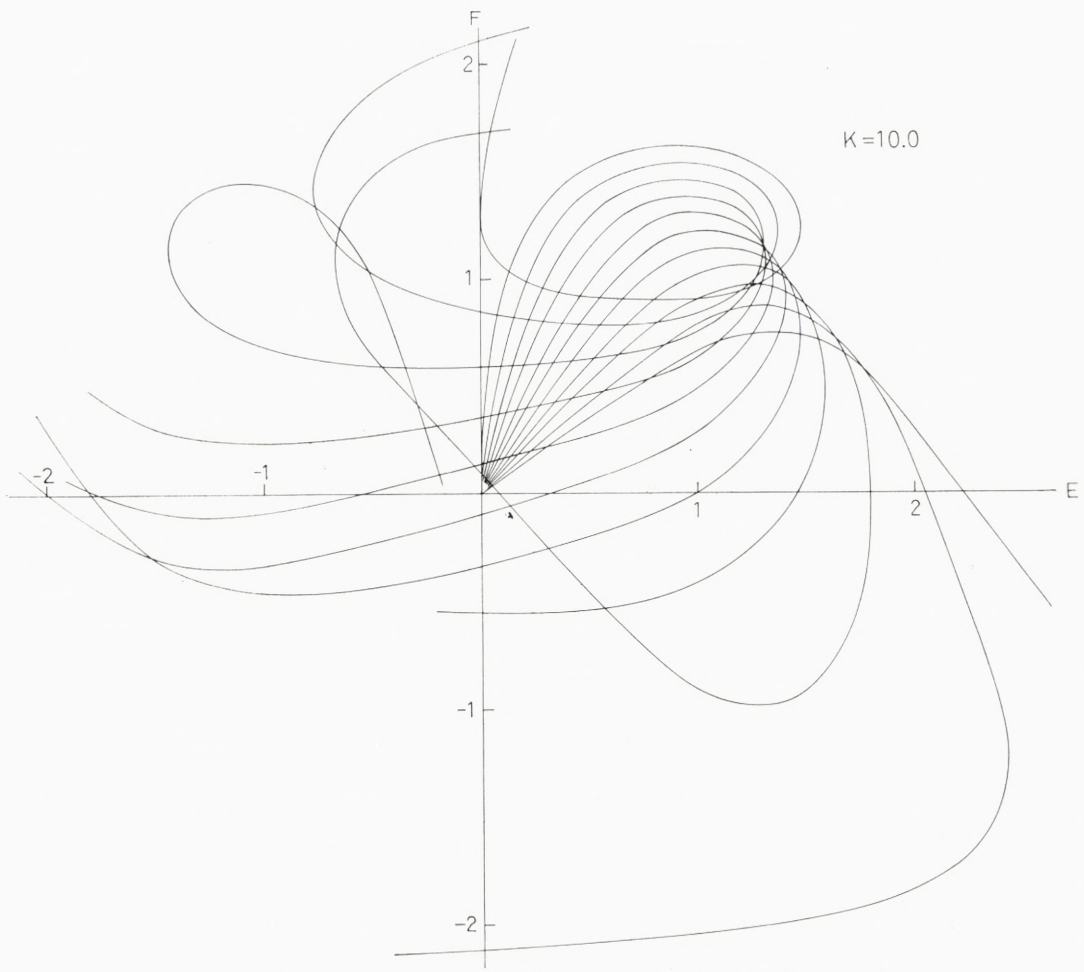

Figure 5 a: Ejection Orbits as a Function of Initial Angle measured from the + F-Axis, 0° to 60°, for $K = 10.0$.

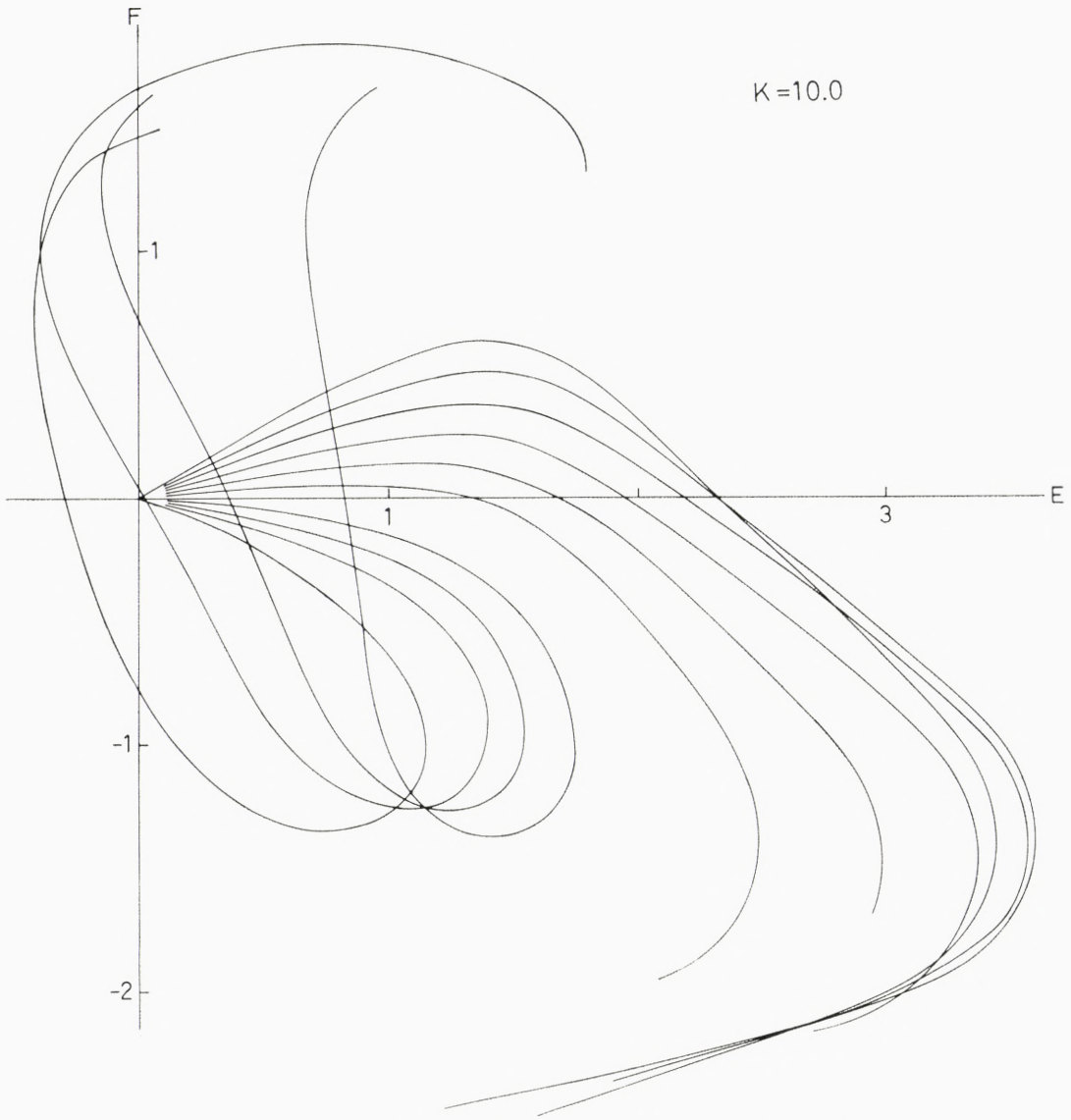

Figure 5 b: Ejection Orbits as a Function of Initial Angle measured from the + F-Axis, 60° to 120°, for $K = 10.0$.

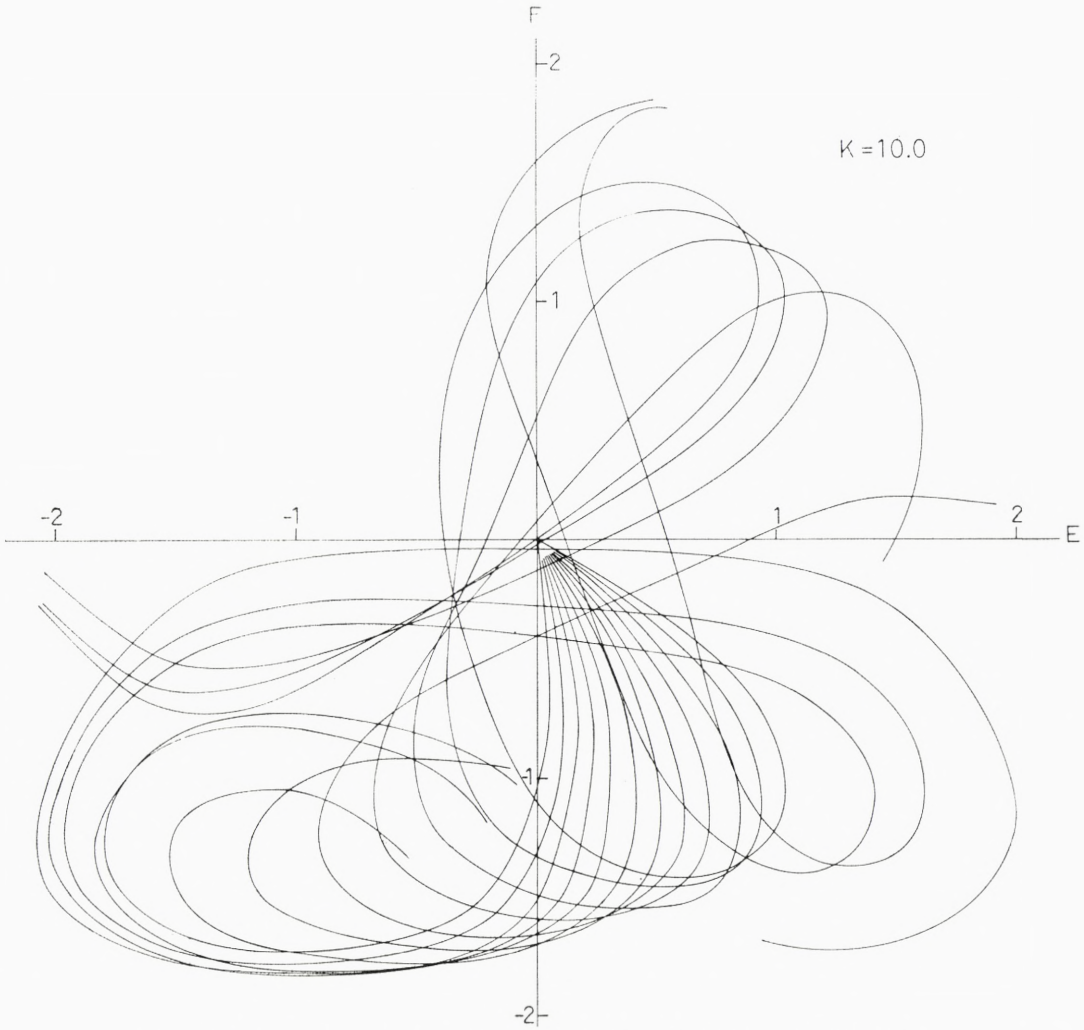

Figure 5 c: Ejection Orbits as a Function of Initial Angle measured from the + F-Axis, 120° to 180°, for $K = 10.0$.

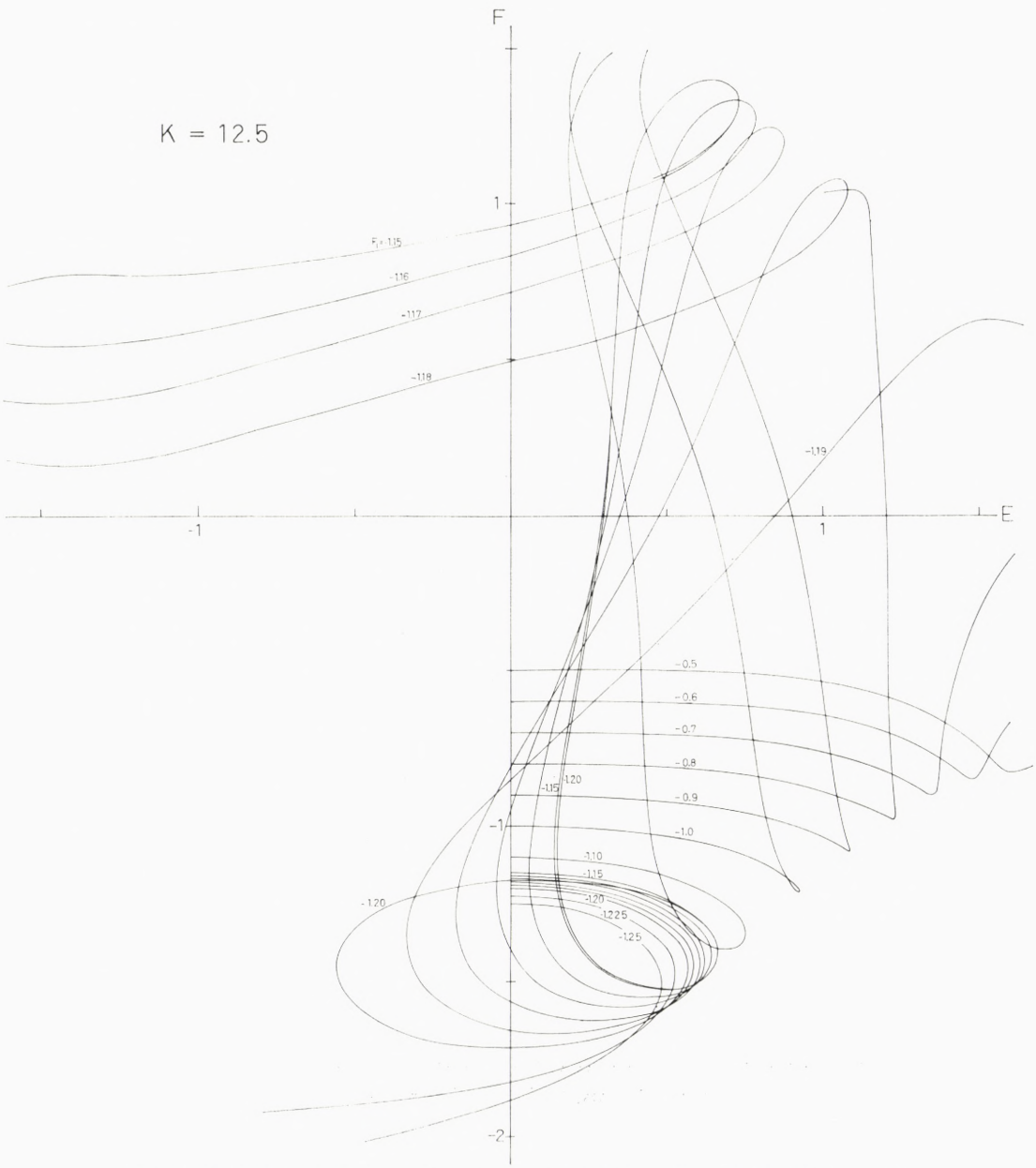

Figure 6 a: Trajectories Normal to the F-Axis, $K = 12.5$, $F_i = -1.25$ to -0.50.
Over the latter part of its course, the trajectory for $F_i = -1.2$ follows rather closely that for $F_i = -1.15$.

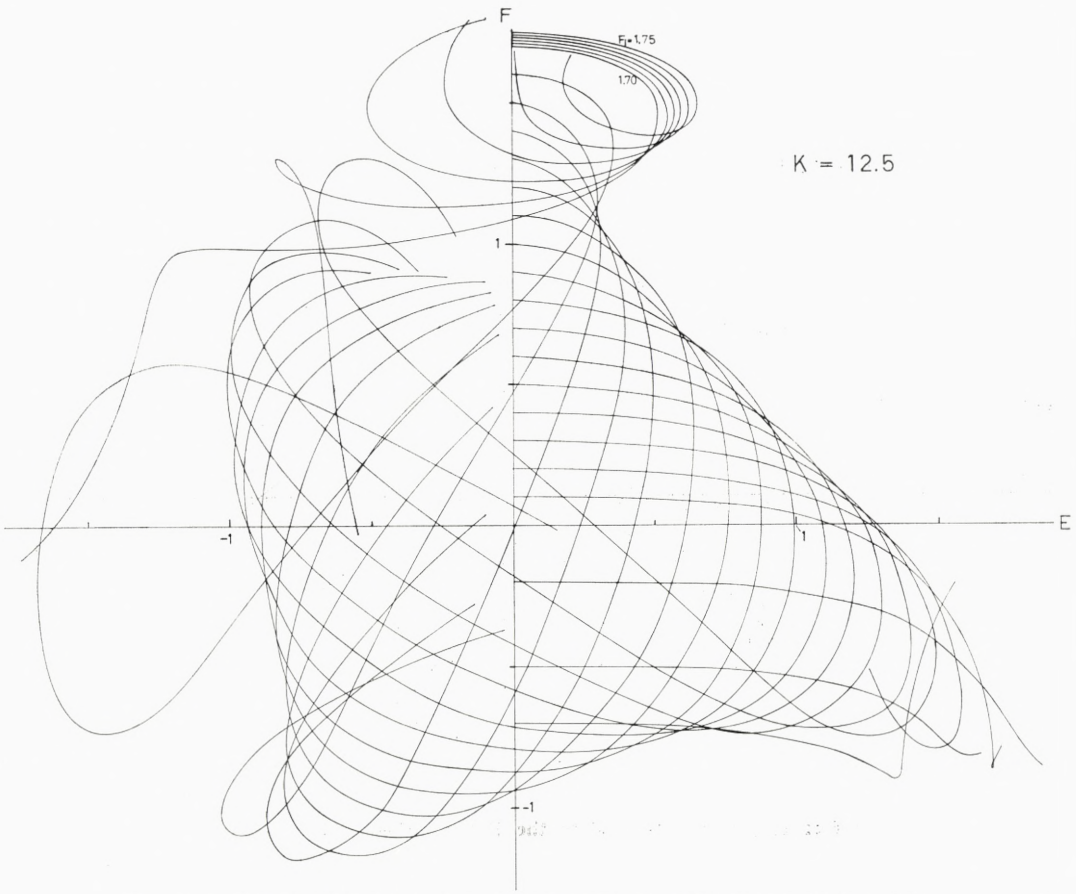

Figure 6 b: Trajectories Normal to the F-Axis, $K = 12.5$, $F_i = -0.70$ to 1.75.

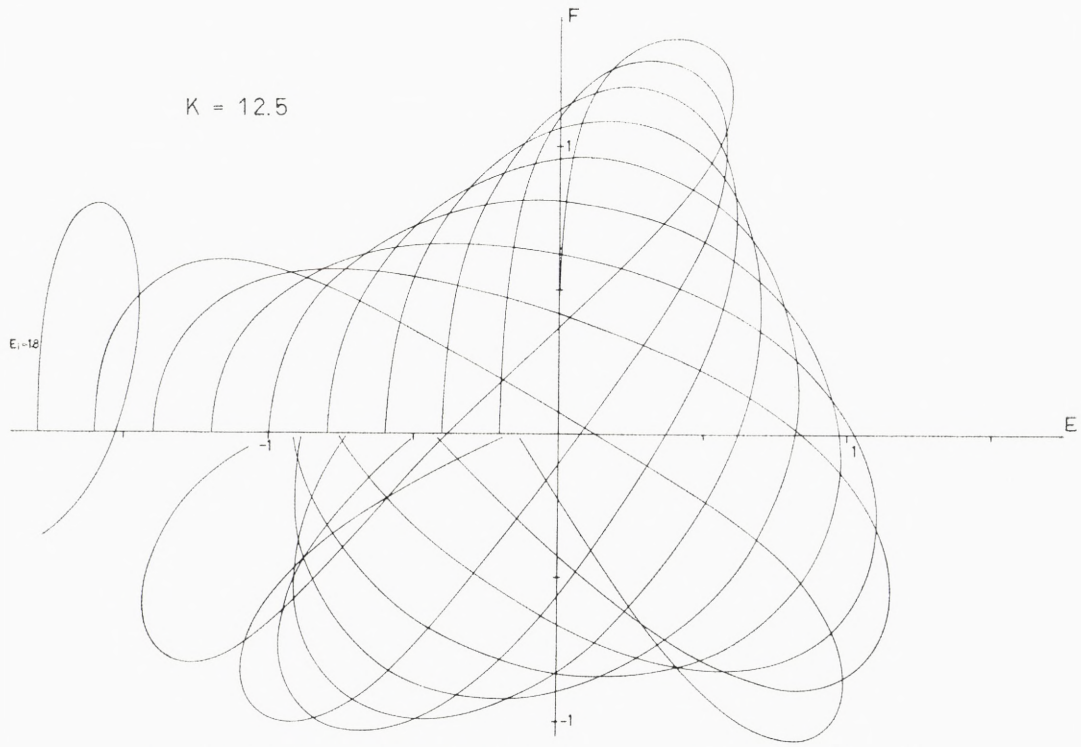

Figure 6 c: Trajectories Normal to the E-Axis, $K = 12.5$, $E_i = -1.80$ to 0.

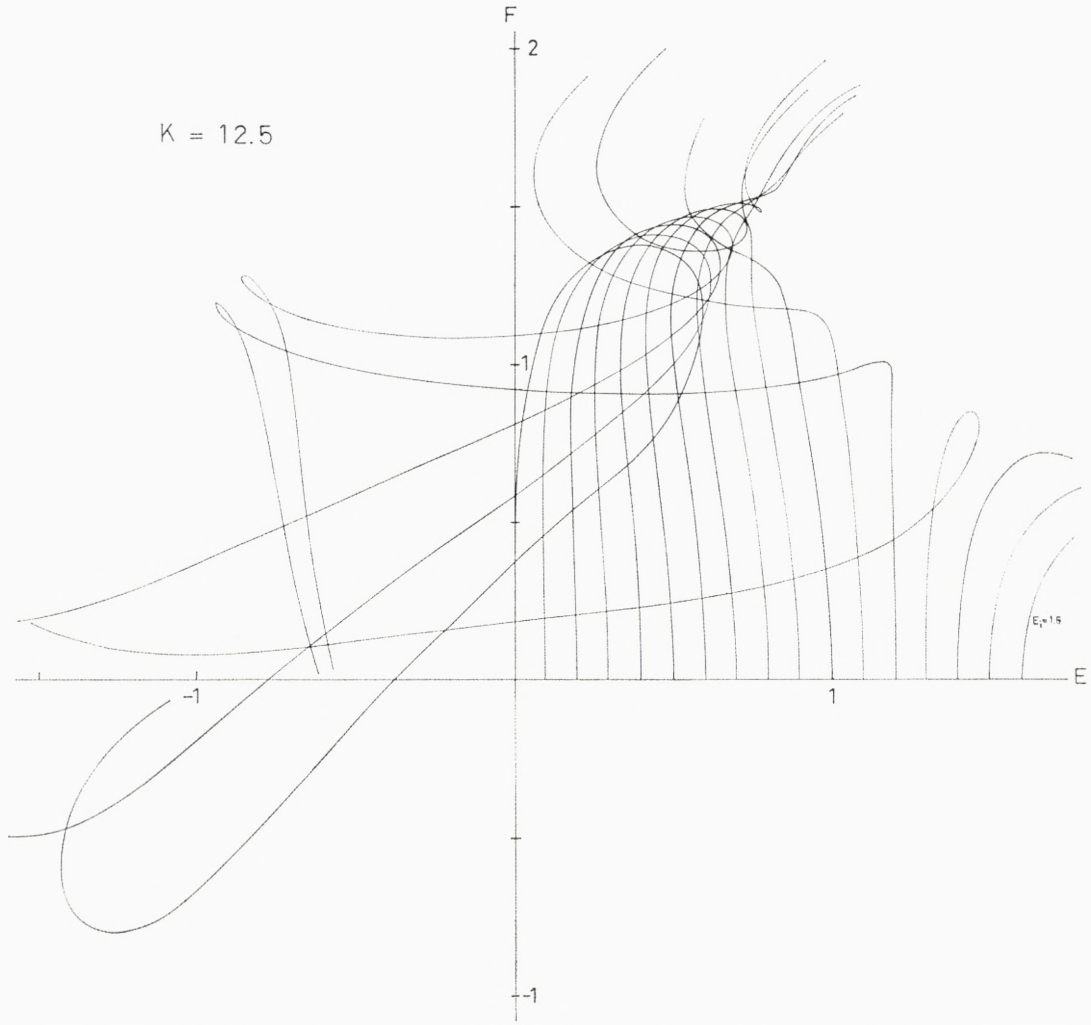

Figure 6 d: Trajectories Normal to the E-Axis, $K = 12.5$, $E_i = 0$ to $+1.60$.

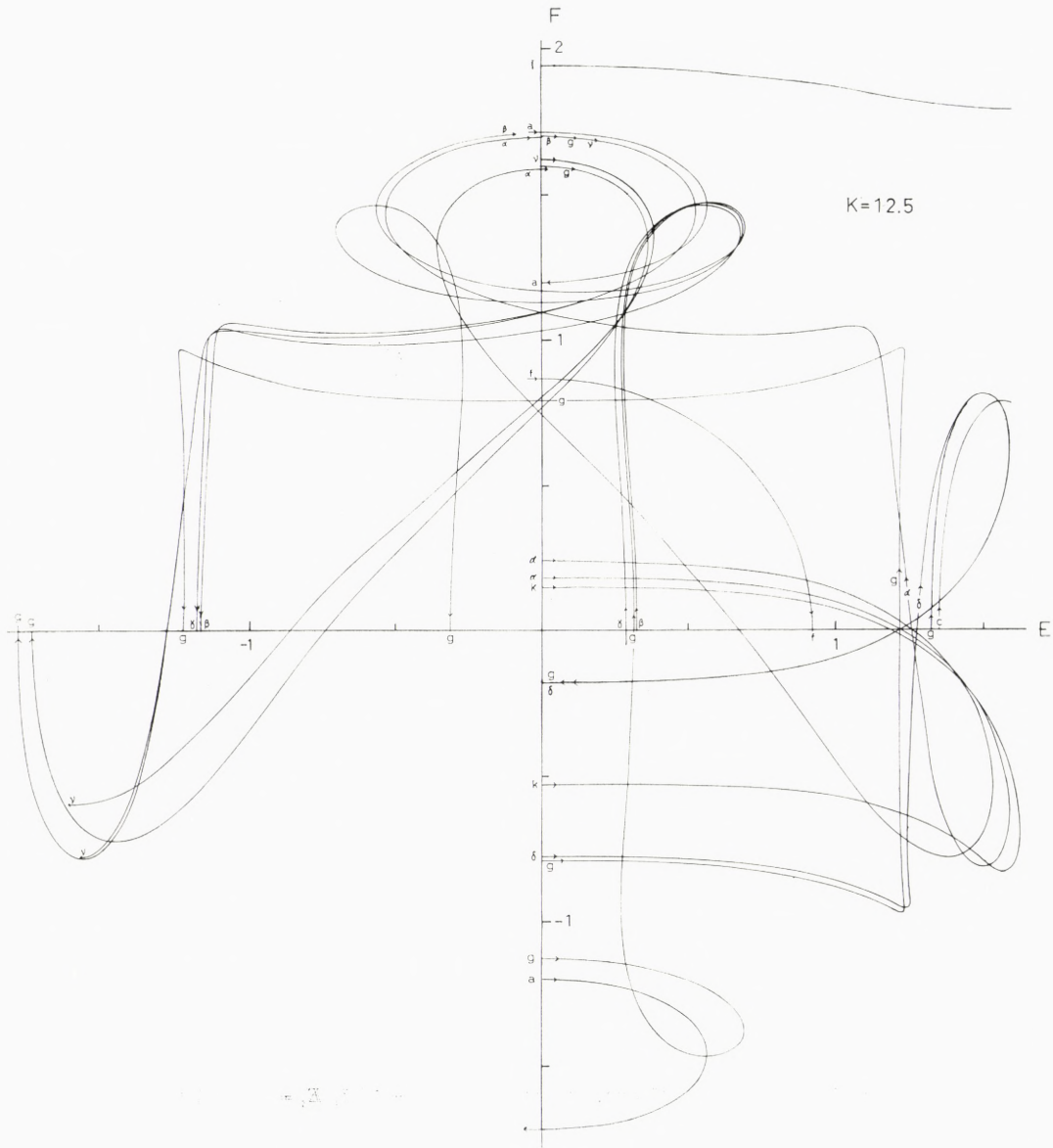

Figure 7: Simple Periodic Orbits for $K = 12.5$.

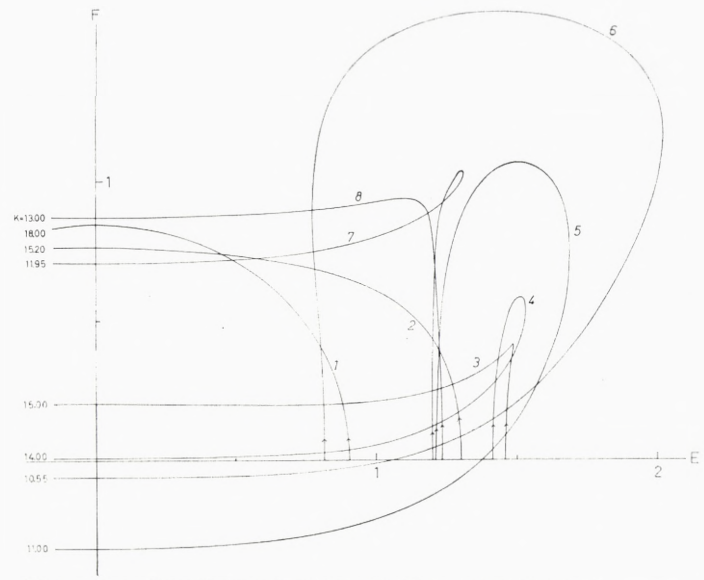

Figure 8 a: Development of the (g) Class, near mass m_2.
The curves are numbered in order along the profile (E or F) starting with 1 near the mass m_2 and increasing until the limiting orbit in Figure 8 c is reached.

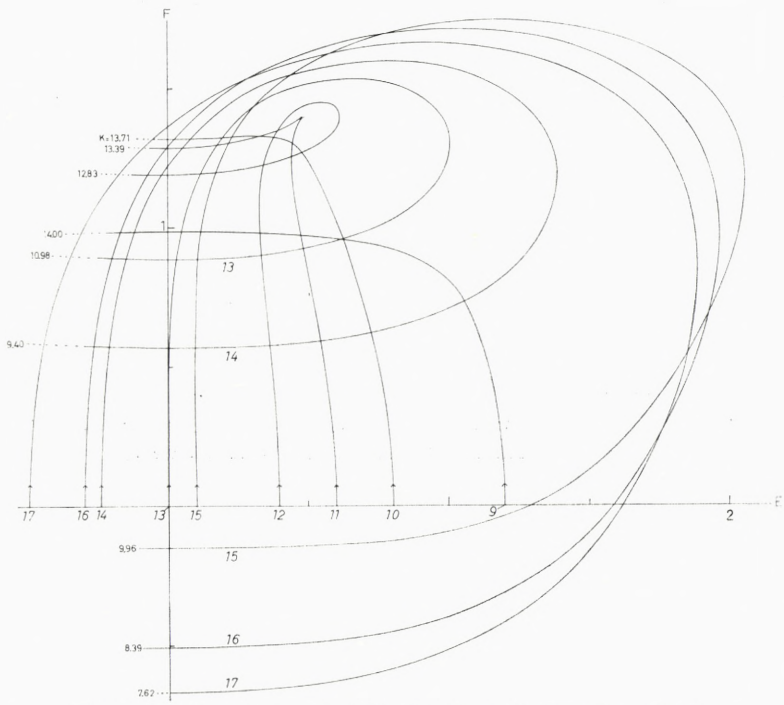

Figure 8 b: Development of the (g) Class, Intermediate Part.

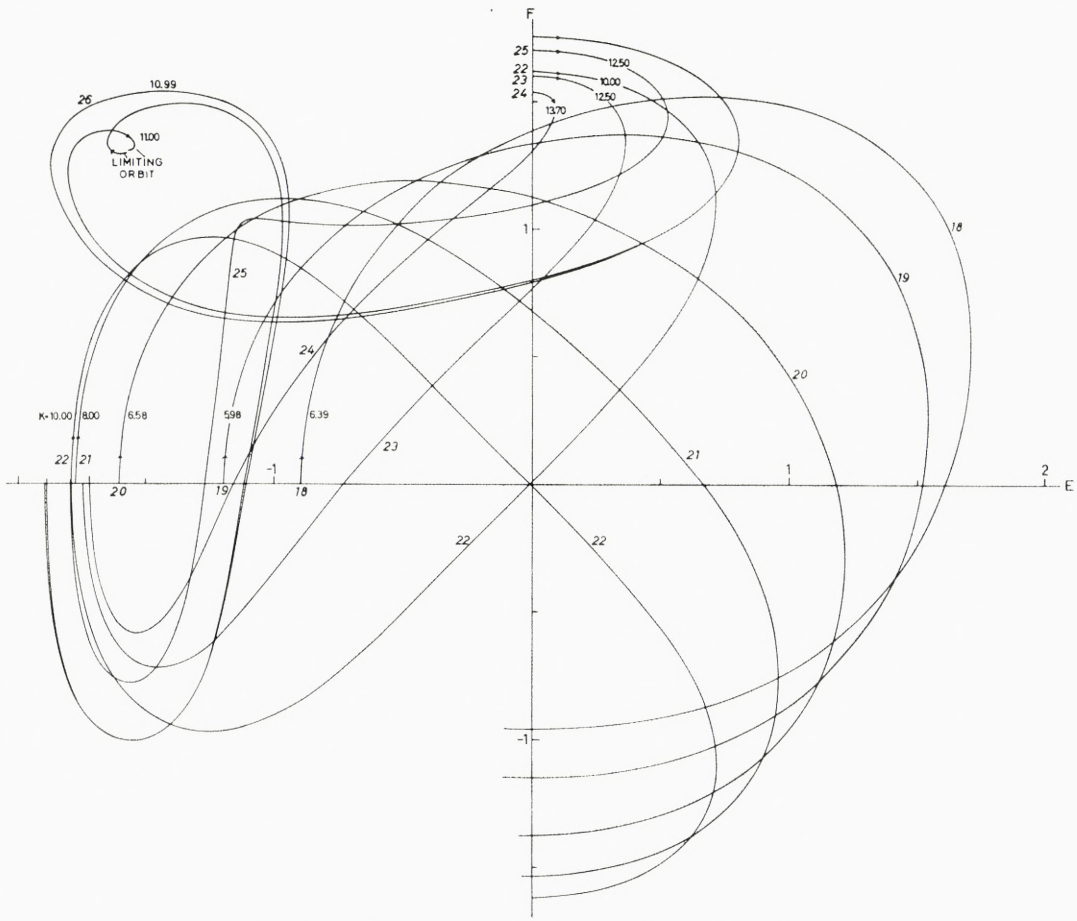

Figure 8 c: Development of the (*g*) Class, Termination.
The curves from 22 onwards are started on the *F*-axis, instead of on the *E*-axis, for clarity of representation and for comparison with Figure 7.

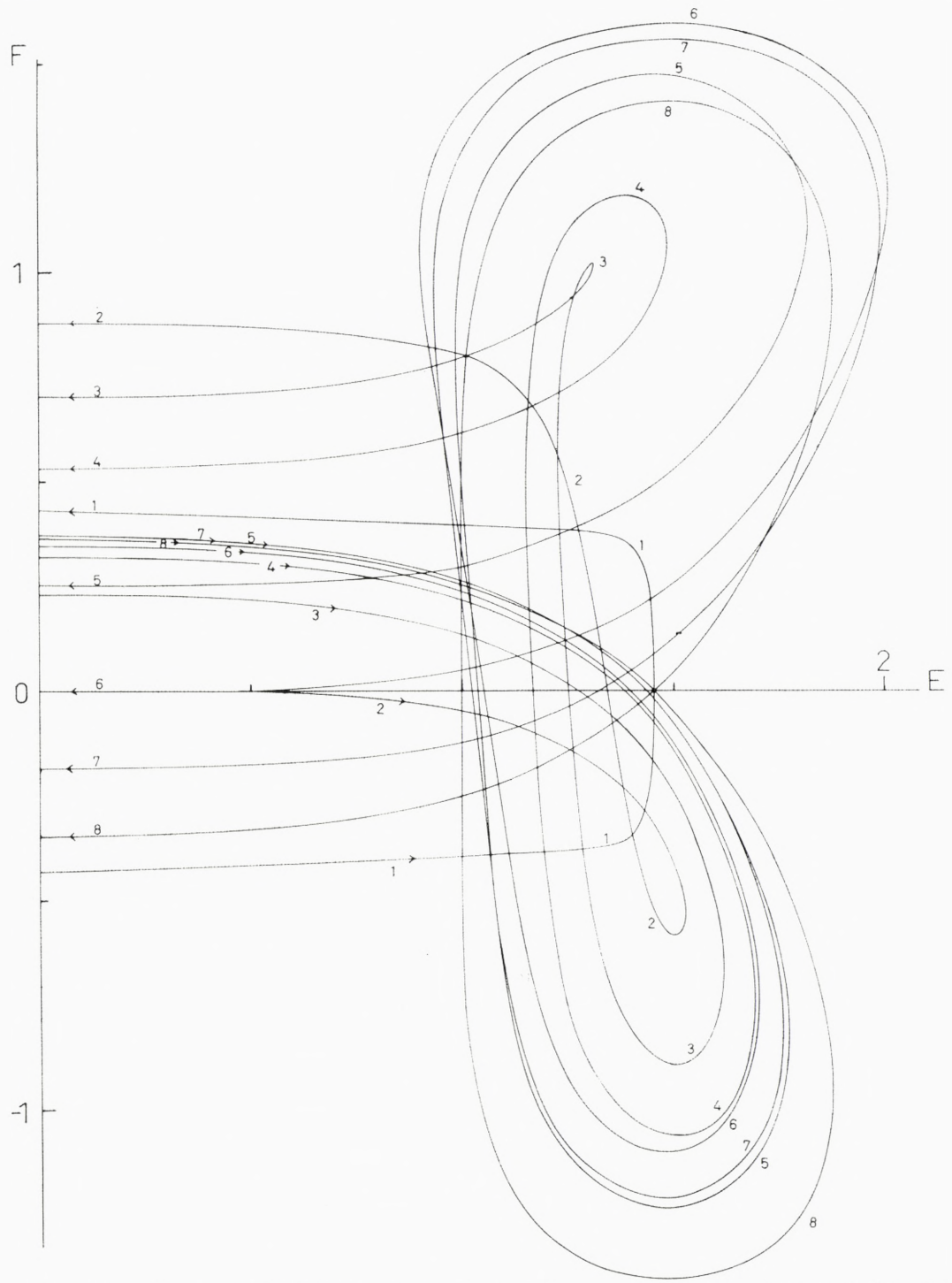

Figure 9: Development of the (δ) Class (a closed group), from maximum K to minimum K. (For the reverse development, take the mirror images about the E-axis).
The curves are numbered consecutively from 1 to 8, and have K-values of 15.428, 13.988, 12.0, 11.0, 10.23, 10.75, 10.30 and 9.915 respectively.

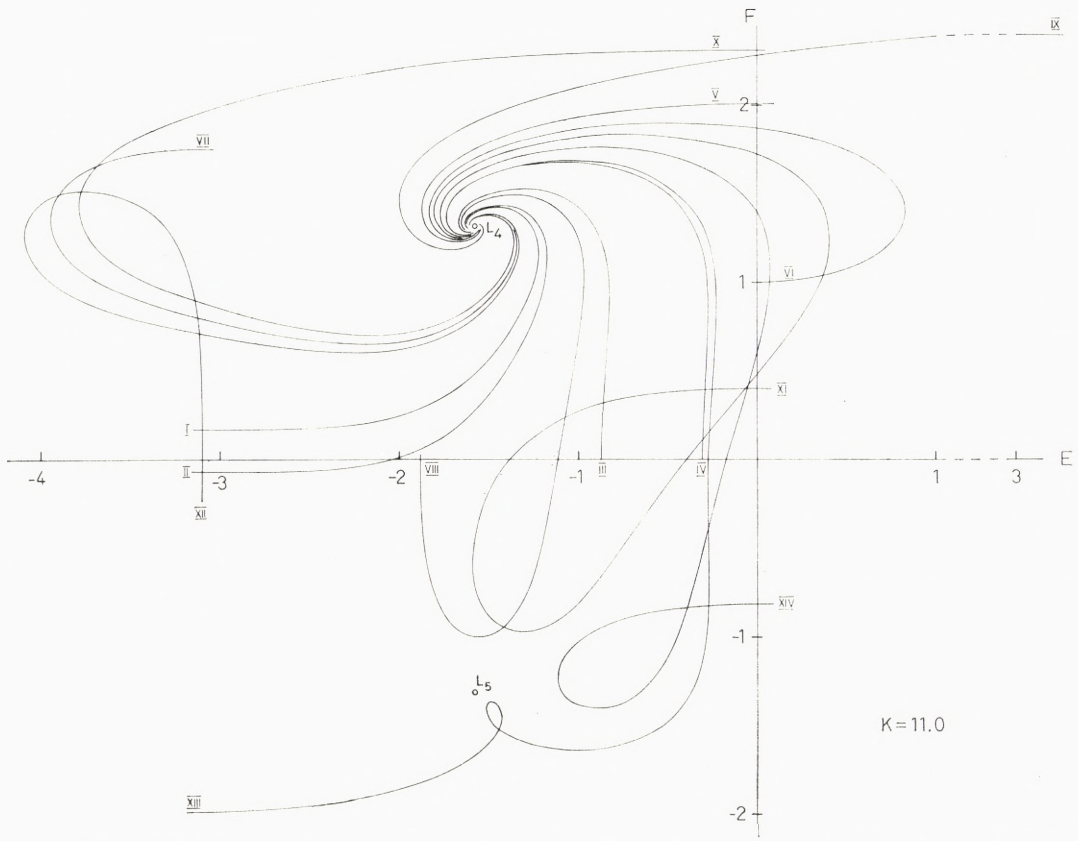

Figure 10: Periodic Limiting Orbits ($K = 11.0$), Symmetric with respect to the E- or F-Axis and Asymptotic to L_4 and L_5. (For complete half-orbits, take the proper mirror images to couple L_4 and L_5). Curves VI, IX–XIV were calculated by C. Wagner.

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THEORY OF FINITE SYSTEMS OF PARTICLES

I. THE GREEN FUNCTION

BY

CLASINE VAN WINTER

København 1964
Kommissionær: Ejnar Munksgaard

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Synopsis

A study is made of the resolvent operator for a system consisting of any finite number of particles. It is assumed that all the forces in the system arise from square-integrable local two-body interactions. The resolvent is considered for complex energies not in the continuous spectrum of the Hamiltonian. It is represented by an integral operator, the kernel of which is called the Green function. In the energy plane cut along the positive real axis, the Green function $G^{(2)}$ for a system of two particles is obtained from an integral equation. Owing to the assumption on the interaction, this equation has a Hilbert-Schmidt kernel. As a result it can be solved by the Fredholm method. With $G^{(2)}$ as a supposedly known quantity, an integral equation for $G^{(3)}$ is constructed which again has a Hilbert-Schmidt kernel, and hence is again soluble. Next the procedure is extended to successively larger systems. For n particles, an integral equation is found from which the Green function $G^{(n)}$ can be obtained once the functions $G^{(2)}, G^{(3)}, \ldots, G^{(n-1)}$ are known. By an induction argument an upper bound is derived for the Schmidt-norm of each successive kernel $K^{(n)}$. This is shown to be finite at every interior point of the energy plane cut along the continuous spectrum of the n-particle Hamiltonian $H^{(n)}$. In the cut plane the Fredholm expressions converge irrespective of the strength of the interaction. The Green function $G^{(n)}$ is regular except for the cut and for possible poles on the negative real axis. These correspond to bound states, the eigenfunctions of $H^{(n)}$ following directly from the residues of $G^{(n)}$. The present method does not give information on the behaviour of the Green function in the neighbourhood of the continuous spectrum. This is the subject of a forthcoming paper on the theory of scattering.

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CONTENTS

1.1. Introduction

This is the first of a series of papers concerned with various general properties of systems of n particles governed by Hamiltonians of the form

$$H'(\boldsymbol{X}) = -\sum_{i=1}^{n} \frac{1}{2\,m_i} \Delta(\boldsymbol{X}_i) + \sum_{i<j} V_{ij}(\boldsymbol{X}_i - \boldsymbol{X}_j). \tag{1.1.1}$$

In eq. (1.1.1) $\boldsymbol{X}_i = (X_{i1}, X_{i2}, X_{i3})$ is the space coordinate of particle i. The three components of $\boldsymbol{X}_i$ range from $-\infty$ to ∞. The system is not enclosed in a finite box, neither are periodic boundary conditions imposed. The symbol Δ stands for the Laplace operator.

The masses of the particles are denoted by m_i. It is assumed that $m_i \neq 0$. The various masses may or may not be equal. The particles are treated as distinguishable. It has been checked that the results of the present paper allow a simple specialization in the case of identical particles, but this point is not pursued here.

In each particular system, the number of particles is kept fixed. No use is made of creation and destruction operators and the techniques associated with these. There are thus distinct problems for $n = 1, 2, 3, \ldots$. Only finite values of n are considered.

The two-body interaction V_{ij} is taken to be real. It is assumed that

$$\int_{-\infty}^{\infty} [V_{ij}(\boldsymbol{X})]^2 d^3\boldsymbol{X} < \infty. \tag{1.1.2}$$

This means, roughly, that at the origin V_{ij} must be less singular than $|\boldsymbol{X}|^{-\frac{3}{2}}$, while at large distances it must tend to zero faster than $|\boldsymbol{X}|^{-\frac{3}{2}}$. The Coulomb interaction is therefore excluded, as are potentials with hard cores.

It is an important point that the relation (1.1.2) does not imply an assumption on the strength of the potential. The results of this and the following papers apply to weak and strong interactions alike, as they are based on methods which go beyond perturbation theory.

In tackling the problem of n particles, the most straightforward starting-point would seem to be the Schrödinger equation

$$H'(\boldsymbol{X})\,\Psi(\boldsymbol{X}) = E\,\Psi(\boldsymbol{X}). \tag{1.1.3}$$

Solving this for Ψ, one would expect that in the case of negative energy only certain discrete values of E are admitted, while for positive E the equation would admit of

a continuum of solutions which satisfy certain outgoing boundary conditions and thereby describe scattering states in which in suitable regions of configuration space the system behaves asymptotically as an assembly of free subsystems. It is of course known that this program works quite well for a system of two particles with spherically symmetric interaction. It must be borne in mind, however, that in this case the success of the method is due to the Schrödinger equation being separable into ordinary differential equations for which methods of solution are readily available. As soon as one passes on to three or more particles, one is always left with partial differential equations. Now, the properties of such equations are quite different from those of ordinary differential equations. As a matter of fact, one does not even have an existence theorem to guarantee that for more-particle systems the desired scattering solutions can actually be found.

It is for this reason that we do not want to go into the question of scattering wave-functions. In the following the Hamiltonian (1.1.1) is considered as an operator which acts on square-integrable functions of $\boldsymbol{X}$, and the n-body problem is approached from the point of view of the theory of Hilbert space. This does not only make it possible to put the formalism on a firm mathematical basis, it also makes available some very powerful computational methods.

One of our principal tools is the resolvent of the Hamiltonian and the Green function G associated with it. As is usual, the resolvent is studied as an analytic function of the energy in the complex plane cut along the real axis from a point M to ∞. At every interior point of the cut plane, we find the Green function for any finite number of particles. To achieve this, we observe first of all that in the cut plane the two-particle Green function $G^{(2)}$ satisfies an integral equation with a Hilbert-Schmidt kernel. Since such an equation is known to be soluble by the methods of the Fredholm theory of integral equations, we can find $G^{(2)}$. It takes the form of a quotient of two series, which are convergent owing to the assumption (1.1.2) that the interactions V_{ij} are square-integrable. The Green function $G^{(2)}$ is now used as a supposedly known quantity in an integral equation for the three-particle function $G^{(3)}$. The point is here that this equation is set up in such a way that it has a Hilbert-Schmidt kernel once again. As a result of this, it can be solved rigorously by the same method as that applied to $G^{(2)}$. Next, $G^{(2)}$ and $G^{(3)}$ are entered into an equation for $G^{(4)}$, and so on. Summarizing, there is an iteration procedure whereby the Green function $G^{(n)}$ for any number of particles can be found once the functions $G^{(m)}$ for $m = 2, 3, \ldots, n-1$ are known. This method of constructing the Green function leads in a natural way to the energies and the wave-functions of bound states. It forms the main contents of the present paper.

In forthcoming papers we shall outline a general theory of scattering, with special emphasis on the channel concept and on sufficient conditions on the interaction to guarantee that a useful scattering formalism can indeed be developed. The next step consists in defining the S-operator, and expressing it in terms of the Green function. The most intricate point to be discussed in this connection concerns the limiting

properties of the Green function as the energy tends to the cut in the complex plane. This limiting behaviour will be shown to be intimately connected with the asymptotic properties of wave-packets at large times, and with the falling-off of the interaction at large distances.

Up to this stage, the formalism is completely general, being capable of describing scattering and reactions among any number of particles or bound fragments. The remaining part of the investigation is devoted to the special case in which both in the distant past and in the remote future the total scattering system is split up into not more than two subsystems. For this case, results will be presented on the analytic properties of scattering amplitudes for fixed momentum transfer, and on dispersion relations. This part of the work also gives information on the asymptotic behaviour of wave-functions for bound states. The last item to be discussed is the scattering of partial waves, for which a new type of resonance formula will be given. The principal feature is here that, along with the well-known Breit-Wigner behaviour in the neighbourhood of an isolated resonance, we find an energy-dependent scattering radius which through a dispersion relation is connected with the absorption.

1.2. The Hamiltonian

1.2.1. Coordinates

In treating the Hamiltonian (1.1.1) it is useful to go over from the coordinates $\boldsymbol{X}$ to new coordinates $\boldsymbol{x}$ so that the energy of the centre-of-mass motion is separated off. This can easily be achieved in various ways, one possibility being the choice(1)

$$\begin{aligned} \boldsymbol{x}_k &= \left(\frac{2\,m_{k+1}}{M_k\,M_{k+1}}\right)^{\frac{1}{2}} \sum_{j=1}^{k} m_j(\boldsymbol{X}_{k+1}-\boldsymbol{X}_j) \quad (k=1,\,2,\,\ldots,\,n-1), \\ \boldsymbol{x}_n &= \frac{\sqrt{2}}{\sqrt{M_n}} \sum_{j=1}^{n} m_j \boldsymbol{X}_j, \\ M_k &= \sum_{j=1}^{k} m_j. \end{aligned} \tag{1.2.1}$$

With this choice of coordinates, the kinetic-energy operator takes the form

$$-\sum_{i=1}^{n} \frac{1}{2\,m_i} \Delta(\boldsymbol{X}_i) = -\sum_{i=1}^{n} \Delta(\boldsymbol{x}_i), \tag{1.2.2}$$

no mixed derivatives appearing. It follows from eq. (1.2.1) that

$$\boldsymbol{X}_i - \boldsymbol{X}_j = \sum_{k=1}^{j-1} c_{ij}^{k} \boldsymbol{x}_k \quad (i<j) \tag{1.2.3}$$

with certain constants c depending on the masses of the particles.

In eq. (1.2.1), $\boldsymbol{x}_n$ is the coordinate of the centre of mass, apart from a scale factor. The coordinates $\boldsymbol{x}_k$ ($k = 1, 2, \ldots, n-1$) describe the internal motion. The Hamiltonian of the internal motion takes the form

$$H'(\boldsymbol{x}) = -\sum_{i=1}^{n-1} \Delta(\boldsymbol{x}_i) + \sum_{i<j} V_{ij}\left(\sum_{k=1}^{j-1} c_{ij}^{k}\, \boldsymbol{x}_k\right). \tag{1.2.4}$$

Here, $\boldsymbol{x}_1$ is proportional to the distance between particles 2 and 1, $\boldsymbol{x}_2$ to the distance between particle 3 and the centre of mass of 2 and 1, and so on. It is easily checked that an alternative system without mixed derivatives in the kinetic energy can be obtained as follows(1). First the system of n particles is split into k subsystems. In each subsystem internal coordinates are introduced according to eq. (1.2.1). Next, a coordinate is used for the distance between the centres of mass of the groups 2 and 1, then a coordinate for the distance between the centres of mass of group 3 and the combined groups 2 and 1, and so on. This takes $n-k$ internal coordinates and $k-1$ relative coordinates between the k groups, so that just one coordinate is left for the centre of mass of the system as a whole. In the following we use all the coordinate systems of this sort, as the need arises.

1.2.2. Self-adjointness

We now want to consider $H'(\boldsymbol{x})$ as an operator in the Hilbert space of square-integrable functions of $\boldsymbol{x}$. This space is denoted by $\mathfrak{L}^2$. In cases of ambiguity we may occasionally write $\mathfrak{L}^2(\boldsymbol{x})$. For the norm and the inner product in $\mathfrak{L}^2$ we use the notations

$$\|f\| = \left[\int |f(\boldsymbol{x})|^2 d\boldsymbol{x}\right]^{\frac{1}{2}}, \quad (g, f) = \int \bar{g}(\boldsymbol{x})\, f(\boldsymbol{x})\, d\boldsymbol{x}. \tag{1.2.5}$$

It is assumed that the reader is familiar with the basic ideas of the theory of Hilbert space, which can be found in the textbooks by ACHIESER and GLASMANN(2), RIESZ and SZ.-NAGY(3), STONE(4), and others.

To get the full benefit of the techniques of Hilbert space, we must define our Hamiltonian more carefully than is implied by eq. (1.2.4). As it stands there, it is too vague, because there does not seem to be a satisfactory criterion for determining the set of functions in $\mathfrak{L}^2$ on which a differential operator can be allowed to act. The way out of this difficulty was indicated by KATO(5) and STUMMEL(6). First the domain of the differential operator was restricted to a dense set in $\mathfrak{L}^2$ consisting of smooth functions which at infinity tend to zero sufficiently rapidly. The operator thus defined is hermitian, but it is not self-adjoint. It was shown, however, that under certain assumptions on the interaction it is essentially self-adjoint, i.e. that it has one and only one self-adjoint extension. It is this self-adjoint extension which we take as our Hamiltonian. It is denoted by H or by $H(\boldsymbol{x})$. The domain of H is denoted by $\mathfrak{D}(H)$.

Let us write the differential operator $H'(\boldsymbol{x})$ as the sum of the kinetic energy and the interaction,

$$H'(\boldsymbol{x}) = H_0'(\boldsymbol{x}) + V(\boldsymbol{x}). \tag{1.2.6}$$

Then, a sufficient condition for essential self-adjointness given by STUMMEL(6) is

$$\left.\begin{aligned} \int_{|\boldsymbol{x}|\leq 1} [V(\boldsymbol{x}-\boldsymbol{y})]^2 \, |\boldsymbol{x}|^{-3n+7-\alpha} \, d^3\boldsymbol{x}_1 \, d^3\boldsymbol{x}_2 \ldots d^3\boldsymbol{x}_{n-1} < C, \\ |\boldsymbol{x}| = (|\boldsymbol{x}_1|^2 + |\boldsymbol{x}_2|^2 + \ldots + |\boldsymbol{x}_{n-1}|^2)^{\frac{1}{2}}, \end{aligned}\right\} \tag{1.2.7}$$

for every $\boldsymbol{y}$, some constant C, and a suitable $\alpha > 0$. This is clearly fulfilled in the present case. For let us take V_{12}. If $n \geq 3$, it satisfies

$$\left.\begin{aligned} &\int_{|\boldsymbol{x}|\leq 1} [V_{12}(c_{12}^1(\boldsymbol{x}_1 - \boldsymbol{y}_1))]^2 \, |\boldsymbol{x}|^{-3n+7-\alpha} \, d^3\boldsymbol{x}_1 \, d^3\boldsymbol{x}_2 \ldots d^3\boldsymbol{x}_{n-1} \\ \leq &\int_{-\infty}^{\infty} [V_{12}(c_{12}^1(\boldsymbol{x}_1 - \boldsymbol{y}_1))]^2 \, d^3\boldsymbol{x}_1 \int_{|\boldsymbol{x}_2|^2 + \ldots + |\boldsymbol{x}_{n-1}|^2 \leq 1} (|\boldsymbol{x}_2|^2 + \ldots + |\boldsymbol{x}_{n-1}|^2)^{-\frac{3}{2}n + \frac{7}{2} - \frac{\alpha}{2}} d^3\boldsymbol{x}_2 \ldots d^3\boldsymbol{x}_{n-1} < C_{12} \end{aligned}\right\} \tag{1.2.8}$$

provided $\alpha < 1$, by virtue of the condition (1.1.2) on V_{ij}. If $n = 2$, the same holds true by an even simpler argument. By a permutation among the coordinates, similar bounds are readily derived for the remaining V_{ij}. The final result then follows from Schwarz's inequality.

It follows from the paper by KATO(5) that $H_0'(\boldsymbol{x})$ has a unique self-adjoint extension H_0. If $\mathfrak{D}(H_0)$ stands for the domain of H_0, it was shown that for every f in $\mathfrak{D}(H_0)$ the quantity Vf belongs to $\mathfrak{L}^2$. It was also shown that

$$\mathfrak{D}(H) = \mathfrak{D}(H_0), \quad H = H_0 + V. \tag{1.2.9}$$

1.2.3. The resolvent

The importance of the Hamiltonian being self-adjoint derives from the fact that this implies that it has a resolvent and a spectral resolution. To the latter concept we come back later. Our first object is the resolvent $R(\lambda)$,

$$R(\lambda) = (H - \lambda)^{-1}, \tag{1.2.10}$$

where λ is a complex number. The resolvent is defined for the set of points λ for which it exists and is a bounded linear operator with domain $\mathfrak{L}^2$. This certainly includes all non-real λ (ACHIESER and GLASMANN(2) section 43). It satisfies (ref.(2) section 44)

$$R(\lambda) - R(\mu) = (\lambda - \mu) \, R(\lambda) \, R(\mu) = (\lambda - \mu) \, R(\mu) \, R(\lambda), \tag{1.2.11}$$

$$R^*(\lambda) = R(\bar{\lambda}), \tag{1.2.12}$$

where the asterisk denotes the adjoint of an operator, and the bar the complex conjugate of a number.

Since $R(\lambda)f$ belongs to $\mathfrak{D}(H)$ whenever f belongs to $\mathfrak{L}^2$, eq. (1.2.9) shows that $H_0R(\lambda)$ and $VR(\lambda)$ are bounded operators. It is therefore justified to write

$$VR(\lambda) = (\lambda - H_0)R(\lambda) + 1. \tag{1.2.13}$$

Applying $R_0(\lambda)$, the resolvent of H_0, to both sides yields the equation

$$R_0(\lambda)VR(\lambda) = R_0(\lambda) - R(\lambda). \tag{1.2.14}$$

It is the main purpose of the present paper to show that in the case under investigation the resolvent is an integral operator,

$$R(\lambda)f(\boldsymbol{x}) = \int G(\boldsymbol{x}, \boldsymbol{y}; \lambda) f(\boldsymbol{y})\, d\boldsymbol{y} \tag{1.2.15}$$

for every f in $\mathfrak{L}^2$ and almost every $\boldsymbol{x}$, and to determine the kernel G. The function G is called the Green function. This agrees with the Green-function concept as used by COURANT and HILBERT(7), and more recently by TITCHMARSH(8). Loosely speaking, G satisfies

$$(H - \lambda)\, G(\boldsymbol{x}, \boldsymbol{y}; \lambda) = \delta(\boldsymbol{x} - \boldsymbol{y}). \tag{1.2.16}$$

In finding the Green function $G^{(n)}$ for n particles, i.e. $(3n-3)$-dimensional $\boldsymbol{x}$ and $\boldsymbol{y}$ $(n = 2, 3, \ldots)$, our starting-point is the fact that in the case of no interaction it is known to exist and to have the form (TITCHMARSH(8) section 13.7)

$$G_0^{(n)}(\boldsymbol{x}, \boldsymbol{y}; \lambda) = \frac{i}{4}\left[\frac{\sqrt{\lambda}}{2\pi|\boldsymbol{x}-\boldsymbol{y}|}\right]^{\frac{3}{2}n-\frac{5}{2}} H^{(1)}_{\frac{3}{2}n-\frac{5}{2}}(\sqrt{\lambda}\,|\boldsymbol{x}-\boldsymbol{y}|) \quad (n = 2, 3, \ldots), \tag{1.2.17}$$

$H^{(1)}$ being the Hankel function of the first kind. If $n = 2$, this reduces to

$$G_0^{(2)}(\boldsymbol{x}, \boldsymbol{y}; \lambda) = \frac{1}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\, e^{i\sqrt{\lambda}|\boldsymbol{x}-\boldsymbol{y}|}. \tag{1.2.18}$$

Here and in the following, λ must always be restricted to

$$0 < \arg\lambda < 2\pi, \quad \operatorname{Im}\sqrt{\lambda} > 0. \tag{1.2.19}$$

1.3. The Green function for two particles

1.3.1. Method of construction

In determining the Green function, it is useful to start with two particles. The methods to be developed for this case are shown later to apply to larger numbers of particles without essential modification. Also, the results are required for the general n-particle problem, as our approach to this involves an iteration procedure.

For two particles, the relative motion depends on a three-dimensional vector $\boldsymbol{x}$. The interaction consists of a single term which, for simplicity, is denoted by $V(\boldsymbol{x})$. In the present section, all superscripts referring to the number of particles are dropped.

If f is any function in $\mathfrak{L}^2$, the functions

$$h(\boldsymbol{x};\lambda) = R(\lambda)f(\boldsymbol{x}), \quad h_0(\boldsymbol{x};\lambda) = R_0(\lambda)f(\boldsymbol{x}) = \int G_0(\boldsymbol{x},\boldsymbol{y};\lambda)f(\boldsymbol{y})\,d\boldsymbol{y} \tag{1.3.1}$$

obviously belong to $\mathfrak{L}^2$. From the resolvent equation (1.2.14) together with our knowledge of $R_0(\lambda)$ contained in eqs. (1.2.15) and (1.2.18), it follows that

$$h(\boldsymbol{x};\lambda) = h_0(\boldsymbol{x};\lambda) - \frac{1}{4\pi}\int \frac{1}{|\boldsymbol{x}-\boldsymbol{y}|}\, e^{i\sqrt{\lambda}|\boldsymbol{x}-\boldsymbol{y}|}\, V(\boldsymbol{y})\, h(\boldsymbol{y};\lambda)\,d\boldsymbol{y}. \tag{1.3.2}$$

Denoting the kernel of this integral equation by K,

$$K(\boldsymbol{x},\boldsymbol{y};\lambda) = -\frac{1}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\, e^{i\sqrt{\lambda}|\boldsymbol{x}-\boldsymbol{y}|}\, V(\boldsymbol{y}), \tag{1.3.3}$$

we observe the important fact that, if $\operatorname{Im}\sqrt{\lambda} > 0$,

$$\left.\begin{aligned} \iint |K(\boldsymbol{x},\boldsymbol{y};\lambda)|^2 d\boldsymbol{x}\,d\boldsymbol{y} &= \frac{1}{16\pi^2}\int [V(\boldsymbol{y})]^2 d\boldsymbol{y} \int \frac{1}{|\boldsymbol{x}-\boldsymbol{y}|^2}\, |e^{i\sqrt{\lambda}|\boldsymbol{x}-\boldsymbol{y}|}|^2 d\boldsymbol{x} \\ &= \frac{1}{8\pi \operatorname{Im}\sqrt{\lambda}} \int [V(\boldsymbol{y})]^2 d\boldsymbol{y} < \infty, \end{aligned}\right\} \tag{1.3.4}$$

owing to the assumption that V is square-integrable, eq. (1.1.2). Kernels which are square-integrable in the sense of eq. (1.3.4) are known as completely continuous, or Hilbert-Schmidt kernels. In the following we denote the set of all Hilbert-Schmidt kernels by $\mathfrak{L}^2$ or $\mathfrak{L}^2(\boldsymbol{x})$.

The importance of this set derives from the fact that for integral equations with kernels in $\mathfrak{L}^2$ the solution is known. As a matter of fact, it follows from the works of CARLEMAN(9), SMITHIES(10), and MICHLIN(11) that with minor alterations the Fredholm theory can be made applicable to these equations (see also SMITHIES(12) ch. VI, and ZAANEN(13) ch. 9, section 17).

To make this clear, let us define

$$\Delta(\lambda) = \sum_{p=0}^{\infty} \Delta_p(\lambda), \quad D(\boldsymbol{x},\boldsymbol{y};\lambda) = \sum_{p=0}^{\infty} D_p(\boldsymbol{x},\boldsymbol{y};\lambda), \tag{1.3.5}$$

where

$$\left.\begin{aligned} \Delta_0(\lambda) &= 1, \quad \Delta_1(\lambda) = 0, \quad D_0(\boldsymbol{x},\boldsymbol{y};\lambda) = K(\boldsymbol{x},\boldsymbol{y};\lambda), \\ \Delta_p(\lambda) &= -\frac{1}{p}\iint K(\boldsymbol{x},\boldsymbol{y};\lambda)\, D_{p-2}(\boldsymbol{y},\boldsymbol{x};\lambda)\,d\boldsymbol{x}\,d\boldsymbol{y} \quad (p \geq 2), \\ D_p(\boldsymbol{x},\boldsymbol{y};\lambda) &= \Delta_p(\lambda)\, K(\boldsymbol{x},\boldsymbol{y};\lambda) + \int K(\boldsymbol{x},\boldsymbol{z};\lambda) D_{p-1}(\boldsymbol{z},\boldsymbol{y};\lambda)\,d\boldsymbol{z} \quad (p \geq 1). \end{aligned}\right\} \tag{1.3.6}$$

It is then shown in the above references that if h_0 belongs to $\mathfrak{L}^2$ and λ is such that $\Delta(\lambda) \neq 0$, the equation (1.3.2) with the kernel (1.3.3) has one and only one solution in $\mathfrak{L}^2$, which takes the form

$$h(\boldsymbol{x};\lambda) = h_0(\boldsymbol{x};\lambda) + \frac{1}{\Delta(\lambda)} \int D(\boldsymbol{x},\boldsymbol{y};\lambda)\, h_0(\boldsymbol{y};\lambda)\, d\boldsymbol{y}. \tag{1.3.7}$$

If for any kernel in $\mathfrak{L}^2$ we denote the $\mathfrak{L}^2$-norm by

$$|K| = \left[\iint |K(\boldsymbol{x},\boldsymbol{y})|^2\, d\boldsymbol{x}\, d\boldsymbol{y}\right]^{\frac{1}{2}}, \tag{1.3.8}$$

we have

$$|\Delta_p(\lambda)| \leq (e/p)^{\frac{1}{2}p} |K(\lambda)|^p \quad (p \geq 1). \tag{1.3.9}$$

This clearly shows that the series for Δ is convergent for all values of λ for which $|K(\lambda)|$ is finite, i.e. for all λ with $\operatorname{Im} \sqrt{\lambda} > 0$ (cf. eq. (1.3.4)). It is to be noted that the convergence properties are independent of the absolute magnitude of the interaction V. As for the series for D, it is known that each kernel D_p belongs to $\mathfrak{L}^2$,

$$|D_p(\lambda)| \leq \sqrt{e}\, (e/p)^{\frac{1}{2}p} |K(\lambda)|^{p+1} \quad (p \geq 1). \tag{1.3.10}$$

From this it follows that D also belongs to $\mathfrak{L}^2$, and that the series for D converges in mean square.

In view of the expressions (1.3.1) for h and h_0, equation (1.3.7) very strongly suggests that

$$R(\lambda) f(\boldsymbol{x}) = \int G_0(\boldsymbol{x},\boldsymbol{z};\lambda) f(\boldsymbol{z})\, d\boldsymbol{z} + \frac{1}{\Delta(\lambda)} \int f(\boldsymbol{z})\, d\boldsymbol{z} \int D(\boldsymbol{x},\boldsymbol{y};\lambda)\, G_0(\boldsymbol{y},\boldsymbol{z};\lambda)\, d\boldsymbol{y}. \tag{1.3.11}$$

If we can justify this, we have thereby established that the resolvent is an integral operator, and we have found an expression for its kernel, the Green function G,

$$G(\boldsymbol{x},\boldsymbol{z};\lambda) = G_0(\boldsymbol{x},\boldsymbol{z};\lambda) + \frac{1}{\Delta(\lambda)} \int D(\boldsymbol{x},\boldsymbol{y};\lambda)\, G_0(\boldsymbol{y},\boldsymbol{z};\lambda)\, d\boldsymbol{y}. \tag{1.3.12}$$

The distinction between eqs. (1.3.7) and (1.3.11) is that in eq. (1.3.11) the integration with respect to $\boldsymbol{y}$ is performed first, while in eq. (1.3.7) this is done last. The problem is therefore to prove that in eq. (1.3.11) the integrations may be interchanged. To show this, let us first take any f and g in $\mathfrak{L}^2$. We know from eq. (1.2.12) that

$$(g, R(\lambda) f) = (R^*(\lambda) g, f) = (R(\bar{\lambda}) g, f), \tag{1.3.13}$$

so that

$$\left.\begin{aligned} \int \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \int G_0(\boldsymbol{x},\boldsymbol{y};\lambda) f(\boldsymbol{y})\, d\boldsymbol{y} &= \int f(\boldsymbol{y})\, d\boldsymbol{y} \int \overline{G}_0(\boldsymbol{y},\boldsymbol{x};\bar{\lambda})\, \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \\ &= \int f(\boldsymbol{y})\, d\boldsymbol{y} \int G_0(\boldsymbol{x},\boldsymbol{y};\lambda)\, \bar{g}(\boldsymbol{x})\, d\boldsymbol{x}, \end{aligned}\right\} \tag{1.3.14}$$

where use has been made of the symmetry properties

$$G_0(\boldsymbol{x}, \boldsymbol{y}; \lambda) = G_0(\boldsymbol{y}, \boldsymbol{x}; \lambda), \tag{1.3.15}$$

$$\overline{G}_0(\boldsymbol{x}, \boldsymbol{y}; \lambda) = G_0(\boldsymbol{x}, \boldsymbol{y}; \bar{\lambda}), \tag{1.3.16}$$

which follow directly from the known expression for G_0.

Equation (1.3.14) shows that with straightforward functions f and g the order of integration may indeed be inverted. For the more complicated case presented by eq. (1.3.11), we note that according to Fubini's theorem (BURKILL(14) section 5.4) $D(\boldsymbol{x}, \boldsymbol{y}; \lambda)$ is square-integrable with respect to $\boldsymbol{y}$ for almost every $\boldsymbol{x}$. The integrations may therefore be interchanged also in this case, for almost every $\boldsymbol{x}$. From this observation the desired equation (1.3.12) for the Green function now follows, as a set of points of measure zero is immaterial in a Hilbert-space formalism.

1.3.2. Symmetry

It is clear from the method of construction that

$$\overline{G}(\boldsymbol{x}, \boldsymbol{y}; \lambda) = G(\boldsymbol{x}, \boldsymbol{y}; \bar{\lambda}). \tag{1.3.17}$$

We now want to show that

$$G(\boldsymbol{x}, \boldsymbol{y}; \lambda) = G(\boldsymbol{y}, \boldsymbol{x}; \lambda). \tag{1.3.18}$$

This is already known to be true for the term G_0 appearing in G. Let us denote the second term in eq. (1.3.12) by F,

$$F(\boldsymbol{x}, \boldsymbol{y}; \lambda) = \frac{1}{\Delta(\lambda)} \int D(\boldsymbol{x}, \boldsymbol{z}; \lambda)\, G_0(\boldsymbol{z}, \boldsymbol{y}; \lambda)\, d\boldsymbol{z}. \tag{1.3.19}$$

Then it is obvious that F belongs to $\mathfrak{L}^2$, since D belongs to $\mathfrak{L}^2$ and G_0 represents a bounded operator. Therefore,

$$\left.\begin{aligned} &\iint |\, \bar{g}(\boldsymbol{x})\, F(\boldsymbol{x}, \boldsymbol{y}; \lambda)\, f(\boldsymbol{y})\, |\, d\boldsymbol{x}\, d\boldsymbol{y} \\ &\leq \left[\iint |\, F(\boldsymbol{x}, \boldsymbol{y}; \lambda)\, |^2 d\boldsymbol{x}\, d\boldsymbol{y} \int |\, g(\boldsymbol{x}')\, |^2 d\boldsymbol{x}' \int |\, f(\boldsymbol{y}')\, |^2 d\boldsymbol{y}' \right]^{\frac{1}{2}} < \infty, \end{aligned}\right\} \tag{1.3.20}$$

so that by Fubini's theorem

$$\int \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \int F(\boldsymbol{x}, \boldsymbol{y}; \lambda)\, f(\boldsymbol{y})\, d\boldsymbol{y} = \int f(\boldsymbol{y})\, d\boldsymbol{y} \int F(\boldsymbol{x}, \boldsymbol{y}; \lambda)\, \bar{g}(\boldsymbol{x})\, d\boldsymbol{x}. \tag{1.3.21}$$

But from eq. (1.3.13) and eqs. (1.3.16) and (1.3.17) we have

$$\left.\begin{aligned} \int \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \int F(\boldsymbol{x}, \boldsymbol{y}; \lambda)\, f(\boldsymbol{y})\, d\boldsymbol{y} &= \int f(\boldsymbol{y})\, d\boldsymbol{y} \int \overline{F}(\boldsymbol{y}, \boldsymbol{x}; \bar{\lambda})\, \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \\ &= \int f(\boldsymbol{y})\, d\boldsymbol{y} \int F(\boldsymbol{y}, \boldsymbol{x}; \lambda)\, \bar{g}(\boldsymbol{x})\, d\boldsymbol{x}. \end{aligned}\right\} \tag{1.3.22}$$

In view of the arbitrariness of f and g in $\mathfrak{L}^2$ and the fact that F belongs to $\mathfrak{L}^2$, this implies that

$$F(\boldsymbol{x}, \boldsymbol{y}; \lambda) = F(\boldsymbol{y}, \boldsymbol{x}; \lambda), \tag{1.3.23}$$

and from this we get eq. (1.3.18). In this argument use is made of the known interchangeability of the integrals to establish the symmetry. Now that we have the symmetry of the Green function, it follows, as in eq. (1.3.14), that

$$\int \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \int G(\boldsymbol{x}, \boldsymbol{y}; \lambda) f(\boldsymbol{y})\, d\boldsymbol{y} = \int f(\boldsymbol{y})\, d\boldsymbol{y} \int G(\boldsymbol{x}, \boldsymbol{y}; \lambda)\, \bar{g}(\boldsymbol{x})\, d\boldsymbol{x}. \tag{1.3.24}$$

According to the resolvent equation (1.2.14), the Green function satisfies

$$\int G(\boldsymbol{x}, \boldsymbol{z}; \lambda) f(\boldsymbol{z})\, d\boldsymbol{z} = \int G_0(\boldsymbol{x}, \boldsymbol{z}; \lambda) f(\boldsymbol{z})\, d\boldsymbol{z} - \int G_0(\boldsymbol{x}, \boldsymbol{y}; \lambda) V(\boldsymbol{y})\, d\boldsymbol{y} \int G(\boldsymbol{y}, \boldsymbol{z}; \lambda) f(\boldsymbol{z})\, d\boldsymbol{z}. \tag{1.3.25}$$

If it is now recalled that $G_0 V$ belongs to $\mathfrak{L}^2$, and if eq. (1.3.24) is taken into account, the argument used in the previous section to get eq. (1.3.11) shows that in eq. (1.3.25) the integrations with respect to $\boldsymbol{y}$ and $\boldsymbol{z}$ may be interchanged. This yields the kernel

$$-\int G_0(\boldsymbol{x}, \boldsymbol{y}; \lambda) V(\boldsymbol{y})\, G(\boldsymbol{y}, \boldsymbol{z}; \lambda)\, d\boldsymbol{y}, \tag{1.3.26}$$

which obviously belongs to $\mathfrak{L}^2$. Likewise, the second term on the right-hand side of eq. (1.3.12) belongs to $\mathfrak{L}^2$. Since both kernels give the same result when multiplied by $f(\boldsymbol{z})$ and integrated over $\boldsymbol{z}$, the two kernels must be equal for almost every $\boldsymbol{x}$ and $\boldsymbol{z}$. In other words, along with eq. (1.3.12) we have

$$G(\boldsymbol{x}, \boldsymbol{z}; \lambda) = G_0(\boldsymbol{x}, \boldsymbol{z}; \lambda) - \int G_0(\boldsymbol{x}, \boldsymbol{y}; \lambda) V(\boldsymbol{y})\, G(\boldsymbol{y}, \boldsymbol{z}; \lambda)\, d\boldsymbol{y}. \tag{1.3.27}$$

1.3.3. Analytic properties

We now pass on to a study of the analytic properties of $D(\boldsymbol{x}, \boldsymbol{y}; \lambda)$ and $\Delta(\lambda)$ considered as functions of λ. To this end, we first observe that, according to eqs. (1.2.11) and (1.2.12),

$$\left.\begin{aligned} \|R(\lambda) f\|^2 &= (R(\lambda) f, R(\lambda) f) = (f, R(\bar{\lambda}) R(\lambda) f) \\ &= \frac{1}{\lambda - \bar{\lambda}} [(f, R(\lambda) f) - (f, R(\bar{\lambda}) f)] \leq \frac{1}{|\operatorname{Im} \lambda|} \|f\|\, \|R(\lambda) f\|. \end{aligned}\right\} \tag{1.3.28}$$

Denoting the norm of $R(\lambda)$ by $\|R(\lambda)\|$, we thus obtain

$$\|R(\lambda)\| \leq \frac{1}{|\operatorname{Im} \lambda|}. \tag{1.3.29}$$

This is a useful bound for non-real λ. However, if there is no interaction the resolvent does not only exist off the real axis, it also exists, and is bounded, for negative real λ. As a matter of fact, in the case of two particles we have

$$\left.\begin{aligned}\int d\boldsymbol{x}\left|\int \frac{e^{i\sqrt{\lambda}|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi|\boldsymbol{x}-\boldsymbol{y}|} f(\boldsymbol{y})\,d\boldsymbol{y}\right|^2 &\le \iiint \frac{e^{-\mathrm{Im}\sqrt{\lambda}|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\,\frac{e^{-\mathrm{Im}\sqrt{\lambda}|\boldsymbol{x}-\boldsymbol{z}|}}{4\pi|\boldsymbol{x}-\boldsymbol{z}|}\,|f(\boldsymbol{y})|\,|f(\boldsymbol{z})|\,d\boldsymbol{x}\,d\boldsymbol{y}\,d\boldsymbol{z}\\ &= \iiint \frac{e^{-\mathrm{Im}\sqrt{\lambda}|\boldsymbol{y}'|}}{4\pi|\boldsymbol{y}'|}\,\frac{e^{-\mathrm{Im}\sqrt{\lambda}|\boldsymbol{z}'|}}{4\pi|\boldsymbol{z}'|}\,|f(\boldsymbol{x}-\boldsymbol{y}')|\,|f(\boldsymbol{x}-\boldsymbol{z}')|\,d\boldsymbol{x}\,d\boldsymbol{y}'\,d\boldsymbol{z}'\\ &\le \left[\int \frac{e^{-\mathrm{Im}\sqrt{\lambda}|\boldsymbol{y}|}}{4\pi|\boldsymbol{y}|}\,d\boldsymbol{y}\right]^2 ||f||^2 = \frac{1}{(\mathrm{Im}\sqrt{\lambda})^4}\,||f||^2,\end{aligned}\right\} \tag{1.3.30}$$

so that here

$$||R_0(\lambda)|| \le \frac{1}{(\mathrm{Im}\sqrt{\lambda})^2}\,. \tag{1.3.31}$$

As we shall see later, this inequality applies also to larger numbers of particles.

Another relation which follows directly from eq. (1.2.11) is

$$\frac{d}{d\lambda}(g, R(\lambda)f) = (g, R(\lambda)R(\lambda)f). \tag{1.3.32}$$

Extending this to higher derivatives yields the power series

$$(g, R(\lambda)f) = \sum_{p=0}^{\infty}(\lambda-\mu)^p(g, [R(\mu)]^{p+1}f), \tag{1.3.33}$$

which converges provided

$$|\lambda-\mu|\;||R(\mu)|| < 1, \tag{1.3.34}$$

and so certainly when λ is inside the circle with centre μ which is tangent to the real axis, by eq. (1.3.29). Clearly the left-hand side of eq. (1.3.33) is regular inside this circle, and by letting μ take all non-real values, it follows that it is in fact regular for all non-real λ. With the additional information supplied by the bound (1.3.31) for $||R_0(\lambda)||$, it follows that $(g, R_0(\lambda)f)$ is even regular in a larger region, viz. inside the λ-plane cut along the real axis from 0 to ∞.

For the purpose of our investigation of the functions $D(\boldsymbol{x}, \boldsymbol{y}; \lambda)$ and $\Delta(\lambda)$, the foregoing is now extended to functions of the form $(g, VR_0(\lambda)f)$. The point is here that in general Vg does not belong to $\mathfrak{L}^2$. However, let us choose a sequence g_N in $\mathfrak{L}^2$ such that Vg_N belongs to $\mathfrak{L}^2$ for every N, while g_N tends to g in mean square,

$$\lim_{N\to\infty} ||g_N - g|| = 0. \tag{1.3.35}$$

Such a sequence certainly exists. For since $\mathfrak{D}(H_0)$ is dense in $\mathfrak{L}^2$, every g in $\mathfrak{L}^2$ can be approximated in mean square by a sequence in $\mathfrak{D}(H_0)$. And if g_N is in $\mathfrak{D}(H_0)$, the function Vg_N belongs to $\mathfrak{L}^2$, by eq. (1.2.9).

For every N, the result (1.3.33) yields the expansion

$$(Vg_N, R_0(\lambda)f) = \sum_{p=0}^{\infty}(\lambda-\mu)^p(Vg_N, [R_0(\mu)]^{p+1}f). \tag{1.3.36}$$

Use can now be made of the relation

$$(Vg_N, R_0(\lambda)f) = (g_N, VR_0(\lambda)f) \tag{1.3.37}$$

and of the fact that $VR_0(\lambda)$ is a bounded operator, again by eq. (1.2.9). Since $VR_0(\lambda)$ is bounded, it follows from eq. (1.3.35) that

$$\lim_{N\to\infty}(g_N, VR_0(\lambda)f) = (g, VR_0(\lambda)f). \tag{1.3.38}$$

Hence, both members of eq. (1.3.37) tend to a limit as N tends to ∞, and so does each term on the right-hand side of eq. (1.3.36). Also, the convergence of the series in eq. (1.3.36) is uniform with respect to N whenever λ satisfies eq. (1.3.34). Then the sum of the limits equals the limit of the sum. Summarizing, we thus get the result

$$(g, VR_0(\lambda)f) = \sum_{p=0}^{\infty}(\lambda-\mu)^p (g, V[R_0(\mu)]^{p+1}f), \tag{1.3.39}$$

which shows that $(g, VR_0(\lambda)f)$ is regular in the same region as $(g, R_0(\lambda)f)$.

The argument is now easily extended to the case in which g itself is a function of λ, and is of the form $R_0(\bar{\lambda})h$ or $R_0(\bar{\lambda})Vh$. By the previous result and eq. (1.2.12), each term of the series in eq. (1.3.39) is still regular, though more complicated than with λ-independent g. The series converges uniformly with respect to λ in any closed region in which λ satisfies eq. (1.3.34). From this it follows as before that the sum is regular in the λ-plane cut from 0 to ∞. The same applies to general expressions of the form

$$(g, R_0(\lambda)[VR_0(\lambda)]^q f),\ (g, [VR_0(\lambda)]^q f)\ (q = 0,1,2,\ldots). \tag{1.3.40}$$

Now by writing out the quantity

$$\int \bar{g}(\boldsymbol{x})\,d\boldsymbol{x}\int D_p(\boldsymbol{x},\boldsymbol{y};\lambda)\,d\boldsymbol{y}\int G_0(\boldsymbol{y},\boldsymbol{z};\lambda)f(\boldsymbol{z})\,d\boldsymbol{z} \tag{1.3.41}$$

with the help of eq. (1.3.6), it can be reduced to functions $\Delta_q(\lambda)$ and expressions of the first form (1.3.40). The latter being regular in a certain region of the λ-plane, we now turn to the functions $\Delta_q(\lambda)$. Let us take in particular

$$\Delta_2(\lambda) = -\frac{1}{2}\iint [G_0(\boldsymbol{x},\boldsymbol{y};\lambda)]^2 V(\boldsymbol{x})V(\boldsymbol{y})\,d\boldsymbol{x}\,d\boldsymbol{y}. \tag{1.3.42}$$

Here we require the fact that the kernel G_0V belongs to $\mathfrak{L}^2$. By virtue of this, it can be developed in mean square in terms of a complete orthonormal set $f_q(\boldsymbol{x})$ $(q = 1, 2, \ldots)$ in $\mathfrak{L}^2$, according to

$$\left.\begin{aligned} -G_0(\boldsymbol{x},\boldsymbol{y};\lambda)V(\boldsymbol{y}) &= \sum_{q,r=1}^{\infty} K_{qr}(\lambda) f_q(\boldsymbol{x})\bar{f}_r(\boldsymbol{y}), \\ K_{qr}(\lambda) &= -\iint \bar{f}_q(\boldsymbol{x})G_0(\boldsymbol{x},\boldsymbol{y};\lambda)V(\boldsymbol{y})f_r(\boldsymbol{y})\,d\boldsymbol{x}\,d\boldsymbol{y}. \end{aligned}\right\} \tag{1.3.43}$$

In terms of the coefficients K_{qr}, the $\mathfrak{L}^2$-norm of $G_0 V$ equals

$$|G_0(\lambda)V| = \left[\sum_{q,r=1}^{\infty} |K_{qr}(\lambda)|^2\right]^{\frac{1}{2}}. \tag{1.3.44}$$

The function Δ_2 takes the form

$$\Delta_2(\lambda) = -\frac{1}{2}\sum_{q,r=1}^{\infty} K_{qr}(\lambda) K_{rq}(\lambda). \tag{1.3.45}$$

Equation (1.3.44) implies the convergence of the series on the right-hand side. In view of this, Schwarz's inequality shows that the series for $\Delta_2(\lambda)$ is absolutely convergent, its partial sums not exceeding $|G_0(\lambda)V|^2/2$.

If we now consider in particular

$$\Delta_2^N(\lambda) = -\frac{1}{2}\sum_{q,r=1}^{N} K_{qr}(\lambda) K_{rq}(\lambda), \tag{1.3.46}$$

we know from the foregoing that it is regular in the λ-plane cut along the real axis from 0 to ∞, for the sum is confined to a finite number of terms, and each term is regular by our previous results. In other words, each function of the sequence $\Delta_2^N(\lambda)$ $(N = 1, 2, \ldots)$ is regular. The sequence tends to $\Delta_2(\lambda)$ as N tends to ∞, and it is bounded uniformly in N in any region in which $|G_0(\lambda)V|$ is bounded, i.e. in any region in which $\operatorname{Im}\sqrt{\lambda} \geq \varepsilon > 0$ (cf. eq. (1.3.4)). From this it follows by Vitali's theorem (TITCHMARSH(15) section 5. 21) that $\Delta_2(\lambda)$ is regular in the region $\operatorname{Im}\sqrt{\lambda} > 0$.

Combining various arguments presented in the foregoing we now easily see that each function $\Delta_p(\lambda)$ is regular in the region $\operatorname{Im}\sqrt{\lambda} > 0$, and that the same applies to the functions

$$\int \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \int f(\boldsymbol{z})\, d\boldsymbol{z} \int D_p(\boldsymbol{x}, \boldsymbol{y}; \lambda)\, G_0(\boldsymbol{y}, \boldsymbol{z}; \lambda)\, d\boldsymbol{y}. \tag{1.3.47}$$

Taking into account the convergence properties of the series for $\Delta(\lambda)$ implied by eq. (1.3.9), a second application of Vitali's theorem yields the result that $\Delta(\lambda)$ is regular in the region $\operatorname{Im}\sqrt{\lambda} > 0$. The same applies to the sum with respect to p of all expressions (1.3.47). If we now recall the expression (1.3.12) for the Green function, we see that

$$(g, R(\lambda) f) = \int \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \int G(\boldsymbol{x}, \boldsymbol{z}; \lambda) f(\boldsymbol{z})\, d\boldsymbol{z} \tag{1.3.48}$$

is regular in any region with $\operatorname{Im}\sqrt{\lambda} > 0$ where $\Delta(\lambda)$ does not vanish.

Obviously, the interest of this conclusion does not derive so much from what it says about the analytic behaviour of the resolvent off the real axis. This already follows from general principles (see the discussion following eq. (1.3.33)). The significant result is the information on the properties of the resolvent in the neighbourhood of

the negative real axis. This is by no means trivial, as it depends on the nature of the interaction. Whereas in general the resolvent of an arbitrary self-adjoint operator exists only for non-real λ, we see here that in the case of two particles with square-integrable interaction it can be continued analytically across the negative real axis. As for the restriction that $\Delta(\lambda)$ must not vanish, since $\Delta(\lambda)$ is regular, its zeros are isolated points. Hence they give rise only to poles of the resolvent. It is these poles to which we now direct our attention.

1.3.4. Bound states

It was remarked above that, if $\Delta(\lambda)$ has zeros, these give rise to poles of the resolvent. However, we saw from eqs. (1.3.29) and (1.3.33) that the resolvent is regular off the real axis, so that the possible zeros of $\Delta(\lambda)$ must be confined to the real axis. In view of the regularity of $\Delta(\lambda)$, they cannot have an accumulation point in the region $\operatorname{Im}\sqrt{\lambda} \geq \varepsilon > 0$, except perhaps the point at infinity. The latter possibility is easily ruled out, however, by the following argument. According to the resolvent equation (1.2.14), we formally have

$$(g, R(\lambda)f) - (g, R_0(\lambda)f) = \sum_{p=1}^{\infty} (-1)^p (g, [R_0(\lambda)V]^p R_0(\lambda)f). \tag{1.3.49}$$

In general this series is not convergent. But if $\operatorname{Im}\sqrt{\lambda}$ is sufficiently large, it follows from eq. (1.3.4) that the $\mathfrak{L}^2$-norm of $R_0 V$ is sufficiently small,

$$|R_0(\lambda)V| < 1 \quad \left(\operatorname{Im}\sqrt{\lambda} > \frac{1}{8\pi}\int [V(\boldsymbol{x})]^2 d\boldsymbol{x}\right). \tag{1.3.50}$$

Under this condition, the series on the right-hand side of eq. (1.3.49) is easily shown to converge and to equal the left-hand side. It thus exhibits the resolvent as a bounded operator, also on the negative real axis. There can therefore be no poles in the neighbourhood of the point at infinity, which is what we wanted to show. Summarizing, we see that on that part of the negative real axis on which $\operatorname{Im}\sqrt{\lambda} \geq \varepsilon > 0$, the function $\Delta(\lambda)$ may have a finite number of zeros at most.

Let us now choose a particular zero $\lambda = \lambda_\alpha$, and let us assume that it is of order q. Then it follows from eq. (1.3.11) that, in the neighbourhood of λ_α, the quantity $(g, R(\lambda)f)$ can be expanded in a Laurent series the most singular term of which is proportional to $(\lambda - \lambda_\alpha)^{-q}$. Hence, in the expansion of $(d/d\lambda)(g, R(\lambda)f)$, the most singular term is proportional to $(\lambda - \lambda_\alpha)^{-q-1}$. But, according to eq. (1.3.32), it is also proportional to $(\lambda - \lambda_\alpha)^{-2q}$, so that $q = 1$. The resolvent can therefore have only simple poles.

At this stage it is convenient to consider the function

$$P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha) = \lim_{\lambda \to \lambda_\alpha} \frac{\lambda - \lambda_\alpha}{\Delta(\lambda)} \int D(\boldsymbol{x}, \boldsymbol{y}; \lambda_\alpha)\, G_0(\boldsymbol{y}, \boldsymbol{z}; \lambda_\alpha)\, d\boldsymbol{y}, \tag{1.3.51}$$

which, according to eq. (1.3.12), is the "residue" of $G(\boldsymbol{x}, \boldsymbol{z}; \lambda)$ at $\lambda = \lambda_\alpha$. From the symmetry relations for the Green function, eqs. (1.3.17) and (1.3.18), it follows that P is real, and that it satisfies

$$P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha) = P(\boldsymbol{z}, \boldsymbol{x}; \lambda_\alpha). \tag{1.3.52}$$

Furthermore, P is a Hilbert-Schmidt kernel. By virtue of all this, P can be developed in mean square in a series of orthonormal eigenfunctions in $\mathfrak{L}^2$ according to (RIESZ and SZ.-NAGY(3) section 97)

$$P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha) = \sum_{q=1}^{\infty} \mu_{\alpha q} \varphi_{\alpha q}(\boldsymbol{x}) \bar{\varphi}_{\alpha q}(\boldsymbol{z}), \tag{1.3.53}$$

$$|P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha)| = \left[\sum_{q=1}^{\infty}{}' \mu_{\alpha q}^2\right]^{\frac{1}{2}}. \tag{1.3.54}$$

Here the eigenvalues μ are real, since P is hermitian. Hence, if φ is an eigenfunction corresponding to a certain eigenvalue μ, so is $\bar{\varphi}$. The above series can therefore be arranged in such a way that the functions $\varphi_{\alpha q}$ are all real. This will always be implied in the following, unless otherwise stated.

It is clear from eq. (1.3.12) that, if $(g, R(\lambda) f)$ is expanded in a Laurent series in powers of $\lambda - \lambda_\alpha$, its principal part takes the form

$$\frac{1}{\lambda - \lambda_\alpha} \int \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \int P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha) f(\boldsymbol{z})\, d\boldsymbol{z}. \tag{1.3.55}$$

Hence, equating the most singular terms in the expansions of $(d/d\lambda)\,(g, R(\lambda) f)$ and $(g, R(\lambda)\, R(\lambda) f)$ yields

$$\left.\begin{aligned} &\int \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \int P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha) f(\boldsymbol{z})\, d\boldsymbol{z} \\ &= -\int \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \int P(\boldsymbol{x}, \boldsymbol{y}; \lambda_\alpha)\, d\boldsymbol{y} \int P(\boldsymbol{y}, \boldsymbol{z}; \lambda_\alpha) f(\boldsymbol{z})\, d\boldsymbol{z}. \end{aligned}\right\} \tag{1.3.56}$$

In view of the arbitrariness of f and g in $\mathfrak{L}^2$, this shows that $-P$ represents a projection. As a result the eigenvalues all satisfy $\mu_{\alpha q} = -1$, the number of independent eigenfunctions is finite by eq. (1.3.54), and eq. (1.3.53) holds for almost every $\boldsymbol{x}$ and $\boldsymbol{z}$.

To get more insight into the properties of the eigenfunctions φ, we consider once more the resolvent equation (1.2.14),

$$R(\lambda) f = R_0(\lambda) f - R_0(\lambda) V R(\lambda) f. \tag{1.3.57}$$

Substituting the Green function on both sides, developing in a Laurent series in powers of $\lambda - \lambda_\alpha$, and equating principal parts yields

$$\int P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha) f(\boldsymbol{z})\, d\boldsymbol{z} = -\int G_0(\boldsymbol{x}, \boldsymbol{y}; \lambda_\alpha) V(\boldsymbol{y})\, d\boldsymbol{y} \int P(\boldsymbol{y}, \boldsymbol{z}; \lambda_\alpha) f(\boldsymbol{z})\, d\boldsymbol{z}. \tag{1.3.58}$$

Taking in particular $f = \varphi_{\alpha q}$ gives

$$\varphi_{\alpha q}(\boldsymbol{x}) = -\int G_0(\boldsymbol{x}, \boldsymbol{y}; \lambda_\alpha) V(\boldsymbol{y}) \varphi_{\alpha q}(\boldsymbol{y})\, d\boldsymbol{y}. \tag{1.3.59}$$

We now want to show that $V\varphi_{\alpha q}$ belongs to $\mathfrak{L}^2$. To do this, we recall first of all that, since $D(\boldsymbol{x}, \boldsymbol{y}; \lambda_\alpha)$ belongs to $\mathfrak{L}^2$, it is a square-integrable function of $\boldsymbol{y}$ for almost every $\boldsymbol{x}$, by Fubini's theorem. Further, $VR_0(\lambda_\alpha)$ is a bounded operator. Denoting its bound by $\| VR_0(\lambda_\alpha) \|$, we deduce from eq. (1.3.51) that

$$\int [V(\boldsymbol{z}) P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha)]^2 d\boldsymbol{z} \leq \text{const.} \| VR_0(\lambda_\alpha) \|^2 \int | D(\boldsymbol{x}, \boldsymbol{y}; \lambda_\alpha) |^2 d\boldsymbol{y}, \tag{1.3.60}$$

$$\iint [V(\boldsymbol{z}) P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha)]^2 d\boldsymbol{z}\, d\boldsymbol{x} \leq \text{const.} \| VR_0(\lambda_\alpha) \|^2 | D(\lambda_\alpha) |^2. \tag{1.3.61}$$

From this it follows with Schwarz's inequality that

$$\left.\begin{aligned} \int | V(\boldsymbol{z}) \varphi_{\alpha q}(\boldsymbol{z}) |^2 d\boldsymbol{z} &= \int | V(\boldsymbol{z}) \int P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha) \varphi_{\alpha q}(\boldsymbol{x})\, d\boldsymbol{x} |^2 d\boldsymbol{z} \\ &\leq \iint [V(\boldsymbol{z}) P(\boldsymbol{x}, \boldsymbol{z}; \lambda_\alpha)]^2 d\boldsymbol{z}\, d\boldsymbol{x} \int | \varphi_{\alpha q}(\boldsymbol{y}) |^2 d\boldsymbol{y} < \infty, \end{aligned}\right\} \tag{1.3.62}$$

which is what we wanted to show.

It is now permitted to apply the operator $H_0 - \lambda_\alpha$ to both sides of eq. (1.3.59). This yields

$$\left.\begin{aligned} (H_0 - \lambda_\alpha) \varphi_{\alpha q}(\boldsymbol{x}) &= -V(\boldsymbol{x}) \varphi_{\alpha q}(\boldsymbol{x}), \\ (H - \lambda_\alpha) \varphi_{\alpha q}(\boldsymbol{x}) &= 0. \end{aligned}\right\} \tag{1.3.63}$$

In other words, φ satisfies the Schrödinger equation. Since it belongs to $\mathfrak{L}^2$, it is the eigenfunction for a bound state, with energy λ_α.

Since in the region with $\operatorname{Im} \sqrt{\lambda} \geq \varepsilon > 0$ the number of poles of the resolvent is finite, the above argument can easily be extended to show that the Green function can be written in the form

$$G(\boldsymbol{x}, \boldsymbol{y}; \lambda) = \sum_{\substack{\alpha=1 \\ \operatorname{Im}\sqrt{\lambda_\alpha} \geq \varepsilon}}^{N(\varepsilon)} \sum_{q_\alpha=1}^{Q_\alpha} \frac{\varphi_{\alpha q_\alpha}(\boldsymbol{x})\, \bar{\varphi}_{\alpha q_\alpha}(\boldsymbol{y})}{\lambda_\alpha - \lambda} + G_B(\boldsymbol{x}, \boldsymbol{y}; \lambda; \varepsilon), \tag{1.3.64}$$

where G_B is determined by the requirement that for $\operatorname{Im} \sqrt{\lambda} \geq \varepsilon > 0$ it be the kernel of a bounded operator. In eq. (1.3.64) Q_α and $N(\varepsilon)$ are certain finite integers. This equation is the analogue of the well-known heuristic expansion in terms of a complete orthonormal set ψ_q $(q = 1, 2, \ldots)$,

$$G(\boldsymbol{x}, \boldsymbol{y}; \lambda) = \sum_{q=1}^{\infty} \frac{\psi_q(\boldsymbol{x}) \bar{\psi}_q(\boldsymbol{y})}{\lambda_q - \lambda}, \tag{1.3.65}$$

which in general can be justified only when the spectrum is purely discrete.

The formalism developed so far does not tell anything about the behaviour of the resolvent in the neighbourhood of the positive real axis. When we pass on to the theory of scattering in a forthcoming paper, we shall see that there is a continuous spectrum from 0 to ∞. It will be discussed how this is related to scattering cross-sections. As regards the interval on the negative real axis where $0 \leq \operatorname{Im} \sqrt{\bar{\lambda}} < \varepsilon$, we should like to know if the number of poles on this is finite or infinite. It is obvious that in the latter case the origin would be the only point of accumulation. It was shown by BARGMANN(16) that, in the case of two particles with a spherically symmetric interaction satisfying

$$\int_{-\infty}^{\infty} \frac{|V(|\boldsymbol{x}|)|}{|\boldsymbol{x}|} d^3\boldsymbol{x} < \infty, \tag{1.3.66}$$

the number of poles is finite. However, Bargmann's method is restricted to separable Hamiltonians, as it is based on the theory of ordinary differential equations. We have not succeeded in recasting his ideas so as to make them applicable to larger numbers of particles. It is for this reason that the behaviour of the resolvent in the neighbourhood of the origin is left out of consideration in the present paper.

1.4. Spectral theory

1.4.1. The integral representation of the resolvent

Before we can pass on to systems of three or more particles, we must give a short summary of some elements of the spectral theory of self-adjoined operators. Most of the material of the present section can be obtained from ACHIESER and GLASMANN(2) or other books on Hilbert space. However, with a view to future applications, we have preferred not to stress the well-known Stieltjes-integral approach to the resolution of the identity. Instead of this a formalism is given mainly in terms of limits of Riemann integrals of resolvents off the real axis. In future sections this will be found to be very useful, as it bridges the gap between the resolvent off the real axis, which is a fairly manageable quantity, and the spectral properties of the Hamiltonian, which have to do with the much more tricky properties of the resolvent in the neighbourhood of the real axis. Our final formulas are essentially the ones given by TITCHMARSH(8) ch. XII, and the present paper owes very much to his book.

Let us start by considering $(f, R(\lambda)f)$ as a function of λ, for fixed f in $\mathfrak{Q}^2$. It was discussed in section 1.3.3 that this function is regular off the real axis. It follows from eqs. (1.2.11) and (1.2.12) that

$$\frac{1}{\operatorname{Im}\lambda} \operatorname{Im}(f, R(\lambda) f) = \frac{1}{\lambda - \bar{\lambda}} (f, [R(\lambda) - R(\bar{\lambda})] f) = (f, R(\bar{\lambda}) R(\lambda) f) \geq 0, \tag{1.4.1}$$

so that in the upper half-plane the function $(f, R(\lambda)f)$ has a non-negative imaginary part. Furthermore, it satisfies

$$|(f, R(\lambda) f)| \leq \frac{1}{|\operatorname{Im} \lambda|} \|f\|^2 \tag{1.4.2}$$

by eq. (1.3.29). From all this it follows that there exists a non-decreasing function of bounded variation $E(l; f, f)$ such that (ACHIESER and GLASMANN(2) section 59)

$$(f, R(\lambda) f) = \int_{-\infty}^{\infty} \frac{dE(l; f, f)}{l - \lambda} \quad (\operatorname{Im} \lambda > 0), \tag{1.4.3}$$

$$\frac{1}{2} E(l-0; f, f) + \frac{1}{2} E(l+0; f, f) = \text{const.} + \lim_{\varepsilon \to 0} \frac{1}{2\pi i} \int_0^l (f, [R(m+i\varepsilon) - R(m-i\varepsilon)] f)\, dm. \tag{1.4.4}$$

If, in addition to satisfying eq. (1.4.4), $E(l; f, f)$ is chosen in such a way that

$$\left.\begin{aligned} E(-\infty; f, f) &\equiv \lim_{l \to -\infty} E(l; f, f) = 0, \\ E(l-0; f, f) &= E(l; f, f), \end{aligned}\right\} \tag{1.4.5}$$

it is uniquely determined.

If we want to consider a general expression of the form $(g, R(\lambda) f)$, it is useful to split this into four terms according to

$$\left.\begin{aligned} 4(g, R(\lambda) f) = (g+f, R(\lambda)[g+f]) - (g-f, R(\lambda)[g-f]) \\ - i(g+if, R(\lambda)[g+if]) + i(g-if, R(\lambda)[g-if]). \end{aligned}\right\} \tag{1.4.6}$$

Here each term allows an integral representation of the form (1.4.3), and so the same holds true for the sum. In other words, there is a relation

$$(g, R(\lambda) f) = \int_{-\infty}^{\infty} \frac{dE(l; g, f)}{l - \lambda} \quad (\operatorname{Im} \lambda > 0), \tag{1.4.7}$$

$E(l; g, f)$ satisfying equations of the forms (1.4.4) and (1.4.5). The function $E(l; g, f)$ is no longer non-decreasing, but since it is a linear combination of non-decreasing functions, it is still of bounded variation.

It follows from eq. (1.4.3) that

$$\left.\begin{aligned} \frac{1}{2\pi i} \int_{-\infty}^{\infty} (f, [R(m+i\varepsilon) - R(m-i\varepsilon)] f)\, dm &= \frac{1}{\pi} \int_{-\infty}^{\infty} dm \int_{-\infty}^{\infty} \frac{\varepsilon}{(m-l)^2 + \varepsilon^2}\, dE(l; f, f) \\ = \frac{1}{\pi} \int_{-\infty}^{\infty} dE(l; f, f) \int_{-\infty}^{\infty} \frac{\varepsilon}{(m-l)^2 + \varepsilon^2}\, dm &= E(\infty; f, f), \end{aligned}\right\} \tag{1.4.8}$$

where the inversion of the integrations is justified by Fubini's theorem for Stieltjes integrals (SAKS(17) ch. III, section 8; also WIDDER(18) ch. I, section 15). If the way

is remembered in which $(g, R(\lambda)f)$ was written as a sum of four terms, eq. (1.4.6), a similar relation is obtained for $E(\infty; g, f)$. Moreover,

$$\frac{2}{\pi}\int_{-\infty}^{\infty} |(g, [R(m+i\varepsilon) - R(m-i\varepsilon)]f)|\, dm$$

$$\leq E(\infty; g+f, g+f) + E(\infty; g-f, g-f) + E(\infty; g+if, g+if) + E(\infty; g-if, g-if), \quad (1.4.9)$$

uniformly in ε. From this it is obvious that as a function of l the integral

$$\frac{1}{2\pi i}\int_0^l (g, [R(m+i\varepsilon) - R(m-i\varepsilon)]f)\, dm \quad (1.4.10)$$

is of bounded variation uniformly with respect to ε. As ε tends to 0, this integral tends to const. $+ [E(l-0; g, f) + E(l+0; g, f)]/2$ (cf. eq. (1.4.4)). Also, $(l-\lambda)^{-1}$ is a continuous function of l. Hence, according to the Helly-Bray theorem on limits of Stieltjes integrals (WIDDER (18) ch. I, theorem 16.4), we have

$$(g, R(\lambda)f) = \lim_{\substack{L\to-\infty \\ T\to\infty}} \int_L^T \frac{dE(l; g, f)}{l-\lambda} = \lim_{\substack{L\to-\infty \\ T\to\infty}} \lim_{\varepsilon\to 0} \frac{1}{2\pi i}\int_L^T (g, [R(l+i\varepsilon) - R(l-i\varepsilon)]f)\frac{dl}{l-\lambda}. \quad (1.4.11)$$

In this formula it is in general necessary to perform the limit with respect to ε first, while the integration interval (L, T) is still finite, because the validity of the Helly-Bray theorem is restricted to finite intervals.

1.4.2. Spectral resolutions

To get more insight into the quantity $E(\infty; g, f)$, we now consider the relation

$$\lambda(g, R(\lambda)f) = -(g, f) + (g, HR(\lambda)f). \quad (1.4.12)$$

With Minkowski's inequality, this yields a bound for the operator $HR(\lambda)$ according to

$$\|HR(\lambda)f\| \leq \|f\| + |\lambda|\,\|R(\lambda)f\| \leq \left[1 + \frac{|\lambda|}{|\mathrm{Im}\,\lambda|}\right]\|f\|. \quad (1.4.13)$$

Now, if g belongs to $\mathfrak{D}(H)$, we clearly have

$$\lim_{\nu\to\infty} (g, HR(i\nu)f) = 0. \quad (1.4.14)$$

But in view of eq. (1.4.13), this must also hold true for any arbitrary g in $\mathfrak{L}^2$. For if we have any g in $\mathfrak{L}^2$, we can always choose a sequence g_N in $\mathfrak{D}(H)$ which tends to g in mean square. In terms of this we get

$$\left.\begin{aligned} &|(g, HR(i\nu)f)| = |(g-g_N, HR(i\nu)f)+(g_N, HR(i\nu)f)| \\ &\leq \|g-g_N\|\,\|HR(i\nu)f\|+|(g_N, HR(i\nu)f)| \leq 2\,\|g-g_N\|\,\|f\|+\|Hg_N\|\,\|R(i\nu)f\|, \end{aligned}\right\} \quad (1.4.15)$$

and this can be made arbitrarily small by choosing first N, next ν sufficiently large.

With eq. (1.4.12) it now follows that

$$\lim_{\nu\to\infty} i\nu(g, R(i\nu)f) = -(g, f). \quad (1.4.16)$$

Combining this with eq. (1.4.7) yields

$$(g, f) = -\lim_{\nu\to\infty} i\nu\int_{-\infty}^{\infty} \frac{dE(l; g, f)}{l-i\nu} = \int_{-\infty}^{\infty} dE(l; g, f) = E(\infty; g, f), \quad (1.4.17)$$

where use is made of the normalization $E(-\infty; g, f) = 0$ (cf. eq. (1.4.5)). By eq. (1.4.4), an alternative way of writing this is

$$(g, f) = \lim_{\substack{L\to-\infty \\ T\to\infty}} \lim_{\varepsilon\to 0} \frac{1}{2\pi i}\int_L^T (g, [R(l+i\varepsilon)-R(l-i\varepsilon)]f)\,dl. \quad (1.4.18)$$

In this form the expression is a generalization of the well-known expansion of (g, f) in terms of a complete orthonormal set of functions in $\mathfrak{L}^2$. For let us consider the simple case that the spectrum is discrete, and such that the resolvent can be represented by a Green function of the form (1.3.65). Under these circumstances we have

$$\left.\begin{aligned} (g, [R(l+i\varepsilon)-R(l-i\varepsilon)]f) &= \sum_{q=1}^{\infty} \bar{g}_q f_q \frac{2i\varepsilon}{(\lambda_q - l)^2+\varepsilon^2}, \\ f_q &= \int \bar{\psi}_q(\boldsymbol{y}) f(\boldsymbol{y})\,d\boldsymbol{y}, \end{aligned}\right\} \quad (1.4.19)$$

so that the expansion (1.4.18) takes the well-known form

$$(g, f) = \sum_{q=1}^{\infty} \bar{g}_q f_q. \quad (1.4.20)$$

We note here without proof that the function $E(l; g, f)$ satisfies an equation of the form

$$E(l; g, f) = (g, E(l)f), \quad (1.4.21)$$

where $E(l)$ is a projection operator with the properties (Achieser and Glasmann(2) section 65)

$$\left.\begin{aligned} &E(l)\,E(m) = E(\min(l, m)), \\ &E(-\infty) = 0, \quad E(\infty) = 1, \\ &E(l-0) = E(l). \end{aligned}\right\} \quad (1.4.22)$$

The operator $E(l)$ is called the resolution of the identity. Some authors normalize $E(l)$ in such a way that $E(l+0) = E(l)$ (see STONE(4) definition 5.1). This will give no confusion in the following. If there is a discrete spectrum with a Green function of the form (1.3.65), we have in any case

$$\left.\begin{aligned}(g,[E(\lambda_p+0)-E(\lambda_p-0)]f) &= \lim_{\delta\to 0}\lim_{\varepsilon\to 0}\frac{1}{\pi}\int_{\lambda_p-\delta}^{\lambda_p+\delta}\left[\sum_{q=1}^{\infty}{}'\bar{g}_q f_q\frac{\varepsilon}{(\lambda_q-l)^2+\varepsilon^2}\right]dl\\ &= \lim_{\delta\to 0}\lim_{\varepsilon\to 0}\frac{1}{\pi}\sum_{q=1}^{\infty}{}'\bar{g}_q f_q\left[\operatorname{arctg}\frac{\lambda_p-\lambda_q+\delta}{\varepsilon}-\operatorname{arctg}\frac{\lambda_p-\lambda_q-\delta}{\varepsilon}\right]=\sum_{\substack{q\\ \lambda_q=\lambda_p}}{}'\bar{g}_q f_q,\end{aligned}\right\}\quad(1.4.23)$$

so that $E(\lambda_p+0)-E(\lambda_p-0)$ is the projection on the subspace of $\mathfrak{L}^2$ spanned by the functions ψ_q with $\lambda_q=\lambda_p$. It will be observed that in the above argument the limits with respect to ε and δ cannot be interchanged.

It is plausible after the foregoing that

$$(g,Hf)=\int_{-\infty}^{\infty} l\,dE(l;g,f),\qquad(1.4.24)$$

provided f belongs to $\mathfrak{D}(H)$, a condition which is expressed by

$$\int_{-\infty}^{\infty} l^2\,dE(l;f,f)<\infty.\qquad(1.4.25)$$

Equation (1.4.24) is discussed in great detail by ACHIESER and GLASMANN(2), section 66. It is another illustration of the fact that, roughly speaking, $E(l+\Delta l)-E(l)$ selects that part of f for which the expectation value of the energy is between l and $l+\Delta l$.

General functions of H are defined by (ref.(2) section 74)

$$(g,F(H)f)=\int_{-\infty}^{\infty}F(l)\,dE(l;g,f),\qquad(1.4.26)$$

provided f is such that

$$\int_{-\infty}^{\infty}|F(l)|^2\,dE(l;f,f)<\infty.\qquad(1.4.27)$$

The expansion of the resolvent, eq. (1.4.7), is a special example of eq. (1.4.26). Also,

$$(g,e^{iHt}f)=\int_{-\infty}^{\infty}e^{ilt}\,dE(l;g,f)=\lim_{\substack{L\to-\infty\\ T\to\infty}}\lim_{\varepsilon\to 0}\frac{1}{2\pi i}\int_{L}^{T}e^{ilt}(g,[R(l+i\varepsilon)-R(l-i\varepsilon)]f)\,dl,\qquad(1.4.28)$$

where the transition from the second to the third member is made with the Helly-Bray theorem, as in the proof of eq. (1.4.11).

If the resolvent can be represented with the help of a Green function with the symmetry property (1.3.17), it is useful to introduce

$$\operatorname{Im}G(\boldsymbol{x},\boldsymbol{y};\lambda)=\frac{1}{2i}[G(\boldsymbol{x},\boldsymbol{y};\lambda)-G(\boldsymbol{x},\boldsymbol{y};\bar{\lambda})].\qquad(1.4.29)$$

Then for any bounded and continuous function F the expansion formula may be written in the form

$$(g, F(H)f) = \lim_{\substack{L\to-\infty \\ T\to\infty}} \lim_{\varepsilon\to 0} \frac{1}{\pi}\int_L^T F(l)\,dl \int \bar{g}(\boldsymbol{x})\,d\boldsymbol{x} \int [\operatorname{Im} G(\boldsymbol{x}, \boldsymbol{y}; l+i\varepsilon)] f(\boldsymbol{y})\,d\boldsymbol{y}. \quad (1.4.30)$$

1.4.3. An upper bound for the resolvent

If the resolvent is regular in a region which includes an interval $L_1 \le l \le L_2$ on the real axis, we have

$$\lim_{\varepsilon\to 0} \int_{L_1}^{L_2} (g, [R(l+i\varepsilon) - R(l-i\varepsilon)] f)\,dl = 0. \quad (1.4.31)$$

In other words, the integral in the expansion formula receives contributions only from the part of the real axis where the resolvent is singular, that is from the spectrum of H. In particular, if the spectrum is bounded below, i.e. if there exists a finite L such that the resolvent is regular in the half-plane $\operatorname{Re}\lambda \le L$, there is no contribution from l-values with $l \le L$. Hence, in this case the limit with respect to L may be omitted from equations such as eq. (1.4.11), provided L is chosen sufficiently small.

If the lower bound of the spectrum is denoted by Λ, it follows from eq. (1.4.4) that $E(l; f, f) = \text{const.}$ in the interval $-\infty < l < \Lambda$. Together with eq. (1.4.5) this yields that, in fact, $E(l; f, f) = 0$ if $-\infty < l \le \Lambda$. Hence, the integral representation of the resolvent may be written in the form

$$(f, R(\lambda)f) = \int_\Lambda^\infty \frac{dE(l; f, f)}{l-\lambda}. \quad (1.4.32)$$

Equation (1.4.1) now gives

$$(R(\lambda)f, R(\lambda)f) = \int_\Lambda^\infty \frac{dE(m; f, f)}{(m-\lambda)(m-\bar{\lambda})}. \quad (1.4.33)$$

If in this expression we write $\lambda = \Lambda + le^{i\varphi}$, then for $\frac{\pi}{2} \le \varphi \le \frac{3}{2}\pi$ we get

$$\left.\begin{aligned} \|R(\Lambda + le^{i\varphi})f\|^2 &= \int_\Lambda^\infty [(m-\Lambda)^2 + l^2 - 2(m-\Lambda)\cos\varphi]^{-1} dE(m; f, f) \\ &\le \frac{1}{l^2}\int_\Lambda^\infty dE(m; f, f) = \frac{1}{l^2}\|f\|^2 \le \frac{1}{l^2 \sin^4 \frac{1}{2}\varphi}\|f\|^2. \end{aligned}\right\} \quad (1.4.34)$$

It is already known from eq. (1.3.29) that

$$\|R(\Lambda + le^{i\varphi})\| \le \frac{1}{|l\sin\varphi|}. \quad (1.4.35)$$

Combining these two inequalities shows that, whenever $0 < \varphi < 2\pi$,

$$\|R(\lambda)\| \le \frac{1}{[\operatorname{Im}\sqrt{(\lambda-\Lambda)}]^2}. \quad (1.4.36)$$

This is a generalization of eq. (1.3.31) for the norm of $R_0(\lambda)$.

1.5. A separable three-body problem

1.5.1. The resolvent

We are now able to tackle the simple three-body problem in which there is an interaction V_{12} between particles 1 and 2, but no interaction between particle 3 and particles 1 and 2. By eq. (1.2.4), the differential operator for the relative motion is in this case

$$\left.\begin{aligned} H'(\boldsymbol{x}_1, \boldsymbol{x}_2) &= H'_{12}(\boldsymbol{x}_1) + H'_0(\boldsymbol{x}_2), \\ H'_{12}(\boldsymbol{x}_1) = -\Delta(\boldsymbol{x}_1) + V_{12}(\boldsymbol{x}_1), &\quad H'_0(\boldsymbol{x}_2) = -\Delta(\boldsymbol{x}_2), \end{aligned}\right\} \tag{1.5.1}$$

the Hamiltonian being the self-adjoint extension of $H'(\boldsymbol{x}_1, \boldsymbol{x}_2)$.

The important point about eq. (1.5.1) is that H' separates into two differential operators which act in different Hilbert spaces. It is therefore useful to consider the spaces $\mathfrak{L}^2(\boldsymbol{x}_1)$, $\mathfrak{L}^2(\boldsymbol{x}_2)$, and $\mathfrak{L}^2(\boldsymbol{x}_1, \boldsymbol{x}_2)$. The extension of $H'_{12}(\boldsymbol{x}_1)$ in $\mathfrak{L}^2(\boldsymbol{x}_1)$ is denoted by $H_{12}(\boldsymbol{x}_1)$, the corresponding resolvent by $R_{12}(\boldsymbol{x}_1; \lambda)$. Likewise, the extension of $H'_0(\boldsymbol{x}_2)$ in $\mathfrak{L}^2(\boldsymbol{x}_2)$ is denoted by $H_0(\boldsymbol{x}_2)$, the resolvent by $R_0(\boldsymbol{x}_2; \lambda)$.

In an obvious way the Hamiltonians $H_{12}(\boldsymbol{x}_1)$ and $H_0(\boldsymbol{x}_2)$ can be considered as operators not only in $\mathfrak{L}^2(\boldsymbol{x}_1)$ and $\mathfrak{L}^2(\boldsymbol{x}_2)$, respectively, but also in $\mathfrak{L}^2(\boldsymbol{x}_1, \boldsymbol{x}_2)$. In this sense, we have

$$H(\boldsymbol{x}_1, \boldsymbol{x}_2) = H_{12}(\boldsymbol{x}_1) + H_0(\boldsymbol{x}_2). \tag{1.5.2}$$

Likewise, the resolvents can be considered as operators in $\mathfrak{L}^2(\boldsymbol{x}_1, \boldsymbol{x}_2)$, with the same bounds as in $\mathfrak{L}^2(\boldsymbol{x}_1)$ and $\mathfrak{L}^2(\boldsymbol{x}_2)$, respectively. In the space $\mathfrak{L}^2(\boldsymbol{x}_1, \boldsymbol{x}_2)$ we write

$$(g(\boldsymbol{x}_1, \boldsymbol{x}_2), R_{12}(\boldsymbol{x}_1; \lambda) f(\boldsymbol{x}_1, \boldsymbol{x}_2)) = \int \bar{g}(\boldsymbol{x}_1, \boldsymbol{x}_2)\, d\boldsymbol{x}_1\, d\boldsymbol{x}_2 \int G_{12}(\boldsymbol{x}_1, \boldsymbol{y}_1; \lambda) f(\boldsymbol{y}_1, \boldsymbol{x}_2)\, d\boldsymbol{y}_1, \tag{1.5.3}$$

and similarly for $R_0(\boldsymbol{x}_2; \lambda)$.

Now, if $\varphi_{12}(\boldsymbol{x}_1)$ is an eigenfunction of $H_{12}(\boldsymbol{x}_1)$, and $\varphi_0(\boldsymbol{x}_2)$ an eigenfunction of $H_0(\boldsymbol{x}_2)$, the product $\varphi_{12}(\boldsymbol{x}_1)\, \varphi_0(\boldsymbol{x}_2)$ is an eigenfunction of $H(\boldsymbol{x}_1, \boldsymbol{x}_2)$. And if the spectra of $H_{12}(\boldsymbol{x}_1)$ and $H_0(\boldsymbol{x}_2)$ were discrete, all the eigenfunctions of $H(\boldsymbol{x}_1, \boldsymbol{x}_2)$ could be obtained in this way. In view of the relation between resolvents, Green functions, and complete orthonormal sets of eigenfunctions brought out by the spectral theory, this suggests that, if the resolvents $R_{12}(\boldsymbol{x}_1; \lambda)$ and $R_0(\boldsymbol{x}_2; \lambda)$ are known, the resolvent $R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda)$ can be constructed therefrom. It is the purpose of the present section to prove that this is indeed the case. As a matter of fact, it is shown that

$$\left.\begin{aligned} &(g(\boldsymbol{x}_1, \boldsymbol{x}_2), R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda) f(\boldsymbol{x}_1, \boldsymbol{x}_2)) \\ &= \frac{1}{2\pi i} \int_C (g(\boldsymbol{x}_1, \boldsymbol{x}_2), R_0(\boldsymbol{x}_2; \lambda - \sigma) R_{12}(\boldsymbol{x}_1; \sigma) f(\boldsymbol{x}_1, \boldsymbol{x}_2))\, d\sigma, \end{aligned}\right\} \tag{1.5.4}$$

where C is a suitable contour in the σ-plane such that the singularities of $R_{12}(\boldsymbol{x}_1; \sigma)$ are on the right of C, and those of $R_0(\boldsymbol{x}_2; \lambda - \sigma)$ on the left of C.

To be explicit, let us choose

$$\lambda = l + i\nu \ (\nu > 0), \quad \sigma = s + \frac{1}{2} i\nu \ (-\infty < s < \infty). \tag{1.5.5}$$

Then, denoting the right-hand side of eq. (1.5.4) by I, we have

$$\left.\begin{aligned} I \leq \frac{1}{2\pi} \Big[\int_{-\infty}^{\infty} || R_0\Big(\boldsymbol{x}_2;\, l - s - \frac{1}{2} i\nu\Big)\, g(\boldsymbol{x}_1, \boldsymbol{x}_2) ||^2 \, ds \Big]^{\frac{1}{2}} \\ \times \Big[\int_{-\infty}^{\infty} || R_{12}\Big(\boldsymbol{x}_1;\, s + \frac{1}{2} i\nu\Big) f(\boldsymbol{x}_1, \boldsymbol{x}_2) ||^2 \, ds \Big]^{\frac{1}{2}}. \end{aligned}\right\} \tag{1.5.6}$$

Our first step is now to establish that $I/(||f||\ ||g||)$ is bounded uniformly in λ in the half-plane $\operatorname{Im}\lambda \geq \varepsilon > 0$. To do this, we note that since $f(\boldsymbol{x}_1, \boldsymbol{x}_2)$ belongs to $\mathfrak{L}^2(\boldsymbol{x}_1)$ for almost every $\boldsymbol{x}_2$, by Fubini's theorem, the spectral theory of section 1.4 can be applied to $R_{12}(\boldsymbol{x}_1; \sigma)$ by keeping $\boldsymbol{x}_2$ fixed at first, and integrating over $\boldsymbol{x}_2$ as a last step. In this way, eqs. (1.4.1) and (1.4.7) give

$$\left.\begin{aligned} I_{12} \equiv \int_{-\infty}^{\infty} || R_{12}\Big(\boldsymbol{x}_1;\, s + \frac{1}{2} i\nu\Big) f(\boldsymbol{x}_1, \boldsymbol{x}_2) ||^2 \, ds \\ = \int_{-\infty}^{\infty} ds \int d\boldsymbol{x}_2 \int \frac{d_m E(\boldsymbol{x}_1;\, m;\, f(\boldsymbol{x}_1, \boldsymbol{x}_2), f(\boldsymbol{x}_1, \boldsymbol{x}_2))}{(m-s)^2 + \frac{1}{4}\nu^2}, \end{aligned}\right\} \tag{1.5.7}$$

where the argument $\boldsymbol{x}_1$ of E denotes that the spectral theorem has been applied in the space $\mathfrak{L}^2(\boldsymbol{x}_1)$. The integration with respect to s may now be performed first, and a bound for I_{12} is obtained of the form

$$I_{12} \leq \frac{2\pi}{\nu} \int d\boldsymbol{x}_2 \, E(\boldsymbol{x}_1;\, \infty;\, f(\boldsymbol{x}_1, \boldsymbol{x}_2), f(\boldsymbol{x}_1, \boldsymbol{x}_2)) = \frac{2\pi}{\nu} \int d\boldsymbol{x}_2 \int |f(\boldsymbol{x}_1, \boldsymbol{x}_2)|^2 \, d\boldsymbol{x}_1 = \frac{2\pi}{\nu} ||f||^2. \tag{1.5.8}$$

As a similar argument applies to $R_0(\boldsymbol{x}_2; \lambda - \sigma)$, it follows that $I/(||f||\ ||g||)$ is bounded if $\nu \geq \varepsilon > 0$, as we wished to show. The useful consequence of this result is that it is sufficient to check the desired relation (1.5.4) for functions f and g in $\mathfrak{D}(H(\boldsymbol{x}_1, \boldsymbol{x}_2))$ only. The final result for all f and g in $\mathfrak{L}^2(\boldsymbol{x}_1, \boldsymbol{x}_2)$ follows with a limiting procedure such as used to get eq. (1.4.16).

Let us choose, then, functions f and g in $\mathfrak{D}(H(\boldsymbol{x}_1, \boldsymbol{x}_2))$. These belong also to $\mathfrak{D}(H_{12}(\boldsymbol{x}_1))$ and $\mathfrak{D}(H_0(\boldsymbol{x}_2))$. Let us further apply the operator

$$1 = R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda)\,[H_{12}(\boldsymbol{x}_1) + H_0(\boldsymbol{x}_2) - \lambda] \tag{1.5.9}$$

to

$$R_0(\boldsymbol{x}_2; \lambda - \sigma)\, R_{12}(\boldsymbol{x}_1; \sigma). \tag{1.5.10}$$

This yields

$$R_0(\boldsymbol{x}_2; \lambda - \sigma) R_{12}(\boldsymbol{x}_1; \sigma) = R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda)\,[R_0(\boldsymbol{x}_2; \lambda - \sigma) + R_{12}(\boldsymbol{x}_1; \sigma)]. \tag{1.5.11}$$

By eq. (1.4.12) we have

$$\left.\begin{aligned}&(g(\boldsymbol{x}_1,\boldsymbol{x}_2), R_{12}(\boldsymbol{x}_1;\sigma) f(\boldsymbol{x}_1,\boldsymbol{x}_2))\\ &= -\frac{1}{\sigma}(g(\boldsymbol{x}_1,\boldsymbol{x}_2), f(\boldsymbol{x}_1,\boldsymbol{x}_2)) + \frac{1}{\sigma}(g(\boldsymbol{x}_1,\boldsymbol{x}_2), R_{12}(\boldsymbol{x}_1;\sigma) H_{12}(\boldsymbol{x}_1) f(\boldsymbol{x}_1,\boldsymbol{x}_2)).\end{aligned}\right\} \quad (1.5.12)$$

Since $H_{12}(\boldsymbol{x}_1) f(\boldsymbol{x}_1, \boldsymbol{x}_2)$ belongs to $\mathfrak{L}^2(\boldsymbol{x}_1, \boldsymbol{x}_2)$ by assumption, we may apply the spectral formula for the resolvent to the second term on the right-hand side of eq. (1.5.12). With this it follows that

$$\left.\begin{aligned}&\int_{-\infty}^{\infty} \frac{ds}{s+\frac{1}{2}i\nu}(g(\boldsymbol{x}_1,\boldsymbol{x}_2), R_{12}\left(\boldsymbol{x}_1; s+\frac{1}{2}i\nu\right) H_{12}(\boldsymbol{x}_1) f(\boldsymbol{x}_1,\boldsymbol{x}_2))\\ &= \int_{-\infty}^{\infty} \frac{ds}{s+\frac{1}{2}i\nu}\int d\boldsymbol{x}_2 \int \frac{1}{m-s-\frac{1}{2}i\nu} d_m E(\boldsymbol{x}_1; m; g(\boldsymbol{x}_1,\boldsymbol{x}_2), H_{12}(\boldsymbol{x}_1) f(\boldsymbol{x}_1,\boldsymbol{x}_2)) = 0.\end{aligned}\right\} \quad (1.5.13)$$

Hence it is only the first term on the right-hand side of eq. (1.5.12) which gives a non-vanishing contribution to the convolution integral I we want to evaluate. A similar argument applies to the contributions from $R_0(\boldsymbol{x}_2; \lambda-\sigma)$. With eq. (1.5.11), I therefore takes the form

$$\left.\begin{aligned}I = -\frac{1}{2\pi i}\int_{-\infty}^{\infty}&\left(\frac{1}{l-s+\frac{1}{2}i\nu}+\frac{1}{s+\frac{1}{2}i\nu}\right)(g(\boldsymbol{x}_1,\boldsymbol{x}_2), R(\boldsymbol{x}_1,\boldsymbol{x}_2; l+i\nu) f(\boldsymbol{x}_1,\boldsymbol{x}_2))\, ds\\ &= (g(\boldsymbol{x}_1,\boldsymbol{x}_2), R(\boldsymbol{x}_1,\boldsymbol{x}_2;\lambda) f(\boldsymbol{x}_1,\boldsymbol{x}_2)),\end{aligned}\right\} \quad (1.5.14)$$

which establishes eq. (1.5.4) for $\operatorname{Im}\lambda > 0$. It can likewise be established for $\operatorname{Im}\lambda < 0$.

In the case at hand, in which the spectra involved are bounded below, the contour in eq. (1.5.4) may be deformed in various ways. If, for instance, $\lambda = l + i\nu$ $(\nu > 0)$ and

$$\sigma = \lambda + Te^{i\varphi} \quad (0 \le \varphi < \pi), \quad (1.5.15)$$

it follows from what we know about the bounds for R_{12} and R_0 that the integrand in eq. (1.5.4) does not exceed

$$\|g\|\,\|f\|\,\frac{1}{[\operatorname{Im}\sqrt{(\lambda-\sigma)}]^2}\,\frac{1}{\operatorname{Im}\sigma} = \|g\|\,\|f\|\,\frac{1}{T\cos^2\frac{1}{2}\varphi}\,\frac{1}{\nu+T\sin\varphi}. \quad (1.5.16)$$

Hence, if we integrate from $\varphi = 0$ to $\varphi = \varphi_0 < \pi$ along the circumference of the circle with centre λ and radius T, the integral so obtained tends to 0 as T tends to ∞. Likewise, denoting the lower bound of the spectrum of $H_{12}(\boldsymbol{x}_1)$ by Λ_{12}, we see that if

$$\sigma = \Lambda_{12} - T + i\tau \quad (\nu < \nu + \varepsilon \le \tau \le T), \quad (1.5.17)$$

the integrand does not exceed

$$\|g\|\,\|f\|\,\frac{1}{|\operatorname{Im}(\lambda-\sigma)|}\,\frac{1}{[\operatorname{Im}\sqrt{(\sigma-\Lambda_{12})}]^2} \le \|g\|\,\|f\|\,\frac{1}{\tau-\nu}\,\frac{1}{T}. \tag{1.5.18}$$

Hence the integral along the straight line from $\Lambda_{12}-T+i\nu+i\varepsilon$ to $\Lambda_{12}-T+iT$ also tends to 0 as T tends to ∞. With arguments of this sort it is easily shown that as our contour we may in fact take any path which does not cross the cuts in the σ-plane caused by the singularities of $R_{12}(\sigma)$ and $R_0(\lambda-\sigma)$.

If λ is in the half-plane $\operatorname{Re}\lambda \le \Lambda_{12}-\varepsilon < \Lambda_{12}$, it is convenient to choose the contour parallel to the imaginary axis. It is easily seen that the integral so obtained converges uniformly with respect to λ. Hence, since the integrand is a regular function of λ, so is the integral. If λ is not real, the integral yields the resolvent, by our previous analysis. Its being regular therefore implies that the resolvent exists, and is regular, throughout the half-plane $\operatorname{Re}\lambda < \Lambda_{12}$. Combining this with previous results shows that the resolvent exists everywhere in the λ-plane cut from Λ_{12} to ∞, and that it is a regular function which can be evaluated by means of a convolution integral according to eq. (1.5.4).

For future reference it is useful to write the right-hand side of eq. (1.5.4) out in the form

$$\frac{1}{2\pi i}\int_C d\sigma \int \bar{g}\,(\boldsymbol{x}_1,\boldsymbol{x}_2)\,R_0(\boldsymbol{x}_2;\,\lambda-\sigma)\,R_{12}(\boldsymbol{x}_1;\,\sigma)\,f(\boldsymbol{x}_1,\boldsymbol{x}_2)\,d\boldsymbol{x}_1\,d\boldsymbol{x}_2, \tag{1.5.19}$$

and to compare this expression with

$$\left.\begin{aligned}&\frac{1}{2\pi}\int_C d\sigma \int |\,\bar{g}\,(\boldsymbol{x}_1,\boldsymbol{x}_2)\,R_0(\boldsymbol{x}_2;\,\lambda-\sigma)\,R_{12}(\boldsymbol{x}_1;\,\sigma)\,f(\boldsymbol{x}_1,\boldsymbol{x}_2)\,|\,d\boldsymbol{x}_1\,d\boldsymbol{x}_2\\ &\qquad\le \frac{1}{2\pi}\int_C d\sigma\,\|g\|\,\|f\|\,\frac{1}{[\operatorname{Im}\sqrt{(\lambda-\sigma)}]^2}\,\frac{1}{[\operatorname{Im}\sqrt{(\sigma-\Lambda_{12})}]^2}.\end{aligned}\right\} \tag{1.5.20}$$

If C is chosen in a suitable way, this integral is certainly convergent. Now in the original convolution expression, $\int_C d\sigma$ was meant to be a Riemann integral. However, if we are willing to interpret it as a Lebesgue integral, it becomes possible to invoke Fubini's theorem to invert the order of integration in the expression (1.5.19). Then we may write

$$R(\boldsymbol{x}_1,\boldsymbol{x}_2;\,\lambda)\,f(\boldsymbol{x}_1,\boldsymbol{x}_2) = \frac{1}{2\pi i}\int_C R_0(\boldsymbol{x}_2;\,\lambda-\sigma)\,R_{12}(\boldsymbol{x}_1;\,\sigma)\,f(\boldsymbol{x}_1,\boldsymbol{x}_2)\,d\sigma. \tag{1.5.21}$$

In this sense there is a convolution integral not only for the inner product $(g,\,R(\lambda)f)$, but also for the function $R(\lambda)f$.

1.5.2. The Green function

The object of the present section is to show that the resolvent $R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda)$ is an integral operator the kernel of which is a Green function of the form

$$G(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \lambda) = \frac{1}{2\pi i}\int_C G_0(\boldsymbol{x}_2, \boldsymbol{y}_2; \lambda - \sigma)\, G_{12}(\boldsymbol{x}_1, \boldsymbol{y}_1; \sigma)\, d\sigma. \qquad (1.5.22)$$

The distinction between this and the results (1.5.4) and (1.5.21) concerning the resolvent is that in the latter expressions certain integrations with respect to the space coodinates are performed first, the integration with respect to σ next, whereas in eq. (1.5.22) it is implied that the integration with respect to σ must be performed first.

To prove eq. (1.5.22), we split G_{12} according to eq. (1.3.27),

$$G_{12}(\boldsymbol{x}_1, \boldsymbol{y}_1; \sigma) = G_0(\boldsymbol{x}_1, \boldsymbol{y}_1; \sigma) - \int G_0(\boldsymbol{x}_1, \boldsymbol{z}_1; \sigma)\, V_{12}(\boldsymbol{z}_1)\, G_{12}(\boldsymbol{z}_1, \boldsymbol{y}_1; \sigma)\, d\boldsymbol{z}_1. \qquad (1.5.23)$$

This corresponds to a splitting of R of the form

$$R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda) = R_0(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda) - [R_0(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda) - R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda)]. \qquad (1.5.24)$$

Here it is known from eq. (1.2.17) that R_0 is an integral operator the kernel of which involves a Hankel function of order 2. In other words, there is a Green function

$$G_0(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \lambda) = \frac{i\lambda}{16\pi^2} \frac{1}{|\boldsymbol{x}_1 - \boldsymbol{y}_1|^2 + |\boldsymbol{x}_2 - \boldsymbol{y}_2|^2} H_2^{(1)}(\sqrt{\lambda}[|\boldsymbol{x}_1 - \boldsymbol{y}_1|^2 + |\boldsymbol{x}_2 - \boldsymbol{y}_2|^2]^{\frac{1}{2}}). \qquad (1.5.25)$$

It is now shown first that this function is obtained when the first term in the right-hand member of eq. (1.5.23) is folded according to eq. (1.5.22). More generally, it is shown that, when λ is not on the positive real axis and $r_1 \neq 0$, $r_2 \neq 0$,

$$\left.\begin{aligned} &-\frac{1}{32\pi i}(2\pi r_1)^{-p}(2\pi r_2)^{-q}\int_C \sigma^{\frac{1}{2}p}(\lambda - \sigma)^{\frac{1}{2}q} H_p^{(1)}(r_1\sqrt{\sigma})\, H_q^{(1)}(r_2\sqrt{(\lambda - \sigma)})\, d\sigma \\ &= \frac{i}{4}\left[\frac{\sqrt{\lambda}}{2\pi(r_1^2 + r_2^2)^{\frac{1}{2}}}\right]^{p+q+1} H_{p+q+1}^{(1)}((r_1^2 + r_2^2)^{\frac{1}{2}}\sqrt{\lambda}) \qquad \left(p, q = \frac{1}{2}, 1, \frac{3}{2}, \ldots\right). \end{aligned}\right\} \qquad (1.5.26)$$

Then it follows with eq. (1.2.17) that

$$\frac{1}{2\pi i}\int_C G_0^{(n_2)}(\boldsymbol{x}_2, \boldsymbol{y}_2; \lambda - \sigma)\, G_0^{(n_1)}(\boldsymbol{x}_1, \boldsymbol{y}_1; \sigma)\, d\sigma = G_0^{(n_1 + n_2 - 1)}(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \lambda). \qquad (1.5.27)$$

In this relation the superscripts n refer to the numbers of particles involved. To describe the relative motion of n particles, $3n - 3$ coordinates are required. In particular, for three particles we need six coordinates. Three of these are used for the relative motion of particles 1 and 2, the remaining three for the motion of 3 with respect to the centre

of mass of 1 and 2. Since formally the latter motion is also of the two-particle type, it is consistent that the three-particle function $G_0^{(3)}$ is obtained from a convolution of two two-particle functions $G_0^{(2)}$. More generally, it is indeed the function for n_1+n_2-1 particles we must expect on the right-hand side of eq. (1.5.27), rather than for n_1+n_2 particles.

In evaluating the integral in eq. (1.5.26), it is convenient to deform the contour C into the positive real axis described twice in opposite directions, the origin being encircled clockwise. Then the integral takes the form

$$-\frac{1}{16\pi i}(2\pi r_1)^{-p}(2\pi r_2)^{-q}\int_0^\infty s^{\frac{1}{2}p}(\lambda-s)^{\frac{1}{2}q}J_p(r_1\sqrt{s})\,H_q^{(1)}(r_2\sqrt{(\lambda-s)})\,ds. \tag{1.5.28}$$

If we now make the substitution

$$H_q^{(1)}(r_2\sqrt{(\lambda-s)}) = \frac{2}{\pi i}e^{-\frac{1}{2}q\pi i}K_{-q}(r_2\sqrt{(s-\lambda)}), \tag{1.5.29}$$

where $\sqrt{(s-\lambda)}$ must be chosen such that its real part is positive, we get an integral of the type studied by SONINE and GEGENBAUER. According to WATSON (19), section 13.47, it is proportional to $K_{-p-q-1}(-i(r_1^2+r_2^2)^{\frac{1}{2}}\sqrt{\lambda})$. If this K-function is again expressed in terms of a Hankel function, the desired relation (1.5.26) immediately follows.

It remains to compare the second terms on the right-hand sides of eqs. (1.5.23) and (1.5.24). According to eq. (1.5.4) and the known representations of $R_0(\boldsymbol{x}_2;\lambda-\sigma)$ and $R_{12}(\boldsymbol{x}_1;\sigma)$, we have

$$\left.\begin{aligned}&(g(\boldsymbol{x}_1,\boldsymbol{x}_2),[R_0(\boldsymbol{x}_1,\boldsymbol{x}_2;\lambda)-R(\boldsymbol{x}_1,\boldsymbol{x}_2;\lambda)]f(\boldsymbol{x}_1,\boldsymbol{x}_2))\\ =&\frac{1}{2\pi i}\int_C d\sigma\int\bar{g}(\boldsymbol{x}_1,\boldsymbol{x}_2)\,d\boldsymbol{x}_1\,d\boldsymbol{x}_2\int G_0(\boldsymbol{x}_2,\boldsymbol{y}_2;\lambda-\sigma)\,[G_0(\boldsymbol{x}_1,\boldsymbol{y}_1;\sigma)-G_{12}(\boldsymbol{x}_1,\boldsymbol{y}_1;\sigma)]\,f(\boldsymbol{y}_1,\boldsymbol{y}_2)\,d\boldsymbol{y}_1\,d\boldsymbol{y}_2\\ =&\frac{1}{2\pi i}\int_C d\sigma\int\bar{g}(\boldsymbol{x}_1,\boldsymbol{x}_2)\,d\boldsymbol{x}_1\,d\boldsymbol{x}_2\int G_0(\boldsymbol{x}_2,\boldsymbol{y}_2;\lambda-\sigma)f(\boldsymbol{y}_1,\boldsymbol{y}_2)\,d\boldsymbol{y}_1\,d\boldsymbol{y}_2\int G_0(\boldsymbol{x}_1,\boldsymbol{z}_1;\sigma)V_{12}(\boldsymbol{z}_1)\,G_{12}(\boldsymbol{z}_1,\boldsymbol{y}_1;\sigma)\,d\boldsymbol{z}_1,\end{aligned}\right\} \tag{1.5.30}$$

the third member following from eq. (1.3.27). To establish $R(\boldsymbol{x}_1,\boldsymbol{x}_2;\lambda)$ as an integral operator, it must be shown that in eq. (1.5.30)

$$\int d\sigma\int d\boldsymbol{x}_1\,d\boldsymbol{x}_2\int d\boldsymbol{y}_1\,d\boldsymbol{y}_2 = \int d\boldsymbol{x}_1\,d\boldsymbol{x}_2\int d\boldsymbol{y}_1\,d\boldsymbol{y}_2\int d\sigma. \tag{1.5.31}$$

Writing

$$F(\boldsymbol{x}_1,\boldsymbol{y}_1;\sigma) = -\int G_0(\boldsymbol{x}_1,\boldsymbol{z}_1;\sigma)\,V_{12}(\boldsymbol{z}_1)\,G_{12}(\boldsymbol{z}_1,\boldsymbol{y}_1;\sigma)\,d\boldsymbol{z}_1, \tag{1.5.32}$$

we know from eqs. (1.3.4) and (1.4.36) that

$$\iint|F(\boldsymbol{x}_1,\boldsymbol{y}_1;\sigma)|^2\,d\boldsymbol{x}_1\,d\boldsymbol{y}_1 \le |R_0(\sigma)V_{12}|^2\,\|R_{12}(\sigma)\|^2 \le \text{const.}\,\frac{1}{\operatorname{Im}\sqrt{\sigma}}\,\frac{1}{[\operatorname{Im}\sqrt{(\sigma-\Lambda_{12})}]^4}. \tag{1.5.33}$$

Substituting the expression for $G_0(\boldsymbol{x}_2, \boldsymbol{y}_2; \lambda-\sigma)$ and introducing $\boldsymbol{x}_2 - \boldsymbol{y}_2 = \boldsymbol{y}_2'$ now yields

$$\left.\begin{aligned}
&\int_C d\sigma \int d\boldsymbol{x}_1\, d\boldsymbol{x}_2 \int d\boldsymbol{y}_1\, d\boldsymbol{y}_2 \,|\, \bar{g}(\boldsymbol{x}_1, \boldsymbol{x}_2)\, G_0(\boldsymbol{x}_2, \boldsymbol{y}_2; \lambda-\sigma)\, F(\boldsymbol{x}_1, \boldsymbol{y}_1; \sigma)\, f(\boldsymbol{y}_1, \boldsymbol{y}_2)\,| \\
&= \frac{1}{4\pi} \int_C d\sigma \int d\boldsymbol{x}_1\, d\boldsymbol{x}_2 \int d\boldsymbol{y}_1\, d\boldsymbol{y}_2' \left| \bar{g}(\boldsymbol{x}_1, \boldsymbol{x}_2)\, \frac{e^{i\sqrt{\lambda-\sigma}\,|\boldsymbol{y}_2'|}}{|\boldsymbol{y}_2'|}\, F(\boldsymbol{x}_1, \boldsymbol{y}_1; \sigma)\, f(\boldsymbol{y}_1, \boldsymbol{x}_2 - \boldsymbol{y}_2') \right| \\
&\leq \frac{1}{4\pi} \int_C d\sigma \int d\boldsymbol{y}_2' \left| \frac{e^{i\sqrt{\lambda-\sigma}\,|\boldsymbol{y}_2'|}}{|\boldsymbol{y}_2'|} \right| \|g\|\, |F(\sigma)|\, \|f\| \\
&\leq \text{const.} \int_C d\sigma\, \frac{1}{[\operatorname{Im}\sqrt{(\lambda-\sigma)}]^2}\, \frac{1}{(\operatorname{Im}\sqrt{\sigma})^{\frac{1}{2}}}\, \frac{1}{[\operatorname{Im}\sqrt{(\sigma-\Lambda_{12})}]^2}\, \|g\|\, \|f\|,
\end{aligned}\right\} \tag{1.5.34}$$

which is certainly finite if C is a suitable contour. Hence, if we interpret $\int_C d\sigma$ as a Lebesgue integral once more, as was done at the end of the previous section, we may invert the order of integration according to eq. (1.5.31) by Fubini's theorem. Then it follows that the resolvent is indeed an integral operator, the kernel of which can be evaluated by means of a convolution integral according to eq. (1.5.22).

1.5.3. Uniqueness of the Green function

It follows from the general theory of Hilbert space that the resolvent is unique. However, this does not imply that it can be represented by a Green function in only one single way. Let us therefore first consider the problem of the uniqueness of the function G_0. According to eq. (1.2.17), there is a function G_0 which depends only on $\boldsymbol{x}-\boldsymbol{y}$, and which is an integrable function of this difference. Let us now imagine that there are two functions G_0 with these properties, and let us denote their difference by Q_0. Then Q_0 satisfies

$$\int |\, Q_0(\boldsymbol{x}-\boldsymbol{y})\,|\, d(\boldsymbol{x}-\boldsymbol{y}) < \infty. \tag{1.5.35}$$

Also, by the uniqueness of the resolvent,

$$\int \bar{g}(\boldsymbol{x})\, d\boldsymbol{x} \int Q_0(\boldsymbol{x}-\boldsymbol{y})\, f(\boldsymbol{y})\, d\boldsymbol{y} = 0 \tag{1.5.36}$$

for every f and g in $\mathfrak{L}^2$. Writing $\boldsymbol{x}-\boldsymbol{y} = \boldsymbol{z}$ and going over to Fourier transforms $\hat{f}$ and $\hat{g}$ yields

$$\iint \bar{\hat{g}}(\boldsymbol{k})\, Q_0(\boldsymbol{z})\, e^{-i\boldsymbol{k}\cdot\boldsymbol{z}}\, \hat{f}(\boldsymbol{k})\, d\boldsymbol{z}\, d\boldsymbol{k} = 0. \tag{1.5.37}$$

In view of the arbitrariness of $\hat{f}$ and $\hat{g}$, it now follows that

$$\int Q_0(\boldsymbol{z})\, e^{-i\boldsymbol{k}\cdot\boldsymbol{z}}\, d\boldsymbol{z} = 0 \tag{1.5.38}$$

for almost every $\boldsymbol{k}$. But this result can easily be extended. For, owing to eq. (1.5.35), the integral in eq. (1.5.38) is absolutely convergent. It is easily shown that as a consequence it is a continuous function of $\boldsymbol{k}$. Hence it vanishes not only for almost every $\boldsymbol{k}$, but in fact for every $\boldsymbol{k}$. From this it now follows that $Q_0(\boldsymbol{z})$ vanishes for almost every $\boldsymbol{z}$ (TITCHMARSH(20) section 6.7), so that the Green function $G_0(\boldsymbol{x}, \boldsymbol{y}; \lambda)$ is in fact unique among all integrable functions of $\boldsymbol{x}-\boldsymbol{y}$. It will be observed that this conclusion does not depend on the number of particles involved.

We now turn to the function G. After the foregoing, it suffices to consider the difference $G-G_0$. It was already used at the end of the preceding section that this depends only on $\boldsymbol{x}_1, \boldsymbol{y}_1$, and $\boldsymbol{x}_2-\boldsymbol{y}_2$, and that it satisfies

$$\int \left[\int | G(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \lambda) - G_0(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \lambda) | \, d(\boldsymbol{x}_2-\boldsymbol{y}_2) \right]^2 d\boldsymbol{x}_1 \, d\boldsymbol{y}_1 < \infty. \quad (1.5.39)$$

Let us now again assume that there are two functions $G-G_0$ with these properties, and let us denote their difference by $Q(\boldsymbol{x}_1, \boldsymbol{y}_1, \boldsymbol{x}_2-\boldsymbol{y}_2)$. This gives

$$\int \bar{g}(\boldsymbol{x}_1, \boldsymbol{x}_2) \, d\boldsymbol{x}_1 \, d\boldsymbol{x}_2 \int Q(\boldsymbol{x}_1, \boldsymbol{y}_1, \boldsymbol{x}_2-\boldsymbol{y}_2) f(\boldsymbol{y}_1, \boldsymbol{y}_2) \, d\boldsymbol{y}_1 \, d\boldsymbol{y}_2 = 0. \quad (1.5.40)$$

Choosing in particular

$$f(\boldsymbol{x}_1, \boldsymbol{x}_2) = a(\boldsymbol{x}_1) f(\boldsymbol{x}_2), \quad g(\boldsymbol{x}_1, \boldsymbol{x}_2) = b(\boldsymbol{x}_1) g(\boldsymbol{x}_2), \quad (1.5.41)$$

we easily get an equation analogous to eq. (1.5.37), viz.

$$\int\int \bar{\hat{g}}(\boldsymbol{k}) \left[\int\int \bar{b}(\boldsymbol{x}_1) Q(\boldsymbol{x}_1, \boldsymbol{y}_1, \boldsymbol{z}) a(\boldsymbol{y}_1) \, d\boldsymbol{x}_1 \, d\boldsymbol{y}_1 \right] e^{-i\boldsymbol{k}\cdot\boldsymbol{z}} \hat{f}(\boldsymbol{k}) \, d\boldsymbol{z} \, d\boldsymbol{k} = 0. \quad (1.5.42)$$

As above, this implies that

$$\int e^{-i\boldsymbol{k}\cdot\boldsymbol{z}} d\boldsymbol{z} \int\int \bar{b}(\boldsymbol{x}_1) Q(\boldsymbol{x}_1, \boldsymbol{y}_1, \boldsymbol{z}) a(\boldsymbol{y}_1) \, d\boldsymbol{x}_1 \, d\boldsymbol{y}_1 = 0 \quad (1.5.43)$$

for almost every $\boldsymbol{k}$, and even for every $\boldsymbol{k}$. From the arbitrariness of a and b it now follows that

$$\int Q(\boldsymbol{x}_1, \boldsymbol{y}_1, \boldsymbol{z}) e^{-i\boldsymbol{k}\cdot\boldsymbol{z}} \, d\boldsymbol{z} = 0 \quad (1.5.44)$$

identically in $\boldsymbol{k}$ for almost every $\boldsymbol{x}_1, \boldsymbol{y}_1$. Also, the integral in eq. (1.5.44) converges absolutely for almost every $\boldsymbol{x}_1, \boldsymbol{y}_1$, by Fubini's theorem and the integrability properties of Q. Hence, for almost every $\boldsymbol{x}_1, \boldsymbol{y}_1$ we have an integrable function of $\boldsymbol{z}$, the Fourier transform of which vanishes identically. Since such a function is known to vanish for almost every $\boldsymbol{z}$, it follows that $Q(\boldsymbol{x}_1, \boldsymbol{y}_1, \boldsymbol{z}) = 0$ for almost every $\boldsymbol{x}_1, \boldsymbol{y}_1, \boldsymbol{z}$. Hence, among all the functions with integrability properties as indicated by the relation (1.5.39), the function $G-G_0$ is unique, with the trivial exception of sets of measure zero. In particular, $G-G_0$ does not depend on the choice of the contour C, as long as $\int_C d\sigma$ converges properly. This was plausible from the outset. But it was not obvious,

say from an argument about contour integration, as we have not discussed the analytic properties of functions which depend not only on λ, but also on variables $\boldsymbol{x}$ and $\boldsymbol{y}$.

It follows from eqs. (1.5.22) and (1.3.17) that

$$\overline{G}(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \lambda) = -\frac{1}{2\pi i}\int_{\overline{C}} G_0(\boldsymbol{x}_2, \boldsymbol{y}_2; \bar{\lambda}-\bar{\sigma})\, G_{12}(\boldsymbol{x}_1, \boldsymbol{y}_1; \bar{\sigma})\, d\bar{\sigma}, \tag{1.5.45}$$

where $\overline{C}$ is the reflection of C in the real axis. Now the right-hand side of eq. (1.5.45) is equal to a function of the form $G(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \bar{\lambda})$. Hence, since the Green function is unique,

$$\overline{G}(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \lambda) = G(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \bar{\lambda}). \tag{1.5.46}$$

Also, by eq. (1.3.18),

$$G(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \lambda) = G(\boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{x}_1, \boldsymbol{x}_2; \lambda). \tag{1.5.47}$$

1.6. The Green function for three particles

1.6.1. The resolvent equation

After the preparations made in the previous sections, it is comparatively easy to find the Green function for a system of three particles in which there are non-vanishing interactions V_{12}, V_{13}, and V_{23}. With the choice of coordinates discussed in section 1.2.1, these are functions

$$V_{12} = V_{12}(c_{12}^1 \boldsymbol{x}_1), \quad V_{13} = V_{13}(c_{13}^1 \boldsymbol{x}_1 + c_{13}^2 \boldsymbol{x}_2), \quad V_{23} = V_{23}(c_{23}^1 \boldsymbol{x}_1 + c_{23}^2 \boldsymbol{x}_2), \tag{1.6.1}$$

where it is essential that the constants c_{ij}^k do not vanish. To save writing, we define $V_{ji} \equiv V_{ij}$ $(i<j)$. The resolvent for the present problem is denoted by $R_{123}^{(3)}$, the upper index indicating that three particles are involved, and the lower index that all the three interactions are present. The resolvent for the three-particle system without interaction is henceforth denoted by $R_0^{(3)}$, the one with interaction V_{ij} only by $R_{ij}^{(3)}$. There is no need to consider a three-particle system with two interaction terms such as $V_{ij} + V_{ik}$.

From the considerations which led to the resolvent equation (1.2.14), it is easily seen that $R_{123}^{(3)}$ satisfies

$$R_{123}^{(3)}(\lambda) = R_{ij}^{(3)}(\lambda) - R_0^{(3)}(\lambda)\Big(\sum_{i<j} V_{ij}\Big) R_{123}^{(3)}(\lambda), \tag{1.6.2}$$

as well as the three equations of the form

$$R_{123}^{(3)}(\lambda) = R_{ij}^{(3)}(\lambda) - R_{ij}^{(3)}(\lambda)(V_{ik} + V_{jk}) R_{123}^{(3)}(\lambda) \quad (i<j,\ i\neq k,\ j\neq k). \tag{1.6.3}$$

Also,

$$R_{ij}^{(3)}(\lambda) = R_0^{(3)}(\lambda) - R_0^{(3)}(\lambda) V_{ij} R_{ij}^{(3)}(\lambda). \tag{1.6.4}$$

Adding the three equations (1.6.3), subtracting twice equation (1.6.2) and using the relations (1.6.4) yields

$$\left.\begin{aligned} R^{(3)}_{123}(\lambda)f(\boldsymbol{x}) &= \sum_{i<j} R^{(3)}_{ij}(\lambda)f(\boldsymbol{x}) - 2\,R^{(3)}_{0}(\lambda)f(\boldsymbol{x}) + \sum_{\substack{i<j\\ i\neq k,\, j\neq k}} [R^{(3)}_{0}(\lambda) - R^{(3)}_{ij}(\lambda)]\,(V_{ik}+V_{jk})\,R^{(3)}_{123}(\lambda)f(\boldsymbol{x}) \\ &= \sum_{i<j} R^{(3)}_{ij}(\lambda)f(\boldsymbol{x}) - 2\,R^{(3)}_{0}(\lambda)f(\boldsymbol{x}) + \sum_{\substack{i<j\\ i\neq k,\, j\neq k}} R^{(3)}_{0}(\lambda)\,V_{ij}\,R^{(3)}_{ij}(\lambda)\,(V_{ik}+V_{jk})\,R^{(3)}_{123}(\lambda)f(\boldsymbol{x}). \end{aligned}\right\} \quad (1.6.5)$$

The point is now that this can be written out as an integral equation for $R^{(3)}_{123}(\lambda)\,f(\boldsymbol{x})$ the kernel of which will be shown to belong to $\mathfrak{L}^2$. This means that from the Hilbert-space point of view eq. (1.6.5) is entirely analogous to the two-particle equation (1.3.2). In particular, it can be solved by the Fredholm technique. And owing to our knowledge of the bounds and the analyticity properties of the resolvents $R^{(3)}_0$ and $R^{(3)}_{ij}$, the symmetries of the associated Green functions, and related matters, all considerations of section 1.3 can be carried over directly to the present problem. We thus find a Green function of the form

$$\left.\begin{aligned} G^{(3)}_{123}(\boldsymbol{x},\boldsymbol{y};\,\lambda) &= \sum_{i<j} G^{(3)}_{ij}(\boldsymbol{x},\boldsymbol{y};\,\lambda) - 2\,G^{(3)}_{0}(\boldsymbol{x},\boldsymbol{y};\,\lambda) \\ &+ \frac{1}{\Delta^{(3)}_{123}(\lambda)} \int D^{(3)}_{123}(\boldsymbol{x},\boldsymbol{z};\,\lambda)\Big[\sum_{i<j} G^{(3)}_{ij}(\boldsymbol{z},\boldsymbol{y};\,\lambda) - 2\,G^{(3)}_{0}(\boldsymbol{z},\boldsymbol{y};\,\lambda)\Big]\,d\boldsymbol{z}, \end{aligned}\right\} \quad (1.6.6)$$

which is entirely analogous to the two-particle Green function discussed in section 1.3. It is obvious that in eq. (1.6.6) $\boldsymbol{x}$, $\boldsymbol{y}$, and $\boldsymbol{z}$ are meant to be six-dimensional coordinates. From the properties of the resolvents $R^{(3)}_{ij}$ it follows that in the three-particle case there is a cut in the λ-plane from $\min(\Delta_{12}, \Delta_{13}, \Delta_{23})$ to ∞, Δ_{ij} being the lower bound of the two-particle spectrum concerned. In the cut plane, the resolvent $R^{(3)}_{123}(\lambda)$ is regular except for possible poles.

1.6.2. An upper bound for the kernel

To return to the equation we have to solve, eq. (1.6.5) is of the form

$$\left.\begin{aligned} h^{(3)}_{123}(\boldsymbol{x};\,\lambda) &= \sum_{i<j} h^{(3)}_{ij}(\boldsymbol{x};\,\lambda) - 2\,h^{(3)}_{0}(\boldsymbol{x};\,\lambda) + \int K^{(3)}_{123}(\boldsymbol{x},\boldsymbol{y};\,\lambda)\,h^{(3)}_{123}(\boldsymbol{y};\,\lambda)\,d\boldsymbol{y}, \\ h^{(3)}_{123}(\boldsymbol{x};\,\lambda) &\equiv R^{(3)}_{123}(\lambda)f(\boldsymbol{x}), \\ h^{(3)}_{ij}(\boldsymbol{x};\,\lambda) &\equiv R^{(3)}_{ij}(\lambda)f(\boldsymbol{x}) = \int G^{(3)}_{ij}(\boldsymbol{x},\boldsymbol{z};\,\lambda)\,f(\boldsymbol{z})\,d\boldsymbol{z}, \\ h^{(3)}_{0}(\boldsymbol{x};\,\lambda) &\equiv R^{(3)}_{0}(\lambda)f(\boldsymbol{x}) = \int G^{(3)}_{0}(\boldsymbol{x},\boldsymbol{z};\,\lambda)\,f(\boldsymbol{z})\,d\boldsymbol{z}, \\ K^{(3)}_{123}(\boldsymbol{x},\boldsymbol{y};\,\lambda) &= \sum_{\substack{i<j\\ i\neq k,\, j\neq k}} [G^{(3)}_{0}(\boldsymbol{x},\boldsymbol{y};\,\lambda) - G^{(3)}_{ij}(\boldsymbol{x},\boldsymbol{y};\,\lambda)]\,[V_{ik}(\boldsymbol{y}) + V_{jk}(\boldsymbol{y})]. \end{aligned}\right\} \quad (1.6.7)$$

It is now shown that each of the three terms in the expression for $K^{(3)}_{123}$ belongs to $\mathfrak{L}^2$. Then the same applies to $K^{(3)}_{123}$ itself. In particular, let us consider the term with $i, j = 1, 2$. For this it follows from eqs. (1.5.22) and (1.5.23) that

$$\left.\begin{aligned} & G_0^{(3)}(\boldsymbol{x},\boldsymbol{y};\,\lambda) - G_{12}^{(3)}(\boldsymbol{x},\boldsymbol{y};\,\lambda) \\ &= \frac{1}{2\pi i}\int_C G_0^{(2)}(\boldsymbol{x}_2,\boldsymbol{y}_2;\,\lambda-\sigma)\,d\sigma \int G_0^{(2)}(\boldsymbol{x}_1,\boldsymbol{z}_1;\,\sigma)\,V_{12}(c_{12}^1\boldsymbol{z}_1)\,G_{12}^{(2)}(\boldsymbol{z}_1,\boldsymbol{y}_1;\,\sigma)\,d\boldsymbol{z}_1 . \end{aligned}\right\} \tag{1.6.8}$$

Repeated application of Schwarz's inequality yields

$$\left.\begin{aligned} I &\equiv \left[\int |G_0^{(3)}(\boldsymbol{x},\boldsymbol{y};\,\lambda) - G_{12}^{(3)}(\boldsymbol{x},\boldsymbol{y};\,\lambda)|^2\,d\boldsymbol{x}_1\,d\boldsymbol{y}_1\,d(\boldsymbol{x}_2-\boldsymbol{y}_2)\right]^{\frac{1}{2}} \\ &\leq \frac{1}{2\pi}\left\{\int_C d\sigma\left[\int |G_0^{(2)}(\boldsymbol{x}_2,\boldsymbol{y}_2;\,\lambda-\sigma)|^2\,d(\boldsymbol{x}_2-\boldsymbol{y}_2)\right]^{\frac{1}{2}}\right. \\ &\times \left.\left[\int\left|\int G_0^{(2)}(\boldsymbol{x}_1,\boldsymbol{z}_1;\,\sigma)\,V_{12}(c_{12}^1\boldsymbol{z}_1)\,G_{12}^{(2)}(\boldsymbol{z}_1,\boldsymbol{y}_1;\,\sigma)\,d\boldsymbol{z}_1\right|^2 d\boldsymbol{x}_1\,d\boldsymbol{y}_1\right]^{\frac{1}{2}}\right\} . \end{aligned}\right\} \tag{1.6.9}$$

With the relation

$$4\pi\int\left|\frac{e^{ir\sqrt{\lambda-\sigma}}}{4\pi r}\right|^2 r^2\,dr \leq \frac{1}{8\pi\,\mathrm{Im}\,\sqrt{(\lambda-\sigma)}} \tag{1.6.10}$$

to be used in connection with $G_0^{(2)}(\boldsymbol{x}_2,\boldsymbol{y}_2;\,\lambda-\sigma)$, and eqs. (1.5.32) and (1.5.33) for the second factor on the right-hand side of eq. (1.6.9), the inequality (1.6.9) can be reduced to

$$\left.\begin{aligned} I &\leq \text{const.}\int_C \frac{1}{[\mathrm{Im}\,\sqrt{(\lambda-\sigma)}]^{\frac{1}{2}}}\,\frac{1}{[\mathrm{Im}\,\sqrt{(\sigma-\Lambda_{12})}]^{\frac{5}{2}}}\,d\sigma \\ &\leq \text{const.}\left[\int_C \frac{d\sigma}{[\mathrm{Im}\,\sqrt{(\lambda-\sigma)}]^3}\right]^{\frac{1}{6}}\left[\int_C \frac{d\sigma}{[\mathrm{Im}\,\sqrt{(\sigma-\Lambda_{12})}]^3}\right]^{\frac{5}{6}}, \end{aligned}\right\} \tag{1.6.11}$$

the third member of eq. (1.6.11) following from Hölder's inequality (TITCHMARSH(15) section 12.42). In passing from eq. (1.5.33) to eq. (1.6.11), use was made of the relation

$$\mathrm{Im}\,\sqrt{(\sigma-\Lambda_{12})} \leq \mathrm{Im}\,\sqrt{\bar{\sigma}}, \tag{1.6.12}$$

which holds true by virtue of Λ_{12} being real and non-positive.

To find an upper bound for I, it is now convenient to write

$$\lambda-\Lambda_{12} = l e^{i\varphi} \tag{1.6.13}$$

and to choose as the contour C the straight line

$$\sigma = s e^{\frac{1}{2}i\varphi} - \frac{1}{2}l + \Lambda_{12} \quad (-\infty < s < \infty) . \tag{1.6.14}$$

This line is tangent to the parabolas $[\mathrm{Im}\,\sqrt{(\sigma-\Lambda_{12})}]^2 = \frac{1}{2}[\mathrm{Im}\,\sqrt{(\lambda-\Lambda_{12})}]^2$ and $[\mathrm{Im}\,\sqrt{(\lambda-\sigma)}]^2 = \frac{1}{2}[\mathrm{Im}\,\sqrt{(\lambda-\Lambda_{12})}]^2$. These parabolas in turn are tangent to one

another, the line in question passing through their point of contact. It follows from a straightforward calculation that on the line (1.6.14)

$$\left.\begin{aligned}[\operatorname{Im}\sqrt{(\sigma-\Lambda_{12})}]^2 &= -\frac{1}{2}\cos\frac{1}{2}\varphi\left(s-\frac{1}{2}l\cos\frac{1}{2}\varphi\right)+\frac{1}{4}l\sin^2\frac{1}{2}\varphi+\frac{1}{2}\left[\left(s-\frac{1}{2}l\cos\frac{1}{2}\varphi\right)^2+\frac{1}{4}l^2\sin^2\frac{1}{2}\varphi\right]^{\frac{1}{2}},\\ [\operatorname{Im}\sqrt{(\lambda-\sigma)}]^2 &= \frac{1}{2}\cos\frac{1}{2}\varphi\left(s-\frac{3}{2}l\cos\frac{1}{2}\varphi\right)+\frac{1}{4}l\sin^2\frac{1}{2}\varphi+\frac{1}{2}\left[\left(s-\frac{3}{2}l\cos\frac{1}{2}\varphi\right)^2+\frac{1}{4}l^2\sin^2\frac{1}{2}\varphi\right]^{\frac{1}{2}}.\end{aligned}\right\} \tag{1.6.15}$$

Substituting this into eq. (1.6.11) yields

$$I \leq \text{const.}\int_{-\infty}^{\infty}\left[t\cos\frac{1}{2}\varphi+\frac{1}{2}l\sin^2\frac{1}{2}\varphi+\left(t^2+\frac{1}{4}l^2\sin^2\frac{1}{2}\varphi\right)^{\frac{1}{2}}\right]^{-\frac{3}{2}}dt. \tag{1.6.16}$$

The change of variables $t=\frac{1}{2}l\sin\frac{1}{2}\varphi\sinh\psi$ now gives

$$I \leq \text{const.}\frac{1}{\sqrt{l}\sin^2\frac{1}{2}\varphi}\int_{-\infty}^{\infty}\cosh\psi\left[\frac{\cos\frac{1}{2}\varphi}{\sin\frac{1}{2}\varphi}\sinh\psi+\frac{1}{\sin\frac{1}{2}\varphi}\cosh\psi+1\right]^{-\frac{3}{2}}d\psi. \tag{1.6.17}$$

At this point it is convenient to write

$$\frac{\cos\frac{1}{2}\varphi}{\sin\frac{1}{2}\varphi}=\sinh\chi,\qquad \frac{1}{\sin\frac{1}{2}\varphi}=\cosh\chi,\qquad \omega=\psi+\chi, \tag{1.6.18}$$

and to go over from the integration variable ψ to ω. Then the inequality for I takes the form

$$I \leq \text{const.}\frac{1}{\sqrt{l}\sin^2\frac{1}{2}\varphi}\int_{-\infty}^{\infty}\left[\frac{1}{\sin\frac{1}{2}\varphi}\cosh\omega-\frac{\cos\frac{1}{2}\varphi}{\sin\frac{1}{2}\varphi}\sinh\omega\right](\cosh\omega+1)^{-\frac{3}{2}}d\omega. \tag{1.6.19}$$

Since the term involving $\sinh\omega$ clearly gives no contribution to the integral, we finally obtain

$$I \leq \text{const.}\frac{1}{\sqrt{l}\sin^3\frac{1}{2}\varphi}=\text{const.}\frac{|\lambda-\Lambda_{12}|}{[\operatorname{Im}\sqrt{(\lambda-\Lambda_{12})}]^3}. \tag{1.6.20}$$

This must now be combined with eq. (1.6.9) and with the last line of eq. (1.6.7). If in the latter expression we use the explicit coordinate-dependence of V_{13} and V_{23} as given by eq. (1.6.1), we get

$$\int |G_0^{(3)}(\boldsymbol{x},\boldsymbol{y};\lambda) - G_{12}^{(3)}(\boldsymbol{x},\boldsymbol{y};\lambda)|^2 |V_{13}(c_{13}^1\boldsymbol{y}_1 + c_{13}^2\boldsymbol{y}_2) + V_{23}(c_{23}^1\boldsymbol{y}_1 + c_{23}^2\boldsymbol{y}_2)|^2 d\boldsymbol{x}_1 d\boldsymbol{y}_1 d(\boldsymbol{x}_2 - \boldsymbol{y}_2) d\boldsymbol{y}_2 \Big| \leq \text{const.} \frac{|\lambda - \Lambda_{12}|^2}{[\text{Im} \sqrt{(\lambda - \Lambda_{12})}]^6}. \Big\} \quad (1.6.21)$$

It will be observed that, as regards the integration with respect to $\boldsymbol{y}_2$, it is essential that c_{13}^2 and c_{23}^2 do not vanish, and that V_{ij} is assumed to be square-integrable.

The inequality (1.6.21) obviously states that in the sum for $K_{123}^{(3)}$ the term with $i, j = 1, 2$ belongs to $\mathfrak{L}^2$ provided λ is an interior point of the complex plane cut from Λ_{12} to ∞. If for a moment we imagine a choice of coordinates adapted to $i, j = 1, 3$ or $2, 3$, we see that these cases can be discussed along exactly the same lines. Hence each term in the sum for $K_{123}^{(3)}$ belongs to $\mathfrak{L}^2$, and so does $K_{123}^{(3)}$ itself, provided λ is inside the complex plane cut from $\min(\Lambda_{12}, \Lambda_{13}, \Lambda_{23})$ to ∞. Moreover, it follows with eq. (1.6.21) that if λ is negative and sufficiently small, the $\mathfrak{L}^2$-norm of $K_{123}^{(3)}$ is less than 1. From this it follows by the argument used in connection with eqs. (1.3.49) and (1.3.50) that the spectrum of $H_{123}^{(3)}$ is bounded below.

Summarizing, we see that the properties of $K_{123}^{(3)}$ are such that in the λ-plane cut from $\min(\Lambda_{12}, \Lambda_{13}, \Lambda_{23})$ to ∞ we can evaluate the Green function $G_{123}^{(3)}$ by the Fredholm method outlined in section 1.3. In the cut plane the resolvent is regular except for possible poles confined to a finite interval of the real axis. Now it will be shown in a forthcoming paper on the theory of scattering that in the present case there is a continuous spectrum from $\min(\Lambda_{12}, \Lambda_{13}, \Lambda_{23})$ to ∞. Hence, if there are no poles in the cut plane and we introduce $\Lambda_{123} \equiv \min(\Lambda_{12}, \Lambda_{13}, \Lambda_{23})$, the Λ_{123} thus defined is the lower bound of the spectrum. And if there are poles, there is still a lower bound Λ_{123}, which is then less than $\min(\Lambda_{12}, \Lambda_{13}, \Lambda_{23})$. In either case it is clear from previous arguments that the norm of $R_{123}^{(3)}$ satisfies

$$\| R_{123}^{(3)}(\lambda) \| \leq \min\left(\frac{1}{[\text{Im} \sqrt{(\lambda - \Lambda_{123})}]^2}, \frac{1}{|\text{Im}\, \lambda|} \right), \quad (1.6.22)$$

cf. eqs. (1.3.29) and (1.4.36). Furthermore, with eq. (1.6.21) it is not difficult to see that

$$|K_{123}^{(3)}(\lambda)| \leq \text{const.} \frac{|\lambda - \Lambda_{123}|}{[\text{Im} \sqrt{(\lambda - \Lambda_{123})}]^3}. \quad (1.6.23)$$

It follows from the foregoing that in the expression (1.6.6) for the Green function $G_{123}^{(3)}$ the last term on the right-hand side belongs to $\mathfrak{L}^2$. Clearly it is the kernel of the integral operator

$$O \equiv R_{123}^{(3)} - \sum_{i<j} R_{ij}^{(3)} + 2 R_0^{(3)}. \quad (1.6.24)$$

But this operator is unique in the sense that, if f and g are any two functions in $\mathfrak{L}^2$, the quantity (g, Of) is uniquely determined. From this it follows with arguments such

as used in section 1.5.3 that, among all the kernels in $\mathfrak{L}^2$, the last term on the right-hand side of eq. (1.6.6) is unique. Also, the Green functions $G_0^{(3)}$ and $G_{ij}^{(3)}$ are unique in the sense specified in section 1.5.3. As a result, $G_{123}^{(3)}$ is unique in the sense that it can be written as a sum of functions with suitable integrability properties in only one way.

As a concluding remark it seems worth while to point out that in the above arguments it is an essential step to consider the somewhat complicated resolvent equation (1.6.5). If we had merely confined ourselves to eq. (1.6.2), we should have had a kernel of the form

$$G_0^{(3)}(\boldsymbol{x}, \boldsymbol{y}; \lambda) \sum_{i<j} V_{ij}(\boldsymbol{y}), \tag{1.6.25}$$

which certainly does not belong to $\mathfrak{L}^2$. For $G_0^{(3)}$ depends only on the difference $|\boldsymbol{x}-\boldsymbol{y}|$, according to eq. (1.5.25), and V_{12} depends only on $\boldsymbol{y}_1$. Hence $G_0^{(3)} V_{12}$ might be a square-integrable function of $\boldsymbol{x}_1-\boldsymbol{y}_1$, $\boldsymbol{x}_2-\boldsymbol{y}_2$, and $\boldsymbol{y}_1$ at best, rather than a function which is square-integrable with respect to four independent variables. However, even square-integrability with respect to three variables does not hold, since for $\boldsymbol{x} = \boldsymbol{y}$ the function $G_0^{(3)}$ has a singularity which prevents it from being square-integrable. Similar remarks apply to $G_0^{(3)} V_{13}$ and $G_0^{(3)} V_{23}$. Apparently the gist of eq. (1.6.5) is that in this equation a first approximation to $R_{123}^{(3)}$ is split off which is so good that the remainder is sufficiently regular and for large $|\boldsymbol{x}|$ and $|\boldsymbol{y}|$ falls off sufficiently rapidly for the equation to be soluble by the Fredholm method.

1.7. General numbers of particles

1.7.1. The resolvent equation

For discussing a general system of n particles, it is convenient to adopt the following notation. The symbol $(n, k)_{p(k)}$ denotes a certain way in which n particles can be split into k groups. Here the subscript $p(k)$ refers to the particular mode of division. Hence $p(k) = 1, 2, \ldots, N(n, k)$, where $N(n, k)$ denotes the number of ways in which n particles can be split into k groups. In the case of a particular division $(n, k)_{p(k)}$, let us imagine that all the interactions between the particles which together form a group are present, but that there are no interactions between particles belonging to different groups. The total interaction present in this way is denoted by $V(n, k)_{p(k)}$. The resolvent for the n-particle system with this interaction is called $R(n, k)_{p(k)}$. It will be shown that it is an integral operator with kernel $G(n, k)_{p(k)}$, the Green function. Comparing this notation with the one used thus far, we have, for example,

$$\left.\begin{aligned} V(n,1) &= \sum_{i<j} V_{ij} = V, & R(n,1) &= R_{12\ldots n}^{(n)} = R, \\ V(n,n) &= 0, & R(n,n) &= R_0^{(n)}. \end{aligned}\right\} \tag{1.7.1}$$

It is also convenient to make use of the symbol $\subset$, where $(n, k+1)_{p(k+1)} \subset (n, k)_{p(k)}$ indicates that the division $(n, k+1)_{p(k+1)}$ is contained in $(n, k)_{p(k)}$ in the sense that it can be obtained from $(n, k)_{p(k)}$ by splitting one group of the latter division into two, the remaining groups being left unchanged.

It is the purpose of the present section to show that for $n \geq 2$ the resolvent satisfies the equation

$$\left.\begin{aligned} R(n,1) &= \sum_{k=2}^{n} \sum_{p(k)=1}^{N(n,k)} (-1)^k (k-1)!\, R(n,k)_{p(k)} \\ &+ (-1)^{n-1} \sum_{\substack{p(n-1),\ldots,p(k),\ldots,p(2) \\ (n,n-1)_{p(n-1)} \subset \cdots \subset (n,k)_{p(k)} \subset \cdots \subset (n,2)_{p(2)}}} \ldots \sum \{ R(n,n) V(n,n-1)_{p(n-1)} R(n,n-1)_{p(n-1)} [V(n,n-2)_{p(n-2)} - V(n,n-1)_{p(n-1)}] \\ &\times \ldots R(n,k+1)_{p(k+1)} [V(n,k)_{p(k)} - V(n,k+1)_{p(k+1)}] \ldots R(n,2)_{p(2)} [V(n,1) - V(n,2)_{p(2)}] \} R(n,1). \end{aligned}\right\} \quad (1.7.2)$$

It will be observed that this equation was already established for $n = 2$ and $n = 3$. One of its features is that with all the groups of particles considered, there are always interactions between all the particles in each group. In other words, for discussing a mode of division in which the particles i, j, and l together form a group, we need the properties of the three-particle system with interaction $V_{ij} + V_{il} + V_{jl}$. But nowhere in the analysis does there occur an "unphysical" system such as the one with interaction $V_{il} + V_{jl}$ only.

In the notation of the preceding sections, eq. (1.7.2) gives an equation for $R^{(4)}_{1234}$ in terms of $R^{(4)}_0$, the six resolvents of the form $R^{(4)}_{ij}$, the four of the form $R^{(4)}_{ijk}$, and the three of the form $R^{(4)}_{ij;\,kl}$. Here $R^{(4)}_{ij;\,kl}$ stands for the resolvent of the four-particle system with interaction $V_{ij} + V_{kl}$ $(i \neq k,\ i \neq l,\ j \neq k,\ j \neq l)$. As will be discussed in some detail later, it can be obtained from a convolution of the resolvents $R^{(2)}_{ij}$, $R^{(2)}_{kl}$, and $R^{(2)}_0$.

Let us now assume that for $n-1$ particles $(n \geq 3)$ eq. (1.7.2) is established by a combinatorial argument based on the set of resolvent equations

$$R(n-1,k)_{p(k)} = R(n-1,l)_{p(l)} - R(n-1,l)_{p(l)} [V(n-1,k)_{p(k)} - V(n-1,l)_{p(l)}] R(n-1,k)_{p(k)} \quad (1.7.3)$$

with fixed $n-1$, the numbers $k, l, p(k), p(l)$ taking all possible values. Then it can be shown that the desired equation for n particles follows on combining resolvent equations of the form (1.7.3), but with $n-1$ replaced by n. For the proof it is convenient to choose a particular mode of division $(n, n-1)_{p(n-1)}$, and to consider the expression

$$\left.\begin{aligned} S(n,n-1)_{p(n-1)} \equiv (-1)^{n-1} \sum_{\substack{p(n-2),\ldots,p(k),\ldots,p(2) \\ (n,n-1)_{p(n-1)} \subset (n,n-2)_{p(n-2)} \subset \cdots \subset (n,2)_{p(2)}}} \ldots \sum \{ & R(n,n-1)_{p(n-1)} [V(n,n-2)_{p(n-2)} - V(n,n-1)_{p(n-1)}] \\ & \times \ldots R(n,2)_{p(2)} [V(n,1) - V(n,2)_{p(2)}] \} R(n,1), \end{aligned}\right\} \quad (1.7.4)$$

which differs from the sum in eq. (1.7.2) in that the factor $R(n,n)\,V(n,n-1)_{p(n-1)}$ and the summation over $p(n-1)$ are left out.

It is obvious that the division $(n,\,n-1)_{p(n-1)}$ must consist of $n-2$ free particles plus a group consisting of two particles, say the particles i and j. Furthermore, the structure of the sum in eq. (1.7.4) is such that in all factors the particles i and j always belong to the same group. Hence if we temporarily consider i and j together as one composite particle, we can say that in a certain sense the multiple sum in eq. (1.7.4) involves only $n-1$ (composite) particles. This suggests that we compare it with the multiple sum which appears in the equation for $n-1$ particles. By assumption, there is a combinatorial argument based on the set of equations (1.7.3) to show that the latter sum is equal to a certain linear combination of resolvents $R(n-1,\,k)_{p(k)}$. Now to each equation (1.7.3) there corresponds an equation

$$\left.\begin{aligned} R(n,k)_{p(k)} = {} & R(n,l)_{p(l)} - R(n,l)_{p(l)}\,[V(n,k)_{p(k)} - V(n,l)_{p(l)}]\,R(n,k)_{p(k)}, \\ & (n,n-1)_{p(n-1)} \subset (n,k)_{p(k)}, \\ & (n,n-1)_{p(n-1)} \subset (n,l)_{p(l)}, \end{aligned}\right\} \tag{1.7.5}$$

which obviously is of the same structure. If we imagine that in the $(n-1)$-particle system there is no particle j, and that the division $(n,k)_{p(k)}$ is obtained from $(n-1,\,k)_{p(k)}$ by adding j and attaching it to i, we can find $V(n,\,k)_{p(k)}$ from $V(n-1,\,k)_{p(k)}$ by merely replacing all terms V_{il} in the latter interaction by $V_{il}+V_{jl}$ and adding V_{ij}. The difference $V(n,k)_{p(k)} - V(n,l)_{p(l)}$ is obtained from $V(n-1,k)_{p(k)} - V(n-1,l)_{p(l)}$ by replacing all terms V_{im} in the latter expression by $V_{im}+V_{jm}$, the remaining terms being left unchanged. Summarizing, it is clear that with a suitable change of notation the combinatorial analysis which led to the $(n-1)$-particle equation can also be applied to the multiple sum in eq. (1.7.4). The result is that

$$S(n,n-1)_{p(n-1)} = -R(n,1) + \sum_{k=2}^{n-1} \sum_{\substack{p(k) \\ (n,n-1)_{p(n-1)} \subset (n,k)_{p(k)}}} (-1)^k (k-1)!\,R(n,k)_{p(k)}. \tag{1.7.6}$$

To this expression we must now apply $\sum_{p(n-1)} R(n,\,n)\,V(n,n-1)_{p(n-1)}$. In doing so, it is convenient to perform the summation with respect to $p(n-1)$ first. This makes it possible to use the relation

$$\sum_{\substack{p(n-1) \\ (n,\,n-1)_{p(n-1)} \subset (n,k)_{p(k)}}} V(n,n-1)_{p(n-1)} = V(n,k)_{p(k)}, \tag{1.7.7}$$

which expresses the fact that if we sum over all two-particle interactions V_{lm} subject to the condition that we only include interactions present in the division $(n,\,k)_{p(k)}$, we get the total $V(n,\,k)_{p(k)}$. Besides eq. (1.7.7), we need the relation

$$R(n,n)V(n,k)_{p(k)}R(n,k)_{p(k)} = R(n,n) - R(n,k)_{p(k)}. \tag{1.7.8}$$

This yields

$$\left.\begin{aligned} &\sum_{p(n-1)} R(n,n)V(n,n-1)_{p(n-1)}S(n,n-1)_{p(n-1)} \\ &= -R(n,n)V(n,1)R(n,1)+\sum_{k=2}^{n-1}\sum_{p(k)}(-1)^k(k-1)!\,R(n,n)V(n,k)_{p(k)}R(n,k)_{p(k)} \\ &= R(n,1)-R(n,n)+\sum_{k=2}^{n-1}\sum_{p(k)}(-1)^k(k-1)!\,R(n,n)-\sum_{k=2}^{n-1}\sum_{p(k)}(-1)^k(k-1)!R(n,k)_{p(k)}, \end{aligned}\right\} \quad (1.7.9)$$

where we recall that it was assumed that $n \geq 3$. This equation is almost equivalent to the desired relation (1.7.2). It only remains to show that

$$\left[1-\sum_{k=2}^{n-1}\sum_{p(k)}(-1)^k(k-1)!\right]R(n,n) = (-1)^n(n-1)!\,R(n,n) \quad (n\geq 3). \quad (1.7.10)$$

To check this, we note that $p(k)$ runs through $N(n,k)$ values, $N(n,k)$ denoting the number of ways in which n particles can be split into k groups. Hence what we want to show is that

$$1-\sum_{k=2}^{n-1}(-1)^k(k-1)!\,N(n,k) = (-1)^n(n-1)! \quad (n\geq 3). \quad (1.7.11)$$

Now any division $(n,k)_{p(k)}$ in which particle n belongs to a group of two or more particles can be obtained from a division $(n-1,k)_{p(k)}$ of the particles $1, 2, \ldots, n-1$ by adding particle n to one of the k groups. And each process of this sort yields a $(n,k)_{p(k)}$. Furthermore, any division $(n,k)_{p(k)}$ in which n forms a group by itself is obtained if to the corresponding division $(n-1,k-1)_{p(k-1)}$ particle n is added as a separate group. Hence

$$N(n,k) = kN(n-1,k)+N(n-1,k-1) \quad (n\geq 2, k\geq 2). \quad (1.7.12)$$

From this it follows that

$$\left.\begin{aligned} &1-\sum_{k=2}^{n-1}(-1)^k(k-1)!\,N(n,k) = 1-\sum_{k=2}^{n-1}(-1)^k k!\,N(n-1,k)-\sum_{k=2}^{n-1}(-1)^k(k-1)!\,N(n-1,k-1) \\ &= 1-(-1)^{n-1}(n-1)!\,N(n-1,n-1)-1!\,N(n-1,1) = (-1)^n(n-1)! \quad (n\geq 3), \end{aligned}\right\} \quad (1.7.13)$$

as we wanted to show.

Starting from the assumption that for $n-1$ particles eq. (1.7.2) had been established by combining various resolvent equations of the form (1.7.3), we have now shown that eq. (1.7.2) also holds true for n particles. In the course of the proof, we only had to combine the sets of resolvent equations (1.7.5) and (1.7.8). Hence what applied to $n-1$ before the proof has now been carried over to n, and we can proceed to $n+1$.

1.7.2. Auxiliary formulas

The reason for using the complicated resolvent equation (1.7.2) is that the operator which on its right-hand side acts on $R(n, 1)$ belongs to $\mathfrak{L}^2$. As a matter of fact, it is discussed in section 1.7.4 that even each separate term in the multiple sum belongs to $\mathfrak{L}^2$. However, before passing on to this point it is useful to start with a few auxiliary formulas.

The first of these concerns the result due to KATO(5) that there are positive constants α and β such that for every f in $\mathfrak{D}(H_0)$

$$\sum_{i<j} || V_{ij} f || < \alpha || H_0 f || + \beta || f ||, \tag{1.7.14}$$

where we may choose α as small as we like. From eq. (1.7.14) it follows in particular that

$$\left.\begin{aligned} || V R_0(\lambda) f || &\leq \alpha || H_0 R_0(\lambda) f || + \beta || R_0(\lambda) f || \\ &\leq \alpha || f || + \alpha |\lambda| \, || R_0(\lambda) f || + \beta || R_0(\lambda) f || \leq \left[\alpha + \frac{\alpha |\lambda| + \beta}{(\operatorname{Im} \sqrt{\lambda})^2}\right] || f ||. \end{aligned}\right\} \tag{1.7.15}$$

Hence if λ is negative and sufficiently small, the norm $|| V R_0(\lambda) ||$ is less than 1. Then the series for $(g, R(\lambda) f)$ in eq. (1.3.49) is convergent, so that the spectrum of H is bounded below. This argument applies to any number of particles.

We know from eq. (1.2.9) that $R(\lambda) f$ belongs to $\mathfrak{D}(H_0)$ for every f in $\mathfrak{L}^2$. Also,

$$H_0 R(\lambda) f = -\sum_{i<j} V_{ij} R(\lambda) f + \lambda R(\lambda) f + f, \tag{1.7.16}$$

so that by Minkowski's inequality

$$|| H_0 R(\lambda) f || \leq \sum_{i<j} || V_{ij} R(\lambda) f || + |\lambda| \, || R(\lambda) f || + || f || \leq \alpha || H_0 R(\lambda) f || + \left[\frac{\beta + |\lambda|}{[\operatorname{Im} \sqrt{(\lambda - \Lambda)}]^2} + 1\right] || f ||, \tag{1.7.17}$$

Λ being the lower bound of the spectrum of H. If we now choose $\alpha < 1$ and subtract $\alpha || H_0 R(\lambda) f ||$ from both sides of eq. (1.7.17), we find with eq. (1.7.14) that

$$\sum_{i<j} || V_{ij} R(\lambda) f || \leq \frac{\alpha}{1 - \alpha} \left[\frac{\beta + |\lambda|}{[\operatorname{Im} \sqrt{(\lambda - \Lambda)}]^2} + 1\right] || f || + \frac{\beta}{[\operatorname{Im} \sqrt{(\lambda - \Lambda)}]^2} || f ||. \tag{1.7.18}$$

From this it follows that the norm $|| V_{ij} R(\lambda) ||$ is uniformly bounded in any region

$$0 < \varepsilon \leq |\lambda - \Lambda|, \qquad 0 < \delta \leq \arg(\lambda - \Lambda) \leq 2\pi - \delta. \tag{1.7.19}$$

This is the required result.

For the following we also need several formulas concerning resolvents of the type $R(n, k)_{p(k)}$. Let us assume in particular that $k = 2$. Then the simplest situation arises if the division $(n, 2)_{p(2)}$ consists of a group of $n - 1$ particles plus a single

particle. In that case it is convenient to choose $n-2$ coordinates $\boldsymbol{x}$ for the internal motion of the $n-1$ particles, plus a coordinate $\boldsymbol{x}_3$ for the distance between the last particle and the centre of mass of the previous ones. If the groups consist of n_1 and n_2 particles with $n_1 \geq 2$, $n_2 \geq 2$, we use internal coordinates $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ within the respective groups, plus a coordinate $\boldsymbol{x}_3$ for the distance between the centres of mass of the groups. In the following we mainly concentrate on the latter case.

For discussing the total Hamiltonian $H(n, 2)_{p(2)}$, we have to consider the Hamiltonians $H(\boldsymbol{x}_1)$, $H(\boldsymbol{x}_2)$, and $H_0(\boldsymbol{x}_3)$ for the internal motion of the groups and their relative motion, respectively. In the first instance, these are defined as self-adjoint operators in the spaces $\mathfrak{L}^2(\boldsymbol{x}_1)$, $\mathfrak{L}^2(\boldsymbol{x}_2)$, and $\mathfrak{L}^2(\boldsymbol{x}_3)$. It was shown by KATO(5) that the domain of $H(\boldsymbol{x}_1)$ consists of all functions $f(\boldsymbol{x}_1)$ in $\mathfrak{L}^2(\boldsymbol{x}_1)$ for which $|\boldsymbol{k}_1|^2 \hat{f}(\boldsymbol{k}_1)$ belongs to $\mathfrak{L}^2(\boldsymbol{k}_1)$, $\hat{f}$ being the Fourier transform of f. With Kato's result, it is not difficult to see that $H(\boldsymbol{x}_1)$ can also be considered as a self-adjoint operator in the space $\mathfrak{L}^2(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$, its domain being the set of functions $f(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$ for which $|\boldsymbol{k}_1|^2 \hat{f}(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3)$ belongs to $\mathfrak{L}^2(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3)$. And similarly for $H(\boldsymbol{x}_2)$ and $H_0(\boldsymbol{x}_3)$. With this interpretation of the Hamiltonians, we have

$$H(n, 2)_{p(2)} \equiv H(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3) = H(\boldsymbol{x}_1) + H(\boldsymbol{x}_2) + H_0(\boldsymbol{x}_3). \tag{1.7.20}$$

Likewise, we can consider the operator $H(\boldsymbol{x}_1) + H(\boldsymbol{x}_2)$, say in the space $\mathfrak{L}^2(\boldsymbol{x}_1, \boldsymbol{x}_2)$. It is of a slightly different structure from the Hamiltonians considered thus far, in that it is not quite the Hamiltonian of a system of particles with two-body interactions. But by Kato's(5) results, it is self-adjoint all the same. Also, it satisfies the crucial relations (1.2.9) and (1.7.14). From this it is easily deduced that the spectrum of $H(\boldsymbol{x}_1) + H(\boldsymbol{x}_2)$ is bounded below, and that there is a resolvent $R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda)$ such that all the operators of the form $V_{ij}(\boldsymbol{x}_1) R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda)$ or $V_{ij}(\boldsymbol{x}_2) R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda)$ are regular and bounded uniformly in λ in a region of the form (1.7.19).

According to eq. (1.5.4), the resolvent $R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda)$ satisfies

$$(g(\boldsymbol{x}_1, \boldsymbol{x}_2), R(\boldsymbol{x}_1, \boldsymbol{x}_2; \lambda) f(\boldsymbol{x}_1, \boldsymbol{x}_2)) = \frac{1}{2\pi i} \int_C (g(\boldsymbol{x}_1, \boldsymbol{x}_2), R(\boldsymbol{x}_2; \lambda - \sigma) R(\boldsymbol{x}_1; \sigma) f(\boldsymbol{x}_1, \boldsymbol{x}_2)) d\sigma. \tag{1.7.21}$$

It is convenient to denote this relationship by

$$R(\boldsymbol{x}_1, \boldsymbol{x}_2) = R(\boldsymbol{x}_1) * R(\boldsymbol{x}_2). \tag{1.7.22}$$

With this notation we have

$$[R(\boldsymbol{x}_1) * R(\boldsymbol{x}_2)] * R_0(\boldsymbol{x}_3) = R(\boldsymbol{x}_1) * [R(\boldsymbol{x}_2) * R_0(\boldsymbol{x}_3)]. \tag{1.7.23}$$

For either side yields the resolvent of $H(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$, which is unique. Hence omitting the square brackets we may write

$$R(n, 2)_{p(2)} \equiv R(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3) = R(\boldsymbol{x}_1) * R(\boldsymbol{x}_2) * R_0(\boldsymbol{x}_3). \tag{1.7.24}$$

It is not difficult to see that in the case of a general division $(n, k)_{p(k)}$ this result can be extended by introducing k sets of internal coordinates for the motion within the k groups, $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_k$, plus a set of $k-1$ three-dimensional coordinates for the relative motion of the groups with respect to each other, $\boldsymbol{x}_{k+1}, \ldots, \boldsymbol{x}_{2k-1}$. As a generalization of eq. (1.7.24) this yields

$$R(n,k)_{p(k)} \equiv R(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k, \boldsymbol{x}_{k+1}, \ldots, \boldsymbol{x}_{2k-1}) = R(\boldsymbol{x}_1) * \ldots * R(\boldsymbol{x}_k) * R_0(\boldsymbol{x}_{k+1}) * \ldots * R_0(\boldsymbol{x}_{2k-1}). \quad (1.7.25)$$

It can be shown with the methods outlined in section 1.3.3 and at the beginning of the present section that all operators $V_{ij} R(n, k)_{p(k)}$ are regular and uniformly bounded in regions of the form (1.7.19). The same applies to operators such as

$$\left.\begin{aligned} & V_{ij}(\boldsymbol{x}_l)\, R(\boldsymbol{x}_1) * \ldots * R(\boldsymbol{x}_k) * R_0(\boldsymbol{x}_p) * \ldots * R_0(\boldsymbol{x}_q) \\ & (l = 1, 2, \ldots, k; \quad k+1 \leq p, \ldots, q \leq 2k-1). \end{aligned}\right\} \quad (1.7.26)$$

We now want to consider operators of the form

$$Q \equiv [R_b(\boldsymbol{x}) * R(\boldsymbol{y})]\, V(\boldsymbol{x})\, [R_a(\boldsymbol{x}) * R(\boldsymbol{y})], \quad (1.7.27)$$

where R_a, R_b, and R may or may not be different resolvents. It is essential that both operators $R(\boldsymbol{y})$ are the same. Also, $\| V(\boldsymbol{x})\, R_p(\boldsymbol{x}) \|$ $(p = a, b)$ must be bounded uniformly in a region of the form (1.7.19) and $\| V(\boldsymbol{x})\, [R_p(\boldsymbol{x}) * R(\boldsymbol{y})] \|$ must be bounded. It is assumed that the respective spectra are bounded below, their lower bounds being denoted by Λ_a, Λ_b, and Λ.

Writing out eq. (1.7.27) and using eq. (1.2.11), we get

$$\left.\begin{aligned} (g, Qf) &= -\frac{1}{4\pi^2} \int_C d\sigma \int_D d\tau\, (g(\boldsymbol{x},\boldsymbol{y}), R_b(\boldsymbol{x};\tau)\, R(\boldsymbol{y};\lambda-\tau)\, V(\boldsymbol{x})\, R_a(\boldsymbol{x};\sigma)\, R(\boldsymbol{y};\lambda-\sigma)\, f(\boldsymbol{x},\boldsymbol{y})) \\ &= -\frac{1}{4\pi^2} \int_C d\sigma \int_D \frac{d\tau}{\sigma-\tau} (g(\boldsymbol{x},\boldsymbol{y}), R_b(\boldsymbol{x};\tau) V(\boldsymbol{x}) R_a(\boldsymbol{x};\sigma) [R(\boldsymbol{y};\lambda-\tau) - R(\boldsymbol{y};\lambda-\sigma)] f(\boldsymbol{x},\boldsymbol{y})). \end{aligned}\right\} \quad (1.7.28)$$

At this point it is convenient to choose as the contours C and D the straight lines

$$\left.\begin{aligned} \sigma &= s e^{i\psi} - s_0 \quad (-\infty < s < \infty), \\ \tau &= t e^{i\psi} - t_0 \quad (-\infty < t < \infty), \end{aligned}\right\} \quad (1.7.29)$$

where we must make sure that

$$-s_0 < \Lambda_a, \quad -t_0 < \Lambda_b, \quad 0 < \delta \leq \psi \leq \pi - \delta. \quad (1.7.30)$$

It is obvious that in choosing ψ we must also take into account the location of the singularities of $R(\boldsymbol{y};\lambda-\sigma)$ and $R(\boldsymbol{y};\lambda-\tau)$. Furthermore, we take $-t_0 < -s_0$, so that the contour D is on the left of C.

It is now easy to evaluate the term on the right-hand side of eq. (1.7.28) which involves $R(\boldsymbol{y}; \lambda - \sigma)$. For the function

$$h(\boldsymbol{x}, \boldsymbol{y}) \equiv V(\boldsymbol{x})\, R_a(\boldsymbol{x}; \sigma)\, R(\boldsymbol{y}; \lambda - \sigma)\, f(\boldsymbol{x}, \boldsymbol{y}) \tag{1.731}$$

does not depend on τ and it belongs to $\mathfrak{L}^2(\boldsymbol{x}, \boldsymbol{y})$. Hence if we consider the expression

$$\int_D \frac{d\tau}{\sigma - \tau} (g(\boldsymbol{x}, \boldsymbol{y}), R_b(\boldsymbol{x}; \tau)\, h(\boldsymbol{x}, \boldsymbol{y})), \tag{1.7.32}$$

we see that its integrand is a regular function of τ in the half-plane on the left of D. Since in this half-plane the integrand tends to zero faster than $1/|\tau|$ when $|\tau|$ tends to ∞, it follows that the integral (1.7.32) vanishes.

To evaluate the remaining term in eq. (1.7.28), we want to invert the order of integration. Performing the integration with respect to σ first, we get a contributon from the pole $\sigma = \tau$ on the left of C. Hence in the abbreviated notation (1.7.22), the final result takes the form

$$[R_b(\boldsymbol{x}) * R(\boldsymbol{y})]\, V(\boldsymbol{x})\, [R_a(\boldsymbol{x}) * R(\boldsymbol{y})] = [R_b(\boldsymbol{x})\, V(\boldsymbol{x})\, R_a(\boldsymbol{x})] * R(\boldsymbol{y}). \tag{1.7.33}$$

It remains to justify the inversion of the order of integration. To check this, we observe that on D the norm $\| V(\boldsymbol{x})\, R_b(\boldsymbol{x}; \tau) \|$ is bounded uniformly in τ, by assumption. Furthermore,

$$\| R_a(\boldsymbol{x}; \sigma) \| \leq \frac{1}{[\operatorname{Im} \sqrt{(\sigma - \Lambda_a)}]^2}, \quad \| R(\boldsymbol{y}; \lambda - \tau) \| \leq \frac{1}{[\operatorname{Im} \sqrt{(\lambda - \tau - \Lambda)}]^2}. \tag{1.7.34}$$

Hence to be able to apply the theorem on the inversion of Riemann integrals (Titchmarsh(15) section 1.85) it suffices to show that

$$I \equiv \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt \frac{1}{|\sigma - \tau|} \frac{1}{[\operatorname{Im} \sqrt{(\sigma - \Lambda_a)}]^2} \frac{1}{[\operatorname{Im} \sqrt{(\lambda - \tau - \Lambda)}]^2} < \infty, \tag{1.7.35}$$

and that the integrals

$$\left.\begin{aligned} I_s &\equiv \int_{-\infty}^{\infty} \frac{1}{|\sigma - \tau|} \frac{1}{[\operatorname{Im} \sqrt{(\lambda - \tau - \Lambda)}]^2} dt, \\ I_t &\equiv \int_{-\infty}^{\infty} \frac{1}{|\sigma - \tau|} \frac{1}{[\operatorname{Im} \sqrt{(\sigma - \Lambda_a)}]^2} ds \end{aligned}\right\} \tag{1.7.36}$$

converge uniformly with respect to s and t, respectively.

As for I, it follows from Hölder's inequality that

$$I \leq \left[\int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt \, \frac{1}{|\sigma-\tau|^{\frac{3}{2}}} \, \frac{1}{[\operatorname{Im}\sqrt{(\sigma-\Lambda_a)}]^3}\right]^{\frac{1}{3}} \left[\int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt \, \frac{1}{|\sigma-\tau|^{\frac{3}{2}}} \, \frac{1}{[\operatorname{Im}\sqrt{(\lambda-\tau-\Lambda)}]^3}\right]^{\frac{1}{3}} \times \left[\int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt \, \frac{1}{[\operatorname{Im}\sqrt{(\sigma-\Lambda_a)}]^3} \, \frac{1}{[\operatorname{Im}\sqrt{(\lambda-\tau-\Lambda)}]^3}\right]^{\frac{1}{3}}. \tag{1.7.37}$$

Now it is easily checked that $\int_{-\infty}^{\infty} |\sigma-\tau|^{-\frac{3}{2}} \, dt$ is bounded uniformly in s. Also $\int_{-\infty}^{\infty} [\operatorname{Im}\sqrt{(\sigma-\Lambda_a)}]^{-3} \, ds$ is convergent by the argument presented in section 1.6.2. Hence the first factor in eq. (1.7.37) is finite, and similarly for the remaining factors. Hence eq. (1.7.35) is satisfied.

In connection with I_t we have

$$\int_T^{\infty} \frac{1}{|\sigma-\tau|} \, \frac{1}{[\operatorname{Im}\sqrt{(\sigma-\Lambda_a)}]^2} \, ds \leq \left[\int_{-\infty}^{\infty} \frac{1}{|\sigma-\tau|^2} \, ds\right]^{\frac{1}{2}} \left[\int_T^{\infty} \frac{1}{[\operatorname{Im}\sqrt{(\sigma-\Lambda_a)}]^4} \, ds\right]^{\frac{1}{2}}, \tag{1.7.38}$$

which clearly demonstrates the required uniform convergence. This completes the proof of eq. (1.7.33).

The proof of eq. (1.7.33) can easily be extended to show that

$$\begin{aligned} &[R_c(\boldsymbol{x}) * R_q(\boldsymbol{y})] V(\boldsymbol{x}) \{[R_b(\boldsymbol{x}) V(\boldsymbol{x}) R_a(\boldsymbol{x})] * [R_q(\boldsymbol{y}) V(\boldsymbol{y}) R_p(\boldsymbol{y})]\} \\ &\quad = [R_c(\boldsymbol{x}) V(\boldsymbol{x}) R_b(\boldsymbol{x}) V(\boldsymbol{x}) R_a(\boldsymbol{x})] * [R_q(\boldsymbol{y}) V(\boldsymbol{y}) R_p(\boldsymbol{y})], \end{aligned} \tag{1.7.39}$$

and similarly for more complicated cases. The essential point about eq. (1.7.39) is that it contains a product $R_q(\boldsymbol{y}) \, R_q(\boldsymbol{y})$ which is reduced to a single factor $R_q(\boldsymbol{y})$. In the course of the proof, it must be assumed that various operators of the form VR are suitably bounded. It is not difficult to see that this condition is fulfilled in all cases in which eq. (1.7.39) is used in the next section.

1.7.3. An analysis of the multiple sum

We are now in a position to study the operator which on the right-hand side of eq. (1.7.2) acts on $R(n, 1)$. Let us choose a particular term of the multiple sum. This is characterized by a certain set $p(n-1), p(n-2), \ldots, p(2)$. Let us further assume that the division $(n, 2)_{p(2)}$ in question consists of two groups of at least two particles each. Then it is convenient to use internal coordinates $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ and a relative coordinate $\boldsymbol{x}_3$ as in section 1.7.2. With this choice of coordinates, eqs. (1.7.22) and (1.7.24) show that

$$R(n, 2)_{p(2)} = R(\boldsymbol{x}_1, \boldsymbol{x}_2) * R_0(\boldsymbol{x}_3). \tag{1.7.40}$$

Since in the expression we are considering $(n,3)_{p(3)} \subset (n,2)_{p(2)}$, the operator $R(n,3)_{p(3)}$ $[V(n,2)_{p(2)} - V(n,3)_{p(3)}]$ which acts on $R(n,2)_{p(2)}$ refers to a further splitting of the two groups of particles. It does not change the situation with respect to $\boldsymbol{x}_3$. Hence the function $V(n,2)_{p(2)} - V(n,3)_{p(3)}$ depends on $\boldsymbol{x}_1, \boldsymbol{x}_2$ but not on $\boldsymbol{x}_3$, and we have essentially

$$R(n,3)_{p(3)}[V(n,2)_{p(2)} - V(n,3)_{p(3)}] = [R(\boldsymbol{x}_1,\boldsymbol{x}_2) * R_0(\boldsymbol{x}_3)]V(\boldsymbol{x}_1,\boldsymbol{x}_2), \quad (1.7.41)$$

where $R(\boldsymbol{x}_1, \boldsymbol{x}_2)$ is some resolvent, not the same as in eq. (1.7.40). Since the operators $R_0(\boldsymbol{x}_3)$ in eqs. (1.7.40) and (1.7.41) are the same, viz. the resolvent for two particles without interaction, we can apply eq. (1.7.33) with the result that

$$\left.\begin{aligned} Q \equiv R(n,3)_{p(3)}[V(n,2)_{p(2)} - V(n,3)_{p(3)}]R(n,2)_{p(2)} \\ = [R(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_1,\boldsymbol{x}_2)R(\boldsymbol{x}_1,\boldsymbol{x}_2)] * R_0(\boldsymbol{x}_3). \end{aligned}\right\} \quad (1.7.42)$$

With the help of eq. (1.7.39) the argument can be extended to the remaining factors in eq. (1.7.2). In the present symbolic notation this finally yields

$$\left.\begin{aligned} (-1)^{n-1}R(n,n)V(n,n-1)_{p(n-1)} \ldots R(n,2)_{p(2)} \\ = -[(-1)^n R(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_1,\boldsymbol{x}_2) \ldots R(\boldsymbol{x}_1,\boldsymbol{x}_2)] * R_0(\boldsymbol{x}_3). \end{aligned}\right\} \quad (1.7.43)$$

We must now analyse the term in square brackets in eq. (1.7.43). Since each resolvent $R(\boldsymbol{x}_1, \boldsymbol{x}_2)$ refers to a system split into groups of particles with coordinates $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, respectively, it can be written in the form of a convolution according to eq. (1.7.22). In particular, if in the division $(n,2)_{p(2)}$ there are n_1 particles with coordinates $\boldsymbol{x}_1$, and n_2 particles with coordinates $\boldsymbol{x}_2$, then the factor $R(\boldsymbol{x}_1, \boldsymbol{x}_2)$ which derives from $R(n,2)_{p(2)}$ can be obtained from a convolution of the resolvents for n_1 and n_2 particles with all their interactions. To bring this out in the notation, we write, with eq. (1.7.40),

$$R(n,2)_{p(2)} = R(\boldsymbol{x}_1; n_1, 1) * R(\boldsymbol{x}_2; n_2, 1) * R(\boldsymbol{x}_3; 2, 2), \quad (1.7.44)$$

where for instance $R(\boldsymbol{x}_3; 2, 2)$ is the resolvent for two particles divided into two groups, i.e. two particles without interaction, which acts on functions of $\boldsymbol{x}_3$.

To go over from the division $(n,2)_{p(2)}$ to $(n,3)_{p(3)} \subset (n,2)_{p(2)}$, it is necessary to split one of the two groups into two. Let this be the group of n_1 particles. Then the division $(n,3)_{p(3)}$ consists of a group of n_2 particles, plus a composite group of n_1 particles which itself consists of two subgroups according to a certain splitting $(n_1,2)_{q(2)}$. In the notation corresponding to eq. (1.7.44), this can be denoted by

$$R(n,3)_{p(3)} = R(\boldsymbol{x}_1; n_1, 2)_{q(2)} * R(\boldsymbol{x}_2; n_2, 1) * R(\boldsymbol{x}_3; 2, 2). \quad (1.7.45)$$

Also, the interaction $V(n,2)_{p(2)} - V(n,3)_{p(3)}$, which is the interaction between the two subgroups, is nothing but $V(\boldsymbol{x}_1; n_1, 1) - V(\boldsymbol{x}_1; n_1, 2)_{q(2)}$. Hence with eq. (1.7.42),

$$\left.\begin{aligned} Q = \{[R(\boldsymbol{x}_1; n_1, 2)_{q(2)} * R(\boldsymbol{x}_2; n_2, 1)]\,[V(\boldsymbol{x}_1; n_1, 1) - V(\boldsymbol{x}_1; n_1, 2)_{q(2)}] \\ \times [R(\boldsymbol{x}_1; n_1, 1) * R(\boldsymbol{x}_2; n_2, 1)]\} * R(\boldsymbol{x}_3; 2, 2). \end{aligned}\right\} \quad (1.7.46)$$

Now we can again apply eq. (1.7.33), with the result that

$$\left.\begin{aligned} Q = \{R(\boldsymbol{x}_1; n_1, 2)_{q(2)}\,[V(\boldsymbol{x}_1; n_1, 1) - V(\boldsymbol{x}_1; n_1, 2)_{q(2)}]\,R(\boldsymbol{x}_1; n_1, 1)\} \\ * R(\boldsymbol{x}_2; n_2, 1) * R(\boldsymbol{x}_3; 2, 2). \end{aligned}\right\} \quad (1.7.47)$$

The division $(n, 4)_{p(4)}$ either implies a further splitting among the n_1 particles, or it splits the group of n_2 particles. In either case it can be treated in the same way as $(n, 3)_{p(3)}$. Similar remarks apply to all further divisions. Since by the time we have reached the division (n, n), the two groups we began with are completely split up into single particles, it is not difficult to see that we finally obtain

$$\left.\begin{aligned} (-1)^{n-1} R(n, n) V(n, n-1)_{p(n-1)} \ldots R(n, 2)_{p(2)} \\ = -[(-1)^{n_1-1} R(n_1, n_1) V(n_1, n_1-1)_{q_1(n_1-1)} \ldots R(n_1, 1)] \\ * [(-1)^{n_2-1} R(n_2, n_2) V(n_2, n_2-1)_{q_2(n_2-1)} \ldots R(n_2, 1)] * R(2, 2), \\ (n, n-1)_{p(n-1)} \subset (n, n-2)_{p(n-2)} \subset \ldots \subset (n, 2)_{p(2)}, \\ (n_1, n_1-1)_{q_1(n_1-1)} \subset (n_1, n_1-2)_{q_1(n_1-2)} \subset \ldots \subset (n_1, 2)_{q_1(2)}, \\ (n_2, n_2-1)_{q_2(n_2-1)} \subset (n_2, n_2-2)_{q_2(n_2-2)} \subset \ldots \subset (n_2, 2)_{q_2(2)}. \end{aligned}\right\} \quad (1.7.48)$$

1.7.4. The kernel

If we compare eqs. (1.7.2) and (1.7.48), we observe that the expressions in square brackets on the right-hand side of eq. (1.7.48) are nothing but terms in the multiple sums in the equations for $R(n_1, 1)$ and $R(n_2, 1)$. Let us therefore assume that by a previous analysis these were shown to be integral operators with kernels of the form

$$F_q^{(m)}(\boldsymbol{x}, \boldsymbol{y}; \lambda) \equiv \int K_q^{(m)}(\boldsymbol{x}, \boldsymbol{z}; \lambda)\, G^{(m)}(\boldsymbol{z}, \boldsymbol{y}; \lambda)\, d\boldsymbol{z} \quad (m = n_1, n_2), \qquad (1.7.49)$$

where $G^{(m)}$ is the Green function corresponding to $R(m, 1)$ and $K_q^{(m)}$ is a kernel belonging to $\mathfrak{L}^2$. Let us also assume that it was established that

$$\left.\begin{aligned} \| R(\lambda; m, 1) \| \leq [\operatorname{Im} \sqrt{(\lambda - \Lambda^{(m)})}]^{-2}, \\ | K_q^{(m)}(\lambda) | \leq \text{const.} \, | \lambda - \Lambda^{(m)} |^{m-2} \, [\operatorname{Im} \sqrt{(\lambda - \Lambda^{(m)})}]^{-\frac{5}{2}m+\frac{9}{2}}, \end{aligned}\right\} \quad (1.7.50)$$

where $\Lambda^{(m)}$ is the lower bound of the spectrum of $H(m, 1)$. These assumptions are in agreement with what we know for $m = 2$ and $m = 3$. In particular, the bound for $| K_q^{(m)} |$ agrees with eqs. (1.3.4) and (1.6.23).

Under the above assumptions we get the equality

$$\left.\begin{aligned} &-(g,[(-1)^{n_1-1}R(n_1,n_1)V(n_1,n_1-1)_{q_1(n_1-1)}\ldots R(n_1,1)] \\ &*[(-1)^{n_2-1}R(n_2,n_2)V(n_2,n_2-1)_{q_2(n_2-1)}\ldots R(n_2,1)]f) \\ =&-\frac{1}{2\pi i}\int_C d\sigma\int\bar{g}(\boldsymbol{x}_1,\boldsymbol{x}_2)\,d\boldsymbol{x}_1\,d\boldsymbol{x}_2\int F_{q_2}^{(n_2)}(\boldsymbol{x}_2,\boldsymbol{y}_2;\lambda-\sigma)\,F_{q_1}^{(n_1)}(\boldsymbol{x}_1,\boldsymbol{y}_1;\sigma)\,f(\boldsymbol{y}_1,\boldsymbol{y}_2)\,d\boldsymbol{y}_1\,d\boldsymbol{y}_2 \end{aligned}\right\}(1.7.51)$$

for any f and g in $\mathfrak{L}^2(\boldsymbol{x}_1,\boldsymbol{x}_2)$. It is now shown first of all that if λ is inside the complex plane cut from $\Lambda^{(n_1)}+\Lambda^{(n_2)}$ to ∞,

$$I\equiv\left\{\int d\boldsymbol{x}_1\,d\boldsymbol{x}_2\int d\boldsymbol{y}_1\,d\boldsymbol{y}_2\left[\int_C|F_{q_2}^{(n_2)}(\boldsymbol{x}_2,\boldsymbol{y}_2;\lambda-\sigma)\,F_{q_1}^{(n_1)}(\boldsymbol{x}_1,\boldsymbol{y}_1;\sigma)|\,d\sigma\right]^2\right\}^{\frac{1}{2}}<\infty. \quad (1.7.52)$$

From this it follows with Fubini's theorem that on the right-hand side of eq. (1.7.51) the integration with respect to σ may be performed first, provided we are willing to consider it as a Lebesgue integration. If this is done, we get an expression of the form

$$\left.\begin{aligned} &-\int\bar{g}(\boldsymbol{x}_1,\boldsymbol{x}_2)\,d\boldsymbol{x}_1\,d\boldsymbol{x}_2\int[F_{q_1}^{(n_1)}*F_{q_2}^{(n_2)}](\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{y}_1,\boldsymbol{y}_2;\lambda)\,f(\boldsymbol{y}_1,\boldsymbol{y}_2)\,d\boldsymbol{y}_1\,d\boldsymbol{y}_2, \\ &[F_{q_1}^{(n_1)}*F_{q_2}^{(n_2)}](\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{y}_1,\boldsymbol{y}_2;\lambda)\equiv\frac{1}{2\pi i}\int_C F_{q_2}^{(n_2)}(\boldsymbol{x}_2,\boldsymbol{y}_2;\lambda-\sigma)\,F_{q_1}^{(n_1)}(\boldsymbol{x}_1,\boldsymbol{y}_1;\sigma)\,d\sigma. \end{aligned}\right\} \quad (1.7.53)$$

If eq. (1.7.52) holds true, the kernel defined in the second line of eq. (1.7.53) belongs to $\mathfrak{L}^2$, its $\mathfrak{L}^2$-norm not exceeding I.

To prove the assertion (1.7.52), we deduce from eq. (1.7.50) that

$$\left.\begin{aligned} &I\leq\text{const.}\int_C|\sigma-\Lambda^{(n_1)}|^{n_1-2}\,[\operatorname{Im}\sqrt{(\sigma-\Lambda^{(n_1)})}]^{-\frac{5}{2}n_1+\frac{5}{2}} \\ &\times|\lambda-\sigma-\Lambda^{(n_2)}|^{n_2-2}[\operatorname{Im}\sqrt{(\lambda-\sigma-\Lambda^{(n_2)})}]^{-\frac{5}{2}n_2+\frac{5}{2}}\,d\sigma. \end{aligned}\right\} \quad (1.7.54)$$

If we now write

$$\lambda-\Lambda^{(n_1)}-\Lambda^{(n_2)}=le^{i\varphi} \quad (1.7.55)$$

and for the contour C take the straight line

$$\sigma=se^{\frac{1}{2}i\varphi}-\frac{1}{2}l+\Lambda^{(n_1)}\quad(-\infty<s<\infty), \quad (1.7.56)$$

then the imaginary parts in eq. (1.7.54) take exactly the forms given on the right-hand sides of eq. (1.6.15). With these expressions, it is not difficult to check that

$$|\sigma-\Lambda^{(n_1)}|\,[\operatorname{Im}\sqrt{(\sigma-\Lambda^{(n_1)})}]^{-2}\leq 4\left(\sin\frac{1}{2}\varphi\right)^{-2}, \quad (1.7.57)$$

and that the same bound applies to the corresponding term with $\lambda-\sigma-\Lambda^{(n_2)}$. Inserting these results in eq. (1.7.54) yields with Hölder's inequality that

$$I \leq \text{const.}\left(\sin\frac{1}{2}\varphi\right)^{-2n+8}\int_{-\infty}^{\infty}\left[t\cos\frac{1}{2}\varphi+\frac{1}{2}t\sin^2\frac{1}{2}\varphi+\left(t^2+\frac{1}{4}t^2\sin^2\frac{1}{2}\varphi\right)^{\frac{1}{2}}\right]^{-\frac{1}{4}n-\frac{31}{2}}dt, \quad (1.7.58)$$

where we have written $n_1+n_2=n$. The reasoning applied to eq. (1.6.16) can now be used to show that

$$I \leq \text{const.}\,|\lambda-\Lambda^{(n_1)}-\Lambda^{(n_2)}|^{n-3}\,[\operatorname{Im}\lambda/(\lambda-\Lambda^{(n_1)}-\Lambda^{(n_2)})]^{-\frac{5}{2}n+5}, \quad (1.7.59)$$

so that eq. (1.7.52) is indeed satisfied.

The conclusion is thus far that if λ is inside the complex plane cut from $\Lambda^{(n_1)}+\Lambda^{(n_2)}$ to ∞, the operator on the left-hand side of eq. (1.7.51) is an integral operator which in the space $\mathfrak{L}^2(\boldsymbol{x}_1,\boldsymbol{x}_2)$ belongs to $\mathfrak{L}^2$. According to eq. (1.7.48), the operator in question plays a prominent part in the equation for $R(n,1)$, eq. (1.7.2). To discuss the latter equation more fully, particularly the term of the multiple sum we are considering in the present section, we note that the factor $V(n,1)-V(n,2)_{p(2)}$ stands for the interaction between the groups of n_1 and n_2 particles which together form the division $(n,2)_{p(2)}$. Consequently, this factor depends in an essential way on the distance between the centres of mass of the two groups, which was denoted by $\boldsymbol{x}_3$. To bring this out explicitly, we note that since $\boldsymbol{x}_1$ describes the internal motion of n_1 particles, it must have n_1-1 three-dimensional components. Let us denote these by $\boldsymbol{x}_{1,r}$ $(r=1,2,\ldots,n_1-1)$, and let us denote the components of $\boldsymbol{x}_2$ by $\boldsymbol{x}_{2,s}$ $(s=1,2,\ldots,n_2-1)$. Then if we take into account all the two-particle interactions between the two groups considered, we get

$$V(n,1)-V(n,2)_{p(2)}=\sum_{i,j}V_{ij}\Big(\sum_r c_{ij}^{1,r}\boldsymbol{x}_{1,r}+\sum_s c_{ij}^{2,s}\boldsymbol{x}_{2,s}+c_{ij}^{3}\boldsymbol{x}_3\Big), \quad (1.7.60)$$

with certain coefficients c. The point is now that none of the coefficients c_{ij}^3 vanishes, owing to the meaning of the interactions V_{ij} involved in eq. (1.7.60). Hence if either side of eq. (1.7.60) is denoted by $V_p(\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{x}_3)$, it follows that $V_p(\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{x}_3)$ belongs to $\mathfrak{L}^2(\boldsymbol{x}_3)$.

Combining this result with eqs. (1.7.48), (1.7.51), (1.7.53), we now consider

$$\left.\begin{aligned}&(g,(-1)^{n-1}R(n,n)V(n,n-1)_{p(n-1)}\ldots R(n,2)_{p(2)}[V(n,1)-V(n,2)_{p(2)}]f)\\&\quad=-\frac{1}{2\pi i}\int_D d\tau\int\bar{g}(\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{x}_3)\,d\boldsymbol{x}_1\,d\boldsymbol{x}_2\,d\boldsymbol{x}_3\int[F_{q_1}^{(n_1)}*F_{q_2}^{(n_2)}](\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{y}_1,\boldsymbol{y}_2;\tau)\\&\qquad\times G_0^{(2)}(\boldsymbol{x}_3,\boldsymbol{y}_3;\lambda-\tau)V_p(\boldsymbol{y}_1,\boldsymbol{y}_2,\boldsymbol{y}_3)f(\boldsymbol{y}_1,\boldsymbol{y}_2,\boldsymbol{y}_3)\,d\boldsymbol{y}_1\,d\boldsymbol{y}_2\,d\boldsymbol{y}_3\end{aligned}\right\} \quad (1.7.61)$$

for any f and g in $\mathfrak{L}^2(\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{x}_3)$. From eqs. (1.6.10) and (1.7.59), it is clear that

$$\left.\begin{aligned}J&\equiv\left\{\int d\boldsymbol{x}\int d\boldsymbol{y}\left[\int_D|[F_{q_1}^{(n_1)}*F_{q_1}^{(n_2)}](\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{y}_1,\boldsymbol{y}_2;\tau)\,G_0^{(2)}(\boldsymbol{x}_3,\boldsymbol{y}_3;\lambda-\tau)V_p(\boldsymbol{y})|\,d\tau\right]^2\right\}^{\frac{1}{2}}\\&\leq\text{const.}\int_D|\tau-\Lambda^{(n_1)}-\Lambda^{(n_2)}|^{n-3}\,[\operatorname{Im}\lambda/(\tau-\Lambda^{(n_1)}-\Lambda^{(n_2)})]^{-\frac{5}{2}n+5}\,[\operatorname{Im}\lambda/(\lambda-\tau)]^{-\frac{1}{2}}\,d\tau.\end{aligned}\right\} \quad (1.7.62)$$

By the method applied to I above, this can be further reduced to

$$J \leq \text{const.} \, |\lambda - \Lambda^{(n_1)} - \Lambda^{(n_2)}|^{n-2} \, [\operatorname{Im} \sqrt{(\lambda - \Lambda^{(n_1)} - \Lambda^{(n_2)})}]^{-\frac{5}{2}n+\frac{9}{2}} . \tag{1.7.63}$$

Hence J is finite if λ is inside the complex plane cut from $\Lambda^{(n_1)} + \Lambda^{(n_2)}$ to ∞. Then in eq. (1.7.61) the integration with respect to τ may be performed first. And if we define

$$K_p^{(n)}(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_3; \lambda)$$
$$\equiv -\frac{1}{2\pi i} \int_D [F_{q_1}^{(n_1)} * F_{q_2}^{(n_2)}] (\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \tau) \, G_0^{(2)}(\boldsymbol{x}_3, \boldsymbol{y}_3; \lambda - \tau) \, V_p(\boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_3) \, d\tau , \tag{1.7.64}$$

it follows that the operator on the left-hand side of eq. (1.7.61) is an integral operator with kernel $K_p^{(n)}$. It belongs to $\mathfrak{L}^2$, and its $\mathfrak{L}^2$-norm does not exceed J.

The foregoing analysis applies to all the terms in the multiple sum in eq. (1.7.2) for which the division $(n, 2)_{p(2)}$ consists of two groups of at least two particles each. In the case of a division into a group of $n-1$ particles plus one single particle, we can confine ourselves to a set of $n-2$ internal coordinates $\boldsymbol{x}$ within the large group, plus a coordinate $\boldsymbol{x}_3$ for the distance between the centre of mass of this group and the last particle. We still want to use eq. (1.7.43), but we may skip equations (1.7.44) to (1.7.48) and (1.7.51) to (1.7.59). For it is easily seen that in the simple case in question the operator in square brackets in eq. (1.7.43) is a term of the multiple sum in the equation for $R(n-1, 1)$. Hence by assumption it is of the form $F_q^{(n-1)}(\boldsymbol{x}, \boldsymbol{y}; \lambda)$ given by eq. (1.7.49), with $K_q^{(n-1)}$ and $R(n-1, 1)$ satisfying eq. (1.7.50). According to this assumption, $F_q^{(n-1)}$ belongs to $\mathfrak{L}^2$, and

$$|F_q^{(n-1)}(\lambda)| \leq \text{const.} \, |\lambda - \Lambda^{(n-1)}|^{n-3} \, [\operatorname{Im} \sqrt{(\lambda - \Lambda^{(n-1)})}]^{-\frac{5}{2}n+5} . \tag{1.7.65}$$

The argument applied to eq. (1.7.61) can now be used to show that corresponding to eq. (1.7.64) we get a kernel

$$K_p^{(n)}(\boldsymbol{x}, \boldsymbol{x}_3, \boldsymbol{y}, \boldsymbol{y}_3; \lambda) \equiv -\frac{1}{2\pi i} \int_D F_q^{(n-1)}(\boldsymbol{x}, \boldsymbol{y}; \tau) \, G_0^{(2)}(\boldsymbol{x}_3, \boldsymbol{y}_3; \lambda - \tau) \, V_p(\boldsymbol{y}, \boldsymbol{y}_3) \, d\tau , \tag{1.7.66}$$

the $\mathfrak{L}^2$-norm of which does not exceed

$$J \leq \text{const.} \, |\lambda - \Lambda^{(n-1)}|^{n-2} \, [\operatorname{Im} \sqrt{(\lambda - \Lambda^{(n-1)})}]^{-\frac{5}{2}n+\frac{9}{2}} . \tag{1.7.67}$$

This is a bound of the same form as eq. (1.7.63), which is thus seen to apply to all the terms in the multiple sum of eq. (1.7.2).

The general result is therefore that the resolvent equation for n particles is equivalent to an equation of the form

$$\left.\begin{aligned} h(\boldsymbol{x};\lambda;n,1) = \sum_{k=2}^{n}\sum_{p(k)=1}^{N(n,k)}(-1)^k(k-1)!\,h(\boldsymbol{x};\lambda;n,k)_{p(k)} + \int \sum_{p} K_p^{(n)}(\boldsymbol{x},\boldsymbol{y};\lambda)\,h(\boldsymbol{y};\lambda;n,1)\,d\boldsymbol{y}, \\ h(\boldsymbol{x};\lambda;n,k)_{p(k)} \equiv R(\boldsymbol{x};\lambda;n,k)_{p(k)}\,f(\boldsymbol{x}), \end{aligned}\right\} \quad (1.7.68)$$

where $\boldsymbol{x}$ now stands for all the space coordinates. If for m particles ($m = 2, 3, \ldots, n-1$) the kernels $K_q^{(m)}$ and the Green function $G^{(m)}$ are known, the kernels $K_p^{(n)}$ in eq. (1.7.68) can be found with convolutions according to eqs. (1.7.49), (1.7.53), and (1.7.64), cq. (1.7.66). All the functions $h(\boldsymbol{x};\lambda;n,k)_{p(k)}$ with $k \geq 2$ can likewise be obtained from the Green functions for less than n particles. For it follows directly from eq. (1.7.25) that the inner product $(g, R(n,k)_{p(k)}\,f)$ can be evaluated by convolutions, and the argument used to get eq. (1.5.21) shows that this result can be carried over to the function $R(n,k)_{p(k)}\,f$ itself. Hence eq. (1.7.68) can be considered as an integral equation for the unknown function $h(\boldsymbol{x};\lambda;n,1)$. And since its kernel belongs to $\mathfrak{L}^2$, it can be solved and further analysed by the methods outlined in section 1.3.

It is obvious that in doing so we have to confine ourselves to the λ-plane cut from a suitable point $M^{(n)}$ to ∞. For in constructing the various kernels $K_p^{(n)}$, we had to observe cuts from $\Lambda^{(n_1)} + \Lambda^{(n_2)}$ to ∞, or from $\Lambda^{(n-1)}$ to ∞. And the convolutions by which we want to find the functions $R(n,k)_{p(k)}\,f$ with $k \geq 2$ necessitate similar cuts. Now the spectrum of $H(n,1)$ has a lower bound, say $\Lambda^{(n)}$. It is discussed in section 1.7.6 that this does not exceed $M^{(n)}$. In particular,

$$\Lambda^{(n)} \leq \Lambda^{(n_1)} + \Lambda^{(n_2)} \quad (n_1 + n_2 = n), \quad \Lambda^{(n)} \leq \Lambda^{(n-1)}. \quad (1.7.69)$$

Hence according to eqs. (1.7.63), (1.7.67) and (1.4.36),

$$\left.\begin{aligned} |K_p^{(n)}(\lambda)| \leq \text{const.}\,|\lambda - \Lambda^{(n)}|^{n-2}\,[\operatorname{Im}\sqrt{(\lambda-\Lambda^{(n)})}]^{-\frac{5}{2}n+\frac{9}{2}}, \\ \|R(\lambda;n,1)\| \leq [\operatorname{Im}\sqrt{(\lambda-\Lambda^{(n)})}]^{-2}, \end{aligned}\right\} \quad (1.7.70)$$

which is of exactly the same form as the assumed relations (1.7.50).

1.7.5. The Green function

It is the purpose of the present section to show that there is a Green function $G^{(n)} \equiv G(n,1)$ such that for every f in $\mathfrak{L}^2$

$$R(\boldsymbol{x};\lambda;n,1)\,f(\boldsymbol{x}) = \int G^{(n)}(\boldsymbol{x},\boldsymbol{y};\lambda)\,f(\boldsymbol{y})\,d\boldsymbol{y}. \quad (1.7.71)$$

Since the kernel of the resolvent equation belongs to $\mathfrak{L}^2$, it follows from the analysis used to obtain eq. (1.3.11) that to prove eq. (1.7.71), it is sufficient to show that there are Green functions for all the resolvents $R(n,k)_{p(k)}$ with $k \geq 2$, and to check that these satisfy symmetry relations analogous to eqs. (1.5.46) and (1.5.47).

To find an expression for the Green functions in question, we rewrite the resolvent equation in the symbolic form

$$R(n,1) = \sum c_k R(n_1,1) * R(n_2,1) * \ldots * R(n_k,1) * R_0 * \ldots * R_0 + K^{(n)} R(n,1), \quad (1.7.72)$$

where for the known resolvents $R(n,k)_{p(k)}$ with $k \geq 2$ we have used eq. (1.7.25). The c_k are certain constants, the summation is to be taken with respect to all possible divisions. It is obvious that in eq. (1.7.72) $n_i \leq n-1$ $(i = 1, 2, \ldots, k)$.

Let us now replace all the resolvents $R(n_i, 1)$ in eq. (1.7.72) by the right-hand sides of their resolvent equations. This yields a multiple sum a typical term of which is of the form

$$[K^{(n_1)} R(n_1,1)] * [K^{(n_2)} R(n_2,1)] * R(n_p,1) * \ldots * R(n_q,1) * R_0 * \ldots * R_0. \quad (1.7.73)$$

It contains a certain number, possibly 0, factors of the form KR, several factors R, and several factors R_0. In the factors R we have $n_p, \ldots, n_q \leq n-2$. To reduce the expression (1.7.73) further, we now replace the resolvents $R(n_p, 1), \ldots, R(n_q, 1)$ by the right-hand sides of their resolvent equations, and so on. In this way we finally obtain a multiple sum consisting of terms of the form

$$[K^{(n_1)} R(n_1,1)] * [K^{(n_2)} R(n_2,1)] * \ldots * [K^{(n_j)} R(n_j,1)] * R_0 * \ldots * R_0. \quad (1.7.74)$$

Here the convolutions may be performed in any desired order. For it was pointed out already in eq. (1.7.23) that this may be done in the case of three or more resolvents. And according to the resolvent equation, the quantities $K^{(n_i)} R(n_i, 1)$ are nothing but sums of resolvents.

Let us therefore begin with the multiple convolution $R_0 * \ldots * R_0$. According to eqs. (1.5.27) and (1.2.17), this yields a certain Hankel function,

$$G_0^{(n')}(\boldsymbol{x}_{j+1}, \boldsymbol{y}_{j+1}; \lambda) = \frac{i}{4}\left[\frac{\sqrt{\lambda}}{2\pi |\boldsymbol{x}_{j+1} - \boldsymbol{y}_{j+1}|}\right]^{\frac{3}{2}n'-\frac{5}{2}} H^{(1)}_{\frac{3}{2}n'-\frac{5}{2}}(\sqrt{\lambda}\,|\boldsymbol{x}_{j+1} - \boldsymbol{y}_{j+1}|), \quad (1.7.75)$$

where the number of dimensions of $\boldsymbol{x}_{j+1}$ and $\boldsymbol{y}_{j+1}$ is $3n'-3$. Obviously $n' \leq n$, the sign of equality applying only if there are no factors KR.

As for the operators KR, we assume as before that these are integral operators with kernels of the form F satisfying eqs. (1.7.49) and (1.7.50). If in general

$$K^{(n_i)} R(n_i,1) f(\boldsymbol{x}_i) = \int F^{(n_i)}(\boldsymbol{x}_i, \boldsymbol{y}_i; \lambda) f(\boldsymbol{y}_i)\, d\boldsymbol{y}_i, \quad (1.7.76)$$

where in the space $\mathfrak{L}^2(\boldsymbol{x}_i)$

$$|F^{(n_i)}(\lambda)|_{\boldsymbol{x}_i} \leq \text{const.}\, |\lambda - \Lambda^{(n_i)}|^{n_i-2} [\operatorname{Im}\sqrt{(\lambda - \Lambda^{(n_i)})}]^{-\frac{5}{2}n_i+\frac{5}{2}}, \quad (1.7.77)$$

then it follows immediately from the reasoning developed in the previous section that $(KR) * (KR)$ is an integral operator,

$$\left.\begin{aligned}&\{[K^{(n_i)}R(n_i,1)] * [K^{(n_j)}R(n_j,1)]\} f(\boldsymbol{x}_i,\boldsymbol{x}_j)\\ &= \int [F^{(n_i)} * F^{(n_j)}](\boldsymbol{x}_i,\boldsymbol{x}_j,\boldsymbol{y}_i,\boldsymbol{y}_j;\lambda) f(\boldsymbol{y}_i,\boldsymbol{y}_j)\, d\boldsymbol{y}_i\, d\boldsymbol{y}_j,\end{aligned}\right\} \quad (1.7.78)$$

where now in the space $\mathfrak{L}^2(\boldsymbol{x}_i,\boldsymbol{x}_j)$

$$|[F^{(n_i)} * F^{(n_j)}](\lambda)|_{\boldsymbol{x}_i,\boldsymbol{x}_j} \leq \text{const.}\,|\lambda - A^{(n_i)} - A^{(n_j)}|^{n_i+n_j-3}\,[\operatorname{Im}\sqrt{(\lambda - A^{(n_i)} - A^{(n_j)})}]^{-\frac{5}{2}(n_i+n_j)+5}. \quad (1.7.79)$$

This result can easily be extended to

$$\left.\begin{aligned}&\{[K^{(n_1)}R(n_1,1)] * [K^{(n_2)}R(n_2,1)] * \ldots * [K^{(n_j)}R(n_j,1)]\} f(\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_j)\\ &= \int [F^{(n_1)} * F^{(n_2)} * \ldots * F^{(n_j)}](\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_j,\boldsymbol{y}_1,\boldsymbol{y}_2,\ldots,\boldsymbol{y}_j;\lambda) f(\boldsymbol{y}_1,\boldsymbol{y}_2,\ldots,\boldsymbol{y}_j)\, d\boldsymbol{y}_1\, d\boldsymbol{y}_2 \ldots d\boldsymbol{y}_j,\end{aligned}\right\} \quad (1.7.80)$$

the norm of the integral kernel satisfying

$$\left.\begin{aligned}&|[F^{(n_1)} * F^{(n_2)} * \ldots * F^{(n_j)}](\lambda)|_{\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_j}\\ &\leq \text{const.}\,|\lambda - \sum_{i=1}^{j} A^{(n_i)}|^{n''-j-1}\,[\operatorname{Im}\sqrt{(\lambda - \sum_{i=1}^{j} A^{(n_i)})}]^{-\frac{5}{2}n''+\frac{5}{2}j},\quad n'' \equiv \sum_{i=1}^{j} n_i.\end{aligned}\right\} \quad (1.7.81)$$

To establish that the operator (1.7.74) is an integral operator, it remains to investigate

$$\left.\begin{aligned}&I \equiv \frac{1}{2\pi}\int_C d\sigma \int d\boldsymbol{x}_1 \ldots d\boldsymbol{x}_j\, d\boldsymbol{x}_{j+1} \int d\boldsymbol{y}_1 \ldots d\boldsymbol{y}_j\, d\boldsymbol{y}_{j+1}\, |\,\bar{g}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_j,\boldsymbol{x}_{j+1})\\ &\times [F^{(n_1)} * \ldots * F^{(n_j)}](\boldsymbol{x}_1,\ldots,\boldsymbol{x}_j,\boldsymbol{y}_1,\ldots,\boldsymbol{y}_j;\sigma)\, G_0^{(n')}(\boldsymbol{x}_{j+1},\boldsymbol{y}_{j+1};\lambda-\sigma) f(\boldsymbol{y}_1,\ldots,\boldsymbol{y}_j,\boldsymbol{y}_{j+1})|.\end{aligned}\right\} \quad (1.7.82)$$

For this we note that

$$\left.\begin{aligned}&|\lambda|^{\frac{3}{4}n'-\frac{5}{4}} \int_0^\infty |H^{(1)}_{\frac{3}{2}n'-\frac{5}{2}}(r\sqrt{\lambda})|\, r^{\frac{3}{2}n'-\frac{3}{2}}\, dr \leq |\lambda|^{\frac{3}{4}n'-\frac{3}{2}} (\operatorname{Im}\sqrt{\lambda})^{\frac{1}{2}} \left| \int_0^\infty H^{(1)}_{\frac{3}{2}n'-\frac{5}{2}}(ir \operatorname{Im}\sqrt{\lambda})\, r^{\frac{3}{2}n'-\frac{3}{2}}\, dr \right|\\ &\leq \text{const.}\,|\lambda|^{\frac{3}{4}n'-\frac{3}{2}} (\operatorname{Im}\sqrt{\lambda})^{-\frac{3}{2}n'+1},\end{aligned}\right\} \quad (1.7.83)$$

where the first inequality follows from an integral representation of the Hankel function (WATSON(19) section 6.12), and the second one from evaluating the integral in the second member. With a change of variables as was made in eq. (1.5.34), it is now readily seen that

$$\left.\begin{aligned}&I \leq \text{const.} \int_C d\sigma\, |\sigma - \sum_{i=1}^{j} A^{(n_i)}|^{n''-j-1}\,[\operatorname{Im}\sqrt{(\sigma - \sum_{i=1}^{j} A^{(n_i)})}]^{-\frac{5}{2}n''+\frac{5}{2}j}\\ &\times |\lambda-\sigma|^{\frac{3}{4}n'-\frac{3}{2}}\,[\operatorname{Im}\sqrt{(\lambda-\sigma)}]^{-\frac{3}{2}n'+1}\, ||\,g\,||\;||\,f\,||,\end{aligned}\right\} \quad (1.7.84)$$

which is finite provided C is a suitable contour and λ is inside the complex plane cut from $\sum_{i=1}^{j} \Lambda^{(n_i)}$ to ∞. Under these circumstances, the operator (1.7.74) can be written as an integral operator the kernel of which is of the form

$$\frac{1}{2\pi i}\int_C [F^{(n_1)} * \ldots * F^{(n_j)}](\boldsymbol{x}_1, \ldots, \boldsymbol{x}_j, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_j; \sigma)\, G_0^{(n')}(\boldsymbol{x}_{j+1}, \boldsymbol{y}_{j+1}; \lambda - \sigma)\, d\sigma. \quad (1.7.85)$$

Since for $k \geq 2$ the resolvents $R(n, k)_{p(k)}$ are linear combinations of operators of the form (1.7.74), it follows that there are Green functions $G(n, k)_{p(k)}$ which are linear combinations of functions of the form (1.7.85).

It is not difficult to see that the kernel given by eq. (1.7.85) depends only on $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_j, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_j$, and $\boldsymbol{x}_{j+1} - \boldsymbol{y}_{j+1}$. It satisfies

$$\left.\begin{aligned}\frac{1}{2\pi}\int d\boldsymbol{x}_1 \ldots d\boldsymbol{x}_j \int d\boldsymbol{y}_1 \ldots d\boldsymbol{y}_j \Big[\int d(\boldsymbol{x}_{j+1} - \boldsymbol{y}_{j+1}) \Big| \int_C [F^{(n_1)} * \ldots * F^{(n_j)}](\boldsymbol{x}_1, \ldots, \boldsymbol{x}_j, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_j; \sigma) \\ \times G_0^{(n')}(\boldsymbol{x}_{j+1}, \boldsymbol{y}_{j+1}; \lambda - \sigma)\, d\sigma \Big|^2 < \infty.\end{aligned}\right\} (1.7.86)$$

This is a situation analogous to the one discussed in section 1.5.3. With the methods outlined there, it is easily shown that the operator (1.7.74) can be written as an integral operator with a kernel satisfying eq. (1.7.86) in only one way. In this sense the kernel (1.7.85) is unique. Since the Green functions $G(n, k)_{p(k)}$ with $k \geq 2$ are linear combinations of functions of the form (1.7.85), they are likewise unique.

If for $m = 2, 3, \ldots, n-1$ the Green functions $G(m, k)_{q(k)}$ $(k = 1, 2, \ldots, m)$ satisfy symmetry relations of the forms (1.5.46) and (1.5.47), then so do the functions $F^{(m)}$, by the resolvent equation. With the argument used to get eqs. (1.5.46) and (1.5.47), it is then easily checked that similar symmetry relations apply to the functions $G(n, k)_{p(k)}$ $(k \geq 2)$. At this point the fact that the kernel $K^{(n)}$ belongs to $\mathfrak{L}^2$ can be used to show that there is a Green function $G^{(n)} \equiv G(n, 1)$ (cf. the proof of eq. (1.3.11)). Also, since the operator $K^{(n)} R(n, 1)$ belongs to $\mathfrak{L}^2$, its kernel is unique among all kernels in $\mathfrak{L}^2$. By the resolvent equation and the uniqueness of the functions $G(n, k)_{p(k)} (k \geq 2)$, this means that $G^{(n)}$ is unique in the sense that it can be written as a linear combination of functions with suitable integrability properties in only one way. It follows with the method of section 1.3.2 that $G^{(n)}$ also satisfies symmetry relations.

1.7.6. The spectrum

We conclude the present investigation with some general remarks on the spectrum of the Hamiltonian $H(n, 1)$. It was assumed in eqs. (1.7.49) and (1.7.50) that for $m = 2, 3, \ldots, n-1$ we know the kernels $K_q^{(m)}$ and the Green functions $G^{(m)}$ in the λ-plane cut from $\Lambda^{(m)}$ to ∞. Under this assumption we are able to evaluate the kernels $K_p^{(n)}$. However, it follows from eqs. (1.7.63) and (1.7.67) that in doing so we have to confine ourselves to the λ-plane cut from $\min(\Lambda^{(n_1)} + \Lambda^{(n_2)}, \Lambda^{(n-1)})$ to ∞, where the

minimum is to be taken with respect to all possible divisions of the n particles into two groups. Now it will be shown in a forthcoming paper on the theory of scattering that there is a continuous spectrum from $\min(A^{(n_1)}+A^{(n_2)}, A^{(n-1)})$ to ∞. From this it follows immediately that the lower bound $A^{(n)}$ of the spectrum of $H(n, 1)$ satisfies

$$A^{(n)} \leq \min(A^{(n_1)}+A^{(n_2)}, A^{(n-1)}) \quad (n_1+n_2=n). \tag{1.7.87}$$

This was already used in eq. (1.7.69).

Let us now consider the convolutions whereby we want to construct the Green functions $G(n, k)_{p(k)}$ with $k \geq 2$. According to eq. (1.7.84), these give rise to various cuts from $\sum_{i=1}^{j} A^{(n_i)}$ to ∞, where $\sum_{i=1}^{j} n_i = n'' \leq n$ $(2 \leq n_i \leq n-1)$. Now if $n'' \leq n-1$, eq. (1.7.87) shows that

$$\min(A^{(n-1)}) \leq \min(A^{(n'')}) \leq \sum_{i=1}^{j} A^{(n_i)}. \tag{1.7.88}$$

Also, if $n''=n$, the sum with respect to i must consist of at least two terms, since $n_i \leq n-1$. Hence in this case we may write

$$A^{(n-n_j)}+A^{(n_j)} \leq \sum_{i=1}^{j-1} A^{(n_i)}+A^{(n_j)} = \sum_{i=1}^{j} A^{(n_i)}, \tag{1.7.89}$$

where now $A^{(n-n_j)}$ refers to the particular system of $n-n_j$ particles which is obtained by putting together the groups of $n_1, n_2, \ldots, n_{j-1}$ particles which appear on the right-hand side of eq. (1.7.89), and taking into account all their interactions. It follows in any case that

$$\min(A^{(n_1)}+A^{(n_2)}, A^{(n-1)}) \leq \sum_{i=1}^{j} A^{(n_i)}. \tag{1.7.90}$$

Hence the cut owing to the kernel contains the cut caused by the construction of the Green functions $G(n, k)_{p(k)}$ with $k \geq 2$. If we define

$$M^{(n)} = \min(A^{(n_1)}+A^{(n_2)}, A^{(n-1)}) \quad (n_1+n_2=n), \tag{1.7.91}$$

the ultimate cut runs from $M^{(n)}$ to ∞. Now it is clear from the method of evaluating the Green function $G^{(n)}$ that $H(n, 1)$ cannot have a continuous spectrum beyond the interval $[M^{(n)}, \infty)$. Hence since there is a continuous spectrum from $M^{(n)}$ to ∞, as was remarked above, it follows that the continuous spectrum of $H(n, 1)$ coincides with the interval $[M^{(n)}, \infty)$. In the λ-plane cut from $M^{(n)}$ to ∞, there may be a discrete spectrum in a finite interval $[A^{(n)}, M^{(n)})$. It is not known if $M^{(n)}$ is a point of accumulation of the discrete spectrum (cf. the discussion at the end of section 1.3.4).

Summarizing, let us assume that for $m=2, 3, \ldots, n-1$ we know the kernels $K_q^{(m)}$ and the Green functions $G^{(m)}$ in the λ-plane cut from $A^{(m)}$ to ∞. Let the quantities $|K_q^{(m)}|$ and $||R(m, 1)||$ satisfy the inequalities (1.7.50). Then we can find the kernels $K_p^{(n)}$ and the Green functions $G(n, k)_{p(k)}$ $(k \geq 2)$ in the λ-plane cut from $M^{(n)}$ to ∞. The quantities $|K_p^{(n)}|$ satisfy the inequality (1.7.50). Also, if all the Green func-

tions $G(m, k)_{q(k)}$ satisfy symmetry relations of the forms (1.5.46) and (1.5.47), then so do the functions $G(n, k)_{p(k)}$ $(k \geq 2)$. Owing to this symmetry combined with the fact that each $|K_p^{(n)}|$ is finite, we can evaluate the Green function $G^{(n)} \equiv G(n, 1)$ for all values of λ not in the spectrum of $H(n, 1)$. In particular, $G^{(n)}$ can be found in the λ-plane cut from $\Lambda^{(n)}$ to ∞. It satisfies the symmetry relations (1.5.46) and (1.5.47). The norm $||R(n,1)||$ satisfies the inequality (1.7.50). We thus see that on the basis of our assumptions for $m = 2, 3, \ldots, n-1$ we can find all the relevant quantities for $m = n$. These satisfy the desired inequalities and symmetry relations. Also, we can evaluate the Green function $G^{(2)} \equiv G(2,1)$ from the known functions $K^{(2)}$ and $G(2,2)$. For $m = 2$ the inequalities and symmetry relations are satisfied. From this we may conclude that by iteration we are able to construct the Green function $G^{(n)}$ for any finite number n.

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A THREE-DIMENSIONAL SPECTRAL CLASSIFICATION OF G AND K STARS

BY

KJELD GYLDENKERNE

København 1964

Kommissionær: Ejnar Munksgaard

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Contents

Synopsis

On the basis of three classification indices k, n and m, related to the break around the H- and K-lines, to the cyanogen absorption at 4200 A and to a broad absorption of the continuum, a system of three independent classification parameters S, L and C has been established for stars of spectral types G 5 – K 3.5 and luminosity classes II–III to IV. The parameter S is closely related to average MK spectral types, parameter L to the luminosity, and C is a third parameter which measures the remaining dispersion and is probably related chiefly to the chemical composition. With systematic dependence also on S, absolute magnitudes $M_V(k, n, m)$ have been derived from L on the basis of M_V given by trigonometric parallaxes (main-sequence stars), cluster parallaxes (Hyades) and M_V(K) determined by the Wilson-Bappu method for a large body of giant stars. The $M_V(k, n, m)$ and M_V(K) values agree with a scatter which corresponds to a mean error of $\pm 0\overset{m}{.}46$ for each of the two sets of absolute magnitudes.

The classification parameters have been compared with the Cambridge intensity ratios and with photoelectric colour indices; furthermore the effect of duplicity has been investigated. The distribution of the parameters and the galactic space-velocity components on the program stars have been studied. It was found that the data of about 160 giants and subgiants in the considered range can be divided into two groups according to C with a limit not much different from the average C value. One of these groups contains young giants evolved from A-type main-sequence stars as well as older stars evolved from the F- and G-type section. The other group includes practically no young giants. This division is also reflected in the velocity distribution of the two groups and is similar to the earlier division of Vyssotsky who used strong-line and weak-line criteria.

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1. Introduction

Quantitative classification of stellar spectra has been carried out extensively during the recent years. A survey of the different methods is given by Strömgren (1963b). For the early type stars, reference should be made to the work of Chalonge and collaborators (cf. Chalonge 1958), Strömgren (1956a, 1956b, 1958a, 1958b), Petrie (1956), Crawford (1958) and T. and J. H. Walraven (1960). Relations between precise classification equivalents of main-sequence B, A and F stars, stellar ages and space velocities have been discussed recently by Strömgren (1962b, 1963a).

The present treatise is concerned with the classification of G and K stars. For these stars we mention the work by Hossack (1954), by Halliday (1955) and by Oke (1957, 1959), who have developed methods for measuring line-depth ratios in photographic spectrograms of 33 A/mm dispersion at H_γ. Wilson and Bappu (1957) used spectra with a dispersion of 10 A/mm and found that the width of the emission component of the H- and K-lines of ionized Ca was a sensitive luminosity indicator for the G, K and M stars, independent of the spectral type; the absolute magnitudes M_v(K) have been calibrated for a number of bright stars (Wilson, 1959).

Improved observational methods have shown the influence of a third parameter, e. g. the cyanogen absorption at 4200 A is affected as could be found through the visual inspection method in the Atlas of Morgan, Keenan and Kellman (1943). It has been further confirmed by Roman (1952) in a classification of a large number of bright G and K stars; she also noticed other differences denoted as strong-line and weak-line characteristics in these spectra. These features are most probably due to differences in the abundances of the metals and of the O, C, N group relative to hydrogen, according to Schwarzschild, Spitzer and Wildt (1951), and are found to be related to differences in space-velocity characteristics (Roman 1952, Keenan and Keller 1953, Keenan 1958, Vyssotsky and Skumanich 1953, Blaauw 1958).

The cyanogen absorption is apparently a sensitive population effect and has been measured quantitatively in photographic spectra by Keenan (1958) and by Yoss (1961, 1962) and photoelectrically using narrow-band techniques by Strömgren and Gyldenkerne (1955) and Gyldenkerne (1958a, 1958b, referred to as Papers I and II in what follows), by Griffin and Redman (1960) and by Crawford (1961). However, already from objective prism observations initiated more than 40 years ago by Lindblad (1922) and carried out extensively at the Stockholm and Uppsala observatories, the cyanogen absorption is known to depend on the luminosity and to a lesser degree on the spectral type. Therefore, in addition to a cyanogen

equivalent, criteria for the spectral type and luminosity should also be determined accurately.

Photoelectric narrow-band measurements of different outstanding features in the G and K type spectra have been made by astronomers at the Cambridge observatory in order to test the sensitivity of these features to the stellar parameters. In addition to the cyanogen observations, GRIFFIN and REDMAN (1960) have published measurements of the G-band, the magnesium b triplet at 5170 A has been measured by DEEMING (1960), and GRIFFIN (1961) has made measurements of the FeI-lines at 5250 A and of the sodium D-lines.

In the method of STRÖMGREN and GYLDENKERNE (1955), three classification indices, similar to three of the Stockholm-Uppsala equivalents were measured by means of interference filters. These quantities are k, which is related to a region close to the K-line of ionized Ca, n, which measures the cyanogen absorption at 4200 A and g, which measures the break at the G-band. The three indices provided a two-dimensional classification, but the analysis of the material of about 250 bright G and K stars clearly showed the effect of a third parameter. BORGMAN (1959) measured the metallic-line index m as defined by STRÖMGREN (1958a) for a few G and K stars and found a separation of high-velocity giants from low-velocity giants in an m, spectral type diagram. Borgman then suggested that it might be possible to separate the three parameters using m together with two of the indices determined by STRÖMGREN and GYLDENKERNE. In 1960–61 the present author measured m for almost all stars for which k, n and g were already available. In a preliminary analysis (GYLDENKERNE 1961) it was found that the spectral type, the luminosity and a third parameter can be determined for G8 to K3 giants by means of k, n and m.

Since the late-type spectra are rich in detail, it should be expected that differences in the spectral transmission regions of the classification indices would influence the sensitivity of the indices to the principal stellar parameters. For the cyanogen index the dependence on the wave length regions has been convincingly demonstrated by YOSS (1962) with reference to the CN ratio measured by GRIFFIN and REDMAN, the present index n and a similar index measured by CRAWFORD (1961). The latter index utilizing filters narrower than n with somewhat different peak wave lengths appeared to be considerably more sensitive for the same measuring accuracy. Similar results may be found for the other indices. Furthermore, the physical significance of an index is not quite clear in every case. For the index k, as an example, it may be that effects other than the K-line contribute considerably to the variation of the index with the stellar parameters (cf. p. 28). In this connection we refer to results obtained by VAN DEN BERGH (1963) for the quantity Δ, covering almost the same spectral range as k.

Further investigations of the dependence of the indices on the spectral transmission regions are in progress at this observatory. However, since through the preliminary analysis it developed that k, n and m, as originally defined, reproduce spectral types and absolute magnitudes in a simple way with good accuracy and

furthermore a third parameter of significant variation appears, we have carried this analysis as far as possible for the available data of G and K stars. The results concerning properties of the classification system as well as its relation to age and kinematics of the program stars are presented in this paper.

The measurements of the index *m* and its relation to spectral types and luminosity classes are described in Section 2. The three-dimensional classification system is established in Section 3. In Sections 4 and 5 the classification parameters are related to other spectrophotometric quantities and to photoelectric colour indices. The properties of the third parameter are discussed in Section 6, and the relations of the three parameters to the space velocity and its galactic components are studied in Section 7. In the final section the results of the analysis are summarized, and the projected extension of the classification program for late type stars is outlined.

2. The Metallic-Line Index *m* for G and K Stars and its relation to MK Spectral Types and Luminosity Classes

The observations of the index *m* have been carried out by means of a two-beam photometer attached to the 20 inch reflecting telescope of the Brorfelde observatory. The photometer, constructed in the observatory workshop under the direction of P. BECHMANN, follows a principle given by STRÖMGREN and quoted by CRAWFORD (1958, Fig. 3, second version). The two beams from the beam splitter pass two field lenses, which image the telescope objective on the thin layers of two interference filters. These images are projected upon the photocathodes of two photomultipliers by a second set of lenses. The anode currents are measured utilizing integrators which were developed and constructed by R. H. WEITBRECHT (1957). A programming unit permits an automatic recording of the two voltages—one after the other—on a one-pen recorder, PHILIPS PR 2210 A/21. Two LALLEMAND 20 stage photomultipliers Gabriel VIII and Norbert VIII have been used without refrigeration throughout the program.

The three intensities were measured through interference filters made by SCHOTT and Genossen, Mainz. These PIL-type filters had the following characteristics:

Wave length of maximum transmission	4050 A	4510 A	4970 A
Width corresponding to one half of maximum transmission	75 A	80 A	90 A
Width corresponding to one tenth of maximum transmission	230 A	250 A	260 A

The maximum transmission of the filters was about 40 per cent.

These filters defined the colour index difference *m* as follows:

$$m = \text{const.} - 2.5 \left\{ [\log I(4970) - \log I(4510)] - [\log I(4510) - \log I(4050)] \right\}$$

The 4050 filter and one 4510 filter were placed in filter holder I (transmitted beam). Another 4510 filter identical with the first one was placed in filter holder II (reflected beam), which also contained the 4970 filter.

The measurements were carried out according to the following scheme:

I	II	
4050	4510	star + sky
4510	4970	star + sky
4050	4510	star + sky
	etc.	
4050	4510	sky
4510	4970	sky

This procedure eliminated effects of varying relative sensitivity of the two parts of the photometer. The number of deflections depends mainly on the quality of the sky. The extinction could vary from one measurement of a pair to the next one, but this effect is practically eliminated by alternating the two colour indices, which almost have equal wave length bases. The integration times varied from 10 to 40 sec for the stars in this program (mainly brighter than $5^{m}.5$).

The observations have been corrected to zenith utilizing an average extinction coefficient, 0.039. Night corrections have been determined from standard star measurements close to zenith each night. The results have been reduced to approximately the same zero point as the one used by Strömgren (1958a) for the F stars. Comparison of measurements of the same stars obtained on different nights yields a mean error of one single observation of $\pm 0^{m}.008$ (mean errors are used throughout in this paper).

The measurements obtained in the described manner have been tested by observing a certain number of the program stars by means of an ordinary single channel photometer together with the three filters. The two sets of observations are in satisfactory agreement.

The values of m for 233 G and K stars and a few stars of other spectral types are given in Table 11.

The relation of the index m to the MK spectral types and luminosity classes is shown in Fig. 1. For stars of class III, mean values of m have been derived and are given in Table 1. The mean values are represented by large dots in Fig. 1*. In the same table are also listed the mean values of k, n and g from Table 1 of Paper II.

Table 1.

Mean values of classification indices for stars of luminosity class III.

MK	$\overline{m}$	number of stars	$\overline{k}$	$\overline{n}$	$\overline{g}$
G8 III	0.354	37	0.342	0.171	0.258
K0 III	0.411	50	0.293	0.198	0.286
K1 III	0.465	14	0.246	0.218	0.312
K2 III	0.522	28	0.206	0.250	0.341
K3 III	0.614	26	0.150	0.284	0.391
K4 III	0.708	8	0.114	0.298	0.432
K5 III	0.790	8	0.105	0.299	0.476

* The dots correspond to star numbers slightly different from those of the table.

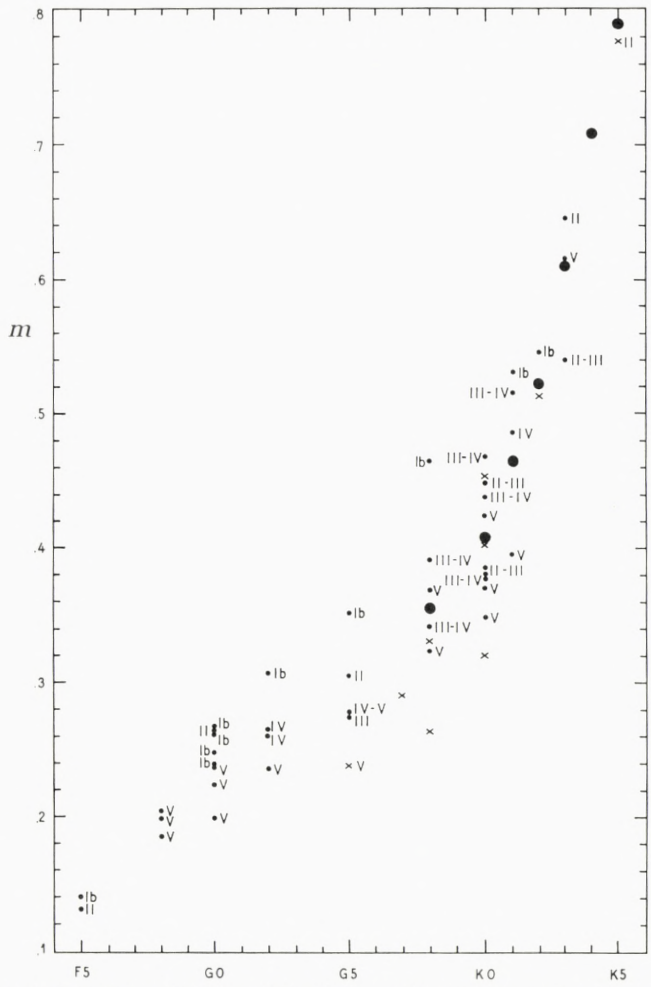

Fig. 1. The metallic-line index m as function of the MK spectral type and luminosity class. Crosses indicate high-velocity stars.

It is seen that the dependence on spectral type is more pronounced for m than for k and g in the whole range G8–K5; the sensitivity of m exceeds that of k and g by a factor of 1.2–2.6.

For the program stars we found the same internal accuracy, $\pm 0^{\mathrm{m}}.008$, of m as of k, n and g. For the mean values of these quantities we provisionally adopted the external mean error $\pm 0^{\mathrm{m}}.010$ in Paper II. Although we have determined m in only one series of measurements we shall consider the mean error $\pm 0^{\mathrm{m}}.010$ as representative for all four quantities in what follows.

Using this mean error we find the accuracy of spectral types determined from m as shown in Table 2. As in earlier cases we have assumed that the range G8 III to K0 III covers one spectral subtype.

TABLE 2.
Mean errors of spectral subtypes determined from m
(unit one spectral subtype).

G8 III – K0 III	±0.18
K0 III – K1 III	±0.19
K1 III – K2 III	±0.18
K2 III – K3 III	±0.11
K3 III – K4 III	±0.11
K4 III – K5 III	±0.12

3. The Three-Dimensional Classification System

In principle it would be desirable to carry out a classification similar to the present one by relating the classification equivalents to computed or measurable stellar atmospheric parameters, such as a measure of the colour temperature, the absolute magnitude and the chemical composition. However, colour equivalents in the normal spectral region as the colour indices $(U-B)$ and $(B-V)$, are expected to be influenced by the abundance effect for the spectral types considered here, and long wave length colour indices are thus far available only for a small number of our stars. Absolute magnitudes based on trigonometric parallaxes are generally quite uncertain for stars in the giant region, and only a few group stars are included in the present program. Abundances, finally, have been published for extremely few G and K giants. Therefore, this analysis has been carried out by separating three independent parameters S, L and C, so that S is closely correlated with average MK spectral types and L with the absolute magnitudes M_v, determined by the method of WILSON and BAPPU (1957), or by the group parallax for the Hyades and the trigonometric parallax for the main-sequence stars; the remaining dispersion defines the third parameter C. An approximate, linear and semi-graphical method has been used.

Figs. 2 and 3 show the distribution of the stars in an (n, k) diagram and a (k, m) diagram. The luminosity class is indicated for the stars of classes Ib to II and IV to V. Dots without indication correspond to stars of luminosity classes II–III, III and III–IV; the large dots correspond to the mean values in Table 1. Crosses indicate stars of high velocity according to KEENAN and KELLER (1953). Both diagrams demonstrate clearly a two-dimensional distribution with the supergiants and main-sequence stars lying on each side of the class III stars. However, the dispersion of the latter stars around a line through the mean points is considerable. Some class III stars lie close to the supergiants, while others lie close to the main-sequence stars. This is very unlikely due to an error in the MK luminosity classification, but should probably be ascribed to the variation of a third parameter, which is assumed to be the initial chemical composition. Extreme abundance-ratio values have been found

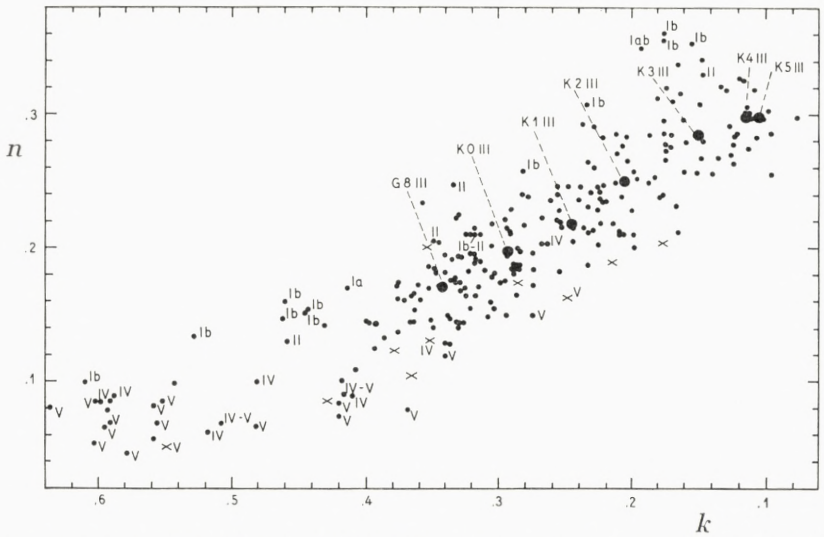

Fig. 2. The cyanogen-absorption index n plotted against the index k. Crosses indicate high-velocity stars.

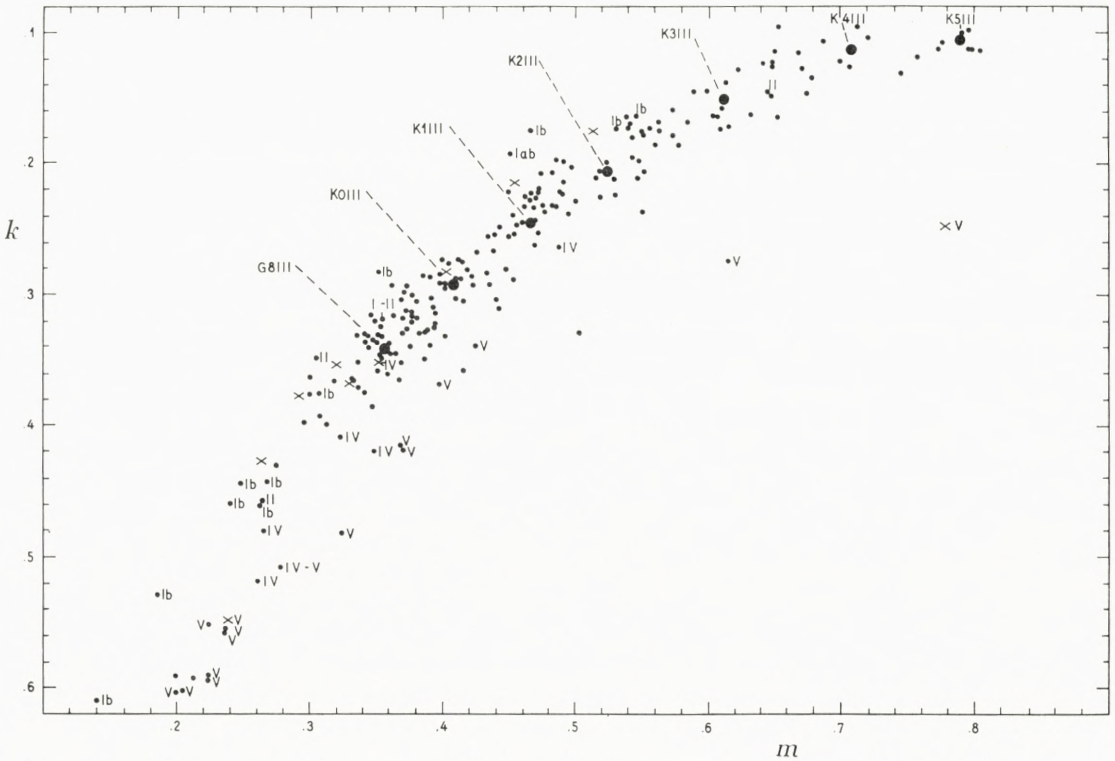

Fig. 3. The index k plotted against the metallic-line index m. Crosses indicate high-velocity stars.

for some class III high-velocity stars, and therefore, these stars should exhibit large deviations from the mean class III stars in the (n, k) and (k, m) diagrams. In the (n, k) diagram the extreme positions of the high-velocity stars (marked by crosses) close to the main-sequence stars have been noticed in Paper II. It is then significant that crosses corresponding to the same high-velocity stars lie close to the supergiants in the (k, m) diagram. This suggests the possibility of separating the chemical composition effect from the luminosity effect by means of the three classification indices.

We have derived the three classification parameters S, L and C by means of the (n, k) diagram and the (k, m) diagram, in the following manner.

In both diagrams we consider the variation along the line through the mean points as related to a first parameter, a measure of the spectral type. Since the mean points in the (n, k) diagram very nearly define a straight line, we determine the quantity giving the spectral type, as a function of n and k:

$$\text{Spectral-type parameter } S = n - 1.70\, k + 1.000\,.$$

With the adopted mean error $\pm 0^{\mathrm{m}}.010$ of n and k and the correlation coefficient -0.83 between them, the mean error of an S value is $\pm 0^{\mathrm{m}}.026$. The mean values of S for different spectral types of luminosity class III are given in Table 3. Accordingly, the mean error of S corresponds to a classification accuracy of one quarter of a spectral subtype from G8 to K3.

TABLE 3.

Mean values of the spectral-type parameter.

	$\bar{S}$
G8 III	$0^{\mathrm{m}}.590$
K0 III	0.700
K1 III	0.800
K2 III	0.900
K3 III	1.029
K4 III	1.104
K5 III	1.121

The second parameter in the two diagrams is measured as the distance from the mean line plus an arbitrary constant. From the (n, k) diagram this parameter x can be expressed through the relation $x = 0.862\, n + 0.507\, k$. For the (k, m) diagram we have determined the distance graphically and adopted the second parameter y as the distance plus 0.100. In the preliminary investigation the material was divided into two groups, corresponding to the intervals in spectral type G8–K1 and K2–K3, and for each part a linear relation between k and m was used. In the present case we have approximated the slightly curved (k, m) relation piecewise by straight lines.

Approximate linear relations have been derived for y as $y = 0.75\, k + 0.66\, m - 0.39$ from G8 to K1, and $y = 0.86\, k + 0.52\, m - 0.35$ from K2 to K3. The accuracy

of the different parameters related to the classification indices, and the scatter in relations between the parameters and other quantities are estimated using an average relation $y = 0.80\,k + 0.60\,m + \text{const}$ and the above relations for x and S. The effect of the correlation moments has been determined by means of correlation coefficients, computed as $\varrho(n, k) = -0.83$, $\varrho(m, k) = -0.64$ and $\varrho(n, m) = +0.54$. Thus, according to the adopted mean error $\pm 0^{m}.010$ of k, n and m, the mean errors of x and y are found to be $\pm 0^{m}.005$ and $\pm 0^{m}.006$ respectively.

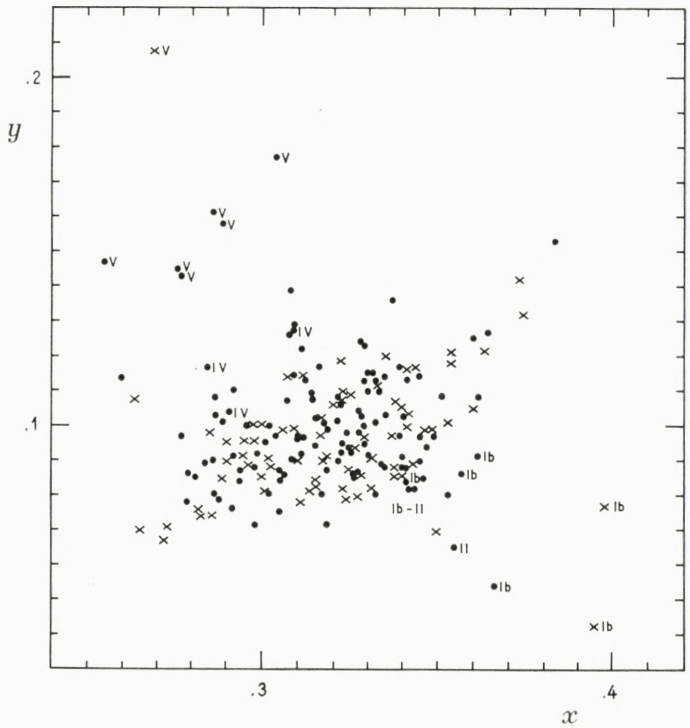

Fig. 4. The dispersion y around the luminosity class III mean-line in the (k, m) diagram, plotted against the corresponding dispersion x in the (n, k) diagram (x and y are both independent of the spectral type). The data are divided into two groups according to the spectral type parameter S. $S < 0.80$, dots; $S > 0.80$, crosses.

In Fig. 4, y is plotted against x. The material is divided into two groups: dots correspond to the region $0.35 < S < 0.80$ and crosses to $0.80 < S < 1.07$. These notations are used throughout in what follows unless otherwise stated. The diagram clearly exhibits a two-dimensional distribution of the stars, and both coordinates x and y are independent of the first parameter S.

Obviously the dispersion in the direction upper left to lower right corner of Fig. 4 is correlated with the luminosity. Accordingly, instead of x and y as second and third parameters we could use $x - y$ and $x + y$, and then $x - y$ would be a luminosity parameter (adopted in the preliminary discussion). However, improved parameters may be obtained as $x - qy$ and $x + 1/q\ y$ if absolute magnitudes are considered.

We have attempted an estimate of q considering stars having approximately the same absolute magnitude but differing significantly with respect to the third parameter. We concentrate the attention on stars with $M_v(K)$ in the range from $0^m.0$ to $1^m.0$, and divide this material into the two groups according to S, each group containing 17 stars. Separate plots of x versus y indicate linear relations for each group and by the least-squares method (errors both in x and y) we find $q = 1.60$ for $S < 0.8$ and $q = 1.89$ for $S > 0.8$. We have made another estimate of q by correcting all the considered giant and subgiant stars to the same absolute magnitude $M_v(\mathrm{K}) = 0.0$. The corrections are made by means of linear relations between M_v and x and y respectively, derived by means of the supergiants and the main-sequence stars. Again we divide the material into two groups and find for $S > 0.8$ the corrections $\Delta x = 0.011\,\Delta M_v$ and $\Delta y = -0.014\,\Delta M_v$, which are used for both groups (for $S < 0.8$ no supergiant can be used). Through least-squares computations of linear relations between the corrected x and y values we find $q = 1.07$ for $S < 0.8$ (47 stars) and $q = 2.08$ for $S > 0.8$ (22 stars). These results indicate a q larger than unity. We have used $q = 1.4$, and thus we define:

$$\text{Luminosity parameter } L = x - 1.40\,y$$
$$\text{Third parameter } C = x + 0.71\,y.$$

In Fig. 5, L is plotted against absolute magnitudes, and the data are divided into two groups with the above-mentioned symbols (the only K3 V star is included in the cross group in this case and also in the above computations of Δx and Δy). The supergiants of the dot group, mainly of the classes G0 Ib–G2 Ib, are omitted, and for the remaining data L appears to be linearly related to the absolute magnitudes. A least-squares solution yields the relation $M_v = 7.61 - 36.1\,L$ for $S < 0.8$, and $M_v = 6.20 - 32.6\,L$ for $S > 0.8$. Thus the L coefficient as well as the constant in the relation varies with S. Adopting the mean value 34.3 for the coefficient, the constant will be $p = M_v + 34.3\,L$, which appears to be linearly correlated with S according to the plot in Fig. 6. Accordingly the absolute magnitude should be represented by a relation of the form $M_v = a + bS + cL$. A least-squares solution for the stars in the range G5–K3.5 provides the relation

$$M_v = 8.28 - 2.28\,S - 32.3\,L$$
$$\pm 0.31 \quad \pm 0.42 \quad \pm 1.6.$$

From the residuals between $M_v(k, n, m)$ computed from this formula and the given M_v values, we find the mean square of the scatter to be 0.43 on the basis of 69 stars of luminosity classes II–III to IV. The mean error of one single determination of $M_v(\mathrm{K})$ is estimated by Wilson to be $\pm 0^m.4$. The average number of observations in the utilized $M_v(\mathrm{K})$ material is 1.8 (Wilson, privately communicated data), and thus the mean error of an $M_v(\mathrm{K})$ value should be $\pm 0^m.3$. Introducing expressions for S and L in the relation, we find the mean error of the computed $M_v(k, n, m)$ to be $\pm 0^m.4$, by using the mean error $\pm 0^m.010$ adopted for k, n and m. Thus the mean

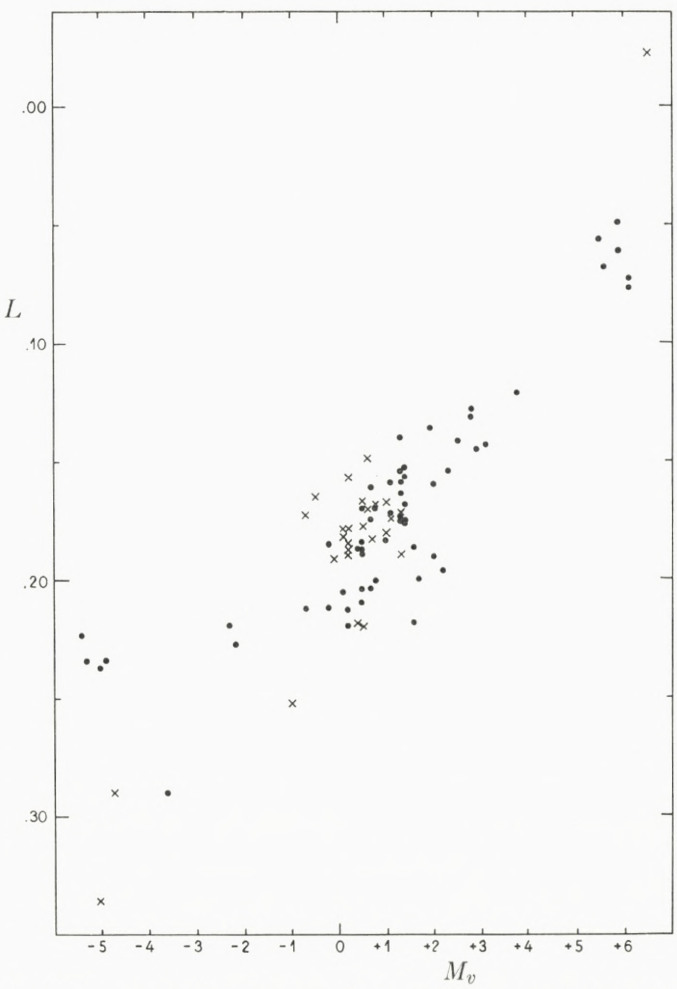

Fig. 5. The luminosity parameter L in relation to the absolute magnitude. $S<0.80$, dots; $S>0.80$, crosses.

square of the scatter due to the uncertainty should be 0.25, and there seems to be a cosmical scatter of $\pm 0^{\mathrm{m}}.42$. WILSON (1959) has estimated the cosmical scatter in the relation between M_v(K) and M_v determined from trigonometric parallaxes to be $\pm 0^{\mathrm{m}}.3$. We have omitted a few extremely large residuals which would, of course, increase the scatter in $M_v(\mathrm{K}) - M_v(k, n, m)$. However, these residuals may be related to an effect of duplicity (cf. Section 5).

The described procedure has essentially used a transformation from the observed indices to the three independent parameters, covering the entire range of spectral types for which S is defined. Then M_v is derived from two of these parameters L and S. M_v depends primarily on L and the dependence on S has the character of a zero-point variation. This might as well be due, at least partly, to a zero-point variation

of M_v(K) with spectral type, but according to WILSON (1959) such effect should be negligible. The third parameter C is assumed to represent the heavy-element-to-hydrogen ratio, but the latter may depend also on S; this question will be discussed in Sections 6 and 7.

An additional number of stars, particularly more supergiants and main-sequence stars, might permit a derivation of a least-squares relation between M_v, S, x and y from which q would be determined (the present data are too inhomogeneously

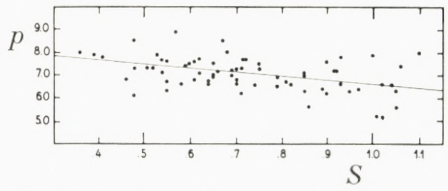

Fig. 6. The constant $p = M_v + 34.3\,L$ plotted against the spectral type parameter S.

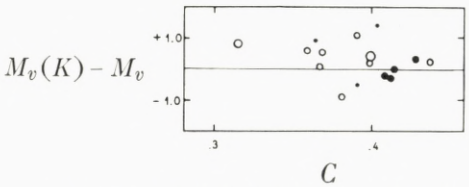

Fig. 7. Absolute magnitudes M_v(K) minus M_v determined from trigonometric parallaxes (open circles) or group parallaxes (dots), plotted against the third parameter C.

distributed relative to the scatter). Then an effect of non-linearity might also be taken into account.

When estimating q and the luminosity parameter L from M_v(K) one should consider that the reversal widths of the K- and H-lines may depend slightly on the chemical composition (cf. a suggestion by VAN DEN BERGH (1962)). This would give a correlation between residuals M_v(K) minus "true" M_v, and the third parameter. In Fig. 7, $M_v(\mathrm{K}) - M_v$ has been plotted against C for group stars and stars with M_v computed from trigonometric parallaxes larger than $0''.040$. The large dots are the Hyades stars, the small dots are the remaining group stars (cf. Table 4); the large open circles are β Gem and α Boo, the small circles the remaining trigonometric parallax stars. Although the data are too limited for a conclusive evaluation, it is indicated that, if real, the effect should be small for the considered range of C. For two of the stars in the program, α Boo and α Ser, representing the smallest and largest C values respectively, $M_v(\mathrm{K}) - M_v$ differs by only $0^{\mathrm{m}}.5$.

An essential result of the preceding analysis is the agreement between $M_v(k, n, m)$ and M_v(K), which corresponds to a mean error of $\pm 0^{\mathrm{m}}.46$ for each of the two sets of absolute magnitudes. It should be mentioned that when changing q from 1.4 to 1.8, the mean square of the residuals is found to be unchanged (0.44). The agreement also justifies the application of the linear method. This is valid for the giant and the subgiant stars. It is probably not strictly valid outside this luminosity range since slight systematic residuals $M_v^{\mathrm{obs}} - M_v(k, n, m)$ are found for the supergiants and the main-sequence stars, on the average $-0^{\mathrm{m}}.4$ in the former and $+0^{\mathrm{m}}.4$ in the latter case.

By means of the expressions for x and y, L and C are found to be related approximately to the classification indices by

$$L = 0.86\ n - 0.61\ k - 0.84\ m + \text{const.}$$
$$C = 0.86\ n + 1.08\ k + 0.43\ m + \text{const.}$$

and the photometric mean error is found to be $\pm 0^{m}.011$ for L and $\pm 0^{m}.006$ for C.

The $M_v(k, n, m)$ values are given in Table 12 for almost all the program stars within the considered region of spectral types and luminosity classes. A few stars which have exhibited peculiarities are omitted, likewise omitted are all stars known to be spectroscopic binaries. Spectroscopic parallaxes have been computed with the aid of the absolute magnitudes together with photoelectric V magnitudes when available or m_v from the Bright Star Catalogue corrected by $-0^{m}.16$ according to a comparison of m_v with V for 29 stars. These parallaxes are also listed in Table 12.

$M_v(k, n, m)$ has been tested by comparing the spectroscopic parallaxes π_s with corresponding trigonometric parallaxes π_t, published in the General Catalogue of Jenkins (1952). In order to have a material approximately homogeneous in accuracy the stars with π ranging from $0''.020$ to $0''.050$ are considered (for smaller parallaxes π_t is uncertain, for large parallaxes $\varepsilon_s = 0.2\ \pi_s$ is exceptionally high). The average mean error for the considered data of 30 stars is $\pm 0''.009$ for π_t according to the General Catalogue and $\pm 0''.006$ for π_s. The mean values for the parallaxes are $0''.0309 \pm 0''.0016$ for π_t and $0''.0297 \pm 0''.0011$ for π_s. The mean error of the scatter in $\pi_t - \pi_s$ is $\pm 0''.0096$ which is even smaller than what corresponds to the mean errors of π_t and π_s; this may be due to the selection. However, it indicates that no serious cosmical scatter should be present.

In the M_v calibration we have used the group parallax values M_v^g for the Hyades as determined from the distance moduli by Heckmann and Johnson (1956), but no particular weight has been given to these stars since the uncertainty of L is of the same order as for the remaining stars. These M_v^g values and, furthermore, the M_v determined for the Eggen group stars included in the program, are shown in Table 4

Table 4.

Comparison of $M_v(k, n, m)$ with M_v^g determined from group parallaxes.

	M_v^g	$M_v(k, n, m)$	
γ Tau	$+0^{m}.68$	$+1^{m}.2$	
δ Tau	+0.66	+0.1	
ε Tau	+0.54	−0.1	
θ^1 Tau	+0.80	+0.4	
$\varkappa$ Per	+1.25	+0.3	Eggen 1962
δ Ari	+1.18	+1.4	" 1962
HR 1327	+0.27	+0.3	" 1958a
ξ CrB	+1.15	+1.2	" 1960b
11 Lac	−0.50	+0.2	" 1960b
HR 5541	+1.05	+2.4	" 1959

together with $M_v(k, n, m)$. For δ Ari, HR 1327 and ξ CrB $M_v(k, n, m)$ agrees well with M_v^g, while for $\varkappa$ Per, HR 5541 and partly also 11 Lac the differences are significant. For γ Tau we have found several indications of peculiarity (cf. p. 46). Without this star the average difference $M_v^g - M_v(k, n, m)$ is $+0^m.5 \pm 0^m.2$ for the Hyades.

For the two giants β Gem and α Boo, having the largest trigonometric parallaxes, $0''.093$ and $0''.090$ respectively, $M_v(k, n, m)$ is found to be $+1^m.8$ and $+0^m.8$. The corresponding values derived from trigonometric parallaxes are $+1^m.0$ and $-0^m.3$. The deviations for these stars have opposite sign of the average deviation for the three Hyades stars. The M_v(K) values do also deviate from the trigonometric M_v for β Gem and α Boo, but the difference is about half that found for $M_v(k, n, m)$.

In Table 12, in which values of S, L, C, $M_v(k, n, m)$ and π_s are given, we have adopted the group parallaxes for the Hyades and the corresponding M_v values. For β Gem and α Boo we have chosen the trigonometric parallaxes and the M_v derived by utilizing these parallaxes.

4. Comparison of the Classification Parameters with the Cambridge Intensity Ratios

We shall test the classification system established in the preceding section by investigating how well other spectrophotometric quantities, i. e. those measured at the Cambridge observatory, can be represented by our classification parameters.

The comparison of the index n with the CN ratio determined by Griffin and Redman (1960) is briefly mentioned in Section 8. The G-band ratio has been measured for 61 of our stars; for 58 of them the luminosity classes are II–III, III and III–IV. A plot of $g' = 2.5 \log$ (G-band ratio) versus S indicates that these quantities are linearly correlated in the range G8 III–K3.5 III. A least-squares solution provides the relation $g' = 1.007 + 0.135\, S$, and the root mean square of the residuals is $\pm 0^m.020$. This scatter is accounted for by the uncertainty of g', according to the estimate made by the Cambridge astronomers. However, the residuals seem to depend somewhat on the right ascension. This effect is also found when all g' data are compared with MK spectral types. For the range G8–K3.5, II–III – III–IV, the average values $\bar{g}'$ have been computed for each MK spectral type. The G-band index, corrected for its dependence on the spectral type, is then $g' - \bar{g}'$. The average values of $g' - \bar{g}'$ for different intervals of right ascension are, 8^h–10^h: $-0^m.013$ (17), 10^h–12^h: $-0^m.012$ (17), 12^h–14^h: $+0^m.005$ (22), 14^h–16^h: $+0^m.006$ (29), 16^h–18^h: $+0^m.007$ (29), 18^h–20^h: $+0^m.004$ (23), (number of stars in parentheses). All G-band observations were carried out in 1958 April–June, and those from the period April 8–23 were rejected by the authors. If we omit all observations with $\alpha < 12^h$ from the common group of stars, we derive the relation $g' = 0.993 + 0.162$ S for data of 39 stars. The root mean square of the residuals is then $\pm 0^m.016$. The residuals are neither correlated with L nor with C.

In Fig. 8 the index $b = 2.5 \log$ (Mg b-line ratio) (Deeming 1960) is plotted against S. It is obvious that b depends both on spectral type and luminosity. From the

mean values of S and b for the class III stars G8–K3 (large open circles in Fig. 8) we derive the linear relation $b = 0.226\,S + 0.743$; hence the quantity $b - 0.226\,S$ measures the variation perpendicular to the regression line. In Fig. 9 this quantity is plotted against $M_v(k, n, m)$. It is evident, that with the exception of a few stars separated from the majority, a good correlation exists between the two quantities. Accordingly, b should be linearly related to two of our parameters S and L and a least-squares solution provides the relation $b = 0.199\,S - 0.901\,L + 0.928$. There seems

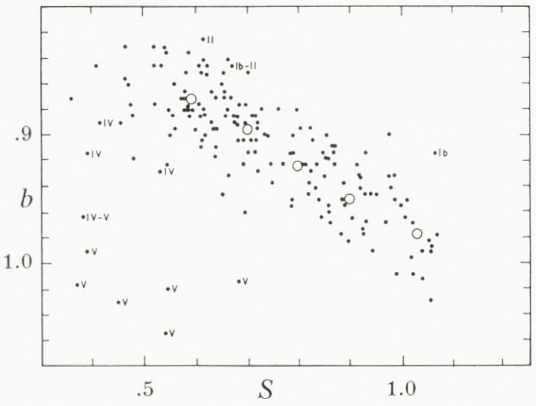

Fig. 8. The magnesium-line index b plotted against the spectral-type parameter S. Large open circles correspond to mean values of b and S for G8 III, K0 III, K1 III, K2 III and K3 III.

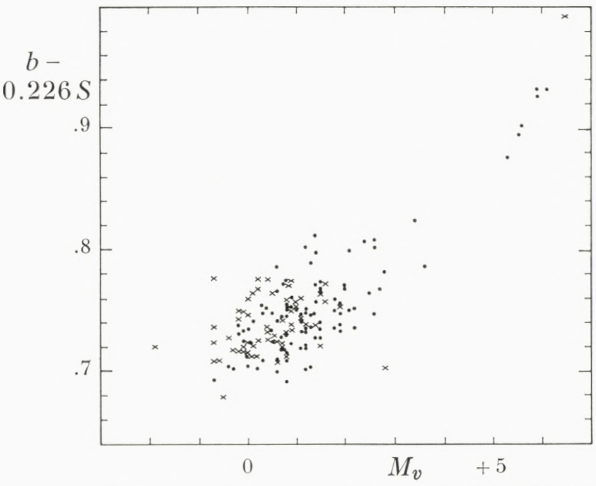

Fig. 9. The magnesium-line index corrected for the spectral-type dependence, $b - 0.226\,S$, plotted against absolute magnitude $M_v(k, n, m)$.

to be no correlation between the residuals $b_{obs} - b_{comp}$ and C. The root mean square is $\pm 0^m.026$. The contribution from b_{comp} should be $\pm 0^m.007$, while the uncertainty from b_{obs} should contribute $\pm 0^m.009$ according to DEEMING (1960). Thus, the total estimated uncertainty $\pm 0^m.011$ does not account for the total scatter; the cosmical scatter is considerable, i.e. $\pm 0^m.024$. An effect of non-linearity should be small. However, a plot of $b - 0.226\,S$ against M_v(K) shows a scatter of the same order as the one found for the relation between $b - 0.226\,S$ and $M_v(k, n, m)$. In both cases the scatter can be explained approximately, if we only assume the accuracy of M_v determined from $b - 0.226\,S$ to be of the same order as the accuracy of $M_v(k, n, m)$ and M_v(K).

The FeI ratio at 5250 A (GRIFFIN 1961) has been measured for 43 stars in our program; 37 stars are of luminosity class III, one of class V and two of class Ib. For the class III stars the index $f = 2.5$ log (FeI ratio) is apparently linearly related to S, and the relation $f = 0.068\,S - 0.006$ is derived. The quantity $f - 0.068\,S$ seems to be related to L, as should be expected from the study of all FeI data measured in

relation to the MK luminosity classes. Apparently there is no correlation between the remaining scatter and C, but the number of stars is too small for a quantitative discussion.

GRIFFIN (1961) has shown that the D-line ratio is related to the spectral type with an appreciable dispersion, which is apparently not correlated with the luminosity. This is also shown in Fig. 10, where $d = 2.5 \log$ (D-line ratio) is plotted against S. The class III stars (dots without indication) are considerably scattered around the

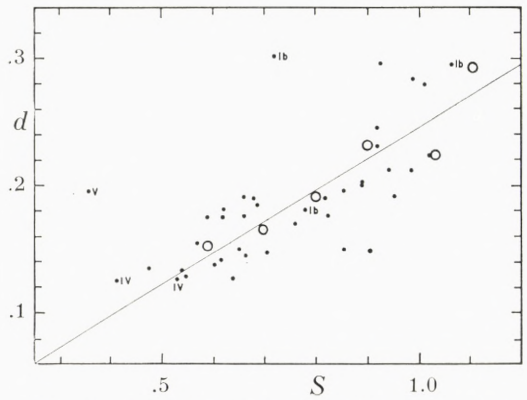

Fig. 10. The D-line index d plotted against the spectral-type parameter S.

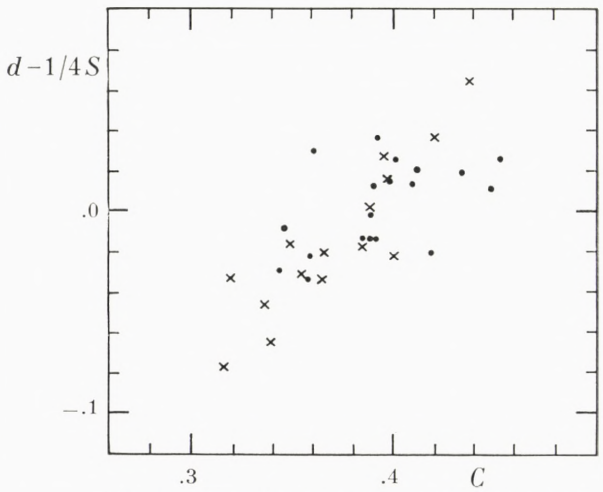

Fig. 11. The D-line index corrected for the spectral-type dependence, $d - 1/4\,S$, plotted against the third parameter C.

mean points (large open circles), and the positions of the few stars of other luminosity classes indicate that the scatter is not due to luminosity variation among the class III stars. The limited data do not justify a substantial evaluation of the dependence of d on S, but the linear relation corresponding to the mean values should be a fair approximation for the considered range. Consequently $d - 1/4\,S$ should be independent of the spectral type. In Fig. 11 this quantity is plotted against C, and it appears that most of the unknown dispersion in the D-line intensity is correlated with our third parameter (the three dot stars with largest C are noted in Table 6).

5. The Relation of the Classification Parameters to Photoelectric Colour Indices

One purpose for a classification of increased accuracy should be to provide precise indicators of intrinsic colours with a view to a determination of colour excesses. In Paper II we considered relations between the colour index $(B - V)$ and k

and g respectively. In the present section we shall make an analysis of $(B-V)$ and $(U-B)$ as well, in terms of our classification parameters, by utilizing additional colour index data. We have based our investigation primarily on data from the following sources: JOHNSON (1955), MORGAN, HARRIS and JOHNSON (1953), JOHNSON and KNUCKLES (1957), JOHNSON and MORGAN (1953), ROMAN (1955), some unpublished observations by HARRIS (private communication), $(B-V)$ transformed from $(P-V)$ measured by EGGEN (1955), $(B-V)$ transformed from $(V-G)$ given by STEBBINS and KRON (1956), and in addition some colour indices published by WILSON and BAPPU (1957). Preference is given in the order in which the sources are presented here (in the remarks to Table 11 the source is indicated for each single star). Hence $(B-V)$ values are available for 80, and $(U-B)$ values for 68 of the stars for which S, L and C have been discussed. Recently ARGUE (1963) has published UBV data for a large number of G and K stars. About 60 stars are common in this series and the above compilation. Except for a small difference, on the average $+0^{\mathrm{m}}.012$ in $(B-V)$ and $-0^{\mathrm{m}}.004$ in $(U-B)$ (ARGUE minus the other sources), the two sets of measurements are in close agreement, the mean square of the residuals being 0.00025 for $(B-V)$ and 0.00027 for $(U-B)$. The first group of observations represents several different series all fitted to the Johnson standard system, while Argue's results are based on two homogeneous series also fitted to the standard values (JOHNSON 1955). In both cases a limited number of stars of the present range of spectral types has been used in the transformations. The close agreement between the two groups for a larger number of stars then demonstrates the reliability of both. We divide the mean square equally among them and adopt the mean errors $\pm 0^{\mathrm{m}}.011$ for $(B-V)$ and $\pm 0^{\mathrm{m}}.012$ for $(U-B)$ as representing the external accuracy of each group. This accuracy is somewhat higher than generally adopted for $(U-B)$ but of the normal order for $(B-V)$. The following relations between colour indices and classification parameters have been derived from the data of the first group. When discussing the interpretation of the residuals we have added 27 stars measured solely by ARGUE, after correcting the colour indices of these stars for the above systematic differences.

The colour indices should depend mainly on the spectral-type parameter, and plots of $(U-B)$ and $(B-V)$ against S indicate linear relations in the considered range. By the least-squares method we have derived the equations $(B-V) = 0.698\,S + 0.549$ from the data of 80 stars, and $(U-B) = 1.552\,S - 0.191$ from 68 stars. The root mean square of the $(B-V)$ residuals is $\pm 0^{\mathrm{m}}.035$. The contribution from the measurement uncertainty should be $\pm 0^{\mathrm{m}}.018$ from S, and $\pm 0^{\mathrm{m}}.011$ from $(B-V)$. Part of the remaining scatter $\pm 0^{\mathrm{m}}.028$ may be attributed to the other parameters L and C. Plots of the $(B-V)$ residuals against these quantities show no significant dependence on the luminosity parameter, but some correlation with the third parameter seems to be present (cf. Fig. 12). A least-squares solution involving both S and C gives the relation

$$\begin{aligned} (B-V) = {} & 0.708\ \mathrm{S} - 0.537\ C + 0.748 \\ & \pm 0.019 \quad \pm 0.109 \quad \pm 0.043 \end{aligned}$$

The root mean square of the residuals is then $\pm 0^{m}.029$, while the contribution from the uncertainty of $(B-V)$, k, n and m is $\pm 0^{m}.022$. Thus the remaining scatter is reduced to $\pm 0^{m}.019$.

In the $(U-B)$ relation the scatter is $\pm 0^{m}.039$ (r.m.s.) which can be explained by the uncertainty of $(U-B)$ and S. Accordingly, the residuals show no dependence on C and L, and the above relation for $(U-B)$ is considered significant

$$\begin{aligned}(U-B) &= 1.552\ \mathrm{S} - 0.191\\ &\pm 0.028 \quad \pm 0.021\end{aligned}$$

A few stars, quoted below in Table 6, have remarkably large positive residuals, both in $(U-B)$ and $(B-V)$; π^{2}UMa shows a large residual in $(B-V)$, while its colour

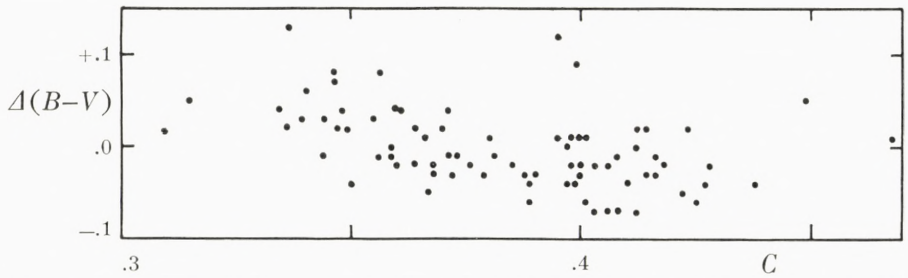

Fig. 12. Residuals $\Delta(B-V)$ from the relation of $(B-V)$ to the spectral type parameter S, plotted against the third parameter C.

index $(U-B)$ is not available. In addition HR 645 has a large negative residual $-0^{m}.12$ in $(U-B)$, but only $-0^{m}.02$ in $(B-V)$. These stars have been omitted in the above evaluation of the scatter. If they are also excluded in the least-squares computations, the first relations are found to be $(B-V) = 0.704\,S + 0.537$ and $(U-B) = 1.559\,S - 0.206$. The scatter is then $\pm 0^{m}.031$ (r.m.s.) in the $(B-V)$ relation and $\pm 0^{m}.038$ in the $(U-B)$ relation. However, since the rejection of certain observations is questionable, and since in the present case it affects the linear relations only very slightly, we adopt the above relations and the corresponding residuals in the following.

It turns out, that the residuals $\Delta(U-B)$ and $\Delta(B-V)$ are correlated, with a correlation coefficient of 0.81. The residuals are plotted in Fig. 13, as dots for the 68 stars. A least-squares solution for these stars gives the relation

$$\Delta(U-B) = 1.50\ \Delta(B-V).$$

There may be a small effect of correlation due to a slight non-linearity in the relations between S and $(U-B)$ and $(B-V)$ respectively. However, even if only stars in the range $0.6 < S < 0.9$ are considered, the correlation between $\Delta(U-B)$ and $\Delta(B-V)$ is still present. If the deviation from linearity should be real, it would influence the two residuals about equally, and would not seriously change the relation between them.

The scatter in the residuals $\Delta(U-B)$ minus $1.50\,\Delta(B-V)$ is found to be $\pm 0^{m}.032$ (r.m.s.), which is much less than would be independently caused by the uncertainty of these quantities. This may be explained by different causes. The two sets of residuals are defined as $\Delta(B-V) = (B-V) - 0.708\,S + 0.537\,C - 0.748$ and $\Delta(U-B) = (U-B) - 1.552\,S + 0.191$, where $(U-B)$ and $(B-V)$ are the observed quantities. Introducing k, n and m through the expression for S on p. 10 and the approximate expression for C on p. 15, the residuals can be expressed as $\Delta(U-B) \sim (U-B) - 1.55\,n + 2.64\,k$ and $\Delta(B-V) \sim (B-V) - 0.25\,n + 0.23\,m + 1.78\,k$. Accord-

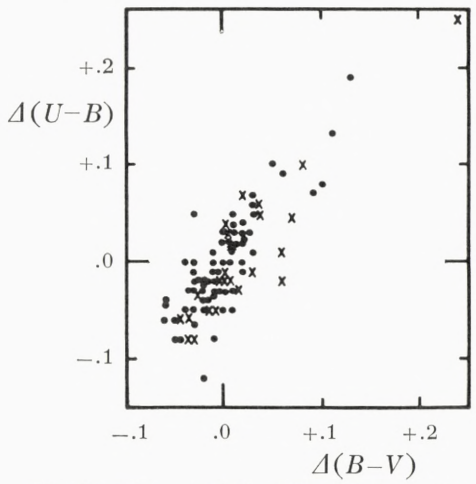

Fig. 13. The residuals $\Delta(U-B)$ from the relation of $(U-B)$ to S, plotted against residuals $\Delta(B-V)$ from the relation of $(B-V)$ to S and C.

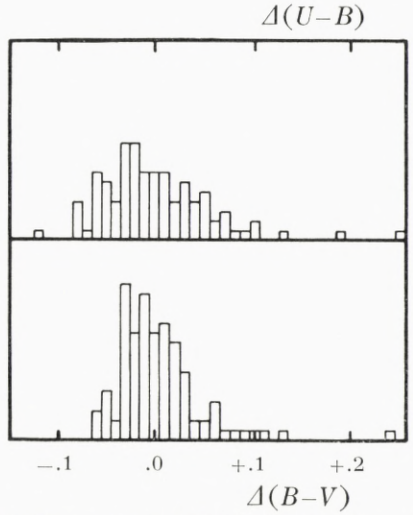

Fig. 14. Histograms of the residuals $\Delta(U-B)$ and $\Delta(B-V)$.

ingly, an error in k will affect $\Delta(U-B)$ and $\Delta(B-V)$ in the same direction, and the two contributions from k will have a ratio of about 1.5. Furthermore, $(U-B)$ and $(B-V)$ are generally measured almost simultaneously. Poor extinction correction would contribute to the mean errors of $(U-B)$ and $(B-V)$ separately, but the single errors two by two would be correlated. Both types of errors could explain the comparatively small scatter in the relation between the residuals. On the other hand it does not seem likely that the uncertainty should cause all the actual variation of the residuals. Even if the large residuals were omitted, we found a remaining scatter in $(B-V)$. When including the residuals determined for the 27 Argue stars, by means of the above relations (crosses in Fig. 13), the correlation is confirmed, but some of the latter residuals contribute to an increase of the scatter. Nevertheless, the total variation of more than $0^{m}.20$ cannot be explained by measurement uncertainties.

The detected colour effect has the characteristic of reddening according to the distribution of the colour residuals for the program stars as shown in Fig. 14. Particularly, we notice the asymmetry in the histogram of $\Delta(B-V)$, which has the smal-

lest measurement uncertainty. Since the stars all belong to the solar vicinity, the average distance being 51 parsecs for the objects with available colour indices, the effect of interstellar absorption should be quite small. We refer particularly to an investigation by STRÖMGREN (1962a) of reddening of nearby B stars, from which it appears that the absorption within 90 parsecs is almost negligible. Therefore, it is probable that effects other than interstellar reddening are responsible for the $\Delta(B-V)$ asymmetry. We also notice that the average ratio between $\Delta(U-B)$ and $\Delta(B-V)$ is obviously larger than the value 0.73 which corresponds to the standard law of interstellar absorption.

In this context we attempt an evaluation of the influence of duplicity on the classification indices and the colour indices. It is obvious that when the components of a double-star system have equal spectral types the system will have the same indices as the single stars and no peculiarity is detected, while the spectroscopic parallax determined from $M_v(k, n, m)$ may be in error, by as much as 35 per cent if the luminosities are also equal. On the other hand, if the spectral types are somewhat different and the brightnesses of the components also differ significantly, the indices for the system will be almost the same as for the most luminous component. The strongest peculiarities will appear when the components are of different spectral types and have brightnesses of the same order.

The question of which combinations of spectral types and luminosities are really possible is related to the problem of the evolution of close binaries. Since the evolutionary paths of the components of such systems may very well be different from those of single stars because of mass exchange and related effects (cf. WOOD 1962), we cannot treat the duplicity problem in a straight-forward manner. However, it is clear that if combinations of giant stars should be frequent, such systems would give peculiarities because of the similarity of the luminosities of these stars. Therefore, we have computed the combined indices k, n, g, m, S, L, C and $(B-V)$ for different systems of class III stars by utilizing the mean values of Table 1 and the corresponding mean values of $(B-V)$ for the range G8–K5, and the values for 31 Com and HR 1327 as representing G0 III and G5 III respectively. In this manner we have considered the entire range for which our classification indices have been determined, although systems with G0 III and G5 III may be unusual. Binaries in which spectral types outside the considered range have significant influence on the composite spectrum should be detectable in the MK classification which has been carried out for the program stars. Concerning the absolute magnitudes we have adopted the MK value at G0 III for 31 Com, the $M_v(k, n, m)$ value for HR 1327, for G8 III–K3 III values computed as averages of $M_v(k, n, m)$ for each spectral type separately, and for K4 III and K5 III average values determined from M_v(K).

The results of the computation are shown in Table 5 for the S range considered throughout this paper. Combined values of S and C are given, and residuals $\Delta(B-V)$ are determined as combined $(B-V)$ minus $(B-V)$ computed by means of the relation on p. 19 from combined S and combined C. It is then remarkable that $\Delta(B-V)$

TABLE 5.
The duplicity effect.

	S	C	$\Delta(B-V)$	Δk	ΔM_v
G 0–G 8	0.389	0.422	0.05	0.042	0.9
G 0–K 0	0.482	0.433	0.06	0.043	1.6
G 0–K 1	0.544	0.441	0.09	0.047	2.2
G 0–K 2	0.625	0.454	0.11	0.059	2.6
G 0–K 3	0.727	0.466	0.14	0.085	3.1
G 0–K 4	0.776	0.480	0.20	0.095	4.1
G 0–K 5	0.806	0.493	0.28	0.121	5.4
G 5–G 8	0.511	0.401	−0.01	0.001	0.6
G 5–K 0	0.585	0.403	−0.01	0.002	0.8
G 5–K 1	0.643	0.406	0.01	0.006	1.2
G 5–K 2	0.713	0.417	0.04	0.015	1.4
G 5–K 3	0.804	0.428	0.06	0.045	1.9
G 5–K 4	0.849	0.438	0.12	0.050	2.6
G 5–K 5	0.874	0.452	0.20	0.081	3.9
G 8–K 0	0.650	0.391	−0.02	0.000	0.9
G 8–K 1	0.703	0.392	0.00	0.002	1.1
G 8–K 2	0.763	0.400	0.02	0.009	1.2
G 8–K 3	0.844	0.408	0.04	0.022	1.6
G 8–K 4	0.886	0.416	0.08	0.035	2.2
G 8–K 5	0.906	0.430	0.16	0.061	3.4
K 0–K 1	0.750	0.387	0.00	0.000	0.9
K 0–K 2	0.803	0.393	0.01	0.006	1.0
K 0–K 3	0.877	0.401	0.03	0.015	1.3
K 0–K 4	0.916	0.407	0.06	0.025	1.8
K 0–K 5	0.933	0.420	0.14	0.050	2.9
K 1–K 2	0.852	0.388	0.02	0.001	0.8
K 1–K 3	0.924	0.393	0.03	0.007	1.1
K 1–K 4	0.963	0.397	0.06	0.014	1.5
K 1–K 5	0.979	0.407	0.13	0.035	2.5
K 2–K 3	0.967	0.393	0.03	0.002	0.8
K 2–K 4	1.005	0.395	0.06	0.008	1.2
K 2–K 5	1.019	0.405	0.12	0.027	2.0
K 3–K 4	1.066	0.390	0.06	0.002	0.8
K 3–K 5	1.076	0.396	0.11	0.015	1.5

is almost exclusively positive and thus the reddening noticed above may be at least partly explained as a duplicity effect. One of our classification indices g has not been used in the classification system. It was found in Paper II (Fig. 4) that g and k are quite closely correlated with only a few stars showing deviations larger than what may be due to the measurement uncertainty. Since duplicity may affect the relation

between these indices we have computed a Δk as combined k minus k determined from the relation by the mean values of k and g of Table 1 using combined g values. These Δk values are also shown in Table 5 and it is again noticeable that Δk is only positive. It should, therefore, be possible to detect the duplicity if all four classification indices k, n, g and m are measured. We notice further in Table 5 that in every case the combined C appears to be larger than the mean value 0.386 determined for all our program stars, and for the systems with one component of the type G0 III or G5 III extremely large C values are found. Finally, ΔM_v in the last column of Table 5

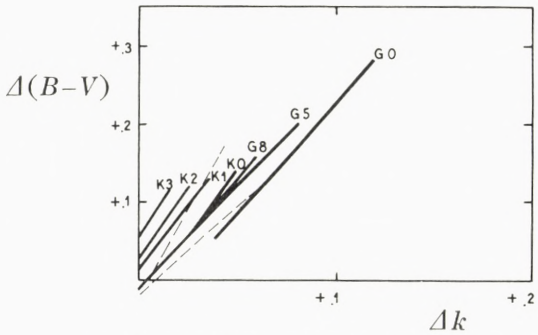

Fig. 15. Residuals $\Delta(B-V)$ for close binaries (see text) plotted against the corresponding residuals Δk.

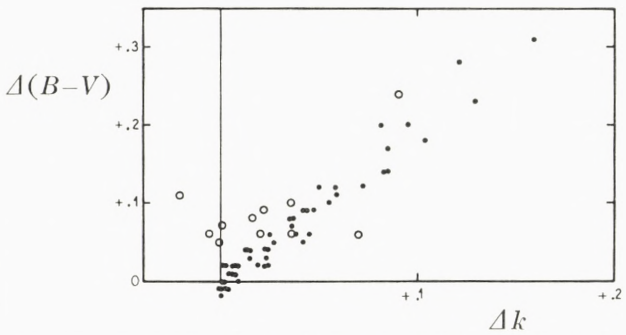

Fig. 16. Residuals $\Delta(B-V)$ for close binaries plotted as dots against corresponding residuals Δk for combined $S<0.9$ (Δm_v, Δm_v+1 and Δm_v-1). The circles correspond to observed values.

is M_v computed from combined S and combined L by means of the relation on p. 12, minus the combined M_v determined directly from the adopted average absolute magnitudes at G0 III, G5 III etc.; also ΔM_v is only positive and will have appreciable values in many cases.

In Fig. 15 we have approximated the relation between $\Delta(B-V)$ and Δk by smooth curves for the systems with one component being G0 III, G5 III, ... K3 III respectively. The G5, G8 and K0 lines are almost merging. In the above computation we have used the magnitude differences Δm_v between the components as determined from the adopted absolute magnitudes*. If we, alternately, use differences Δm_v+1 or Δm_v-1 we get lines in Fig. 15 with somewhat deviating tilts, as demonstrated for the G5, G8, K0 case by the dotted lines; largest $\Delta(B-V)/\Delta k$ corresponds to Δm_v+1.

In Table 6 we have listed the program stars with $\Delta(B-V)$ larger than $+0^{\mathrm{m}}.04$. When attempting a distinction between interstellar and duplicity reddening one should, of course, consider the uncertainty of Δk, and an improved classification accuracy with increased sensitivity of g and k may give better separation of the two effects than is possible at present. However, for stars as 132 Tau and 73 Leo with very large Δk values and also exceptionally large values of C, $\Delta(B-V)$ is very likely due to duplicity. In fact, 73 Leo is denoted as spectroscopic binary in the General Catalogue of Stellar Radial Velocities, and for 132 Tau we have found an indication of varying spectral type (Paper I, p. 28). One additional star, HR 8485, for which

* For k, n, g and m the corresponding Δm_b has been used.

TABLE 6.
Program stars with $\Delta(B-V)$ larger than $+0^{m}.04$.

HR		S	C	$\Delta(B-V)$	Δk	$M_v(k, n, m) - M_v(\mathrm{K})$	gal. latitude	distance pc
				m		m		
163	ε And	0.359	0.346	+0.06	+0.020	−0.1	−33°	37
1907	φ^2 Ori	0.481	0.346	+0.05	−0.001	+0.1	−12	20
2002	132 Tau	0.625	0.492	+0.06	+0.070		− 2	101
2805	66 Aur	0.858	0.374	+0.08	+0.016		+23	111
3403	π^2 UMa....	0.860	0.356	+0.06	− 0.006	+0.9	+36	42
4301	α UMa ...	0.658	0.449	+0.09	+0.022	+1.0	+51	16
4365	73 Leo	0.664	0.496	+0.24	+0.091		+64	119
4377	ν UMa ...	1.010	0.395	+0.13	+0.018	+1.1	+69	43
4608	o Vir.....	0.477	0.398	+0.10	+0.036	+1.4	+69	19
4928	9 Dra	0.872	0.336	+0.11	−0.021		+51	91
5480	31 Boo	0.621	0.454	+0.06	+0.036		+58	63
6199		0.679	0.434	+0.07	+0.001		+41	45

$(B-V)$ has not yet been measured, has $\Delta k = 0.073$ and $C = 0.474$ and is known to be a binary. α UMa has an appreciable although not very large value of Δk but C is extremely large, and this star is known to have a close visual companion ($\Delta m = 2.94$ according to KUIPER). 31 Boo is peculiar since Δk and C are large and $\Delta(U-B)$ is $-0^{m}.03$ (large $\Delta(B-V)$ and C to some extent correlated). o Vir has a high Δk value, and HR 6199 has a C value at the upper limit of the general dispersion of our data. However, for small and for moderate values of Δk a study also of the S values should increase the possibility for detecting duplicity. As apparent from Fig. 15, Δk as indicator of duplicity is most useful for the early-type systems of Table 5. In Fig. 16 the dots correspond to all the systems of Table 5 and of similar tables computed with $\Delta m_v + 1$ and $\Delta m_v - 1$ for which the combined S is smaller than 0.9. These dots are distributed fairly even along a straight line. The open circles denote the stars of Table 6 with S actually being smaller than this limit. It is then noteworthy that the stars with small Δk values all lie above the region of the dots. With due regard to the uncertainty of Δk and to the approximate character of this duplicity estimate we suggest that for 9 Dra and π^2 UMa and maybe also for φ^2 Ori and HR 6199 the colour excess $\Delta(B-V)$ is due to interstellar reddening. For ε And, 66 Aur and α UMa part of the effect may be interstellar. The duplicity may also be traceable from the absolute magnitudes. We are not able to estimate the effect upon $M_v(\mathrm{K})$ but, according to Table 5, we could expect that if stars of Table 6 have large positive residuals $M_v(k, n, m) - M_v(\mathrm{K})$ this may give additional indication of duplicity. For the six stars with available residuals these are negligible for ε And and φ^2 Ori but about 1^{m} for the other stars. Generally, duplicity may contribute to the remaining scatter of the M_v relation on p. 12.

One star in Table 6, ν UMa, has $S > 0.9$, and it is then impossible to see from Δk whether the large $\Delta(B-V)$ is due to interstellar or duplicity reddening. The M_v

residual indicates duplicity, but it would be important to make a more detailed spectroscopic analysis in this case. For if this star is not a binary its position in the vicinity of the B star 33 LMi, investigated by Strömgren (1962a), is interesting. The two stars are located in a comparatively high galactic latitude with an angular distance of about 10 degrees. Their distance from the Sun is found to be almost the same, about 50 parsecs, and the mutual linear distance is then less than 10 parsecs. The stars show the same, considerably high colour excess $+0^{m}.15$ (it is reasonable to add $0^{m}.02$ to the $\Delta(B-V)$ of ν UMa according to the histogram of Fig. 14). However, if we ascribe the reddening in both cases to interstellar matter being within a small distance from the Sun, this matter should not necessarily belong to a single cloud, since two other stars in the direction between ν UMa and 33 LMi show no reddening. These stars are 46 LMi and 46 UMa with $\Delta(B-V)$ equal to $-0^{m}.06$ and $-0^{m}.03$ and distances of 29 and 62 parsecs respectively. Investigations of more stars in small angular distances from 33 LMi and ν UMa are desirable. However, if these stars are not binaries their location relative to the other stars together with the $\Delta(B-V)$ values, indicates a steep increase of the interstellar absorption. If ν UMa should be a binary as is possible according to the above analysis*, the steep increase of $\Delta(B-V)$ for 33 LMi is still remarkable.

6. The Third Parameter

On the basis of the classification indices k, n and m we have derived three independent empirical parameters S, L and C, where S and L are closely related to the spectral type and the absolute visual magnitude. Concerning the third parameter C we are at present not able to relate it quantitatively to any physical or chemical quantity of the stars, but we shall assume that C varies mainly with the chemical composition.

In the high-dispersion analysis by M. and B. Schwarzschild, Searle and Meltzer (1957) the abundance estimate has been concentrated on the high-velocity giant φ^2 Ori, and it was concluded that this star deviates from the low-velocity giants in having a lower metal abundance by approximately a factor of 4 and a lower abundance of the oxygen group by a similar, but possibly somewhat smaller, factor. The C value of this star is 0.346 and for the low-velocity giants investigated in the analysis and measured also in our program, the average value of C is found to be 0.385. Thus a small value of C should correspond to a comparatively small metal content. Furthermore, according to the abundance analysis similar deviations as for φ^2 Ori, though of a smaller amount, appear to hold for the high-velocity giant stars 14 And and α Boo. However, for the latter star we find a considerably smaller value of C, 0.315, than for φ^2 Ori, but this discrepancy is possibly not real. The remark on the abundance for 14 And and α Boo is made from a judgement of the spectral deviation of these stars from low-velocity giants relative to the deviations for φ^2 Ori. In fact, the

* Recent measurements in other spectral regions support this assumption (note added in proof).

TABLE 7.
Mean values of the third parameter for different spectral types.

MK	$\bar{C}$	number of stars
G 8 III	.386	36
K 0 III	.386	48
K 1 III	.383	13
K 2 III	.387	29
K 3 III	.396	20

iron-to-hydrogen ratio should be directly related to the average equivalent width W of weak FeI lines. Among the 16 high- and low-velocity stars studied, nine stars are common to our program, and for eight of them the relation $W = 0.051\ S + 0.177\ C - 0.003$ is derived. The scatter of the W residuals is ± 0.006. The additional common star γ Tau is known to exhibit peculiarities and it also shows a large W residual, but there is no discrepancy for φ^2 Ori, 14 And and α Boo.

According to the estimate for φ^2 Ori the abundance factor corresponding to the dispersion of C for our program stars should be of the same order as the one found by STRÖMGREN (1963a) for the late F- and early G-type main-sequence field stars.

The average values of C for different MK spectral types of luminosity class III are given in Table 7. It appears, as we should expect, that $\bar{C}$ is nearly constant in the whole range, and only a small increase from K2 to K3 is noticed. The dispersion in C is considerably larger than what corresponds to the uncertainty of this parameter, and it is of the same order for different spectral types as shown in Fig. 17. To some extent differences in abundance and in temperature may similarly influence the

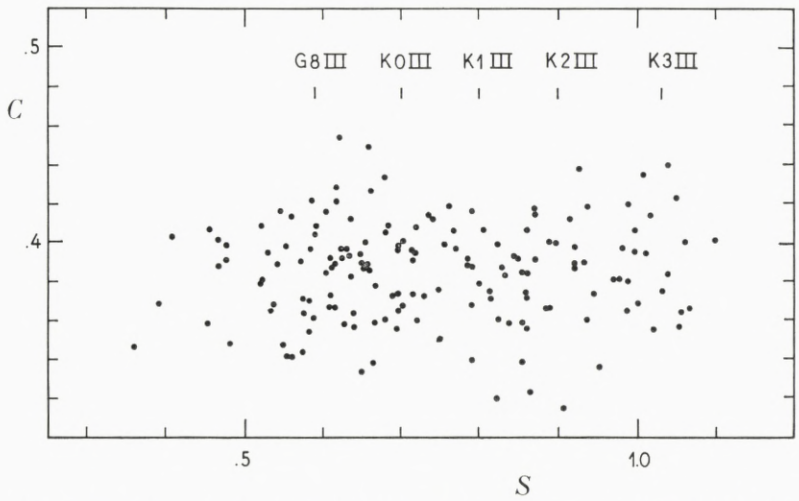

Fig. 17. The third parameter C plotted against the spectral-type parameter S; the stars with the largest C values are excluded here and in the computations for Table 7 (cf. p. 24–25).

individual spectral type estimates (cf. PAGEL 1962). The parameter S is defined by means of average spectral types and should be expected to be mainly a temperature parameter and C mainly an abundance parameter. However, as already emphasized, the correct relation between the heavy-element-to-hydrogen ratio and C may also involve the parameter S.

In this connection we shall consider again the colour index relations from the preceding section. From the $(U-B)$ and $(B-V)$ relations it appears, that C increases with decreasing intensity of the V region relative to the intensities of the U and B regions. If we assume that S and C are mainly parameters for the temperature and heavy element abundance respectively, we may interpret the variation of C with V so that for a certain value of S, the metallic line effect on the U and B region is so heavy that a further increase of the line absorption is small for these regions compared with the effect on the V region. This would again suggest that the increase of C with m (cf. p. 15) is due to a decrease of I (4970) relative to I (4050) and I (4510), rather than to a decrease of I (4050) relative to I (4510) and I (4970) as for the F stars.

The relation of k to C (p. 15) is also quite remarkable. If k is a measure of the K-line intensity an increase of k would correspond to an increase of I (3920) relative to I (4070) (cf. the definition of k in Paper I), and thus to a decrease of the K-line intensity. Consequently the composition effect on the K-line would be reversed. However, it may be questionable whether the k-index is primarily a measure of the K-line intensity. In this connection we recall the results of Paper II (p. 19), i.e. that k is well correlated with the break around the K-line, as measured by WESTERLUND (1953), while there is considerable scatter in the relation between k and the K-line intensity determined by this author. VAN DEN BERGH (1963) has recently shown that for main-sequence F and G stars the quantity Δ, measuring a discontinuity at 4000 A, is a sensitive metal-abundance equivalent. Since Δ covers almost the same spectral region as k it may well be that the Δ effect is of higher influence on this classification index than the K-line. In this connection we should recall that the spectral region of the short wave length filter (peak around 3910–3920 A) has a relatively large width of about 120 A and is not quite symmetrical; the "wing" transmission is higher on the ultraviolet side than on the red side of the maximum. This asymmetry is partly reduced by the decrease of the photocathode spectral response and the field lens transmission against shorter wave lengths. The ultraviolet part has turned out to affect the k-index considerably; attempts with a noviol filter (CHANCE OY 10) in addition to the 3920 filter gave an index of some 24 per cent smaller sensitivity than the first k although the half width was only slightly reduced. The two indices are closely correlated within the measurement uncertainty. The difference is a kind of colour effect but may be ascribed to a difference in the Δ effect as well. Recent tests utilizing a new filter for the short wave length region with peak at 3910 A and half width 60 A have shown that the corresponding k-index is about 1.7 times as sensitive as the present k. Some additional scatter is present, but a preliminary estimate indicates that

the new k can be evaluated satisfactorily in terms of S, L and C. This has not appeared to be possible if the short wave length region is centred at 3850 A (CN-absorption) or at 3930 A (K-line).

However, for a given colour index or spectral type, Δ is smaller for metal-deficient main-sequence stars than for stars of normal metal abundance, and if k chiefly measures the same effect as Δ, and if C is primarily an abundance parameter, the relation of k to C would indicate that for the giant stars the discontinuity dependence on the metal deficiency is reversed. This would be similar to what is found from the UBV relations.

Quite a few giant stars are listed in Table 1 of VAN DEN BERGH's paper and only 9 stars are common with our Table 12 (two others are spectroscopic binaries). For these stars, Δ is found to be closely related to S through a least-squares linear relation $\Delta = 0.456\ S + 0.435$. The residuals range from -0.04 to $+0.03$ and the C values from 0.315 to 0.414. When the stars with the four smallest and the four largest C values are considered, the average values for the two groups are

$\bar{C}$	$\overline{\Delta_o - \Delta_c}$
0.336	$+0.02$
0.405	-0.01

indicating a variation of Δ with C which is in agreement with what is suggested from the k variation.

It should be emphasized that these interpretations are based on the assumption that the dependence of S on the abundance and of C on the temperature, is small, and if this condition is not fulfilled the above picture will, of course, be changed.

Also we have considered the relation of our classification parameters to the long wave length colour index $(R-I)$ as determined by STEBBINS and KRON (1956), although only limited data are available. By comparing $(R-I)$ and S for 28 of our program stars, it appears that this colour index depends linearly on S, and the relation $(R-I) = 0.384\ S - 0.094$ is derived. The scatter of the residuals is $\pm 0^{m}.029$, which is considerably more than is expected from the uncertainty of $(R-I)$ and S. Plots of the residuals against L and C indicate some correlation with C, and the following relation is then derived:

$$\begin{aligned}(R-I) = {} & 0.405\ \mathrm{S} - 0.335\ C + 0.024 \\ & \pm 0.029 \quad \pm 0.181 \quad \pm 0.069\end{aligned}$$

We notice that $(R-I)$ depends relatively on S and C in a similar manner as $(B-V)$; almost the same ratio of the C and S coefficients are found in the two cases, -0.76 for $(B-V)$ and -0.83 for $(R-I)$. However, the uncertainty of the ratios, mainly in the latter case, is quite large. It may be expected that $(R-I)$ is influenced considerably less by the abundance effect than $(B-V)$ and therefore may provide a more pure colour equivalent. If $(R-I)$ should not depend on the abundance at all, this would

imply that S and C could be expressed as $S \sim S' + 0.8\,C'$ and $C \sim C' - 0.8\,S'$, where S' and C' are pure equivalents for the temperature and abundance respectively. However, this strong correction from (S, C) to (S', C') does not seem likely. In fact, through the analysis in the next section, it is found that the dependence of S and C on abundance and temperature respectively, must be much weaker.

Calibration through high-dispersion analysis of selected stars is clearly desirable but may be uncertain due to complications in the theory of stellar atmospheres for giant stars. Perhaps the relations between S and C and the stellar atmospheric parameters could be established most precisely in an empirical way by extending the classification measurements to stars in groups and clusters covering the entire range of giant spectral types.

The situation may be even more complicated if we consider a result of Strömgren (1963a) for the main-sequence stars. The metallic-line index m_1 exhibits a large dispersion for the A stars which cannot be due to abundance differences, and since A stars evolve into the giant branch it might be that effects other than the abundance do influence m. Our third parameter depends only partly on this index, but it is found in the next section that C has a considerable variation also for the giants evolved from the A stars. Thus groups and clusters of intermediate as well as high ages should be observed in order to elucidate the significance of the third parameter.

The direct relation between $(U-B)$ and $(B-V)$ is $(U-B) = 2.035\ (B-V) - 1.212$, computed from data of the 68 stars. The residuals u of this relation are plotted against the third parameter in Fig. 18. An increase of u with C is clearly apparent in this figure. This is not surprising since $(-u)$ would be a measure of the "ultraviolet excess" and C should increase with increasing metal content. However, according to the above discussion, the decrease of u (related to a decrease of C) should be due to a decrease of V relative to U and B, rather than to a decrease of U relative to B and V. Furthermore, the scatter in Fig. 18 is quite large. The dots surrounded by circles

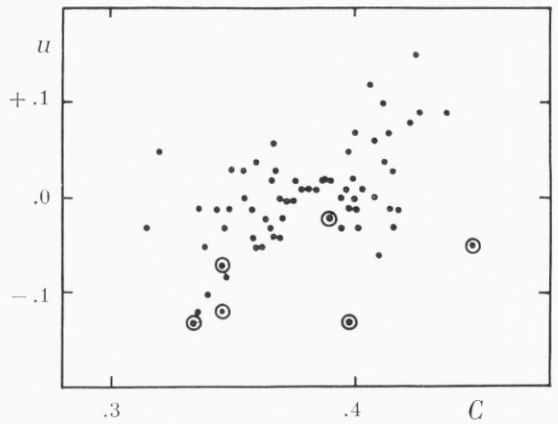

Fig. 18. Residuals u from the relation between $(U-B)$ and $(B-V)$, plotted against the third parameter C.

correspond to 6 stars with extremely large positive $\Delta(U-B)$ and $\Delta(B-V)$, and thus the effects of the third parameter and the reddening (interstellar or duplicity) will interfere in the (u, C) diagram. Furthermore, substituting in the expression $u = (U-B)_{obs} - (U-B)_{comp} = (U-B) - 2.035\ (B-V) + 1.212$, the linear relations for $(U-B)$ and $(B-V)$ as functions of S and C found above, we get $u = 0.111\ S + 1.093\ C - 0.501$, which shows, that u should depend also on S.

Although we are not able at present to relate C correctly to the stellar atmospheric parameters, we consider this quantity as an empirical characteristic similar to the weak-line, strong-line, weak-CN, and 4150 features used earlier. We shall examine how it is distributed among the program stars, relative to the distribution of the two other astrophysical parameters and to the space velocity and its galactic components. Instead of considering the independent parameters S and L, we use $(B-V)$ as directly measured or as derived from S and C, and M_v as given in Table 12. In this way we investigate the distribution of the stars in the colour-magnitude diagram relative to well known cluster sequences.

7. The Classification Parameters and their Relation to Space Velocities for the Program Stars

During recent years it has become increasingly clear that the kinematic situation for the stars in the solar vicinity is complex and rich in systematic features related to the physical characteristics of the stars. Delhaye (1948) found an indication of a preferential motion of A and F stars in the direction of the Ursa Major cluster velocity. Parenago (1950) determined the solar velocity and the apex coordinates, the vertex direction, and the axes of the velocity ellipsoid for different spectral types of the main sequence and concluded that the O–F stars form a flattened subsystem, and that the G–M stars form an intermediate subsystem. Through extensive investigations of space velocities and partly on the basis of spectroscopic population criteria, Vyssotsky and collaborators (cf. Vyssotsky 1957) have separated the neighbouring stars into two groups. The one exhibits a small dispersion of peculiar velocities and a vertex deviation, and the other, including stars with a larger dispersion in the velocities, shows no vertex deviation. Investigations of the vertex deviation have been presented in a number of papers (Strömberg 1946, Hins and Blaauw 1948, Delhaye 1952, Alexander 1958, van Rijn 1960). The deviation seems to characterize the motion of the stars that move close to the galactic plane and may be detected for stars as faint as 13^m (Vyssotsky 1957). It has been interpreted as being due to streaming, perturbations or to the evolution of spiral arms, and by Lindblad (1958) in terms of dispersion orbits, i.e. orbits along which an association of stars tends to disperse in the central field of the Galaxy. Lindblad suggested that the young stars showing the deviation may have originated in a vast cloud, which, according to Oort (1958), may be part of a spiral arm.

The spectroscopic population criteria used by VYSSOTSKY were the strength of the G-band and the hydrogen lines, the 4227-line of neutral calcium, and for dwarf M stars emission lines of hydrogen or ionized calcium. Part of the data was subdivided according to the weak-line and strong-line criteria of ROMAN (1952). BLAAUW (1958) has carried further the weak-line and strong-line differentiation for selected spectral types, and has found that the strong-line G8 III giants exhibit two concentrations of the projected velocity vectors in the galactic plane, similar to the concentrations for A0–A9 stars demonstrated by DELHAYE (1948, op. cit.). The K0 III strong-line giants show a concentration between the two G8 III groups. This picture indicates kinematic similarities between stellar types having approximately equal ages according to current theories of stellar evolution.

WOOLLEY and EGGEN (1958) have classified the stars within 20 parsecs of the Sun according to the closeness with which they approach the galactic centre. The colour-luminosity arrays of the classes indicate a decreasing pericentric distance with age, from the youngest class with an array similar to the Pleiades and nearly circular orbits, to the oldest M 67-like stars penetrating to regions within 3.5 kpc from the centre. From galactic velocity components determined by EGGEN (1962), EGGEN, LYNDEN-BELL and SANDAGE (1962) have computed orbital eccentricities and angular momenta for 221 dwarf stars and have shown that correlations exist between the observed ultraviolet excess for these stars, recognized as measuring the metal abundance, and the eccentricity, the angular momentum and the velocity component perpendicular to the plane, respectively. A correlation between the Z velocity component and the metal-to-hydrogen ratio is also found by WALLERSTEIN (1962). YOSS (1962) has indicated evidence of a correlation between the CN-anomaly for giant stars and the dispersion of the three velocity components.

In his series of stellar group investigations EGGEN (1958b) found indications of non-random distributions of the galactic plane velocity components for G1–K5 main-sequence stars when the data are subdivided according to the component perpendicular to the plane. EGGEN (1960a) further studied the components in the plane of AV stars and has detected evidence for the existence of subgroups, whose stars have a common value of the component in the direction of rotation. According to KING (1961) such stars may have originated simultaneously in a region with the same distance from the centre as our present distance; the age should be equal to the epicycle period $\pi/\sqrt{B(B-A)}$, where A and B are the Oort constants.

Such kinematic features are related to comparatively young stars and indicate a common origin; they should be expected among the older stars in the solar vicinity only under special circumstances. The high-velocity stars may be an example of this. VAN WIJK (1956) has discussed the origin of the disk high-velocity stars and has shown that these stars have probably been formed close to the perigalacticon of their orbits, a smaller fraction of them close to the apogalacticon.

The relation between kinematic and age properties of field stars are more prominent when observational methods of increased accuracy are used. We refer to

results from high-dispersion quantitative abundance analysis of selected stars by GREENSTEIN and collaborators, and particularly to the very extended investigations of nearby B, A and F stars made by STRÖMGREN and associates, using narrow-band and intermediate-band techniques. STRÖMGREN (1962b) obtained data for about 1200 A2–G2 stars brighter than 6^m5 in the u, v, b, y four-colour system and calibrated the measurements in terms of metal abundance and age. It was found that the average speed relative to the local standard of rest, is correlated with the age and the chemical composition respectively, for stars of small and intermediate velocities. For the region F4–G2 and luminosity classes IV and V, stars as old as the galactic cluster M 67 definitely have a higher average velocity than younger stars, and there is further an increase in the average velocity with decreasing metal content. On the basis of the same data of A and F stars, supplemented with results for B8–B9 stars (CRAWFORD 1963) the distribution of the velocity components in the galactic plane was studied by STRÖMGREN (1963a) for different age groups. Certain features for stars of ages between 200 and 600 million years, already noticeable in earlier similar investigations by DELHAYE (1948), are clearly outstanding and are presumably related to star formation in spiral arms.

When attempting similar studies for the giant and subgiant region we encounter serious difficulties in the age determination due to the funnel effect, and, to some extent, to the overlapping of evolutionary sequences corresponding to quite different ages. However, kinematic features similar to the afore-mentioned features for evolved main-sequence stars might be found also for stars in the giant region and might support a segregation of age groups there.

In comparison with the A and F main-sequence observations described above, the present data are limited by a smaller accuracy of the location in the HR diagram and of the tangential velocity, and the third parameter needs further interpretation and calibration. Furthermore, the comparatively small number of stars should make a detection of age groups uncertain. The following, therefore, gives only a provisional kinematic picture for stars of the solar neighbourhood in the giant and subgiant regions.

The space velocities have been computed utilizing the parallaxes determined in Section 3, the radial velocities from the General Catalogue by R. E. WILSON (1953) and proper motions provided in the following way. For about one hundred stars, the proper motions listed in the FK4 catalogue or its supplement have been used. For about fifty of the remaining stars, the N30 proper motions have been corrected to the FK3 system utilizing the tables of H. R. MORGAN (1953) and then to the FK4 system by means of tables of the differences FK4 minus FK3 (provided in advance of publication by W. GLIESE). For the remaining stars (about thirty) the Boss GC proper motions have been corrected to the FK3 system by means of the tables of KOPFF (1939) and then from FK3 to FK4. The space velocity and its galactic components determined in the 1958 system are reduced to the local standard of rest utilizing the standard solar motion (note, p. 54). The total velocity Q and the components X,

Y and Z are given in Table 12. Z is perpendicular to the galactic plane, positive towards the north pole, Y is the component in the anticentre direction, and X in the direction of the rotation (unit km/sec).

In considering the third parameter in relation to the total space velocity, we have divided the data into three groups according to C with an equal number of stars in each group. The average space velocities for these groups are shown in Table 8, where the first section comprises only stars of small and intermediate velocities, while the last section includes also the high-velocity stars. We have chosen the limit at the velocity 63 km/sec (where the asymmetry in the distribution of the plane components begins).

TABLE 8.

Average space velocities in relation to the third parameter.

C	$Q<63$		all Q values included	
	$\bar{Q}$	number of stars	$\bar{Q}$	number of stars
0.315 – 0.373	30	42	43	54
0.374 – 0.397	25	49	28	53
0.397 – 0.468	26	53	27	54

It is seen that there is practically no change in $\bar{Q}$ for C larger than 0.375, while $\bar{Q}$ increases when C decreases below this limit. This is quite clear when the high-velocity stars are included, but also if only stars with $Q<63$ are considered the effect should be real since the mean error of each of the $\bar{Q}$ values is about 1–2 km/sec.

If we interpret C as a measure of the chemical composition the results for the high-velocity stars agree with what is generally expected from the properties of these stars. For the low- and intermediate-velocity stars the tendency is in agreement with STRÖMGREN's results for the F4–G2 main-sequence stars, but the effect is more pronounced in the latter case. In his similar division STRÖMGREN (1962b) finds $\bar{Q}$ to be 28.5, 32 and 36.5 km/sec respectively. We shall return to this point later.

Fig. 19 shows C histograms for all the program stars and for the weak-line and strong-line stars included in the program. The first histogram indicates that the distribution of C is not quite symmetrical. From the weak-line and strong-line histograms some correlation appears in the sense that weak lines correspond to small C values and strong lines to large C values. As shown in Table 9 the average values of C for the two groups are clearly different. The difference is not very pronounced, but our data include somewhat less than half of the G and K stars for which the weak-line and strong-line characteristics have actually been indicated. These are only G8–K1 stars while the present discussion comprises the types from G5 to K3.5. The difference in C for the cyanogen criteria also given in Table 9, is quite significant.

From the plot of the velocity component Z against C in Fig. 20 we see a marked difference in the dispersion of Z for small and large C values. Again we refer to what

TABLE 9.
Mean values of the third parameter for Roman's spectroscopic groups.

	$\bar{C}$	number of stars
weak-line stars	0.378	55
strong-line stars	0.394	43
weak-CN stars	0.352	9
"4150" stars	0.406	11

has been found for the A2–G2 main-sequence stars (STRÖMGREN 1963a, p. 34), that among the 1217 stars measured in the u, v, b, y photometry the few stars having velocity components at right angles to the galactic plane larger than 35 km/sec all have a comparatively small metal content (smaller than 0.3 times that of the Hyades stars).

In the investigations of dwarf and subdwarf stars (WALLERSTEIN 1962, EGGEN, LYNDEN-BELL and SANDAGE 1962), a steady increase of the dispersion σ_Z with decreasing metal content or increasing ultraviolet excess has been found. Fig. 20 and Table 10, in which the mean values $|\bar{Z}|$ and the σ_Z values have been computed for successive intervals of C, indicate that for the present data there is rather an approximately constant dispersion in Z for C larger than a limit around $C = 0.38$, and a steep increase in the dispersion below this limit.

In view of this result and furthermore with the indications of the average speed $\bar{Q}$ in Table 8 and the histograms of Fig. 19 in mind, we proceed in a manner similar to

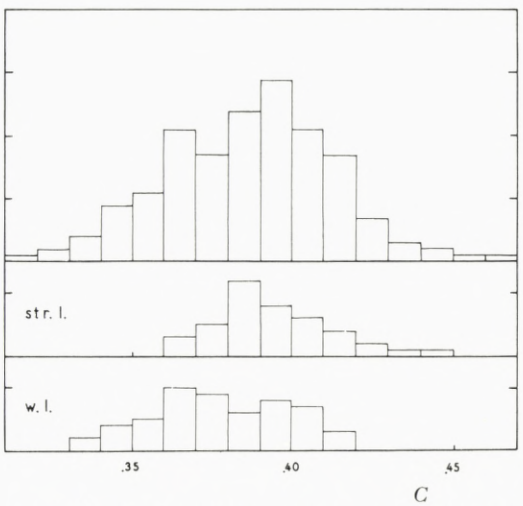

Fig. 19. Histogram of the third parameter C for all stars and for the strong-line and weak-line stars separately (binaries included).

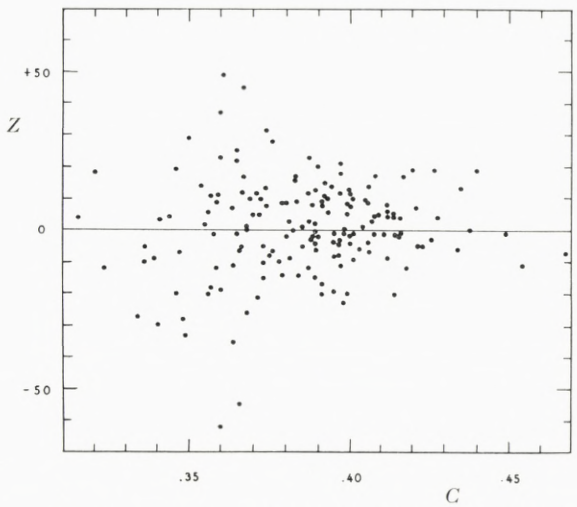

Fig. 20. The space-velocity component Z perpendicular to the galactic plane, plotted against the third parameter C.

TABLE 10.

Mean values of the numerical Z velocity component (perpendicular to the galactic plane) and values of the Z dispersion for different intervals of the third parameter.

C	$\lvert\bar{Z}\rvert$	σ_Z	number of stars
0.340–0.349	16	20	7
0.350–0.359	12	15	11
0.360–0.369	22	29	21
0.370–0.379	12	15	17
0.380–0.389	8	10	24
0.390–0.399	10	13	29
0.400–0.409	7	9	20
0.410–0.419	7	10	11
0.420–0.429	9	12	7

VYSSOTSKY and collaborators; we divide the program stars into two main groups A and B according to the value of the third parameter and tentatively set the limit at $C = 0.38$. When considering the colour-magnitude diagrams of the two groups we notice a striking difference. Group A, including the stars with C larger than 0.380, populates the diagram above the level of the sequence of the galactic cluster M 11, while group B contains very few stars above the Hyades sequence. We interpret the difference so that the group A contains a number of young giants having evolved from A-type stars, while group B consists mainly of stars of small masses evolved from the F and early G types of the main sequence. In other words, below a certain limit of our third parameter no young giants are found in our program.

If we consider only the region above the Hyades level the number of stars for successive intervals of C are 2 for the range 0.360–0.369, 5 for 0.370–0.379, 14 for 0.380–0.389, 12 for 0.390–0.399, 11 for 0.400–0.409 and 8 for 0.410–0.419. The smallest value of C is 0.366. Remembering the photometric uncertainty it seems reasonable to adopt the limit at 0.380. In group A we then include stars with $C > 0.380$, and in addition five of the seven stars above the Hyades level with $C < 0.380$. These five stars all have $|Z|$ values below the dispersion $\sigma_Z = 10$ km/sec found for all stars with $C > 0.380$. The remaining stars with $C < 0.380$ are included in group B. With the duplicity effect in mind, we exclude all stars with $C > 0.430$ from the following discussion.

The two colour-magnitude diagrams are then shown in Fig. 21. We have constructed these diagrams using $(B - V)$ from the sources quoted in Section 5, or computed from S and C by means of the equation on p. 19. The giant sequences of some galactic clusters are shown in the diagram. The M 67 and NGC 188 curves are drawn through the normal points corrected for reddening, published by SANDAGE (1962). The Hyades line is based on the data used in Table 12 (reference p. 15), and the NGC 752 and M 11 sequences are reproduced from an earlier paper of SANDAGE (1957).

Group B contains about 60 stars, while group A consists of a little less than 100 stars. VYSSOTSKY's groups A and B have about equal numbers of stars, but refer only to G5–K1 stars of luminosity classes II–III, III and III–IV, while our investigation extends as far as K3.5 and also includes a few stars of luminosity class IV (and the separation criterion is not determined quantitatively in VYSSOTSKY's work). Our data are probably subject to a selection effect since the absolute brightest stars, being so numerous in group A, have been favoured in our program ($m_v < 5.5$, mainly),

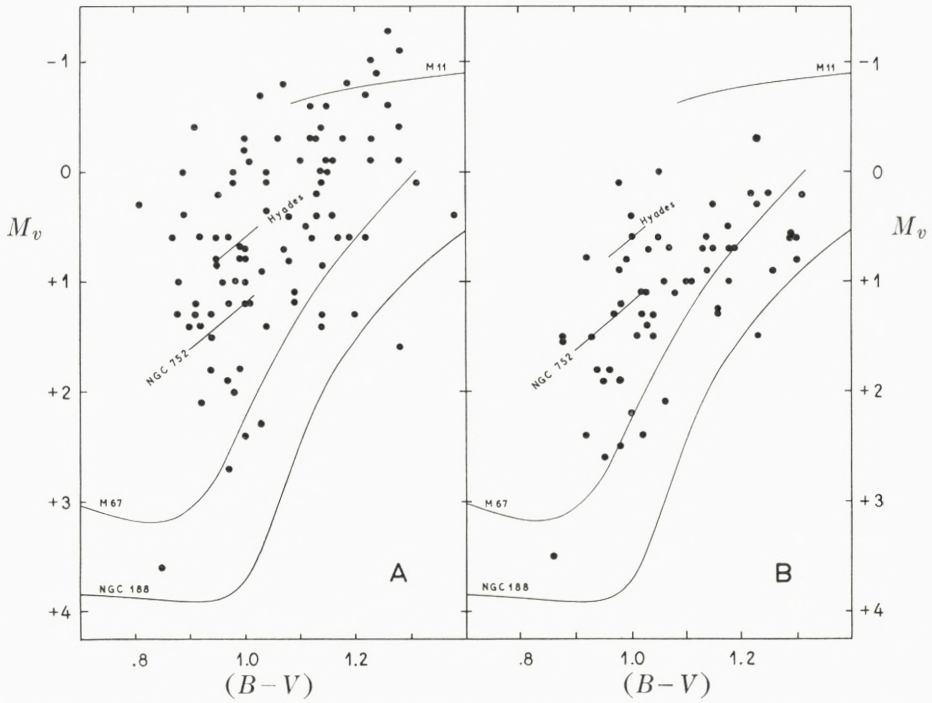

Fig. 21. Colour-magnitude diagrams for group A ($C > 0.38$) and group B ($C < 0.38$).

and the colour-magnitude diagram of field stars in the giant region should be most abundantly populated at about $M_v = 1.0$ according to HALLIDAY (1955) and SANDAGE (1957). From evolutionary considerations the latter author estimated that about 70 per cent of the present K0–K2 giants were originally F2–F7 dwarfs, while most of the remaining 30 per cent were originally A0–A5 main-sequence stars. The velocity dispersions, as shown by SANDAGE (1957) by means of data compiled by PARENAGO (1950), indicate that the majority of the K0–K2 giants evolved from the F dwarfs.

However, this was mainly an age and mass division, while our division pertains to the chemical composition, and group A apparently includes also a number of stars evolved from the F- and G-type main sequence. According to the location in the colour-magnitude diagrams some stars of groups A and B have approximately the same age, as high as M 67 or even more, and have quite different C values, ranging from 0.35 to 0.40. A single star, HR 4181, lying below the NGC 188 sequence in the

$(B-V, M_v)$ diagram of group A, has the C value 0.383, which is close to the limit between the two groups. This picture is an agreement with what has been found by STRÖMGREN (1963a) and by other investigators, that low as well as high metal content is found among very old stars, indicating that heavy element synthesis has occurred at an early state of the evolution of the Galaxy.

Returning to Table 9 and the question of the average speed in relation to C we recall that STRÖMGREN's subdivision is concerned with stars from F4 to G2 of the main sequence. The number of stars in our data, definitely known as evolved from this region, is far too small for a conclusive discussion of the relation between C and Q, and, furthermore, some of these stars have comparatively large Z values. Table 8 presents chiefly a distinction between group A and group B with $\bar{Q} = 28$ and $\bar{Q} = 43$ respectively when the high-velocity stars are included. If for $Q < 63$ km/sec only the stars below the Hyades level are considered, the $\bar{Q}$ values are practically unchanged. For the total number (90) of these stars $\bar{Q}$ is 28 km/sec while STRÖMGREN finds $\bar{Q} = 32$ for the F4–G2 stars. This indicates that a number of the considered stars have evolved from late A and early F stars as should be expected.

The above differentiation of two main groups A and B presents some uncertainty in the interpretation of our third parameter. For the old stars, say older than NGC 752, C would be a measure of the chemical composition with a possible correction depending on S taken into account. However, for the young giants evolved from A-type stars, no variation of the initial abundance (cf. STRÖMGREN 1963a) should be expected, but for these stars the C variation is still quite significant. If we consider only the stars above the Hyades level in the group A colour-magnitude diagram we find a dispersion of C of $\pm 0^{m}.014$ (about 50 stars), which is considerably greater than the photometric mean error of C (cf. p. 15). This should be compared with the scatter of Δm_1 determined by STRÖMGREN (1963a). This quantity has a comparatively small range in the region of early F stars and the dispersion increases in the direction of the later F stars due to increasing dispersion in the chemical composition. For A stars the variation of Δm_1 for a certain spectral type is again very strong and here the interpretation is not quite clear. It would, furthermore, be a matter for discussion whether the effect suggested for explaining the difference in dispersion between early F and late A-type stars, viz. the existence or non-existence of a deep outer convection zone (STRÖMGREN 1963a), is also found in the giant region.

In this connection we notice that the four Hyades giants which belong to group A have practically equal C values for γ Tau, δ Tau and ε Tau, on the average 0.411, while for θ^1 Tau C is 0.428. In the estimate of the dispersion for the young giants we have omitted stars with C larger than 0.430 with the duplicity effect in mind (cf. p. 24). It may be that part of the dispersion is due to the duplicity systematically causing large C values; the θ^1 Tau deviation in C from the other Hyades might be explained in this way.

In order to elucidate the significance of the variation of the third parameter for young giants, an increased classification accuracy would be desirable, and, in ad-

dition, extended observations of other spectrophotometric equivalents should be made. As mentioned on p. 18 part of the variation of the D-line intensity seems to be correlated with C. However, measurements of the D-line ratio are available for only few giants above the Hyades level. It is found that two of these stars with negative values of $d-1/4\ S$, on the average -0.016, have a mean value of C of 0.385, while three stars with positive $d-1/4\ S$, average value $+0.041$, have $C = 0.435$. This indicates a real scatter also for $d-1/4\ S$ for the young giants.

Furthermore, it should be emphasized that the stars above the Hyades level may not be termed young giants in every case. Some of the stars in this region, pre-

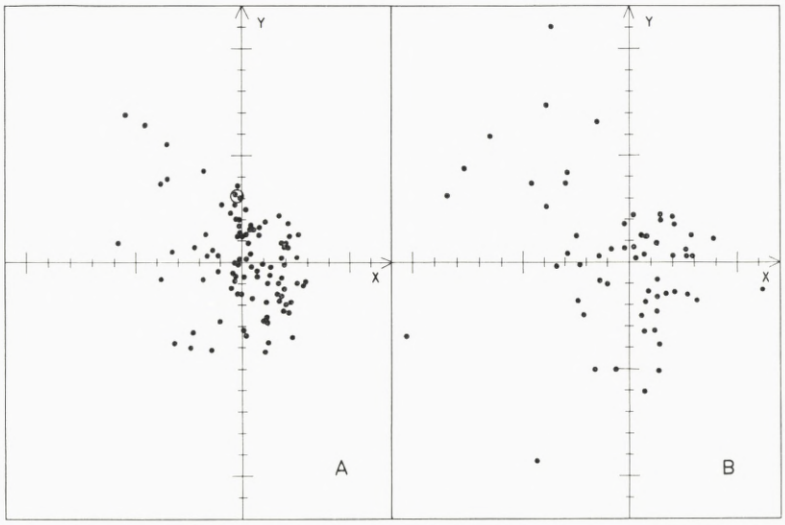

Fig. 22. Velocity components in the galactic plane for stars of group A ($C > 0.38$) and group B ($C < 0.38$). X-axis, rotational direction. Y-axis, anticentre direction. Unit 10 km/sec.

sumably a small fraction, may be old stars in late giant phases, passing from the right to the left side of the HR diagram, and for these stars the third parameter could be related to the abundance. Giants of the types belonging to intermediate-age clusters such as NGC 2158 (Arp 1962) would also partly appear above the Hyades level.

However, our interpretation of the absolute bright members of group A as being mainly evolved A-type stars is supported by the (X, Y) distribution in Fig. 22. Group A (including the Hyades shown by a circle), shows a remarkable concentration in the (X, Y) plane with the characteristic vertex deviation. In fact, when comparing Fig. 22 with Fig. 4 of the paper of Vyssotsky (1957) and taking into account the different solar motion used in the two cases, the stars of group A appear to be located mainly within the region of the early A-type stars (although this region is not entirely occupied). Group B exhibits much less concentration in the (X, Y) plane. The (X, Y) distribution of the two groups gives a picture similar to the one found by Vyssotsky, except for the relatively small number of stars in group B.

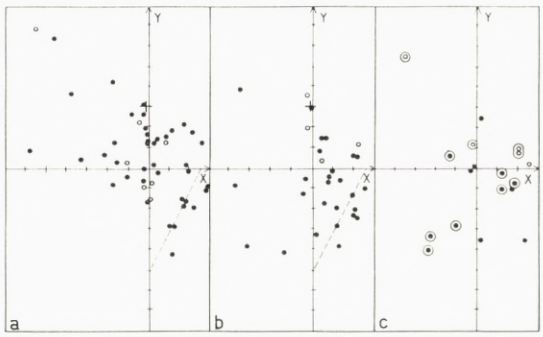

Fig. 23. Velocity components in the galactic plane for subgroups of group A: (a) stars above the Hyades level in the colour-magnitude diagram, (b) stars between the Hyades and NGC 752, (c) stars below the NGC 752 level. The open circles are stars with $|Z| > 15$ km/sec; the dots and open circles surrounded by large circles correspond to stars below or to the right of the M 67 sequence.

Following Strömgren (1963a) we have attempted a subdivision of group A into age groups as follows: a) the stars in the $(B-V, M_v)$ diagram located above the Hyades line and its extension, b) the stars between this line and the corresponding NGC 752 level and c) the stars below the NGC 752 sequence and its extension. The ages of these clusters, 4×10^8 years and 10^9 years, provide approximate age limits for the three groups. Although they are somewhat different from Strömgren's limits for the main-sequence stars and much less precisely defined, similar features as those found by Strömgren may be detected also in the (X, Y) diagram in Fig. 23. The youngest giants(a) show a tendency of concentration close to the Ursa Major stream line (dotted in the figures) and also some alignment along the Y-axis with the head at the Hyades (cross); for the main-sequence stars the corresponding concentration appears to be slightly curved or tilted. For the older stars in Fig. 23b we again find an indication of a concentration along the Ursa Major line, as Strömgren found for the 400–600 million years main sequence and a concentration along the Y-axis. The lower left quadrant is not as sparsely populated as this quadrant in the three

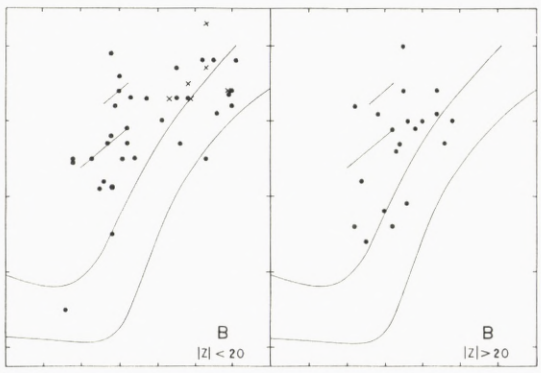

Fig. 24. Colour-magnitude diagrams for stars of group B divided into two subgroups according to the $|Z|$ value.

STRÖMGREN diagrams. These indications are only weak and additional data are needed. It should be noticed that among the three stars with space velocity larger than 63 km/sec in Fig. 23a, two are in the region of high-velocity stars originated at the apogalacticon according to VAN WIJK (1956).

Since the stars of group B are probably all comparatively old, any evolutionary and kinematic significance of the velocity distribution of these stars would be different from the one found for the young stars of group A. We divide the stars in group B into two subgroups according to $|Z|$ with the limit 20 km/sec. The colour-magnitude diagrams (Fig. 24) indicate some age division. The stars with the largest $|Z|$ values are preferably distributed around the M 67 sequence, while the stars with small

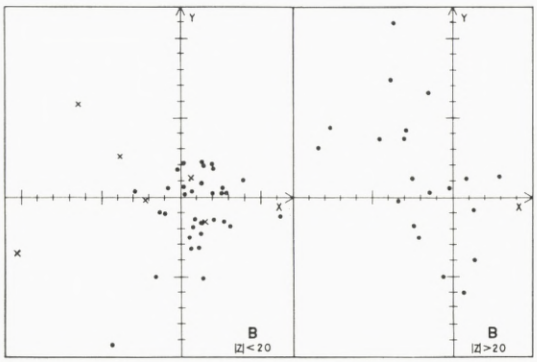

Fig. 25. (X, Y) diagram for stars of group B divided into two subgroups according to the $|Z|$ value.

$|Z|$ values are located elsewhere, mainly in three groups. The 20 stars with $|Z| > 20$ km/sec have approximately the same value of C, on the average 0.350. These stars may have some vertex shift (Fig. 25), but large as well as moderate $|Z|$ values, and high as well as low Q values are included in this grouping. The star with the highest space velocity is among those close to the Hyades in the $(B-V, M_v)$ diagram. The stars with $|Z| < 20$ represent quite different C values. The crosses in the diagrams of these stars are those with the smallest C values, on the average 0.328.

The five dot stars with $|Z| < 20$, close to NGC 188 in Fig. 24 and thus apparently very old, show similarities in their velocity data and have almost the same C, about 0.360. This indicates some kind of grouping. However, two of these stars have residuals $M_v(k, n, m) - M_v(K)$ of about $+1^m$ and one has $\Delta(B-V) = +0.06$ (cf. the duplicity estimate in Section 5); a further discussion requires more accurate data.

Among the subgiants in groups A and B, three are common with the investigation of PAGEL (1963). For these stars, γ Cep, η Cep and β Aql, no appreciable difference is noted for [Fe/H] while the ultraviolet excess is 0.00, 0.06 and 0.07 respectively. These results are in close relative agreement with the C values which are 0.399, 0.365 and 0.368 respectively.

Concluding the discussion of this section we note that the division of the giants and subgiants into two main groups with the described properties is interpreted satisfactorily in the light of current theories of stellar evolution. The separation is made by means of the third parameter without any correction, and, in fact, the division implies that a correction depending strongly on S is very improbable. If we, tentatively, repeat the above analysis using a quantity $C' = C + 0.5\,S$ instead of C (cf. p. 30), we find a (Z, C') diagram with a much less pronounced limit in the dispersion of Z, and a larger scatter in C' for the stars with $|Z|$ larger than 35 km/sec. Even more convincingly, if we attempt a division into two groups we find young giants in both groups whatever the separation value of C' within reasonable limits, and, as a consequence of the dependence of C' on S, the two groups are restricted almost exclusively to two separated intervals of $(B-V)$. This result is, of course, quite unlikely from an evolutionary point of view.

8. Summary

An empirical three-dimensional spectral classification of bright field giant and subgiant stars of the range G5–K3.5 has been established by means of the classification indices k, n and m, related to a region close to the K-line of ionized Ca, to the cyanogen absorption at 4200 A, and to the metallic line effect on the continuum, respectively. The classification parameters, S for the spectral type, L for the luminosity, and a third parameter C, have turned out to represent other spectrophotometric quantities for the stars in question with good accuracy, and absolute magnitudes $M_v(k, n, m)$ derived from L and S agree with M_v(K) determined from the K- and H-line reversals with a scatter corresponding to a mean error $\pm 0^{\mathrm{m}}.5$ for the two sets of magnitudes. The classification parameters have further been related to photoelectric colour indices, and it was found that $(U-B)$ depends only on S, while $(B-V)$ depends on S and on C as well. The remaining scatter of these relations may be due to duplicity or to absorption by interstellar matter, and evidence of interstellar reddening is indicated for two of the program stars. The classification parameters are quite sensitive to duplicity effects. However, duplicity should be detectable, at least for spectral types earlier than K2, when measuring the G-band index in addition to the other classification indices. The detectability may be sharpened if the sensitivity of the indices can be increased by means of filters with smaller band widths; observations of known binaries consisting of giant stars would be a valuable test.

The variation of the third parameter C is assumed to be related mainly to abundance differences. The distribution of the parameter C for the program stars and its relation to the distribution of the stars in the colour-magnitude diagram and to the galactic velocity components have been studied. It is found that the value $C = 0.38$, close to the average value for the program stars, divides the data into two main groups so that a considerable fraction of the stars in the group with $C > 0.38$ are giants evolved

from A-type main-sequence stars, while the group with $C < 0.38$ consists probably chiefly of stars evolved from the F- and G-type section. The dispersion in C for A-type giants of the first group is significant, a result which should be compared with the variation of the index m_1 found by STRÖMGREN for the A stars. This indicates that effects other than the abundance may influence the third parameter. Duplicity may contribute to this dispersion in C. On the other hand, the results of the discussion in Section 7 implies that for the giants evolved from the F- and early- G-type main-sequence, C should represent the chemical composition; a possible correction depending on S should be small.

It is important to extend this investigation to a large number of near-by stars of the types studied and, if possible, also of the late-type giants. However, as already emphasized in the introduction, our classification system is to be considered as a provisional one, giving a first approach along these lines in the age and population discussion of the giant stars. It is desirable to attempt an improvement of the classification accuracy, and we shall mention some results of the investigations in progress for the filter method.

It appeared through measurements made by CRAWFORD (1961) and measurements made at this observatory that halving the width of the cyanogen filter increases the sensitivity of the index n considerably. The peaks of the filters of the new and the old index are also somewhat different. The two indices are correlated with a scatter which corresponds to an external mean error of the two series of $\pm 0^{m}.014$ when K4 and K5 stars are excluded. These stars and a few other stars, for instance γ Tau (peculiar, cf. p. 46), clearly exhibit systematic deviations. When comparing the present n with the Cambridge CN ratio a considerable scatter is also found, and systematic deviations for the K4 and K5 stars are even much more pronounced. In connection with the comparison of different series of cyanogen measurements we again refer to the work of Yoss (1962).

The systematic deviations for the K4 and K5 stars indicate that the relation between two cyanogen indices is also dependent on the spectral type. Generally, each of the three classification indices depends on all three parameters, and slight changes of the transmission bands corresponding to the indices will have no serious effect if the new indices, in common, define the three parameters without any new scatter. The relations between different series of measurements of an index will be discussed in connection with an account of the definite classification system.

The step from the present to an improved n-index may contribute to an increased accuracy of M_v and of the third parameter. This may, however, require also improvement of the other indices in our classification parameters. A third cyanogen index with peaks defined as for the second index but with small band width of both filters (about 40 A) is now being investigated. In this connection we measure also a new index for the G-band, defined by the long wave length intensity of the cyanogen index and an intensity for a region of similar width at 4360 A. It should be noticed here that it has not been profitable to replace k by the index g already available

(Papers I and II) in the classification system used above. A second index g measured together with the second n used only slightly differing filter widths and has appeared to be only slightly more sensitive than the first g.

A possible improvement of the sensitivity of the other indices is still questionable. A metallic-line index m_1 obtained through STRÖMGREN's four colour-system is linearly correlated with the present index m and very nearly has the same sensitivity. Some remaining scatter is present. An index with the same peaks as the four-colour m_1 but smaller widths will be tested.

As already mentioned the significance of the index k is not quite clear. Several series of standard observations of k have been carried out utilizing the original 3920 filter together with the 4070 filter or other filters of similar half width but with peak wave lengths differing by 10–30 A. Also different phototubes have been used. These series are in agreement within the adopted measurement accuracy ($\pm 0^{m}.010$) and show only weakly varying sensitivity of the index. Thus the original index k could be used in an extended program, but attempts to reproduce this index by means of other filters may meet difficulties. Furthermore, in case of fainter stars the effect of interstellar reddening would not be well defined, and we test indices with filters of smaller widths centred on different wave lengths in the surrounding of 3920 A (cf. p. 28).

In this connection we may notice that it has been difficult to obtain filters at these wave lengths with small width and fair peak transmission. In the cyanogen- and G-band regions filters can now be produced with half widths of about 40 A, very precise peak wave lengths and peak transmissions of 50–70 per cent. Reduction of the width is then at least partly compensated by a doubling of the transmission, and the limiting magnitude would not be much changed. For the present equipment it has been $7–7^{1}/_{2}$ mag. (one minute exposure time; no cooling),

When attempting an improvement and an extension of the classification one should stress the importance of adding observations of other equivalents such as the Cambridge intensity ratios. For instance we recall the luminosity sensitivity of the FeI lines at 5250 A and the relation of the D-line intensity to our third parameter. Observations of different features covering limited regions of the spectra, strong lines and bands, combined with observations of the four-colour system might throw light on different questions raised through the preceding analysis, such as the significance of the dispersion of C for the young giants.

A powerful tool in selecting the most effective system of equivalents may be a scanning of the spectra such as the one carried out by MEINEL and GOLSON (1959).

Finally, we may emphasize the importance of group stars and cluster stars as objects for calibrating absolute magnitudes and possibly also for establishing a precise relation between the third parameter and the spectral-type parameter on one hand, and the chemical composition and the temperature on the other hand. Abundance determinations needed for a calibration of the composition equivalent are in progress

(WALLERSTEIN, private communication). Abundances of extreme population II giants relative to abundances of normal giants are available through the work of WALLERSTEIN, GREENSTEIN, PARKER, HELFER and ALLER (1963).

Acknowledgments

The author expresses his sincere gratitude to Dr. O. C. WILSON for providing M_v(K) data in advance of publication, which have given the substantial basis for the present calibration of $M_v(k, n, m)$. I am much indebted to Dr. W. GLIESE for helping me with proper motion data as mentioned on p. 33, and to Dr. D. L. CRAWFORD for making unpublished n and g results available for comparison with the present data. The observations have been carried out by the author, but in the reductions and computations in various steps and in the making of drawings I have been assisted effectively by Miss BODIL HELT, Miss KAREN T. JOHANSEN, Mr. P. DICKOW, Mr. P. U. B. S. JACOBSEN, Mr. L. H. JENSEN, Mr. K. JEPSEN, Mr. R. WEST, and Mr. F. WISSING. I also want to express my gratitude to the director of the Copenhagen and Brorfelde observatories, Professor A. REIZ, for his continued interest and support during this work. Finally, it is a pleasure to thank Professor B. STRÖMGREN for valuable discussions and for reading the manuscript.

Copenhagen University Observatory. Brorfelde.

TABLE 11.

The metallic-line index m together with the number of observation nights, listed according to the Harvard-Revised-Photometry or Bright-Star number.

The MK spectral types were given in the catalogue of Paper II (GYLDENKERNE 1958a).

In the Remarks the sources of the U, B, V observations are indicated (cf. also p. 19):

A	ARGUE (1963)	MHJ	MORGAN, HARRIS and JOHNSON (1953)
E	EGGEN (1955)	R	ROMAN (1955)
J	JOHNSON (1955)	SK	STEBBINS and KRON (1956)
JK	JOHNSON and KNUCKLES (1957)	W	WILSON and BAPPU (1957)
JM	JOHNSON and MORGAN (1953)	H	D. L. HARRIS, private communication

In the Remarks further SB denotes spectroscopic binary and an asterisk denotes peculiarity. The latter has been discussed in Section 5 (Table 6) for some stars. The remaining peculiarities are commented as follows:

HR

1346 γ Tau The star is found to be variable (JOHNSON and HARRIS 1954). The index k may be variable (Paper I, p. 28). The star has a discrepancy between the present n and a new n-index (cf. p. 43), and a large residual in the W, S, C relation (p. 27).

1409 ε Tau The index k may be variable (cf. Paper I, p. 28).

3905 μ Leo Large b, S, L residual.

4695 16 Vir Peculiar location in the u, C diagram, Fig. 18.

8498 1 Lac Large b, S, L residual.

HR		m		Remarks
163.....	ε And	.264	3	R
165.....	δ And	.648	3	W
166.....	54 Psc	.424	2	J
168	α Cas	.449	12	SK
175.....	32 And	.332	3	JK
253.....	υ^1 Cas	.542	3	
265.....	υ^2 Cas	.342	3	
285.....		.550	2	SK
294.....	ε Psc	.341	3	E
321.....	μ Cas	.239	3	J
351.....	χ Psc	.370	3	
352.....	τ Psc	.469	3	
360.....	φ Psc	.423	2	SB
390.....	ξ And	.468	3	
399.....	ψ Cas	.438	3	
430.....	49 And	.398	2	
434.....	μ Psc	.654	3	R
437.....	η Psc	.348	3	J
442.....	χ Cas	.347	3	
458.....	υ And	.204	2	JM
464.....	51 And	.603	12	J
469.....	χ And	.308	3	
483.....		.236	3	J
489.....	ν Psc	.649	2	
493.....	107 Psc	.396	3	J

(continued)

TABLE 11 (continued).

HR		m		Remarks		HR		m		Remarks	
510.....	o Psc	.352	3			1739.....	109 Tau	.360	2	A	
511.....		.371	3	MHJ		1907.....	φ^2 Ori	.332	3	R	
549.....	ξ Psc	.355	3			1963.....	51 Ori	.461	2	R	
592.....	49 Cas	.354	2			1995.....	τ Aur	.352	2		
617.....	α Ari	.491	14	J		2002.....	132 Tau	.416	2	A	*
643.....	60 And	.707	2			2012.....	ν Aur	.475	2		
645.....		.320	3	R	SB	2047.....	χ^1 Ori	.224	2	JK	
694.....	64 And	.378	3			2077.....	δ Aur	.399	6	J	
699.....	65 And	.757	3			2152.....	37 Cam	.391	3		
743.....		.337	2			2219.....	$\varkappa$ Aur	.374	2	R	
800.....	14 Per	.268	3			2289.....	ψ^1 Aur	.450	1		
824.....	39 Ari	.472	2			2427.....	ψ^2 Aur	.540	2	R	
843.....	17 Per	.796	2			2459.....	ψ^4 Aur	.791	2	R	
882.....	24 Per	.543	2			2473.....	ε Gem	.465	2	A	
918.....		.386	2			2477.....	13 Lyn	.378	2		
937.....	ι Per	.224	2	J		2478.....	30 Gem	.482	3		
941.....	$\varkappa$ Per	.403	2			2487.....	ψ^6 Aur	.442	2	A	
947.....	ω Per	.452	2			2506.....	18 Mon	.455	2		
951.....	δ Ari	.433	3			2516.....	ψ^7 Aur	.562	2	R	
969.....		.305	3		SB	2527.....		.744	2		
999.....		.669	2			2649.....		.651	3	A	
1017.....	α Per	.140	9	JM		2697.....	τ Gem	.563	2	A	
1030.....	o Tau	.300	3	J		2715.....	18 Lyn	.471	2		
1052.....	σ Per	.649	3			2793.....	65 Aur	.414	2		
1135.....	ν Per	.131	3			2805.....	66 Aur	.471	2	A	
1256.....	37 Tau	.434	3			2808.....	57 Gem	.363	2	A	
1303.....	μ Per	.240	2			2821.....	ι Gem	.410	3	H	
1327.....		.275	2	JK		2864.....	6 CMi	.541	3		
1343.....	54 Per	.377	3			2990.....	β Gem	.435	3	J	
1346.....	γ Tau	.390	3	J	*	3149.....	χ Gem	.495	2	A	SB
1348.....	φ Tau	.483	3			3176.....	μ Cnc	.261	2	H	
1373.....	δ Tau	.402	2	J		3249.....	β Cnc	.712	2	J	
1396.....	π Tau	.350	3			3275.....	31 Lyn	.790	2	H	
1407.....	75 Tau	.519	3			3403.....	π^2 UMa	.519	2	SK	
1409.....	ε Tau	.407	3	J	*	3418.....	σ Hya	.523	2		
1411.....	θ^1 Tau	.366	3			3461.....	δ Cnc	.453	2	H	
1457.....	α Tau	.796	3	J		3508.....	35 Lyn	.345	11	A	
1523.....		.611	3			3522.....	ϱ^1 Cnc	.459	1	A	
1577.....	ι Aur	.645	6	W		3547.....	ζ Hya	.381	2	H	
1580.....	o^2 Ori	.485	2			3612.....		.356	3	A	
1603.....	β Cam	.262	3			3627.....	ξ Cnc	.371	2	A	SB
1729.....	λ Aur	.237	2	JM		3731.....	$\varkappa$ Leo	.578	2	A	
						3751.....		.675	3		

(*continued*)

TABLE 11 (continued).

HR		m		Remarks
3771.....	24 UMa	.265	2	
3773.....	λ Leo	.798	2	A
3800.....	10 LMi	.341	3	H
3815.....	11 LMi	.369	2	J
3839.....	27 UMa	.405	2	
3851.....	43 Lyn	.355	2	A
3873.....	ε Leo	.264	2	SK–A
3905.....	μ Leo	.584	2	H *
4126.....		.379	3	
4178.....	38 UMa	.560	2	SB
4181.....		.679	2	
4246.....	44 UMa	.589	2	A
4247.....	46 LMi	.439	11	H
4258.....	46 UMa	.460	2	H
4291.....	58 Leo	.485	2	H
4301.....	α UMa	.402	8	J *
4335.....	ψ UMa	.490	7	J
4365.....	73 Leo	.503	2	A SB
4377.....	ν UMa	.610	4	J
4461.....	2 Dra	.355	2	
4495.....	92 Leo	.394	2	A
4496.....	61 UMa	.324	3	JM
4504.....	3 Dra	.556	2	
4518.....	χ UMa	.474	6	H
4521.....		.632	3	A
4608.....	o Vir	.348	3	H *
4667.....	7 Com	.361	3	H
4668.....		.470	3	H SB
4695.....	16 Vir	.454	2	R *
4697.....	11 Com	.374	3	H
4716.....	5 CVn	.319	3	H
4728.....	6 CVn	.391	2	H
4737.....	γ Com	.516	6	H
4783.....		.392	2	A
4785.....	β CVn	.199	2	J
4883.....	31 Com	.212	3	A
4928.....	9 Dra	.491	2	R
4932.....	ε Vir	.370	2	H
4954.....	41 Com	.773	2	H
4983.....	β Com	.223	4	J
4997.....		.419	3	H
5013.....		.648	4	A
5072.....	70 Vir	.278	3	J
5200.....	υ Boo	.804	4	H
5201.....	6 Boo	.672	2	H
5247.....	9 Boo	.688	2	H
5330.....	15 Boo	.378	2	A
5340.....	α Boo	.514	13	J
5370.....	20 Boo	.609	2	A
5429.....	ϱ Boo	.613	4	J
5430.....	5 UMi	.700	3	
5480.....	31 Boo	.387	2	A *
5502.....	o Boo	.371	2	A
5541.....		.410	2	R
5563.....	β UMi	.721	4	MHJ
5602.....	β Boo	.349	12	MHJ
5681.....	δ Boo	.343	2	J
5744.....	ι Dra	.548	2	J
5854.....	α Ser	.547	2	J
5901.....	$\varkappa$ CrB	.453	2	H
5947.....	ε CrB	.539	2	J
5966.....	5 Her	.383	2	R
6018.....	τ CrB	.440	3	MHJ SB
6103.....	ξ CrB	.416	2	A
6126.....		.483	2	
6132.....	η Dra	.337	2	MHJ
6199.....		.442	2	A
6220.....	η Her	.332	3	A
6299.....	$\varkappa$ Oph	.529	2	MHJ
6603.....	β Oph	.552	2	J
6688.....	ξ Dra	.551	6	MHJ
6703.....	ξ Her	.368	3	H
6705.....	γ Dra	.776	6	J
6872.....	$\varkappa$ Lyr	.497	2	A
6895.....	109 Her	.524	2	R
6945.....	42 Dra	.466	2	
7137.....		.296	2	
7180.....	υ Dra	.461	2	
7295.....	53 Dra	.395	3	A
7309.....	54 Dra	.530	2	A
7310.....	δ Dra	.372	5	MHJ
7328.....	$\varkappa$ Cyg	.364	2	MHJ
7352.....	τ Dra	.616	3	SB
7462.....	σ Dra	.349	4	J
7468....		.387	3	A

(*continued*)

TABLE 11 (continued).

HR		m		Remarks	HR		m		Remarks
7517.....	15 Cyg	.336	3	A	8468.....	24 Cep	.300	3	
7576.....	20 Cyg	.653	3	E	8475.....		.488	2	
7602.....	β Aql	.323	3	JM	8485.....		.550	5	SB
7615.....	η Cyg	.415	8	H	8498.....	1 Lac	.606	3	*
7685.....	ϱ Dra	.599	2		8538.....	β Lac	.381	2	
7796.....	γ Cyg	.185	1		8551.....	35 Peg	.422	3	R
7806.....	39 Cyg	.641	3	R	8632.....	11 Lac	.573	2	
7949.....	ε Cyg	.400	9	J SB	8656.....	13 Lac	.373	2	
7955.....		.199	1		8684.....	μ Peg	.351	3	SK
7957.....	η Cep	.353	3	J	8694.....	ι Cep	.426	3	
8085.....	61 Cyg A	.778	3	J	8702.....		.622	2	SK
8173.....	1 Peg	.477	2	J	8779.....		.573	3	
8228.....	71 Cyg	.393	2		8780.....	3 And	.412	2	
8232.....	β Aqr	.248	3	JM	8796.....	56 Peg	.514	2	SB
8252.....	ϱ Cyg	.313	2	JK	8832.....		.615	3	J
8255.....	72 Cyg	.449	3	R	8852.....	γ Psc	.291	3	R
8308.....	ε Peg	.546	3	JM	8874.....	11 And	.395	3	
8313.....	9 Peg	.352	3	JM	8916.....	θ Psc	.447	3	E
8317.....	11 Cep	.500	3		8923.....	70 Peg	.362	3	
8324.....		.469	2		8930.....	14 And	.402	3	R
8414.....	α Aqr	.307	3	JM	8974.....	γ Cep	.487	9	J
8465.....	ζ Cep	.531	13	SB	9008.....	τ Cas	.465	3	

TABLE 12.

HR	S	L	C	M_v	π	X	Y	Z	Q
163....	.359	.186	.346	$+1^{m}.5$	$''.027$	− 44	− 93	+ 19	105
165....	1.055	.179	.423	+ 0.1	.023	− 13	+ 6	− 5	15
166....	.542	.073	.379						
168....	.898	.252	.400	− 1.9	.014	+ 2	+ 2	− 2	3
175....	.520	.174	.379	+ 1.5	.017	+ 13	− 16	+ 9	22
253....	.919	.174	.389	+ 0.6	.014	+ 1	− 32	− 4	32
265....	.555	.162	.341	+ 1.8	.027	− 16	− 50	+ 3	53
285....	.996	.218	.406	− 1.0	.0085	− 3	+ 32	+ 9	33
294....	.579	.177	.344	+ 1.2	.024	+ 31	− 18	+ 4	36
351....	.701	.227	.400	− 0.7	.0082	+ 8	+ 16	− 4	18
352....	.800	.170	.379	+ 1.0	.020	+ 21	+ 18	− 14	31
360....	.716	.179	.411						
390....	.833	.191	.383	+ 0.2	.012	+ 1	− 7	+ 17	18

(*continued*)

TABLE 12 (continued).

HR	S	L	C	M_v	π	X	Y	Z	Q
399....	.768	.190	.397	$+0^m.4$	″.013	− 11	+ 3	+ 21	24
430....	.717	.203	.395	+ 0.1	.0097	− 1	− 16	− 8	18
437....	.622	.212	.397	0.0	.019	+ 18	+ 2	− 3	18
442....	.628	.200	.358	+ 0.4	.014	+ 27	− 15	− 1	31
464....	1.017	.188	.414	− 0.1	.018	+ 8	+ 13	− 20	25
469....	.476	.192	.391	+ 1.0	.016	+ 25	− 10	+ 9	28
489....	1.056	.162	.364	+ 0.6	.016	+ 21	− 14	+ 7	26
493....	.452	.049	.359						
510....	.630	.209	.397	+ 0.1	.014	+ 17	+ 22	+ 12	30
511....	.370	.061	.400						
549....	.612	.193	.387	+ 0.6	.015	+ 26	+ 13	− 12	31
592....	.591	.191	.404	+ 0.8	.014	+ 19	− 13	+ 1	23
617....	.853	.174	.359	+ 0.7	.053	− 10	− 10	+ 11	18
645....	.599	.241	.410						
694....	.655	.189	.389	+ 0.7	.012	− 5	− 12	0	13
743....	.530	.181	.401	+ 1.2	.016	+ 20	− 20	+ 10	30
800....	.400	.237	.418						
824....	.861	.199	.372	− 0.1	.012	− 58	+ 9	+ 5	59
882....	.945	.184	.374	+ 0.2	.012	+ 14	− 51	+ 13	54
918....	.714	.205	.374	0.0	.010	+ 7	− 60	+ 31	68
941....	.714	.196	.396	+ 0.3	.020	− 18	+ 43	− 8	47
947....	.829	.206	.387	− 0.3	.010	+ 28	− 11	+ 3	30
951....	.714	.161	.391	+ 1.4	.026	+ 2	+ 25	+ 8	26
969....	.613	.264	.401						
1030....	.535	.219	.368	0.0	.019	+ 11	− 42	0	43
1052....	1.053	.157	.357	+ 0.8	.019	+ 26	+ 3	+ 11	28
1256....	.792	.203	.387	− 0.1	.013	− 22	+ 7	+ 12	26
1327....	.409	.218	.403	+ 0.3	.010	+ 11	− 28	− 6	31
1343....	.617	.183	.421	+ 1.0	.016	+ 12	− 38	+ 7	40
1346....	.637	.174	.412	+ 0.68	.0253	− 2	+ 31	+ 4	31
1373....	.718	.203	.408	+ 0.66	.0239	− 2	+ 31	+ 5	31
1396....	.650	.220	.389	− 0.3	.0096	+ 4	+ 15	− 15	22
1407....	.845	.152	.393	+ 1.4	.018	+ 20	+ 9	+ 6	23
1409....	.734	.209	.414	+ 0.54	.0253	− 1	+ 31	+ 5	31
1411....	.617	.200	.428	+ 0.80	.0245	− 2	+ 32	+ 4	32
1523....	1.000	.158	.369	+ 0.9	.014	+ 13	− 23	+ 10	28
1580....	.863	.174	.323	+ 0.7	.021	+ 17	− 15	− 12	26
1603....	.363	.234	.426						
1739....	.558	.170	.413	+ 1.5	.020	− 4	+ 7	− 3	9
1907....	.481	.141	.346	+ 2.6	.050	− 39	+ 74	− 20	86
1963....	.791	.159	.340	+ 1.3	.019	− 15	+ 66	− 30	74
1995....	.551	.170	.398	+ 1.5	.025	+ 11	− 28	− 1	30

(continued)

TABLE 12 (continued).

HR	S	L	C	M_v	π	X	Y	Z	Q
2002....	.625	.169	.492						
2012....	.848	.196	.392	$0^{m}.0$	$''.016$	+ 19	− 1	+ 8	21
2077....	.702	.183	.367	+ 0.8	.026	− 8	+ 6	+ 12	16
2152....	.697	.187	.365	+ 0.6	.012	+ 29	+ 13	+ 25	40
2219....	.650	.170	.334	+ 1.3	.025	− 25	+ 12	− 27	39
2289....	1.021	.333	.432						
2427....	.977	.208	.381	− 0.7	.0079	− 17	+ 13	+ 3	22
2473....	1.056	.336	.425						
2477....	.608	.156	.367	+ 1.9	.021	+ 13	+ 9	+ 16	22
2478....	.885	.202	.366	− 0.3	.011	− 11	− 4	− 5	13
2487....	.824	.218	.399	− 0.6	.0072	+ 17	− 18	+ 5	25
2506....	.798	.183	.382	+ 0.5	.016	+ 9	− 1	0	9
2516....	.998	.205	.395	− 0.6	.0075	− 55	+ 69	− 19	90
2697....	.979	.195	.397	− 0.3	.012	− 1	+ 14	− 3	14
2715....	.786	.163	.391	+ 1.2	.016	− 35	+ 55	− 20	68
2793....	.691	.162	.373	+ 1.5	.020	+ 15	+ 20	− 5	25
2805....	.858	.199	.374	− 0.1	.0090	+ 2	+ 13	+ 8	15
2808....	.455	.113	.407	+ 3.6	.054	+ 13	− 2	+ 3	13
2821....	.693	.168	.373	+ 1.3	.033	+ 7	+ 4	− 10	13
2864....	.987	.213	.380	− 0.9	.0076	+ 10	− 28	− 2	30
2990....	.696	.152	.399	+ 1.0	.093	+ 20	+ 7	− 20	29
3149....	.840	.178	.412						
3403....	.860	.149	.356	+ 1.5	.024	+ 26	+ 6	+ 6	27
3418....	.937	.209	.418	− 0.6	.010	− 6	+ 8	+ 6	12
3461....	.787	.179	.388	+ 0.7	.022	− 38	− 8	− 2	39
3508....	.581	.176	.354	+ 1.3	.018	+ 29	+ 3	+ 14	32
3522....	.549	.056	.430						
3547....	.654	.189	.400	+ 0.7	.032	+ 4	+ 15	+ 8	17
3612....	.669	.227	.400						
3627....	.674	.215	.414						
3731....	.931	.149	.390	+ 1.3	.023	− 2	+ 12	+ 20	23
3800....	.522	.176	.408	+ 1.4	.024	+ 11	− 19	− 1	22
3815....	.383	.068	.401						
3839....	.767	.227	.406	− 0.8	.0062	− 16	+ 3	− 7	18
3851....	.592	.191	.408	+ 0.8	.012	− 5	+ 23	+ 17	29
3873....	.351	.219	.409						
3905....	1.023	.212	.425						
4126....	.648	.187	.394	+ 0.8	.015	+ 21	+ 7	+ 14	26
4178....	.969	.196	.413						
4181....	1.038	.134	.383	+ 1.6	.020	+ 12	− 10	+ 9	18
4246....	1.032	.197	.375	− 0.4	.0076	− 3	+ 27	− 8	28
4247....	.748	.160	.350	+ 1.4	.034	− 21	− 25	+ 29	44

(*continued*)

TABLE 12 (continued).

HR	S	L	C	M_v	π	X	Y	Z	Q
4258....	.789	.168	.368	$+1^m.1$	″.016	− 2	+ 6	− 26	27
4291....	.815	.160	.371	+ 1.3	.019	+ 9	− 14	+ 12	21
4301....	.658	.185	.449	+ 0.8	.063	+ 4	− 7	− 1	8
4335....	.855	.183	.385	+ 0.4	.030	+ 7	− 4	+ 1	8
4365....	.664	.095	.496						
4377....	1.010	.172	.395	+ 0.4	.023	+ 18	− 7	− 4	19
4461....	.613	.186	.367	+ 0.9	.014	− 6	− 50	+ 45	68
4495....	.618	.151	.392	+ 2.0	.022	− 2	− 1	+ 11	11
4504....	.970	.191	.381	− 0.1	.0082	+ 21	+ 18	− 9	29
4518....	.854	.182	.339	+ 0.5	.023	+ 6	+ 13	− 9	17
4521....	1.038	.185	.440	− 0.1	.0085	+ 3	− 21	+ 19	28
4608....	.477	.140	.398	+ 2.7	.053	+ 20	+ 9	− 23	32
4667....	.574	.160	.371	+ 1.8	.024	+ 13	− 8	− 21	26
4668....	.818	.170	.349						
4695....	.823	.178	.320	+ 0.7	.014	− 65	+ 59	+ 18	90
4697....	.589	.148	.361	+ 2.2	.031	+ 8	+12	+ 49	51
4716....	.542	.205	.389	+ 0.4	.013	+ 16	− 15	− 6	23
4728....	.604	.157	.416	+ 1.8	.022	− 1	+ 1	+ 4	4
4737....	.913	.201	.412	− 0.3	.012	− 33	+ 5	+ 8	34
4783....	.666	.176	.378	+ 1.1	.015	+ 6	− 25	− 10	28
4928....	.872	.176	.336	+ 0.6	.011	− 39	+ 26	− 10	48
4932....	.586	.175	.422	+ 1.3	.050	+ 5	+ 15	− 5	17
4997....	.762	.213	.418	− 0.3	.0092	− 1	+ 13	− 12	18
5330....	.633	.180	.393	+ 1.0	.014	− 32	− 38	+ 10	51
5340....	.905	.167	.315	− 0.3	.090	−103	− 35	+ 4	109
5370....	.988	.167	.420	+ 0.6	.014	− 2	+ 36	+ 19	41
5429....	1.020	.165	.355	+ 0.6	.025	+ 14	+ 22	+ 2	26
5480....	.621	.186	.454	+ 0.9	.016	+ 13	+ 3	− 11	17
5502....	.615	.176	.389	+ 1.2	.022	− 4	− 5	+ 2	7
5541....	.639	.136	.364	+ 2.4	.024	− 29	+ 42	− 35	62
5602....	.604	.195	.385	+ 0.6	.027	− 3	− 6	− 5	8
5681....	.549	.159	.347	+ 1.9	.051	+ 8	− 19	− 7	22
5744....	.920	.172	.398	+ 0.6	.029	+ 7	− 7	0	10
5854....	.926	.189	.438	+ 0.1	.032	+ 34	− 17	0	38
5901....	.696	.132	.397	+ 2.4	.036	− 24	− 40	− 11	48
5947....	.951	.179	.336	+ 0.3	.018	− 23	− 1	− 5	24
5966....	.583	.138	.370	+ 2.5	.030	+ 20	+ 21	+ 5	29
6018....	.662	.128	.401						
6103....	.684	.171	.409	+ 1.2	.021	− 1	+ 30	+ 5	30
6126....	.869	.208	.417	− 0.4	.0073	− 3	− 9	+ 17	19
6132....	.572	.196	.390	+ 0.6	.038	+ 4	− 2	− 2	5
6199....	.679	.147	.434	+ 2.0	.022	+ 2	+ 5	− 6	8
6220....	.521	.175	.380	+ 1.4	.039	+ 19	− 23	+ 9	31

(*continued*)

TABLE 12 (continued).

HR	S	L	C	M_v	π	X	Y	Z	Q
6299....	.890	.170	.400	$+0^m.8$	″.032	− 35	+ 39	+ 13	54
6603....	.925	.180	.427	+ 0.4	.033	+ 22	+ 12	+ 19	31
6688....	.935	.168	.360	+ 0.7	.025	+ 2	+ 7	− 19	20
6703....	.546	.154	.416	+ 2.1	.049	+ 17	− 10	− 1	20
6872....	.920	.216	.389	− 0.8	.010	− 1	+ 17	+ 13	21
6895....	.888	.164	.366	+ 1.0	.027	− 34	− 2	− 54	64
6945....	.837	.188	.359	+ 0.3	.012	+ 62	− 12	− 12	64
7137.. .	.467	.204	.388	+ 0.6	.014	+ 22	− 19	+ 8	30
7180....	.862	.215	.384	− 0.6	.0085	+ 11	+ 19	− 14	26
7295....	.661	.185	.426	+ 0.8	.014	+ 3	+ 10	− 3	11
7309....	.861	.155	.406	+ 1.3	.017	− 10	− 28	− 4	30
7310....	.666	.190	.359	+ 0.6	.032	+ 39	+ 11	+ 9	42
7328....	.653	.204	.388	+ 0.2	.019	− 9	+ 27	− 3	29
7352....	1.026	.192	.450						
7462....	.360	.077	.379						
7468....	.609	.154	.392	+ 1.9	.024	+ 2	− 35	+ 15	38
7517....	.610	.210	.373	+ 0.1	.011	+ 2	+ 22	− 15	27
7576....	1.057	.189	.468	− 0.2	.0091	− 4	− 43	− 7	44
7602....	.392	.121	.368	+ 3.5	.091	− 29	+ 4	+ 1	29
7615....	.727	.182	.372	+ 0.7	.023	− 13	− 9	+ 10	19
7685....	1.061	.215	.400	− 1.1	.0076	− 2	+ 20	+ 12	23
7806....	1.067	.176	.366	+ 0.2	.014	+ 3	+ 2	− 5	6
7949....	.706	.175	.344						
7957....	.532	.145	.365	+ 2.4	.062	− 84	+ 31	+ 22	92
8173....	.812	.167	.376	+ 1.0	.024	− 46	+ 37	+ 28	65
8228....	.656	.172	.387	+ 1.2	.016	− 3	+ 20	+ 23	31
8232....	.397	.234	.418						
8252....	.465	.184	.401	+ 1.3	.029	+ 21	− 24	− 1	32
8255....	.805	.201	.406	0.0	.010	− 46	+ 64	+ 14	80
8313....	.780	.290	.404						
8317....	.871	.192	.415	+ 0.1	.012	− 38	+ 37	− 2	53
8324....	.790	.175	.416	+ 0.8	.013	− 14	− 41	− 1	43
8414....	.535	.223	.401						
8465....	1.064	.290	.453						
8468....	.531	.231	.395	− 0.4	.0090	− 3	0	− 1	3
8475....	.870	.195	.391	0.0	.0089	0	− 15	− 17	23
8485....	.888	.174	.474						
8498....	.932	.113	.341						
8538....	.639	.165	.357	+ 1.5	.026	+ 7	− 32	− 18	37
8551....	.679	.143	.360	+ 2.1	.029	+ 14	− 39	− 62	75
8632....	.985	.180	.365	+ 0.2	.014	− 2	+ 18	− 1	18
8656....	.678	.213	.405	− 0.1	.0092	+ 29	− 10	+ 10	32

(continued)

TABLE 12 (continued).

HR	S	L	C	M_v	π	X	Y	Z	Q
8684....	.575	.170	.364	$+1^m.5$	″.040	+ 20	+ 3	− 11	23
8694....	.747	.182	.376	+ 0.7	.027	+ 12	− 32	− 7	35
8702....	1.100	.220	.401	− 1.3	.0060	− 18	− 8	− 9	22
8779....	1.006	.213	.435	− 0.9	.0056	0	+ 6	+ 13	14
8780....	.718	.175	.360	+ 1.0	.018	− 30	+ 37	+ 37	60
8832....	.682	− .022	.417						
8852....	.480	.199	.348	+ 0.8	.026	− 37	+111	− 28	120
8874....	.635	.157	.383	+ 1.8	.020	+ 25	+ 2	+ 16	30
8916....	.739	.169	.412	+ 1.1	.024	+ 23	− 35	+ 6	42
8923....	.585	.174	.397	+ 1.3	.023	+ 4	+ 4	+ 18	19
8930....	.694	.172	.356	+ 1.1	.015	− 77	+ 44	− 20	91
8974....	.754	.131	.399	+ 2.3	.066	− 23	− 33	+ 8	41
9008....	.824	.181	.360	+ 0.6	.014	− 14	+ 3	+ 23	27

Notes to Table 12 and Figures 20–25.

Stars within the considered limits of S and L are included (HR 8702 is outside the limits), but for SB stars (cf. Table 11) and for stars with large (b, S, L) residuals, M_v, π, X, Y, Z and Q are not published. For the SB stars HR 360, 3149, 3627, 4668 these data were computed, and the stars are included in the plots of Figures 20–25, but are excluded from the computations pertaining to Tables 8 and 10.

For HR 4301, HR 4608, HR 4695 and HR 5480 (asterisk, Table 11), and for HR 2808 ($M_v(k,n,m) - M_v(\mathrm{K}) = +2.0$) the data may be unreliable.

X, Y, Z and Q were first computed utilizing the "basic solar motion" (Vyssotsky and Janssen 1951); later +5 and +1 were added to X and Z respectively (and new Q values computed) in order to correct to the "standard solar motion". Deviations of 1 km/sec will occur in some cases between the given X, Z and Q and corresponding values computed by means of the solar motion adopted by Allen (1963). All data in Table 12 are preliminary, and improved values will probably be obtained through more accurate classification measurements and through a better calibration.

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THEORY OF FINITE SYSTEMS OF PARTICLES

II. SCATTERING THEORY

BY

CLASINE VAN WINTER

København 1965
Kommissionær: Ejnar Munksgaard

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Synopsis

A scattering theory is presented for a non-relativistic system consisting of a finite number of particles with local two-body interactions. The behaviour of the system is studied from the point of view of the theory of Hilbert space. The formalism aims at expressing the scattering of wave-packets in terms of the resolvent of the Hamiltonian.

The starting-point is Jauch's theory of wave-operators, which is summarized. It is explained that this theory is particularly well suited for describing multi-channel processes. It permits an unambiguous definition of reaction channels and is sufficiently general to discuss the scattering, both elastic and inelastic, of any finite number of particles or bound fragments.

In Jauch's theory, there is a condition on the time development of the system. In order that there exist wave-operators, the system must split into mutually independent fragments as the time tends to ∞ or $-\infty$. In the present paper, this condition is translated into a condition on the two-body interactions. It is shown that for the existence of wave-operators it is sufficient, roughly speaking, if the two-body interactions are locally square-integrable and at large distances tend to 0 faster than the Coulomb interaction. This result applies to general multi-channel processes.

If the interaction satisfies sufficient conditions, the wave-operators can easily be related to the resolvent. This is done with the spectral theory of self-adjoint operators. It is found, however, that the theory of the scattering operators still meets with practical difficulties. These have to do with repeated limits that cannot be interchanged. To obtain workable expressions for the scattering operators, some further conditions are imposed upon the interaction. Also, the discussion is restricted to wave-packets that satisfy certain smoothness criteria. The scattering of smooth wave-packets is described by the limit of a sequence of linear functionals. In this sequence, the wave-function plays the part of a test-function. Each functional contains the resolvent for complex energies in the neighbourhood of the continuous spectrum. The limit refers to the energy tending to real values. The limiting behaviour is discussed in detail.

For systems with spherically symmetric two-body interactions, particular attention is devoted to scattering events in which both in the distant past and in the remote future there are only two fragments. For such events, it is shown how from the general expression for the scattering of a wave-packet, one can extract a scattering matrix the elements of which are functions of a real energy-parameter. Also, a study is made of the scattering of a collimated beam. This is not described by a plane wave, but by a statistical mixture of wave-packets. For the total scattering intensity to be finite, it is sufficient if the interaction between scattered fragments is locally square-integrable and at large distances tends to 0 faster than the inverse distance squared. Under this condition it is possible to define the amplitudes for scattering through a fixed angle. For real energies, these quantities are discussed in detail. In particular, it is shown how they are related to the resolvent and to sums of scattering-matrix elements. In a forthcoming paper the present results will be used to continue the scattering amplitudes into the complex plane, and to investigate their analytic properties.

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CONTENTS

2.1. Introduction

2.1.1. General outline

In a previous paper with the subtitle "The Green Function" (1), a study was made of the resolvent operator for a system consisting of any finite number of particles. This operator was considered for complex energies not in the continuous spectrum of the Hamiltonian. Under the assumption that in the system there are only square-integrable local two-body interactions, it was shown that the resolvent is an integral operator the kernel of which can be evaluated explicitly. The kernel in question was called the Green function. In the energy plane cut along the real axis from some point M to ∞, the resolvent is analytic, regular except for possible poles on the real axis. If there are poles, these are located at the energies of bound states, the corresponding eigenfunctions following from the residues of the resolvent. Since in the cut energy plane the resolvent can be evaluated explicitly, the bound states of the system considered have thus been made accessible to further investigation. By contrast, the previous paper does not give any information on the structure of the continuous spectrum, nor, in fact, does it determine its location. Since obviously there is an intimate relationship between the existence of a continuous spectrum and the occurrence of scattering phenomena, we therefore continue our investigation of finite systems of particles with a paper on the theory of scattering.

In a scattering process there is a number of fragments which in the distant past were very far apart and consequently behaved as if they were free. In the course of time, the fragments approach each other, and a collision takes place. This may cause the fragments to change their velocities. It may also give rise to reactions. After the collision there will in any case emerge a number of fragments. In the remote future these will be free again. It is the object of the scattering theory, firstly, to say what states can occur as initial and final states in a scattering event and, secondly, to evaluate the probability for transitions between these states. In the course of years numerous papers have been devoted to this subject. However, in none of these did we find a rigorous treatment that takes us from first principles to explicit expressions for observable quantities related to the continuous spectrum.

The formalism of the present paper has as its starting-point a theory due mainly to Jauch (2, 3), which expresses in a precise mathematical form the essential features

of a scattering process. Jauch's theory is concerned with the time development of suitably chosen wave-packets, which are required to tend to free packets as the time tends to ∞ or $-\infty$. The requirement that there should be limits makes it possible to define the wave-operators and, subsequently, the scattering operators, which determine the transition probabilities. For the simple case of one-channel scattering, this is summarized in section 2.2.

It is one of the beautiful features of Jauch's theory that it makes possible an unambiguous description of multi-channel processes. This is explained in section 2.3. From this section it will become clear that the theory is a considerable improvement on the usual heuristic scattering formalism, in which there are always difficulties associated with the possibility for reactions to take place. In particular, it is no longer necessary to restrict the discussion to processes in which the total scattering system is not separated into more than two fragments. Neither need there be an exterior region in configuration space in which there is no interaction between the fragments. The most important improvement, however, is concerned with the channel concept. In the usual formalism, reaction channels are defined via a discussion of the wave-function in the external region. In this region an expansion is made in terms of channel wave-functions which are, however, not strictly orthogonal. As a result the decomposition into channels is not really unique. If the system is in channel a, this does not in general exclude its being in channel b. This ambiguity is completely avoided in the formalism to be summarized in section 2.3, the point being that in Jauch's theory one concentrates on the ergodic properties of the system, rather than on its asymptotic behaviour in configuration space.

Sections 2.2 and 2.3 are completely formal in the sense that it is simply assumed that the properties of the system are such that, as the time tends to ∞ or $-\infty$, the wave-function tends to well-behaved limits. This is equivalent to the assumption that there exist wave-operators and scattering operators. As it stands this requirement is fairly abstract. However, for one-channel problems it was shown by Cook(4), Jauch and Zinnes(5), and Kuroda(6) that this point can be traced back to the interaction in the system. This is discussed in section 2.4, in which we also treat the multi-channel case. It is found that for the existence of the scattering operators it is sufficient, roughly speaking, that the interaction between scattered fragments is locally square-integrable and at large distances falls off more rapidly than the Coulomb interaction. For a large class of interactions it is shown that the set of states that can occur as initial or final states in a scattering event is uniquely determined. This means that within the framework of the present formalism there is one and only one way in which channels can be defined. The channels are mutually orthogonal, according to section 2.3.

In section 2.5 the wave-operators are expressed in terms of the resolvent. This is done with the spectral theory developed in section 1.4 of our previous paper(1). Since by the previous paper the resolvent can be evaluated explicitly, section 2.5 makes it possible, in principle, to compute the wave-operators.

When in section 2.6 we try to extend the methods of section 2.5 to the scattering operators, an unexpected difficulty presents itself. There appears a repeated limit which in general is completely unmanageable. It is found, however, that, if the relative motion of the scattered fragments and their mutual interaction are what we call admissible, one limit can be performed explicitly. There then remains a limit which involves the resolvent and essentially refers to the energy of the system approaching the continuous spectrum through non-real values. This limit exists owing to the fact that, as the time tends to ∞ or $-\infty$, the system splits into independent fragments sufficiently rapidly. This splitting, in turn, is due to the interaction between the fragments decreasing sufficiently rapidly as their distance increases. We thus see that there is an intimate relationship between the behaviour of the resolvent in the neighbourhood of the continuous spectrum, the time development of scattered wave-packets, and the properties of the interaction. In some of our formulas there is an analogy with the work of LIPPMANN and SCHWINGER(7) and GELL-MANN and GOLDBERGER(8), but the general point of view is entirely different.

The requirement that the interaction and the relative motion of the scattered fragments be admissible is discussed in sections 2.6.3 to 2.6.6. For the interaction, sufficient conditions are found which are only slightly more restrictive than the mere existence of the scattering operators. For the relative motion, wave-functions are chosen which in momentum space are smooth and vanish outside bounded regions. The more detailed results of the present paper all refer to such wave-functions. The scattering of smooth wave-packets is described by the limit of a sequence of linear functionals. In the terminology of the theory of distributions, the wave-function plays the role of the test-function. Each member of the sequence contains the resolvent for complex energies in the neighbourhood of the continuous spectrum. In the limit the energy tends to the real axis, as mentioned above. It is obvious that the formalism must yield the conservation of energy during the scattering process. This comes out in a natural way, without the intermediary of δ-functions. Also, there are no normalization difficulties.

The formulas of section 2.6 apply to the scattering of any number of fragments. It is discussed in section 2.7 that considerable simplifications become possible if we restrict ourselves to scattering events in which both in the distant past and in the remote future there are only two fragments. For systems with spherically symmetric two-body interactions, particular attention is devoted to the scattering of partial waves. It is shown how this can be described with the help of a matrix, the elements of which are functions of a real energy-parameter. Under suitable conditions this $\mathcal{S}$-matrix is unitary and symmetric.

Whereas the $\mathcal{S}$-matrix refers to one single wave-packet, section 2.8 discusses the scattering of what we call a beam. By this we mean a certain statistical mixture of wave-packets. By analogy with a plane wave, a beam can be decomposed into a sum of partial waves. The requirement that this sum be convergent imposes the restriction that, as the distance between scattered fragments increases, their interaction decreases

faster than the inverse distance squared. If this condition is fulfilled, it is possible to define the amplitudes for scattering through a fixed angle. These determine the cross section. A beam as defined here provides a good description of a collimated stream of projectiles. It is, in fact, much more appropriate than a plane wave. Mathematically a beam can be handled more easily. Since it consists of a mixture of wave-packets, it is also more acceptable physically than a plane wave.

Qualitatively, the result that there is an $\mathcal{S}$-matrix and scattering amplitudes is what one expects from more heuristic theories. It must be remarked, however, that a correct definition of these quantities requires a careful handling of limits and integrals that cannot be interchanged. In the present treatment an element of the $\mathcal{S}$-matrix comes out as the derivative of the limit of a sequence of integrals. A scattering amplitude is defined as the sum of a series which converges in mean square. With the help of section 2.6 the $\mathcal{S}$-matrix and the scattering amplitudes are related to the resolvent. Mathematically this is also a subtle affair.

The insight we have gained into the limiting properties of the resolvent in the neighbourhood of the continuous spectrum is very useful for further research. In a forthcoming paper it will make it possible to consider the $\mathcal{S}$-matrix elements and the scattering amplitudes as the boundary values of analytic functions that depend on a complex energy. It will be shown that the boundary behaviour is sufficiently smooth for these analytic functions to satisfy dispersion relations. Because of the dispersion relations, there is also a parameter expansion for the $\mathcal{S}$-matrix. This nicely describes the qualitative features of the scattering. In particular, it exhibits resonances against a background of direct reactions.

2.1.2. Notation and basic assumptions

In the following our previous paper (1) is denoted by I. We use the same notation. Since in I all sections and formulas were given numbers beginning with 1, they can simply be referred to by the original numbers.

We recall from I that the present investigation is concerned with systems consisting of n distinguishable particles, the Hamiltonian being derived from

$$H'(\boldsymbol{X}) = -\sum_{i=1}^{n} \frac{1}{2\,m_i} \Delta(\boldsymbol{X}_i) + \sum_{i<j} V_{ij}(\boldsymbol{X}_i - \boldsymbol{X}_j) \tag{2.1.1}$$

(cf. eq. (1.1.1)). As was the case in I, it is useful to split off the motion of the centre of mass. If this is done through the introduction of new coordinates $\boldsymbol{x}$ according to eq. (1.2.1), the operator for the relative motion takes the form

$$H'(\boldsymbol{x}) = -\sum_{i=1}^{n-1} \Delta(\boldsymbol{x}_i) + \sum_{i<j} V_{ij}\left(\sum_{k=1}^{j-1} c_{ij}^{k} \boldsymbol{x}_k\right), \tag{2.1.2}$$

with certain constants c (cf. eq. (1.2.4)).

It was explained in section 1.2.2 that, under suitable assumptions on the functions V_{ij}, there is a unique way of extending $H'(\boldsymbol{x})$ to a self-adjoint operator in the Hilbert space of square-integrable functions of $\boldsymbol{x}$. This self-adjoint extension is taken as the Hamiltonian. It is denoted by H or $H(\boldsymbol{x})$. Its domain is denoted by $\mathfrak{D}(H)$. If there is no interaction, H reduces to the operator H_0 with domain $\mathfrak{D}(H_0)$.

For the Hilbert space of square-integrable functions of $\boldsymbol{x}$ we use the notation $\mathfrak{L}^2$ or $\mathfrak{L}^2(\boldsymbol{x})$. If f and g are any two functions in $\mathfrak{L}^2$, the norm of f is denoted by $||f||$, the inner product of f and g by (g,f),

$$||f|| = [\int |f(\boldsymbol{x})|^2 d\boldsymbol{x}]^{\frac{1}{2}}, \qquad (g,f) = \int \bar{g}(\boldsymbol{x}) f(\boldsymbol{x}) d\boldsymbol{x}. \tag{2.1.3}$$

It is assumed throughout the present paper that the operator $H'(\boldsymbol{x})$ is essentially self-adjoint, i. e. that it has one and only one self-adjoint extension. This point was discussed in great detail by KATO(9). It was shown first that $H_0'(\boldsymbol{x})$ is essentially self-adjoint, the domain $\mathfrak{D}(H_0)$ of the self-adjoint extension H_0 consisting of all functions $f(\boldsymbol{x})$ in $\mathfrak{L}^2(\boldsymbol{x})$ whose Fourier transforms $\hat{f}(\boldsymbol{k})$ are such that $|\boldsymbol{k}|^2 \hat{f}(\boldsymbol{k})$ belongs to $\mathfrak{L}^2(\boldsymbol{k})$. Next it was shown by KATO that for $H'(\boldsymbol{x})$ to be essentially self-adjoint, it is sufficient if there are constants α and β, with $\alpha < 1$, such that, for every f in $\mathfrak{D}(H_0)$, the quantity $V_{ij}f$ satisfies

$$\sum_{i<j} ||V_{ij} f|| < \alpha ||H_0 f|| + \beta ||f|| \tag{2.1.4}$$

(cf. eq. (1.7.14)). If this condition is fulfilled, we have

$$\mathfrak{D}(H) = \mathfrak{D}(H_0), \qquad H = H_0 + \sum_{i<j} V_{ij} \tag{2.1.5}$$

(cf. eq. (1.2.9)). In the present paper it is assumed throughout that eqs. (2.1.4) and (2.1.5) are satisfied.

It follows from the work of KATO(9) and STUMMEL(10) that eq. (2.1.4) holds true for a large class of interactions. Obviously it is fulfilled whenever V_{ij} is bounded. It is also satisfied if

$$\int [V_{ij}(\boldsymbol{X})]^2 (1 + |\boldsymbol{X} - \boldsymbol{Y}|)^{-1+\zeta} d^3\boldsymbol{X} < \text{const.} \tag{2.1.6}$$

for some ζ with $0 < \zeta < 1$, and every $\boldsymbol{Y}$. If this relation holds true, the constant α in eq. (2.1.4) may be chosen as close to 0 as we like.

Equation (2.1.6) gives a typical condition on V_{ij} that is often imposed from section 2.4 onwards. In later sections some further restrictions are required. These are indicated as the need arises.

2.2. The scattering of two particles

2.2.1. The time development of the system

As a simple example of a system in which scattering can take place, we consider two particles the interaction of which depends only on their mutual distance. For the Hamiltonian of the relative motion we write H, the corresponding Hamiltonian for the system without interaction being denoted by H_0.

If in the Schrödinger representation the wave-function for the relative motion is equal to f_+ at time $t = 0$, it takes the form $\exp(-iHt)f_+$ at time t. Here f_+ must belong to the Hilbert space $\mathfrak{L}^2$. The operator $\exp(-iHt)$ can most easily be defined through the spectral theory given in section 1.4.

We imagine that the time development of the system is such that in the distant past the two particles were very far apart, and that they behaved approximately as free particles, according to a wave-function $\exp(-iH_0t)f$, with some f in $\mathfrak{L}^2$. That is, we assume that there are functions f_+ and f such that

$$\lim_{t\to-\infty} (e^{-iHt}h,\ e^{-iHt}f_+ - e^{-iH_0t}f) = 0 \tag{2.2.1}$$

for every h in $\mathfrak{L}^2$. A second assumption is that in the course of time the norm of the wave-function does not change,

$$||f_+|| = ||f||. \tag{2.2.2}$$

It follows from eqs. (2.2.1) and (2.2.2) that

$$\left.\begin{aligned} &\lim_{t\to-\infty} ||f_+ - e^{iHt}e^{-iH_0t}f||^2 \\ &= \lim_{t\to-\infty} [||f_+||^2 + ||f||^2 - (e^{-iHt}f_+, e^{-iH_0t}f) - (e^{-iH_0t}f, e^{-iHt}f_+)] \\ &= ||f||^2 - ||f_+||^2 = 0. \end{aligned}\right\} \tag{2.2.3}$$

In other words, we assume in fact that there is a function f_+ which is the limit in mean of the sequence $\exp(iHt)\exp(-iH_0t)f$,

$$f_+ = \text{l.i.m.}_{t\to-\infty} e^{iHt}e^{-iH_0t}f. \tag{2.2.4}$$

With a view to discussing the behaviour of the system in the remote future, we likewise assume that there is a funtion f_- such that

$$f_- = \text{l.i.m.}_{t\to\infty} e^{iHt}e^{-iH_0t}f. \tag{2.2.5}$$

For future reference it is convenient to define

$$\Omega(t) = e^{iHt}e^{-iH_0t}. \tag{2.2.6}$$

If f is such that $\Omega(t)f$ has a limit as t tends to $-\infty$, it is not obvious that there is also a limit as t tends to ∞. However, in all practical cases in which we are interested in the following, it turns out that if one limit exists, so does the other. For simplicity we therefore assume that this is so from the outset. While there is a feeling that this point is related to invariance under time reversal (JAUCH(2) footnote p. 136), it seems that it is not well understood. However this may be, let us denote the set of functions f for which both limits exist by $\mathfrak{C}$. Then it is not difficult to see that $\mathfrak{C}$ is a closed set. For let us choose a sequence f_N in $\mathfrak{C}$ which tends in mean to some function f in $\mathfrak{L}^2$. Then we want to prove that for f the limits (2.2.4) and (2.2.5) exist, so that it belongs to $\mathfrak{C}$. For this it is sufficient to show that, given a positive δ, there is a number T such that

$$||\Omega(s)f - \Omega(t)f|| < \delta \qquad (s,t < -T;\ s,t > T). \tag{2.2.7}$$

If eq. (2.2.7) is satisfied, it follows from the fact that the space $\mathfrak{L}^2$ is closed, that there must be a function f_+ in $\mathfrak{L}^2$ such that, as t tends to $-\infty$, the sequence $\Omega(t)f$ tends in mean to f_+. And similarly for f_-. Hence f belongs to $\mathfrak{C}$, and $\mathfrak{C}$ is closed.

To check eq. (2.2.7), we write

$$\left.\begin{aligned} ||\Omega(s)f - \Omega(t)f|| &= ||[\Omega(s) - \Omega(t)](f - f_N) + [\Omega(s) - \Omega(t)]f_N|| \\ &\leq ||[\Omega(s) - \Omega(t)](f - f_N)|| + ||\Omega(s)f_N - f_{N\pm}|| + ||\Omega(t)f_N - f_{N\pm}|| \\ &< 2||f - f_N|| + ||\Omega(s)f_N - f_{N\pm}|| + ||\Omega(t)f_N - f_{N\pm}||, \end{aligned}\right\} \tag{2.2.8}$$

$f_{N\pm}$ being the limit of $\Omega(t)f_N$ as t tends to $\mp\infty$. By choosing first N sufficiently large, next s and t sufficiently small, c. q. sufficiently large, the right-hand side of eq. (2.2.8) can be made less than δ. Hence eq. (2.2.7) is satisfied, and our assertion is proved.

In the following the set of functions f_+ which are limits in the sense of eq. (2.2.4) is denoted by $\mathfrak{R}_+$, the corresponding set of functions f_- is denoted by $\mathfrak{R}_-$. Taking into account the fact that $\mathfrak{C}$ is closed, it is easily shown that the sets $\mathfrak{R}_\pm$ are also closed.

2.2.2. The wave-operators

Since the set $\mathfrak{C}$ is closed, every function h in $\mathfrak{L}^2$ can uniquely be decomposed according to

$$h = f + g, \quad f \in \mathfrak{C}, \quad g \perp \mathfrak{C}, \tag{2.2.9}$$

where $g \perp \mathfrak{C}$ means that g belongs to the orthogonal complement of $\mathfrak{C}$. With the help of this decomposition, we now introduce operators $\Omega_\pm$ defined by

$$\Omega_\pm h = \underset{t \to \mp\infty}{\text{l.i.m.}}\, \Omega(t)f. \tag{2.2.10}$$

These operators are called wave-operators. They are bounded operators with domains $\mathfrak{L}^2$ and ranges $\mathfrak{R}_\pm$. The wave-operators have uniquely determined adjoints $\Omega_\pm^*$, which satisfy

$$(k,\Omega_{\pm}^{*}h) = (\Omega_{\pm}k,h) \tag{2.2.11}$$

for every h and k in $\mathfrak{L}^2$. It follows from eq. (2.2.11) that $\Omega_{\pm}^{*}h = 0$ whenever $h \perp \mathfrak{R}_{\pm}$. Also, $(k,\Omega_{\pm}^{*}h)$ vanishes if $k \perp \mathfrak{C}$, by eqs. (2.2.10) and (2.2.11). Hence, if $\Omega_{\pm}^{*}h$ does not vanish, it belongs to $\mathfrak{C}$.

We now want to show that the operator $\Omega_{\pm}^{*}\Omega_{\pm}$ is the projection operator with range $\mathfrak{C}$. In the notation of eq. (2.2.9), this statement is equivalent to

$$(k,\Omega_{\pm}^{*}\Omega_{\pm}h) = (k,f) \tag{2.2.12}$$

for every k in $\mathfrak{L}^2$. If $k \perp \mathfrak{C}$, eq. (2.2.12) is obvious. In this case either side vanishes. If $k \in \mathfrak{C}$, we have

$$\left.\begin{aligned} |(k,\Omega_{\pm}^{*}\Omega_{\pm}h) - (k,f)| &= |(\Omega_{\pm}k,\Omega_{\pm}f) - (k,f)| \\ = \lim_{s,t \to \mp\infty} |(\Omega(s)k,\Omega(t)f) - (\Omega(t)k,\Omega(t)f)| &\leq \lim_{s,t \to \mp\infty} ||[\Omega(s) - \Omega(t)]k||\,||f|| = 0. \end{aligned}\right\} \tag{2.2.13}$$

Hence in this case eq. (2.2.12) is also satisfied. It follows that $\Omega_{\pm}^{*}\Omega_{\pm}$ is the projection onto $\mathfrak{C}$, as we wished to prove. With this result it is easily seen that the operators $\Omega_{\pm}\Omega_{\pm}^{*}$ are likewise projections. Their ranges are $\mathfrak{R}_{\pm}$. Summarizing, we have

$$\Omega_{\pm}^{*}\Omega_{\pm} = P(\mathfrak{C}), \tag{2.2.14}$$

$$\Omega_{\pm}\Omega_{\pm}^{*} = P(\mathfrak{R}_{\pm}), \tag{2.2.15}$$

where $P(\mathfrak{C})$ and $P(\mathfrak{R}_{\pm})$ denote the projections onto $\mathfrak{C}$ and $\mathfrak{R}_{\pm}$, respectively.

2.2.3. The intertwining property

If f belongs to $\mathfrak{C}$, we have

$$\lim_{s \to \mp\infty} ||e^{iHt}f_{\pm} - e^{iHs}e^{-iH_0s}e^{iH_0t}f|| = \lim_{s \to \mp\infty} ||e^{iHt}f_{\pm} - e^{iHt}e^{iH(s-t)}\,e^{-iH_0(s-t)}f|| = 0. \tag{2.2.16}$$

Hence $\exp(iH_0t)f$ also belongs to $\mathfrak{C}$, and the operators $\Omega_{\pm}$ have the intertwining property

$$\Omega_{\pm}e^{iH_0t}f = e^{iHt}\Omega_{\pm}f \qquad (f \in \mathfrak{C}). \tag{2.2.17}$$

Conversely, if $\exp(iH_0t)f$ belongs to $\mathfrak{C}$, then so does f. This means that if $f \perp \mathfrak{C}$, we also have $\exp(iH_0t)f \perp \mathfrak{C}$. In the latter case either side of eq. (2.2.17) vanishes, so that this equation is again satisfied. Since every f in $\mathfrak{L}^2$ can be decomposed into a component in $\mathfrak{C}$ and a component orthogonal to $\mathfrak{C}$, it follows that eq. (2.2.17) holds in fact for every f in $\mathfrak{L}^2$. In other words,

$$\Omega_{\pm}e^{iH_0t} = e^{iHt}\Omega_{\pm}. \tag{2.2.18}$$

From eq. (2.2.18) it follows that, if the quantity $\Omega_{\pm}h$ does not vanish, it cannot be an eigenfunction of H. For let us assume the contrary, i. e. let us assume that

$$e^{iHt}\Omega_{\pm}h = e^{i\lambda t}\Omega_{\pm}h \tag{2.2.19}$$

for every t and some real λ. Then

$$\Omega_{\pm}e^{iH_0t}h = \Omega_{\pm}e^{i\lambda t}h. \tag{2.2.20}$$

Since $\Omega_{\pm}h \neq 0$ by assumption, h must have a component f in $\mathfrak{C}$. Applying $\Omega_{\pm}^{*}$ to both sides of eq. (2.2.20), we obtain

$$e^{iH_0t}f = e^{i\lambda t}f. \tag{2.2.21}$$

From this it follows that

$$\lim_{t\to 0}||\frac{1}{t}(e^{iH_0t}-1)f|| = \lim_{t\to 0}||\frac{1}{t}(e^{i\lambda t}-1)f|| = ||\lambda f||. \tag{2.2.22}$$

Next it follows from the existence of the limit in eq. (2.2.22) that f belongs to the domain of H_0 (RIESZ and SZ.-NAGY(11) section 137). Also,

$$\text{l.i.m.}_{t\to 0}\frac{1}{it}(e^{iH_0t}-1)f = H_0f = \lambda f, \tag{2.2.23}$$

so that f is an eigenfunction of H_0. But since H_0 is known not to have eigenfunctions in $\mathfrak{L}^2$, this result is invalid. Hence the assumption that $\Omega_{\pm}h$ is an eigenfunction of H must be incorrect.

It follows from eq. (2.2.18) that

$$\Omega_{\pm}R_0(\lambda) = R(\lambda)\Omega_{\pm} \qquad (\text{Im}\lambda \neq 0), \tag{2.2.24}$$

where R and R_0 stand for the resolvents of H and H_0, respectively. One method of proving this relation makes use of the formula

$$(g,R(\lambda)f) = \frac{1}{2\pi}\int_{-\infty}^{\infty}(g,e^{iHt}f)dt\int_{-\infty}^{\infty}\frac{1}{l-\lambda}e^{-ilt}dl \tag{2.2.25}$$

given by STONE(12). From eq. (2.2.24) it follows immediately that

$$E_0(l;\Omega_{\pm}^{*}g,f) = E(l;g,\Omega_{\pm}f) \tag{2.2.26}$$

for every f and g in $\mathfrak{L}^2$. Here E and E_0 are the spectral functions associated with H and H_0 which were defined in section 1.4.1. If in eq. (2.2.26) we choose f in $\mathfrak{C}$ and take $g = \Omega_{\pm}f$, we obtain

$$E_0(l;f,f) = E(l;\Omega_{\pm}f,\Omega_{\pm}f). \tag{2.2.27}$$

Now since the spectrum of H_0 is continuous, the left-hand side of eq. (2.2.27) is a continuous function of l. Hence so is the right-hand side. This shows again that $\Omega_{\pm}f$ cannot be an eigenfunction of H. As a matter of fact, if H has eigenfunctions in $\mathfrak{L}^2$,

eq. (2.2.27) implies that $\Omega_{\pm}f$ is orthogonal to these (cf. STONE(13) theorem 5.13).

If, given a certain l, there is a function f in $\mathfrak{C}$ such that l is not an interior point of an interval in which $E_0(l;f,f) = \text{const.}$, then l certainly belongs to the continuous spectrum of H_0. By eq. (2.2.27), l also belongs to the continuous spectrum of H. Hence the continuous spectrum of H contains the set of points l for which there is a function f with the property mentioned. In practical cases, this set consists of all points l in the spectrum of H_0. The continuous spectrum of H then contains the spectrum of H_0.

For future reference we note that, according to eq. (2.2.26),

$$\Omega_{\pm}E_0(l) = E(l)\Omega_{\pm}, \tag{2.2.28}$$

$E(l)$ and $E_0(l)$ denoting the resolutions of the identity associated with H and H_0, respectively (cf. eq. (1.4.21)). If f belongs to $\mathfrak{C}$, it follows with eq. (1.4.22) that

$$\left.\begin{aligned} ||\Omega_{\pm}E_0(l)f||^2 &= ||E(l)\Omega_{\pm}f||^2 = (\Omega_{\pm}f, E(l)\Omega_{\pm}f) \\ &= (\Omega_{\pm}^{*}\Omega_{\pm}f, E_0(l)f) = (f, E_0(l)f) = ||E_0(l)f||^2. \end{aligned}\right\} \tag{2.2.29}$$

Hence, if f belongs to $\mathfrak{C}$, so does $E_0(l)f$, by eq. (2.2.14). Now $E_0(l)f$ belongs to $\mathfrak{D}(H_0)$ (cf. section 1.4.2 and ACHIESER and GLASMANN(14) section 66). If l tends to ∞, the function $E_0(l)f$ tends in mean to f. This means that, if f belongs to $\mathfrak{C}$, it can be approximated in mean square by a function which belongs both to $\mathfrak{C}$ and to $\mathfrak{D}(H_0)$.

If f belongs both to $\mathfrak{C}$ and to $\mathfrak{D}(H_0)$, it follows from eqs. (2.2.26) and (1.4.24) that

$$\Omega_{\pm}H_0f = H\Omega_{\pm}f. \tag{2.2.30}$$

With an argument as used in eq. (2.2.29), it is easily shown that in this case H_0f also belongs to $\mathfrak{C}$.

2.2.4. The scattering operator

From the beginning of section 2.2.1 we recall that at time t the wave-function in the Schrödinger representation is of the form

$$e^{-iHt}f_{+} = e^{-iHt}\Omega_{+}f \qquad (f\in\mathfrak{C}). \tag{2.2.31}$$

Now we imagine that in the remote future the system we are considering will behave asymptotically as a free system. Let us therefore determine the probability of finding it in the state $\exp(-iH_0t)g$, where g belongs to $\mathfrak{C}$. This probability is equal to

$$|(e^{-iH_0t}g, e^{-iHt}\Omega_{+}f)|^2. \tag{2.2.32}$$

If t tends to ∞, this quantity tends to

$$\lim_{t\to\infty}|(e^{iHt}e^{-iH_0t}g, \Omega_{+}f)|^2 = |(\Omega_{-}g, \Omega_{+}f)|^2 = |(g, \Omega_{-}^{*}\Omega_{+}f)|^2. \tag{2.2.33}$$

Hence the probability for a transition from the state $\exp(-iH_0t)f$ at $t = -\infty$ to the state $\exp(-iH_0t)g$ at $t = \infty$ is determined by the operator

$$S = \Omega_-^* \Omega_+, \tag{2.2.34}$$

which is called the scattering operator.

Since $\Omega_+ f$ belongs to $\mathfrak{R}_+$, and $\Omega_- g$ to $\mathfrak{R}_-$, it is obvious that there are no transitions from f to g if $\mathfrak{R}_+$ and $\mathfrak{R}_-$ are orthogonal. More generally, let us imagine that there exists a function h_+ in $\mathfrak{R}_+$ which is orthogonal to $\mathfrak{R}_-$. By the definition of $\mathfrak{R}_+$, there must be a function h in $\mathfrak{C}$ such that $h_+ = \Omega_+ h$. This function has the property that $(\Omega_- g, \Omega_+ h)$ vanishes for every g in $\mathfrak{L}^2$. Hence, if the wave-function takes the form $\exp(-iH_0t)h$ at $t = -\infty$, a situation arises in which there is no possibility for the system to become free as t approaches ∞. Conversely, if there is a function h_- in $\mathfrak{R}_-$ and orthogonal to $\mathfrak{R}_+$, there is a function h in $\mathfrak{C}$ such that the wave-function $\exp(-iH_0t)h$ cannot occur as the outcome of a scattering process. Since either case seems to be pathological, it was required by JAUCH (2) that

$$\mathfrak{R}_+ = \mathfrak{R}_-. \tag{2.2.35}$$

2.2.5. Unitarity

The relation (2.2.35) is directly related to the unitarity of the S-operator. As a matter of fact, if $\mathfrak{R}_+ = \mathfrak{R}_-$, it follows from eqs. (2.2.14), (2.2.15), and (2.2.34) that

$$\left.\begin{aligned} S^*S &= \Omega_+^* \Omega_- \Omega_-^* \Omega_+ = \Omega_+^* P(\mathfrak{R}_-) \Omega_+ = \Omega_+^* P(\mathfrak{R}_+) \Omega_+ = \Omega_+^* \Omega_+ = P(\mathfrak{C}), \\ SS^* &= \Omega_-^* \Omega_+ \Omega_+^* \Omega_- = \Omega_-^* P(\mathfrak{R}_+) \Omega_- = \Omega_-^* P(\mathfrak{R}_-) \Omega_- = \Omega_-^* \Omega_- = P(\mathfrak{C}). \end{aligned}\right\} \tag{2.2.36}$$

Hence S can be considered as a unitary operator in $\mathfrak{C}$. In all cases which were investigated explicitly thus far, $\mathfrak{C}$ was the whole space $\mathfrak{L}^2$. Hence S was unitary whenever $\mathfrak{R}_+ = \mathfrak{R}_-$.

It is easily seen from eq. (2.2.36) that for S to be unitary it is not merely sufficient, but it is also necessary that $\mathfrak{R}_+ = \mathfrak{R}_-$. Thus special studies were devoted to this problem by KURODA (6, 15) and IKEBE (16). For the case of two particles, hence three-dimensional $\boldsymbol{x}$, it was shown by KURODA (6, 15) that S is unitary if the interaction $V(\boldsymbol{x})$ is both integrable and square-integrable. If $V(\boldsymbol{x})$ is spherically symmetric, it is sufficient if there is a positive ζ such that $V(|\boldsymbol{x}|)(1 + |\boldsymbol{x}|)^{-\frac{1}{2}+\zeta}$ is square-integrable (KURODA (6)). IKEBE (16) established the unitarity of the S-operator under the assumption that $V(\boldsymbol{x})$ is Hölder-continuous except for a finite number of singularities, is square-integrable, and as $|\boldsymbol{x}|$ tends to ∞ is of the order $O(|\boldsymbol{x}|^{-2-\eta})$, with some positive η. Under these assumptions he was also able to show that the space $\mathfrak{R}_+ = \mathfrak{R}_-$ is the orthogonal complement of the space spanned by the eigenfunctions of H, if these exist. Hence, under Ikebe's assumptions on the interaction, every function which is orthogonal to the eigenfunctions of H can occur as the wave-function in a scattering process. In section 2.2.3 we saw already that in a scattering experiment we never

get the eigenfunctions of H. This follows from the result that $\Omega_{\pm} f$ is orthogonal to these eigenfunctions (cf. eq. (2.2.27)).

2.2.6. Integral representations of the wave-operators

For future reference we note that it was shown by JAUCH (2) that, if the limits (2.2.4) and (2.2.5) exist,

$$\left.\begin{aligned} f_+ &= \operatorname*{l.i.m.}_{\varepsilon \to 0} \varepsilon \int_{-\infty}^{0} e^{\varepsilon t} \Omega(t) dt f, \\ f_- &= \operatorname*{l.i.m.}_{\varepsilon \to 0} \varepsilon \int_{0}^{\infty} e^{-\varepsilon t} \Omega(t) dt f, \end{aligned}\right\} \tag{2.2.37}$$

it being understood that ε tends to 0 through positive values.

Since for fixed f and g the quantity $(g, \Omega(t)f)$ is a bounded and continuous function of t, the integrals

$$\mp \varepsilon \int_{0}^{\mp\infty} e^{-\varepsilon|t|} (g, \Omega(t) f) dt \tag{2.2.38}$$

exist and are bounded. Hence, in virtue of the Riesz-Fréchet theorem (ACHIESER and GLASMANN (14) section 21), there are bounded operators $\Omega_{\pm\varepsilon}$, which conveniently may be written as

$$\Omega_{\pm\varepsilon} = \mp \varepsilon \int_{0}^{\mp\infty} e^{-\varepsilon|t|} \Omega(t) dt, \tag{2.2.39}$$

such that

$$\mp \varepsilon \int_{0}^{\mp\infty} e^{-\varepsilon|t|} (g, \Omega(t) f) dt = \mp \varepsilon \left(g, \int_{0}^{\mp\infty} e^{-\varepsilon|t|} \Omega(t) dt f \right). \tag{2.2.40}$$

This defines the integrals in eq. (2.2.37).

Now if, given a positive δ, there exists a number T such that

$$||f_+ - \Omega(t) f|| < \delta \tag{2.2.41}$$

whenever $t < -T$, it follows that

$$\left.\begin{aligned} ||f_+ - \varepsilon \int_{-\infty}^{0} e^{\varepsilon t} \Omega(t) dt f|| &= \varepsilon || \int_{-\infty}^{0} e^{\varepsilon t} dt [f_+ - \Omega(t) f]|| \\ < \varepsilon \int_{-\infty}^{-T} e^{\varepsilon t} ||f_+ - \Omega(t) f|| dt + \varepsilon \int_{-T}^{0} e^{\varepsilon t} ||f_+ - \Omega(t) f|| dt &< \delta + 2(1 - e^{-\varepsilon T}) ||f||. \end{aligned}\right\} \tag{2.2.42}$$

By choosing ε sufficiently small, this can be made less than 2δ, say. The first statement of eq. (2.2.37) then follows. The second one can be justified similarly.

2.3. Multi-channel scattering

2.3.1. The channel concept

To discuss the scattering in a system of more than two particles, we consider the case that in the distant past the system was split into m fragments which were very far apart. In this situation it is convenient to introduce m' sets of internal coordinates to describe the motion within the m' fragments that consist of two or more particles, $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_{m'} (m' \leq m)$, plus a set of $m-1$ three-dimensional coordinates, $\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}$, for the motion of the fragments with respect to each other. It follows from section 1.2.1 that this can be done in such a way that the differential operator for the relative kinetic energy of the m fragments with respect to each other takes the form $-\sum_{j=m+1}^{2m-1} \Delta(\boldsymbol{x}_j)$.

To bring out the assumption that in the distant past the m fragments were very far apart, and that effectively there was no interaction between them, we introduce the operator

$$H'_a(\boldsymbol{x}) = -\sum_{j=m+1}^{2m-1} \Delta(\boldsymbol{x}_j) + \lambda_a , \tag{2.3.1}$$

where λ_a is a real number to be determined in the course of the following. In the space $\mathfrak{L}^2(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{m'}, \boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$ the operator $H'_a(\boldsymbol{x})$ has a unique self-adjoint extension. This we denote by H_a (cf. the discussion in section 1.7.2). Now the idea is that H_a represents the effective energy of the system at time $t = -\infty$. That is, we imagine that in the distant past the system behaved according to some wave-function $\exp(-iH_a t) f_a$, and we require the existence of

$$f_{a\pm} = \underset{t \to \mp\infty}{\text{l.i.m.}}\, e^{iHt} e^{-iH_a t} f_a . \tag{2.3.2}$$

In this picture, λ_a plays the role of the intrinsic energy of the m fragments. Under very general assumptions on the interaction between the fragments, it is shown in section 2.4.3 that, for the limit in eq. (2.3.2) to exist, it is necessary that λ_a is of the form

$$\lambda_a = \sum_{j=1}^{m'} \lambda_{(j)} , \tag{2.3.3}$$

where the numbers $\lambda_{(j)}$ are eigenvalues of the Hamiltonians $H_{(j)}(\boldsymbol{x}_j)$ for the internal motions of the respective fragments. It is also shown that, if to each $\lambda_{(j)}$ in the series (2.3.3) there corresponds only one eigenfunction $\varphi_{(j)}(\boldsymbol{x}_j)$, the function f_a must be of the form

$$f_a(\boldsymbol{x}) = \prod_{j=1}^{m'} \varphi_{(j)}(\boldsymbol{x}_j) f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}). \tag{2.3.4}$$

If $\lambda_{(1)}$ is degenerate, with orthonormal eigenfunctions $\varphi_{(1)1}(\boldsymbol{x}_1)$ and $\varphi_{(1)2}(\boldsymbol{x}_1)$ say, we find it convenient to write $H_a = H_b$, and to consider separately

$$\left.\begin{aligned} f_a(\boldsymbol{x}) &= \varphi_{(1)1}(\boldsymbol{x}_1) \prod_{j=2}^{m'} \varphi_{(j)}(\boldsymbol{x}_j) f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}), \\ f_b(\boldsymbol{x}) &= \varphi_{(1)2}(\boldsymbol{x}_1) \prod_{j=2}^{m'} \varphi_{(j)}(\boldsymbol{x}_j) f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}). \end{aligned}\right\} \quad (2.3.5)$$

And similarly for more degenerate cases.

If asymptotically the system behaves according to the wave-function $\exp(-iH_at)f_a$, it is said to be in channel a. With the notation outlined in the previous paragraph, we have $H_a \neq H_b$, except possibly if $f_a \perp f_b$. The case $H_a = H_b$, $f_a \perp f_b$ also covers the exceptional situation that λ_a can be decomposed into a sum of the form (2.3.3) in more than one way.

2.3.2. The wave-operators

In line with section 2.2.2 we denote the set of functions f_a for which the limits (2.3.2) exist by $\mathfrak{C}_a$, the sets of functions $f_{a\pm}$ by $\mathfrak{R}_{a\pm}$. These sets are all closed. Decomposing a general function h in $\mathfrak{L}^2$ according to

$$h = f_a + g_a, \quad f_a \in \mathfrak{C}_a, \quad g_a \perp \mathfrak{C}_a, \quad (2.3.6)$$

we define the wave-operators $\Omega_{a\pm}$ by

$$\Omega_{a\pm} h = \underset{t \to \mp\infty}{\text{l.i.m.}}\, \Omega_a(t) f_a, \quad (2.3.7)$$

where

$$\Omega_a(t) = e^{iHt} e^{-iH_a t}. \quad (2.3.8)$$

In analogy to eqs. (2.2.14) and (2.2.15), we have

$$\Omega_{a\pm}^* \Omega_{a\pm} = P(\mathfrak{C}_a), \quad (2.3.9)$$

$$\Omega_{a\pm} \Omega_{a\pm}^* = P(\mathfrak{R}_{a\pm}). \quad (2.3.10)$$

Also,

$$\Omega_{a\pm} e^{iH_a t} = e^{iHt} \Omega_{a\pm}. \quad (2.3.11)$$

With trivial changes of notation, the conclusions which were drawn from the corresponding equation (2.2.18) apply also in the present case. In particular, if R_a denotes the resolvent of H_a, there is a relation analogous to eq. (2.2.24). The spectrum of H contains the spectrum of H_a if, given a point l in the spectrum of H_a, there is a function f_a in $\mathfrak{C}_a$ such that l is not an interior point of an interval in which $E_a(l; f_a, f_a) = \text{const}$. If f_a belongs to $\mathfrak{C}_a$, the function $E_a(l) f_a$ belongs both to $\mathfrak{C}_a$ and to $\mathfrak{D}(H_a)$.

If at time $t = -\infty$ the system was in the state $\exp(-iH_at)f_a$, the probability of finding it in the state $\exp(-iH_bt)g_b$ at time $t = \infty$ is given by

$$\lim_{t \to \infty} |(e^{-iH_b t} g_b, e^{-iHt} \Omega_{a+} f_a)|^2 = |(g_b, \Omega_{b-}^* \Omega_{a+} f_a)|^2. \quad (2.3.12)$$

In evaluating this expression in practical cases, it will be necessary to express H_b and g_b in the coordinate system adapted to H_a and f_a, or vice versa. This may give awkward formulas, but we shall not bother about that in the following.

It follows from eq. (2.3.12) that the transitions from channel a to channel b are determined by the operator

$$S_{ba} = \Omega_{b-}^{*}\Omega_{a+}. \tag{2.3.13}$$

If $\mathfrak{R}_{a+} \perp \mathfrak{R}_{b-}$, no transitions are possible.

2.3.3. Orthogonality of the channels

In connection with the foregoing, the question arises whether there is an ambiguity in the channel concept in the sense that the statement that the system is in channel b does not exclude its being in channel c. Let us assume for a moment that the system can be in two channels at the same time. Or rather, let us assume that there is a function h which belongs to $\mathfrak{R}_{a+}$, and also to both $\mathfrak{R}_{b-}$ and $\mathfrak{R}_{c-}$. By definition, this assumption means that there are functions h_a, h_b, and h_c such that

$$h = \Omega_{a+}h_a = \Omega_{b-}h_b = \Omega_{c-}h_c. \tag{2.3.14}$$

If we now consider the wave-function $\exp(-iHt)\Omega_{a+}h_a$, we find

$$\left.\begin{aligned} \lim_{t\to\infty} ||e^{-iHt}\Omega_{a+}h_a - e^{-iH_bt}h_b|| &= 0, \\ \lim_{t\to\infty} ||e^{-iHt}\Omega_{a+}h_a - e^{-iH_ct}h_c|| &= 0. \end{aligned}\right\} \tag{2.3.15}$$

According to this result, the wave-function in question would tend to $\exp(-iH_bt)h_b$, and also to $\exp(-iH_ct)h_c$. Hence, at $t = \infty$, the system would be in two different channels. It is clear that the root of this undesirable situation is the idea that there is an overlap between the sets $\mathfrak{R}_{b-}$ and $\mathfrak{R}_{c-}$. It is therefore important that

$$\mathfrak{R}_{a+} \perp \mathfrak{R}_{b+}, \qquad \mathfrak{R}_{a-} \perp \mathfrak{R}_{b-}, \qquad (a \neq b), \tag{2.3.16}$$

so that the above ambiguity does not occur. Obviously we do not expect a relation of the form $\mathfrak{R}_{a+} \perp \mathfrak{R}_{b-}$, because this would exclude the possibility of transitions from one channel to another in the course of time.

Equation (2.3.16) is due to Jauch (3). For the proof it suffices to show that

$$(\Omega_{b\pm}g_b, \Omega_{a\pm}f_a) = 0 \qquad (a \neq b) \tag{2.3.17}$$

for every f_a in $\mathfrak{C}_a$ and every g_b in $\mathfrak{C}_b$. Now,

$$\left.\begin{aligned} |(\Omega_b(t)g_b, \Omega_a(t)f_a) - (\Omega_{b\pm}g_b, \Omega_{a\pm}f_a)| &= |(\Omega_b(t)g_b, [\Omega_a(t) - \Omega_{a\pm}]f_a) \\ + ([\Omega_b(t) - \Omega_{b\pm}]g_b, \Omega_{a\pm}f_a)| &\leq ||g_b||\,||[\Omega_a(t) - \Omega_{a\pm}]f_a|| + ||[\Omega_b(t) - \Omega_{b\pm}]g_b||\,||f_a||. \end{aligned}\right\} \tag{2.3.18}$$

Since the right-hand side of this relation tends to 0 as t tends to $\mp\infty$, it follows that

$$(\Omega_{b\pm}g_b, \Omega_{a\pm}f_a) = \lim_{t\to\mp\infty} (\Omega_b(t)g_b, \Omega_a(t)f_a). \tag{2.3.19}$$

Hence, by the definition of $\Omega(t)$,

$$(\Omega_{b\pm}g_b, \Omega_{a\pm}f) = \lim_{t\to\mp\infty} (e^{-iH_bt}g_b, e^{-iH_at}f_a) = \lim_{t\to\mp\infty} (g_b, e^{-i(H_a-H_b)t}f_a), \tag{2.3.20}$$

where the third member is justified by the fact that H_a and H_b commute.

We must now distinguish two cases. Firstly the case that $H_a = H_b$. Then the right-hand side of eq. (2.3.20) vanishes because f_a and g_b are orthogonal (cf. the discussion at the end of section 2.3.1). Hence eq. (2.3.17) is satisfied. Secondly we consider the case that $H_a \neq H_b$. With the definition $H_a - H_b = K$, it is then a question of

$$\lim_{t\to\mp\infty} (g_b, e^{-iKt}f_a). \tag{2.3.21}$$

Now the quantity $(g_b,\exp(-iKt)f_a)$ is bounded, and it is known to tend to a limit as t tends to $\mp\infty$, by eq. (2.3.20). From this it follows that we must have

$$\lim_{t\to\mp\infty} (g_b, e^{-iKt}f_a) = \lim_{t\to\mp\infty} \frac{1}{t}\int_0^t (g_b, e^{-iKs}f_a)ds. \tag{2.3.22}$$

But, according to one of the ergodic theorems of VON NEUMANN (17), the right-hand side of eq. (2.3.22) is equal to (g_b,Pf_a), where P is the projection operator onto the subspace of $\mathfrak{L}^2$ spanned by the functions h with $\exp(-iKt)h = h$. These functions are eigenfunctions of K satisfying $Kh = 0$ (cf. the argument following eq. (2.2.21)). However, it is not difficult to see that K has no eigenfunctions in $\mathfrak{L}^2$. Hence P is in fact the zero operator. Thus the expression (2.3.21) vanishes, and eq. (2.3.17) is again satisfied. Taking into account that $\Omega^*_{b\pm}\Omega_{a\pm}f_a$ belongs to $\mathfrak{C}_b$, by eq. (2.2.11), it follows that

$$\Omega^*_{b\pm}\Omega_{a\pm}f_a = \delta_{ba}f_a. \tag{2.3.23}$$

This settles the orthogonality of the channels. It is not claimed that $\mathfrak{C}_a \perp \mathfrak{C}_b$ if $a \neq b$. As a matter of fact, a relation of this sort does in general not hold true, nor is there a reason why we should want it to be satisfied. Indeed, the functions f_a and g_b are only auxiliary quantities. What counts is the wave-function, which is of the form $\exp(-iHt)\Omega_{a+}f_a$. The crucial point is that this can be decomposed unambiguously into mutually orthogonal components corresponding to the various channels. The decomposition is brought about by the projection operators $\Omega_{b-}\Omega^*_{b-}$, which project onto the sets $\mathfrak{R}_{b-}$. The component corresponding to channel b is given by

$$\Omega_{b-}\Omega^*_{b-}e^{-iHt}\Omega_{a+}f_a = e^{-iHt}\Omega_{b-}\Omega^*_{b-}\Omega_{a+}f_a. \tag{2.3.24}$$

In fact, owing to the relation

$$\lim_{t\to\infty} ||e^{-iH_b t}\Omega^*_{b-}\Omega_{a+}f_a - e^{-iHt}\Omega_{b-}\Omega^*_{b-}\Omega_{a+}f_a|| = 0, \tag{2.3.25}$$

either side of eq. (2.3.24) tends to $\exp(-iH_b t)\Omega^*_{b-}\Omega_{a+}f_a$ as t tends to ∞. Otherwise stated, the component of $\exp(-iHt)\Omega_{a+}f_a$ which at $t = \infty$ will be in channel b is its projection onto $\mathfrak{R}_{b-}$. It follows from eq. (2.3.11) that the projection operator $\Omega_{b-}\Omega^*_{b-}$ commutes with $\exp(-iHt)$. This means that the decomposition according to channels does not depend on the time at which it is made. Also, it is unambiguous, in virtue of the orthogonality of the sets $\mathfrak{R}_{b-}$.

It is often convenient to write the wave-function $\exp(-iHt)\Omega_{a+}f_a$ as the sum of an incident wave plus a scattered wave, the latter taking the form

$$e^{-iHt}\Omega_{a+}f_a - e^{-iH_a t}f_a. \tag{2.3.26}$$

If the scattered wave is decomposed according to channels, it follows with eq. (2.3.11) that the probability of scattering into channel b is given by

$$||\Omega^*_{b-}(e^{-iHt}\Omega_{a+}f_a - e^{-iH_a t}f_a)||^2 = ||\Omega^*_{b-}(\Omega_{a+} - e^{iHt}e^{-iH_a t})f_a||^2. \tag{2.3.27}$$

If t tends to ∞, this tends to

$$||\Omega^*_{b-}(\Omega_{a+} - \Omega_{a-})f_a||^2 = ||(S_{ba} - \delta_{ba})f_a||^2. \tag{2.3.28}$$

2.3.4. Completeness of the channel description

Since the space $\mathfrak{L}^2$ is separable and the closed sets $\mathfrak{R}_{b\pm}$ are mutually orthogonal, the number of channels is finite or denumerably infinite. In the former case it is obvious that the operators $\sum_b \Omega_{b\pm}\Omega^*_{b\pm}$ are projections. In the latter case it can be shown that, if N tends to ∞, the sequences of projections $\sum_{b=1}^{N}\Omega_{b\pm}\Omega^*_{b\pm}$ tend to operators which are again projections. Indeed, according to Stone's (13) theorem 2.40, there exist projections $P_\pm$, which may be denoted by $\sum_b \Omega_{b\pm}\Omega^*_{b\pm}$, such that

$$\lim_{N\to\infty} ||\left[\sum_{b=1}^{N}\Omega_{b\pm}\Omega^*_{b\pm} - \sum_b \Omega_{b\pm}\Omega^*_{b\pm}\right]f|| = 0 \tag{2.3.29}$$

for every f in $\mathfrak{L}^2$. From this result it is obvious that

$$(g, \sum_b \Omega_{b\pm}\Omega^*_{b\pm}f) = \sum_b (g, \Omega_{b\pm}\Omega^*_{b\pm}f). \tag{2.3.30}$$

The ranges of the two limit-projections are the sets $\mathfrak{R}_\pm = \sum_b \oplus \mathfrak{R}_{b\pm}$, that is the closed sets determined by the sums $\mathfrak{R}_{1\pm} + \mathfrak{R}_{2\pm} + \ldots$. In other words,

$$\sum_b \Omega_{b\pm}\Omega^*_{b\pm} = P(\mathfrak{R}_\pm). \tag{2.3.31}$$

Now we expect on physical grounds that, if b runs through all channels,

$$\sum_b \Omega_{b-}\Omega_{b-}^{*}\Omega_{a+}f_a = \Omega_{a+}f_a, \tag{2.3.32}$$

so that $\Omega_{a+}f_a$ does not have components which do not correspond to some channel b. Since $\Omega_{a+}f_a$ runs through $\Re_{a+}$ when f_a runs through $\mathfrak{C}_a$, it is clear that, for eq. (2.3.32) to be satisfied for every f_a in $\mathfrak{C}_a$, it is necessary that

$$\Re_{a+} \subseteq \Re_{-}. \tag{2.3.33}$$

On the other hand, in order that every function of the form $\exp(-iH_at)f_a$ can be realized as the result of a scattering event, we must have

$$\Re_{+} \supseteq \Re_{a-}. \tag{2.3.34}$$

Hence, combining eqs. (2.3.33) and (2.3.34), we expect that

$$\Re_{+} = \Re_{-}. \tag{2.3.35}$$

This is a generalization of eq. (2.2.35).

It is not known at present if this relation holds true in practical cases. There is no reason to believe that it does not. But only in one fairly special multi-channel example has it been possible to check it (18, 19). For the general case of a system of n particles with two-body interactions depending only on the distances between the particles, no methods for investigating this problem seem to be known.

2.3.5. Unitarity

In the multi-channel case there is a connection between the relation (2.3.35) and unitarity in the following sense. Let $\mathfrak{H}$ be the set of all column-matrices $f = \{f_a\}$ which have a function $f_a \in \mathfrak{C}_a$ in row a, with $\sum_a ||f_a||^2 < \infty$. If the inner product is defined by

$$(g,f) = \sum_a (g_a, f_a), \tag{2.3.36}$$

and if addition and multiplication by a constant are defined in the natural way, $\mathfrak{H}$ is a Hilbert space. We now consider the operator-matrix $\mathcal{S}$ which transforms $\{f_a\}$ according to

$$\mathcal{S}\{f_a\} = \{\sum_b S_{ab}f_b\} = \{\sum_b \Omega_{a-}^{*}\Omega_{b+}f_b\}. \tag{2.3.37}$$

In case the number of channels is infinite, there is a convergence problem involved in this equation. However, in virtue of eqs. (2.3.17) and (2.3.9),

$$||\sum_{b=M}^{N} \Omega_{b+}f_b||^2 = \sum_{b=M}^{N} ||\Omega_{b+}f_b||^2 = \sum_{b=M}^{N} ||f_b||^2. \tag{2.3.38}$$

If M and N tend to ∞, this tends to 0, by the assumption that $\sum_a ||f_a||^2$ converges. Hence the quantity $\sum_{b=1}^{N} \Omega_{b+} f_b$ tends in mean to a function in $\mathfrak{L}^2$, which we denote by $\sum_b \Omega_{b+} f_b$. Applying the operator Ω_{a-}^* to this function, we obtain a function in $\mathfrak{C}_a$ (cf. the discussion following eq. (2.2.11)). Also, since Ω_{a-}^* is bounded and therefore continuous,

$$\Omega_{a-}^* \sum_b \Omega_{b+} f_b = \underset{N\to\infty}{\text{l.i.m.}} \sum_{b=1}^{N} \Omega_{a-}^* \Omega_{b+} f_b = \sum_b \Omega_{a-}^* \Omega_{b+} f_b . \tag{2.3.39}$$

This defines the third member of eq. (2.3.37) for the case of an infinite number of channels. It follows that in this expression the function in row a belongs to $\mathfrak{C}_a$.

As regards the norm of $\mathcal{S}f$ we have

$$\left.\begin{aligned} (\mathcal{S}f, \mathcal{S}f) &= \sum_b \Big(\Omega_{b-}^* \sum_c \Omega_{c+} f_c , \Omega_{b-}^* \sum_a \Omega_{a+} f_a \Big) \\ &= \Big(\sum_c \Omega_{c+} f_c , P(\mathfrak{R}_-) \sum_a \Omega_{a+} f_a \Big) \leq \Big|\Big| \sum_a \Omega_{a+} f_a \Big|\Big|^2 = \sum_a ||f_a||^2 < \infty . \end{aligned}\right\} \tag{2.3.40}$$

Hence $\mathcal{S}$ is a bounded operator in $\mathfrak{H}$.

In the above argument the sign of equality applies if and only if the relation (2.3.33) holds true for every a. In this case we have

$$(\mathcal{S}g, \mathcal{S}f) = \Big(\sum_c \Omega_{c+} g_c , \sum_a \Omega_{a+} f_a \Big) = \sum_a (g_a, f_a) = (g, f), \tag{2.3.41}$$

which is equivalent to $\mathcal{S}^* \mathcal{S} = \mathcal{J}$, $\mathcal{J}$ denoting the unit matrix.

The adjoint operator $\mathcal{S}^*$ satisfies

$$(\mathcal{S}^* g, f) = (g, \mathcal{S}f) = \sum_a \Big(g_a , \sum_b \Omega_{a-}^* \Omega_{b+} f_b \Big). \tag{2.3.42}$$

This can easily be transformed into

$$(\mathcal{S}^* g, f) = \sum_b \Big(\Omega_{b+}^* \sum_a \Omega_{a-} g_a , f_b \Big), \tag{2.3.43}$$

from which it follows that

$$(\mathcal{S}^* g, \mathcal{S}^* f) = \sum_b \Big(\Omega_{b+}^* \sum_a \Omega_{a-} g_a , \Omega_{b+}^* \sum_c \Omega_{c-} f_c \Big). \tag{2.3.44}$$

Hence we obtain

$$(\mathcal{S}^* g, \mathcal{S}^* f) = \Big(\sum_a \Omega_{a-} g_a , \sum_c \Omega_{c-} f_c \Big) = \sum_a (g_a, f_a) = (g, f) \tag{2.3.45}$$

if and only if eq. (2.3.34) holds true for every a. Summarizing, the unitarity relations $\mathcal{S}^* \mathcal{S} = \mathcal{J}$ and $\mathcal{S}\mathcal{S}^* = \mathcal{J}$ are satisfied if and only if eq. (2.3.35) is fulfilled.

To avoid confusion, we remark that the matrix $\mathcal{S}$ does not occur in Jauch's paper (3). In particular, it is not the quantity JAUCH denotes by S. Although there is a certain analogy between the present $\mathcal{S}$-matrix and the operator S discussed in

sections 2.2.4 and 2.2.5, it must be observed that there does not seem to be a sensible way of writing $\mathcal{S}$ as the product of a matrix Ω_-^* times a matrix Ω_+ in such a way that the Ω-matrices are limits of suitable time-dependent matrices which involve Hamiltonians.

2.3.6. Conjugation and symmetry

For the systems in which we are interested in the present paper, the relations (2.3.33) and (2.3.34) are not independent. This is due to the fact that there is an operator of conjugation C,

$$(Cg, Cf) = (f, g), \qquad C^2 f = f, \tag{2.3.46}$$

such that

$$CHf = HCf \qquad CH_a f = H_a C f \tag{2.3.47}$$

for every f in $\mathfrak{D}(H)$, or every f in $\mathfrak{D}(H_a)$, as the case may be. Indeed, if C is defined by the relation $Cf(\boldsymbol{x}) = \bar{f}(\boldsymbol{x})$ for every f in $\mathfrak{L}^2$, then eqs. (2.3.46) and (2.3.47) are satisfied.

It follows from eq. (2.3.47) that

$$R(\lambda) = CR(\bar{\lambda})C \tag{2.3.48}$$

(Achieser and Glasmann (14) section 45). Hence, if f and g are any two functions in $\mathfrak{L}^2$, eq. (1.4.28) yields

$$\left.\begin{aligned}(g, Ce^{iHt}f) = (e^{iHt}f, Cg) &= -\frac{1}{2\pi i}\lim_{U_\pm \to \pm\infty}\lim_{\zeta \to 0}\int_{U_-}^{U_+} e^{-iut}([R(u+i\zeta) - R(u-i\zeta)]f, Cg)du \\ &= \frac{1}{2\pi i}\lim_{U_\pm \to \pm\infty}\lim_{\zeta \to 0}\int_{U_-}^{U_+} e^{-iut}(g, [R(u+i\zeta) - R(u-i\zeta)]Cf)du = (g, e^{-iHt}Cf).\end{aligned}\right\} \tag{2.3.49}$$

Since in this relation f and g are arbitrary,

$$Ce^{iHt} = e^{-iHt}C. \tag{2.3.50}$$

Now let g be any function in $\mathfrak{R}_{a+}$. Then there is a function f_a in $\mathfrak{C}_a$ such that

$$\lim_{t \to -\infty} ||g - e^{iHt}e^{-iH_a t}f_a|| = 0. \tag{2.3.51}$$

But from this it follows that

$$\lim_{t \to \infty} ||Cg - e^{iHt}e^{-iH_a t}Cf_a|| = 0. \tag{2.3.52}$$

Hence, if g belongs to $\mathfrak{R}_{a+}$, then Cg belongs to $\mathfrak{R}_-$. More generally, if g belongs to $\mathfrak{R}_+$, then Cg belongs to $\mathfrak{R}_-$, and vice versa.

Let us now assume that eq. (2.3.33) holds true for every a. Then, if g belongs

to $\mathfrak{R}_+$, it also belongs to $\mathfrak{R}_-$. We know already that, if h is any function in $\mathfrak{R}_-$, the function Ch belongs to $\mathfrak{R}_+$. If eq. (2.3.33) is satisfied, it follows that Ch also belongs to $\mathfrak{R}_-$. Hence h belongs to $\mathfrak{R}_+$. But this means that $\mathfrak{R}_- \subseteq \mathfrak{R}_+$, i. e. that eq. (2.3.34) holds true. We thus see that in problems which admit a conjugation, eq. (2.3.34) is a consequence of eq. (2.3.33). Conversely, eq. (2.3.33) is a consequence of eq. (2.3.34).

If channel a is not degenerate, it follows unambiguously from eq. (2.3.52) that

$$C\Omega_{a+}f_a = \Omega_{a-}Cf_a. \tag{2.3.53}$$

If there are degenerate channels $a,b,\ldots$ with $H_a = H_b = \ldots$, the function Cf_a does not necessarily belong to $\mathfrak{C}_a$. However, by an appropriate choice of the channels, there will in many cases be pairs of channels a,a', with $H_a = H_{a'}$, such that the conjugation C transforms a function f_a in $\mathfrak{C}_a$ into a function in $\mathfrak{C}_{a'}$, a function $f_{a'}$ in $\mathfrak{C}_{a'}$ into a function in $\mathfrak{C}_a$. If this is so, we have

$$C\Omega_{a\pm}f_a = \Omega_{a'\mp}Cf_a, \qquad C\Omega_{a'\pm}f_{a'} = \Omega_{a\mp}Cf_{a'}. \tag{2.3.54}$$

In the matrix notation of the previous section we now define

$$\mathscr{C}f = \mathscr{C}\{f_a\} = \{Cf_{a'}\}. \tag{2.3.55}$$

After some rearrangements this yields

$$\left.\begin{aligned} (g, \mathscr{C}\mathscr{S}^*\mathscr{C}f) = (\mathscr{C}f, \mathscr{S}\mathscr{C}g) = \sum_{a,b}(Cf_{a'}, \Omega^*_{a-}\Omega_{b+}Cg_{b'}) \\ = \sum_{a,b}(C\Omega_{b+}Cg_{b'}, C\Omega_{a-}Cf_{a'}) = \sum_{a,b}(g_{b'}, \Omega^*_{b'-}\Omega_{a'+}f_{a'}) = (g, \mathscr{S}f). \end{aligned}\right\} \tag{2.3.56}$$

It is appropriate to call $\mathscr{C}\mathscr{S}^*\mathscr{C}$ the transpose of $\mathscr{S}$. In this sense we can say that the transpose of $\mathscr{S}$ is equal to $\mathscr{S}$, hence that $\mathscr{S}$ is symmetric with respect to the conjugation $\mathscr{C}$.

2.3.7. The optical theorem

For future reference we want to say a few words about the optical theorem and its connection with the unitarity of the S-operator (cf. Messiah (20) ch. XIX, section 31). In its simplest form, the optical theorem gives a relation between the total intensity scattered from any particular channel, and the amplitude for scattering into the channel itself. In the one-channel case, one usually argues as follows.

In the Schrödinger representation the scattered wave has the form

$$e^{-iHt}\Omega_+ f - e^{-iH_0t}f. \tag{2.3.57}$$

In the interaction representation it is

$$e^{iH_0t}e^{-iHt}\Omega_+ f - f. \tag{2.3.58}$$

As t tends to ∞, this is supposed to tend to

$$\underset{t\to\infty}{\text{l.i.m.}}\, e^{iH_0t}e^{-iHt}\Omega_+f - f = \Omega_-^{\ast}\Omega_+f - f = Sf - f, \tag{2.3.59}$$

a relation which in fact only holds true if $\mathfrak{R}_- \supseteq \mathfrak{R}_+$. Now if $S^*S = 1$,

$$||[S-1]f||^2 = ||Sf||^2 + ||f||^2 - (Sf,f) - (f,Sf) = 2\mathrm{Re}(f,[1-S]f). \tag{2.3.60}$$

Hence one expects that, as t tends to ∞, the intensity of the scattered wave tends to the right-hand side of eq. (2.3.60). If this is confirmed by experiments, it might be taken to indicate that $S^*S = 1$, hence that $\mathfrak{R}_- \supseteq \mathfrak{R}_+$. But such a conclusion would be premature. For what one observes experimentally is the intensity at a very large but finite time t. This is

$$||e^{-iHt}\Omega_+f - e^{-iH_0t}f||^2 = ||\Omega_+f - e^{iHt}e^{-iH_0t}f||^2. \tag{2.3.61}$$

If t tends to ∞, the intensity tends to

$$||\Omega_+f - \Omega_-f||^2 = 2||f||^2 - (\Omega_+f,\Omega_-f) - (\Omega_-f,\Omega_+f) = 2\mathrm{Re}(f,[1-S]f). \tag{2.3.62}$$

Hence there is a limit of the form (2.3.62) irrespective as to whether S is unitary.

In obtaining this result, the crucial point is that the intensity is determined first, the limit next. This corresponds to the experimental situation. In a multi-channel problem, it is in general not even possible to determine the limit first. For the quantity

$$e^{iH_at}e^{-iHt}\Omega_{a+}f_a - f_a \tag{2.3.63}$$

does in general not tend to a limit. Hence there is no multi-channel analogue to eq. (2.3.59). At the same time, the intensity of the wave scattered from channel a is given by

$$||e^{-iHt}\Omega_{a+}f_a - e^{-iH_at}f_a||^2 = ||\Omega_{a+}f_a - e^{iHt}e^{-iH_at}f_a||^2. \tag{2.3.64}$$

If t tends to ∞, this tends to

$$||\Omega_{a+}f_a - \Omega_{a-}f_a||^2 = 2\mathrm{Re}(f_a,[1-S_{aa}]f_a), \tag{2.3.65}$$

analogously to eq. (2.3.62).

With the methods of section 2.3.4, it is easily checked that

$$\sum_b ||(S_{ba}-\delta_{ba})f_a||^2 = 2\mathrm{Re}(f_a,[1-S_{aa}]f_a) \tag{2.3.66}$$

if and only if $\mathfrak{R}_- \supseteq \mathfrak{R}_{a+}$. Hence it is only under this condition that the total scattering intensity is the sum of the intensities scattered into the separate channels. If eq. (2.3.66) holds true for every a, we have

$$||[\mathcal{S}-\mathcal{J}]f||^2 = 2\mathrm{Re}\big(f,[\mathcal{J}-\mathcal{S}]f\big). \tag{2.3.67}$$

This is the multi-channel analogue of eq. (2.3.60). It is the point of the present section that in this expression it is the right-hand side which is simply related to the total scattering intensity, rather than the left-hand side, as one might be inclined to think.

It is shown in section 2.8.9 how in special cases the intensity of the scattered wave is connected with the forward scattering amplitude.

2.4. The existence of the wave-operators

2.4.1. A general condition

For the remaining part of the present investigation, we restrict ourselves explicitly to the class of n-particle systems described in section 2.1.2. For this class we first find sufficient conditions on the interaction under which there exist wave-operators. The method for obtaining such conditions is mainly due to JAUCH and ZINNES (5). However, because we have restricted ourselves from the outset to interactions satisfying eq. (2.1.5), we need only a simplified version of the argument of these authors.

Let us observe first of all that, if we want to show that there is a limit of the form (2.3.2) for all functions f_a in a certain closed set $\mathfrak{C}_a$, it suffices to check the existence of the limit for the functions f_a in a set $\mathfrak{C}'_a$ which is everywhere dense in $\mathfrak{C}_a$. The result for the closed set $\mathfrak{C}_a$ then follows with the reasoning given in section 2.2.1. It also follows from that section that it is in fact sufficient to show that, for every f_a in $\mathfrak{C}'_a$ and every positive δ, there is a number T such that

$$||\Omega_a(s)f_a - \Omega_a(t)f_a|| < \delta \qquad (s,t < -T; s,t > T). \tag{2.4.1}$$

Here T may depend on f_a.

Let us now imagine that we want to establish eq. (2.4.1) for a function f_a in $\mathfrak{D}(H_0)$. If f_a belongs to $\mathfrak{D}(H_0)$, so does $\exp(-iH_at)f_a$, since H_a commutes with H_0. The function $\exp(-iH_at)f_a$ then also belongs to $\mathfrak{D}(H)$, by eq. (2.1.5). Owing to this, we have

$$\lim_{\tau \to 0} ||\frac{1}{\tau}[e^{iH(t+\tau)}e^{-iH_a(t+\tau)} - e^{iHt}e^{-iH_at}]f_a - ie^{iHt}(H - H_a)e^{-iH_at}f_a|| = 0 \tag{2.4.2}$$

(RIESZ and SZ.-NAGY (11) section 137). Hence, for every g in $\mathfrak{L}^2$,

$$\frac{d}{dt}(g, \Omega_a(t)f_a) = i(g, e^{iHt}[H - H_a]e^{-iH_at}f_a), \tag{2.4.3}$$

$$(g, [\Omega_a(t) - \Omega_a(s)]f_a) = i\int_s^t (g, e^{iHu}[H - H_a]e^{-iH_au}f_a)du. \tag{2.4.4}$$

The particular choice $g = [\Omega_a(t) - \Omega_a(s)]f_a$ yields

$$\left.\begin{aligned} ||[\Omega_a(t) - \Omega_a(s)]f_a||^2 &= \int_s^t du \int_s^t dv (e^{iHv}[H - H_a]e^{-iH_a v} f_a, e^{iHu}[H - H_a]e^{-iH_a u} f_a) \\ &< \left[\int_s^t ||(H - H_a)e^{-iH_a u} f_a|| du\right]^2. \end{aligned}\right\} \tag{2.4.5}$$

Hence, if f_a belongs to $\mathfrak{D}(H_0)$, a sufficient condition for eq. (2.4.1) to be satisfied is

$$\int_{-\infty}^{\infty} ||(H - H_a)e^{-iH_a t} f_a|| dt < \infty. \tag{2.4.6}$$

2.4.2. Sufficient conditions on the interaction

Using the notation of section 2.3.1, we proceed to derive sufficient conditions on the functions V_{ij} under which eq. (2.4.6) is satisfied for a suitable set of functions f_a. For the Hamiltonian H we write

$$H = \sum_{j=1}^{m'} H_{(j)}(\boldsymbol{x}_j) + H_a(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}) - \lambda_a + \sum_{p,q} V_{pq}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{2m-1}). \tag{2.4.7}$$

We recall that m denotes the number of fragments into which the system is split when it is in channel a. The operators $H_{(j)}(\boldsymbol{x}_j)$ are the Hamiltonians of the m' fragments which consist of at least two particles each. The symbol $H_a(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$ stands for the operator H_a defined in section 2.3.1. From the meaning of the various quantities involved it is obvious that the summation with respect to p and q must include only interactions between particles belonging to different fragments.

Let us now consider a particular term V_{pq}. In general, this depends on $\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}$. On the other hand, as regards the coordinates $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{m'}$ it depends only on the internal coordinates of the fragments to which the particles p and q belong. Let us denote these by $\boldsymbol{x}_{j(p)}$ and $\boldsymbol{x}_{j(q)}$. Furthermore, let us recall that, if fragment $j(p)$ consists of $n_{j(p)}$ particles, the coordinate $\boldsymbol{x}_{j(p)}$ has $n_{j(p)} - 1$ three-dimensional components. If these are denoted by $\boldsymbol{x}_{j(p),r}$, the corresponding components of $\boldsymbol{x}_{j(q)}$ by $\boldsymbol{x}_{j(q),s}$, the function V_{pq} in question is of the form

$$V_{pq}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{2m-1}) = V_{pq}\left(\sum_r d_r \boldsymbol{x}_{j(p),r} + \sum_s d_s \boldsymbol{x}_{j(q),s} + \sum_{j=m+1}^{2m-1} c_j \boldsymbol{x}_j\right). \tag{2.4.8}$$

Here it will be understood that, if fragment $j(p)$ consists of only one particle, the term with $\boldsymbol{x}_{j(p)}$ may simply be dropped from eq. (2.4.8).

It is an essential point that at least one of the constants c_j does not vanish. If in particular $c_h \neq 0$, it is convenient to write symbolically

$$V_{pq}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{2m-1}) = V_{pq}(c\boldsymbol{x}_h + d\boldsymbol{x}_{j \neq h}) \qquad (m+1 \leq h \leq 2m-1). \tag{2.4.9}$$

In the following the quantity $|\boldsymbol{x}_h|$ is denoted by x_h, and similarly for other vectors.

We now study the integral (2.4.6) for functions of the general product-form given by eq. (2.3.4). In line with the previous section, we restrict the function $f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$ of eq. (2.3.4) to the set $\mathfrak{E}$ consisting of all linear combinations of functions

$$f_{\boldsymbol{y}}(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}) = \prod_{j=m+1}^{2m-1} f_{\boldsymbol{y}_j}(\boldsymbol{x}_j) \tag{2.4.10}$$

the Fourier transforms of which are of the form

$$\prod_{j=m+1}^{2m-1} \hat{f}_{\boldsymbol{y}_j}(\boldsymbol{k}_j) = \prod_{j=m+1}^{2m-1} [k_{j1} k_{j2} k_{j3} \exp(-k_j^2 - i\boldsymbol{k}_j \cdot \boldsymbol{y}_j)]. \tag{2.4.11}$$

In this expression k_{j1}, k_{j2}, k_{j3} are the three components of the vector $\boldsymbol{k}_j$. The symbol k_j stands for $|\boldsymbol{k}_j|$. The vector $\boldsymbol{y}_j$ is a parameter the three components of which may take any finite values. With a view to one-channel scattering, the set of functions $\mathfrak{E}$ was introduced by KURODA (6). It follows from Wiener's theorem on the closure of the translations of a function in $\mathfrak{L}^2$ that $\mathfrak{E}$ is dense in the space $\mathfrak{L}^2(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$ (WIENER (21) section 15). More precisely, given a function $f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$ in $\mathfrak{L}^2$ and a positive δ, there is an integer A, a set of constants a_α and a set of vectors $\boldsymbol{y}(\alpha)$ such that

$$||f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}) - \sum_{\alpha=1}^{A} a_\alpha f_{\boldsymbol{y}(\alpha)}(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})|| < \delta. \tag{2.4.12}$$

It is obvious that all functions in $\mathfrak{E}$ belong to $\mathfrak{D}\big(H_0(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})\big)$. Furthermore, since $\varphi_{(j)}(\boldsymbol{x}_j)$ is an eigenfunction of $H_{(j)}(\boldsymbol{x}_j)$, it belongs to $\mathfrak{D}\big(H_{(j)}(\boldsymbol{x}_j)\big)$. Hence, by the assumption that eq. (2.1.5) is satisfied, it belongs to $\mathfrak{D}\big(H_0(\boldsymbol{x}_j)\big)$. From this it is easily seen that, if f_a is equal to $\prod_{j=1}^{m'} \varphi_{(j)}(\boldsymbol{x}_j)$ times a function in $\mathfrak{E}$, it belongs to $\mathfrak{D}\big(H_0(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{m'}, \boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})\big)$. In other words, all the functions f_a we consider in the present context belong to $\mathfrak{D}(H_0)$. They can therefore be used in the argument of the previous section.

Owing to our particular choice for the functions f_a, the study of eq. (2.4.6) reduces to a study of expressions of the form

$$\int_{-\infty}^{\infty} ||V_{pq}(c\boldsymbol{x}_h + d\boldsymbol{x}_{j \neq h}) \prod_{j=1}^{m'} \varphi_{(j)}(\boldsymbol{x}_j) \prod_{j=m+1}^{2m-1} [\exp[i\Delta(\boldsymbol{x}_j)t] f_{\boldsymbol{y}_j}(\boldsymbol{x}_j)]||dt. \tag{2.4.13}$$

If these are finite, it follows that there exist wave-operators $\Omega_{a\pm}$, the closed sets $\mathfrak{C}_a$ containing all functions of the form (2.3.4), where now $f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$ may be any square-integrable function of its arguments.

With eq. (2.4.11) it is not difficult to evaluate $\exp[i\Delta(\boldsymbol{x}_j)t] f_{\boldsymbol{y}_j}(\boldsymbol{x}_j)$ explicitly. This was done by KURODA (6), who showed that

$$|\exp[i\Delta(\boldsymbol{x}_j)t] f_{\boldsymbol{y}_j}(\boldsymbol{x}_j)| < \text{const.} \frac{|\boldsymbol{x}_j - \boldsymbol{y}_j|^3}{(1+t^2)^{\frac{9}{4}}} \exp\left[-\frac{|\boldsymbol{x}_j - \boldsymbol{y}_j|^2}{4(1+t^2)}\right]. \tag{2.4.14}$$

From this it follows that, if ζ is in the interval $0 < \zeta < 1$, we may write

$$|\exp[iA(\boldsymbol{x}_j)t]f_{\boldsymbol{y}_j}(\boldsymbol{x}_j)| < \text{const.}(1+t^2)^{-\frac{1}{2}-\frac{1}{4}\zeta}(1+|c\boldsymbol{x}_j - c\boldsymbol{y}_j|)^{-\frac{1}{2}+\frac{1}{2}\zeta}, \qquad (2.4.15)$$

c being the constant used in eqs. (2.4.9) and (2.4.13).

Let us now assume that there is a ζ with $0 < \zeta < 1$ such that

$$\iiint |V_{pq}(c\boldsymbol{x}_h + d\boldsymbol{x}_{j\neq h})\varphi_{(j(p))}(\boldsymbol{x}_{j(p)})\varphi_{(j(q))}(\boldsymbol{x}_{j(q)})|^2(1+|c\boldsymbol{x}_h - c\boldsymbol{y}_h|)^{-1+\zeta}d\boldsymbol{x}_{j(p)}d\boldsymbol{x}_{j(q)}d\boldsymbol{x}_h < M(\boldsymbol{y}_h), \qquad (2.4.16)$$

where $M(\boldsymbol{y}_h)$ is finite for every finite $\boldsymbol{y}_h$, and independent of the coordinates $\boldsymbol{x}_j$ on which the integral on the left may still depend. In evaluating the norm in eq. (2.4.13), it is then convenient to perform the integrations with respect to $\boldsymbol{x}_{j(p)}, \boldsymbol{x}_{j(q)}$, and $\boldsymbol{x}_h$ first. In an obvious notation, this yields

$$\left.\begin{aligned} &||V_{pq}(c\boldsymbol{x}_h + d\boldsymbol{x}_{j\neq h})\prod_{j=1}^{m'}\varphi_{(j)}(\boldsymbol{x}_j)\prod_{j=m+1}^{2m-1}[\exp[iA(\boldsymbol{x}_j)t]f_{\boldsymbol{y}_j}(\boldsymbol{x}_j)]||_{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_{m'},\boldsymbol{x}_{m+1},\ldots,\boldsymbol{x}_{2m-1}} \\ &\quad < \text{const.}[M(\boldsymbol{y}_h)]^{\frac{1}{2}}(1+t^2)^{-\frac{1}{2}-\frac{1}{4}\zeta}\prod_{\substack{j=1\\ j\neq j(p),\,j(q)}}^{m'}{}'||\varphi_{(j)}(\boldsymbol{x}_j)||_{\boldsymbol{x}_j}\prod_{\substack{j=m+1\\ j\neq h}}^{2m-1}{}'||f_{\boldsymbol{y}_j}(\boldsymbol{x}_j)||_{\boldsymbol{x}_j}. \end{aligned}\right\} \qquad (2.4.17)$$

Hence in eq. (2.4.13) the integral with respect to t converges. From this it follows that there exist wave-operators $\Omega_{a\pm}$ whenever eqs. (2.4.16) and (2.1.5) are satisfied.

In obtaining this result, it was tacitly assumed that the fragments $j(p)$ and $j(q)$ consist of at least two particles each. If this is not so, we simply omit, say, $\varphi_{(j(p))}(\boldsymbol{x}_{j(p)})$ and the integration with respect to $\boldsymbol{x}_{j(p)}$ from eq. (2.4.16), and the argument can be carried through essentially unchanged.

In the case of scattering of only two fragments, $\boldsymbol{x}_h$ must necessarily be $\boldsymbol{x}_3$. There is no coordinate $\boldsymbol{x}_j$ on which the integral in eq. (2.4.16) might depend. Now for $\boldsymbol{y}_3 = 0$, the condition (2.4.16) implies

$$\iiint |V_{pq}(\sum_r d_r\boldsymbol{x}_{1,r} + \sum_s d_s\boldsymbol{x}_{2,s} + c_3\boldsymbol{x}_3)\varphi_{(1)}(\boldsymbol{x}_1)\varphi_{(2)}(\boldsymbol{x}_2)|^2(1+|c_3|x_3)^{-1+\zeta}d\boldsymbol{x}_1\,d\boldsymbol{x}_2\,d\boldsymbol{x}_3 < M. \qquad (2.4.18)$$

If this holds true, it follows from the inequality

$$(1+|c_3\boldsymbol{x}_3 - c_3\boldsymbol{y}_3|)^{-1+\zeta} < (1+|c_3|x_3)^{-1+\zeta}(1+|c_3|y_3)^{1-\zeta} \qquad (2.4.19)$$

that eq. (2.4.16) is also satisfied for general vectors $\boldsymbol{y}_3$, with

$$M(\boldsymbol{y}_3) = M(1+|c_3|y_3)^{1-\zeta}. \qquad (2.4.20)$$

It is true that $M(\boldsymbol{y}_3)$ is not bounded uniformly in y_3, but this does not matter. For in using functions $f_{\boldsymbol{y}}(\boldsymbol{x})$ according to eq. (2.4.12), we can always restrict ourselves to a finite number of bounded vectors $\boldsymbol{y}_3$. Hence for two-fragment channels the simplified equation (2.4.18) already gives a sufficient condition for the existence of wave-operators.

In scattering problems in which three or more fragments are involved, V_{pq} depends in general not only on $\boldsymbol{x}_h$, but also on one or more of the remaining vectors $\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}$. Then the condition that there must be a bound $M(\boldsymbol{y}_h)$ independent of $\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}$ becomes significant. It implies in fact that $M(\boldsymbol{y}_h)$ must be independent of $\boldsymbol{y}_h$. Conversely, if $M(\boldsymbol{y}_h)$ is independent of $\boldsymbol{y}_h$, it follows that it cannot depend on any $\boldsymbol{x}_j$ either. It is therefore convenient to demand simply that eq. (2.4.16) be satisfied by a constant $M = M(\boldsymbol{y}_h)$.

For eq. (2.4.16) to hold true it is obviously sufficient if

$$\int [V_{pq}(\boldsymbol{X})]^2 (1 + |\boldsymbol{X} - \boldsymbol{Y}|)^{-1+\zeta} d^3\boldsymbol{X} < \text{const.} \tag{2.4.21}$$

for some ζ with $0 < \zeta < 1$, and every $\boldsymbol{Y}$. We recall that a relation of this form was already discussed at the end of section 2.1.2 in connection with the Hamiltonian being self-adjoint. It is clearly fulfilled if $V_{pq}(\boldsymbol{X})$ belongs to $\mathfrak{L}^2(\boldsymbol{X})$. More generally, for eq. (2.4.21) to hold true it is sufficient if there are positive constants R and η such that

$$\int\limits_{X \leq R} [V_{pq}(\boldsymbol{X})]^2 d^3\boldsymbol{X} < \infty, \quad |V_{pq}(\boldsymbol{X})| < \text{const.} X^{-1-\eta} \qquad (X > R). \tag{2.4.22}$$

If $\eta > \frac{1}{2}$, eq. (2.4.22) implies that $V_{pq}(\boldsymbol{X})$ belongs to $\mathfrak{L}^2(\boldsymbol{X})$. If $0 < \eta \leq \frac{1}{2}$, it is convenient to choose in eq. (2.4.21) $\zeta = \eta$. It is then a question of

$$\int\limits_{X \leq R} [V_{pq}(\boldsymbol{X})]^2 (1 + |\boldsymbol{X} - \boldsymbol{Y}|)^{-1+\eta} d^3\boldsymbol{X} + \text{const.} \int\limits_{X \geq R} X^{-2-2\eta} (1 + |\boldsymbol{X} - \boldsymbol{Y}|)^{-1+\eta} d^3\boldsymbol{X}, \tag{2.4.23}$$

which is bounded uniformly in $\boldsymbol{Y}$ in virtue of Hölder's inequality (Burkill (22) section 5.6). Hence, roughly speaking, it is sufficient if V_{pq} is locally square-integrable and falls off more rapidly than the Coulomb interaction. This is a generalization of the multi-channel result due to Hack (23), according to which it is sufficient if V_{pq} is square-integrable.

As for the scattering of two particles without internal coordinates, it is sufficient if

$$\int [V_{pq}(\boldsymbol{X})]^2 (1 + X)^{-1+\zeta} d^3\boldsymbol{X} < \infty \tag{2.4.24}$$

for some ζ with $0 < \zeta < 1$. This condition was found by Kuroda (6). It is a special case of eq. (2.4.18).

2.4.3. The set of asymptotic wave-functions

It follows from the previous section that, if the interaction satisfies suitable conditions, there exist wave-operators $\Omega_{a\pm}$. The set $\mathfrak{C}_a$ of asymptotic wave-functions f_a contains all functions of the form (2.3.4), where $f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$ may be any square-integrable function of its arguments. Under the assumption that

$$\int [V_{pq}(\boldsymbol{X})]^2(1 + |\boldsymbol{X} - \boldsymbol{Y}|)^{-3+\zeta} d^3\boldsymbol{X} < \text{const.} \tag{2.4.25}$$

for some positive ζ, uniformly in $\boldsymbol{Y}$, we now show that $\mathfrak{C}_a$ is not larger than the set of wave-functions of the form (2.3.4). The assumption (2.4.25) is very mild. Indeed, it is satisfied whenever $V_{pq}(\boldsymbol{X})$ is locally square-integrable and of the order $O(X^{-\eta})$ as X tends to ∞, with some positive η. It is much less stringent than the condition (2.4.21) for the existence of the wave-operators $\Omega_{a\pm}$. In the course of this section it will become clear that, if the operator $H'_a(\boldsymbol{x})$ is restricted to the general form (2.3.1), with some real λ_a, there are not more channels than we have considered thus far.

To prove our assertion, it is sufficient to show that, if f_a belongs to $\mathfrak{C}_a$ and to $\mathfrak{D}(H_0)$, $E_a(l)f_a$ is of the form (2.3.4) for every real l, $E_a(l)$ denoting the resolution of the identity associated with H_a. Now if f_a belongs to $\mathfrak{C}_a$, so does $H_aE_a(l)f_a$, by the end of section 2.2.3. Hence

$$\lim_{t \to \mp\infty} ||(H\Omega_{a\pm} - e^{iHt}e^{-iH_at}H_a)E_a(l)f_a|| = 0, \tag{2.4.26}$$

owing to eq. (2.2.30). Also, if R stands for the resolvent of H, the operator $R(\mu)H$ is bounded whenever μ is not real. Therefore

$$\lim_{t \to \mp\infty} ||R(\mu)H(\Omega_{a\pm} - e^{iHt}e^{-iH_at})E_a(l)f_a|| = 0. \tag{2.4.27}$$

Combining this with the previous equation yields

$$\lim_{t \to \mp\infty} ||R(\mu)e^{iHt}(H - H_a)e^{-iH_at}E_a(l)f_a|| = 0. \tag{2.4.28}$$

Hence, in view of eq. (2.4.7) and the fact that f_a belongs to $\mathfrak{D}(H_0)$,

$$\lim_{t \to \mp\infty} ||R(\mu)\left[\sum_{j=1}^{m'} H_{(j)}(\boldsymbol{x}_j) - \lambda_a + \sum_{p,q} V_{pq}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{2m-1})\right]e^{-iH_at}E_a(l)f_a|| = 0. \tag{2.4.29}$$

Using the symbolic notation of eq. (2.4.9), we now show that

$$\lim_{t \to \mp\infty} ||R(\mu)V_{pq}(c\boldsymbol{x}_h + d\boldsymbol{x}_{j \neq h})e^{-iH_at}E_a(l)f_a|| = 0. \tag{2.4.30}$$

Since $R(\mu)V_{pq}$ is a bounded operator, by eqs. (2.1.4) and (2.1.5), it is sufficient to prove that there is a set of functions f in $\mathfrak{D}(H_0)$ which is dense in $\mathfrak{L}^2$ and such that

$$\lim_{t \to \mp\infty} ||R(\mu)V_{pq}(c\boldsymbol{x}_h + d\boldsymbol{x}_{j \neq h})e^{-iH_at}f|| = 0 \tag{2.4.31}$$

for every f in the set. Let us therefore consider the set consisting of all linear combinations of functions of the form

$$f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{m'}, \boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}) = g(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{m'}) \prod_{j=m+1}^{2m-1} f_{\boldsymbol{y}_j}(\boldsymbol{x}_j), \tag{2.4.32}$$

where g is any function in $\mathfrak{L}^2(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{m'})$ and $f_{\boldsymbol{y}_j}(\boldsymbol{x}_j)$ is the function introduced in eq. (2.4.10). This set has a subset in $\mathfrak{D}(H_0)$ which is dense in $\mathfrak{L}^2$. If $0 < \zeta < 1$,

$$|\exp[i\Delta(\boldsymbol{x}_h)t]f_{\boldsymbol{y}_h}(\boldsymbol{x}_h)| < \text{const.}(1+t^2)^{-\frac{1}{4}\zeta}(1+|c\boldsymbol{x}_h - c\boldsymbol{y}_h|)^{-\frac{3}{2}+\frac{1}{2}\zeta}, \tag{2.4.33}$$

by eq. (2.4.14). Hence, in view of eq. (2.4.25),

$$\left.\begin{aligned} &||V_{pq}(c\boldsymbol{x}_h + d\boldsymbol{x}_{j\neq h})e^{-iH_a t}f||^2_{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_{m'},\boldsymbol{x}_{m+1},\cdots,\boldsymbol{x}_{2m-1}} \\ &< \text{const.}(1+t^2)^{-\frac{1}{2}\zeta}||g||^2_{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_{m'}} \prod_{\substack{j=m+1\\ j\neq h}}^{2m-1}{}' ||f_{\boldsymbol{y}_j}(\boldsymbol{x}_j)||^2_{\boldsymbol{x}_j} \int [V_{pq}(c\boldsymbol{x}_h + d\boldsymbol{x}_{j\neq h})]^2(1+|c\boldsymbol{x}_h - c\boldsymbol{y}_h|)^{-3+\zeta}d\boldsymbol{x}_h \\ &< \text{const.}(1+t^2)^{-\frac{1}{2}\zeta}||g||^2_{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_{m'}}. \end{aligned}\right\} \tag{2.4.34}$$

From this it is obvious that eq. (2.4.31) holds true for every f in the set under discussion, and also for every f in $\mathfrak{D}(H_0)$.

Since $R_0(\mu)(H-\mu)$ is a bounded operator, again by eq. (2.1.5), it now follows from eq. (2.4.29) that

$$\lim_{t\to\mp\infty} ||R_0(\mu)\left[\sum_{j=1}^{m'} H_{(j)}(\boldsymbol{x}_j) - \lambda_a\right]e^{-iH_a t}E_a(l)f_a|| = 0. \tag{2.4.35}$$

Hence, since H_a commutes both with $H_{(j)}(\boldsymbol{x}_j)$ and with $R_0(\mu)$,

$$||R_0(\mu)\left[\sum_{j=1}^{m'} H_{(j)}(\boldsymbol{x}_j) - \lambda_a\right]E_a(l)f_a|| = 0, \tag{2.4.36}$$

from which it is obvious that

$$\left[\sum_{j=1}^{m'} H_{(j)}(\boldsymbol{x}_j) - \lambda_a\right]E_a(l)f_a = 0. \tag{2.4.37}$$

This equation can only be fulfilled if λ_a is of the form given in eq. (2.3.3). Also, if the eigenvalues $\lambda_{(j)}$ are not degenerate, $E_a(l)f_a$ must be of the form (2.3.4). In the case of degenerate eigenvalues, $E_a(l)$ might be a linear combination of functions of the form (2.3.4). But if we then further specify the channel concept as was explained in eq. (2.3.5), the functions $E_a(l)f_a$ for the various channels a with the same λ_a are again restricted to the form (2.3.4). Since $E_a(l)f_a$ tends to f_a if l tends to ∞, the function f_a must also be of the form (2.3.4). Hence we may conclude that the set $\mathfrak{C}_a$ is not larger than the set of functions of the form (2.3.4). Since by the previous section it is not smaller, it follows that $\mathfrak{C}_a$ must be equal to the set (2.3.4). This result holds true whenever eqs. (2.1.5), (2.4.25), and the general sufficient condition (2.4.16) are fulfilled. If we restrict the operators $H_a(\boldsymbol{x})$ to the general form of eq. (2.3.1), there are no channels besides the ones we have considered in the foregoing.

2.4.4. The continuous spectrum

Now that we can use the theory of wave-operators, we can justify the statement of section 1.7.6 concerning the continuous spectrum of the Hamiltonian $H^{(n)}$ for a system consisting of n particles with square-integrable two-body interactions. In section 1.7.6 we considered a splitting of the system into fragments of n_1 and n_2 particles ($n_1 + n_2 = n$). The lower bounds of the spectra of $H^{(n_1)}$ and $H^{(n_2)}$ were denoted by $\Lambda^{(n_1)}$ and $\Lambda^{(n_2)}$, respectively. It was asserted that the continuous spectrum of $H^{(n)}$ runs from $M^{(n)}$ to ∞, with

$$M^{(n)} = \min(\Lambda^{(n_1)} + \Lambda^{(n_2)}, \Lambda^{(n-1)}) \qquad (n_1, n_2 \geq 2,\ n_1 + n_2 = n), \tag{2.4.38}$$

the minimum being taken with respect to all possible splittings.

According to paper I, $M^{(n)}$ is not smaller than the minimum in eq. (2.4.38). To justify our assertion, we now show that $M^{(n)}$ is not larger either. The proof is based on the result of section 2.3.2, according to which the continuous spectrum of H contains the spectrum of H_a if, given a point l in the spectrum of H_a, there is a function f_a in $\mathfrak{C}_a$ such that l is not an interior point of an interval in which $E_a(l; f_a, f_a) = \text{const}$. It is obvious that this condition is fulfilled for all channels considered in this paper. Indeed, H_a is nothing but $H_0(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}) + \lambda_a$, and f_a may contain any function in $\mathfrak{L}^2(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$ as a factor.

For the purpose of the present section, it is convenient to call a splitting which yields the minimum in eq. (2.4.38) a minimum-splitting. It is also convenient to define $\Lambda^{(1)} = 0$, and to drop the restriction $n_1, n_2 \geq 2$. This formally makes $\Lambda^{(n-1)}$ equal to a quantity of the form $\Lambda^{(n_1)} + \Lambda^{(n_2)}$.

Let us now consider a minimum-splitting into n_1 and n_2 particles. The simplest situation arises if $\Lambda^{(n_1)}$ and $\Lambda^{(n_2)}$ are the eigenvalues of the bound states $\varphi_{(1)}(\boldsymbol{x}_1)$ and $\varphi_{(2)}(\boldsymbol{x}_2)$, respectively. Then it is useful to consider the scattering of two fragments in these bound states, the Hamiltonian H_a taking the form $H_0(\boldsymbol{x}_3) + \Lambda^{(n_1)} + \Lambda^{(n_2)}$. From the fact that the spectrum of this Hamiltonian H_a runs from $\Lambda^{(n_1)} + \Lambda^{(n_2)}$ to ∞, it follows that $M^{(n)}$ cannot exceed $\Lambda^{(n_1)} + \Lambda^{(n_2)}$. Combining this with the result that $M^{(n)}$ is not less than the minimum in eq. (2.4.38), we see that eq. (2.4.38) is fulfilled.

To cover the case that $\Lambda^{(n_1)}$ and $\Lambda^{(n_2)}$ do not both correspond to bound states, we proceed by induction. We first consider the scattering of two particles. For this $H_a = H_0(\boldsymbol{x}_1)$. Hence the continuous spectrum of $H^{(2)}$ coincides with the spectrum of H_0. Since this runs from 0 to ∞, it follows that $M^{(2)} = 0$. Formally we have $M^{(2)} = \Lambda^{(1)} + \Lambda^{(1)}$, hence eq. (2.4.38) holds true for $n = 2$.

As our next step we consider a minimum-splitting for three particles. This involves a lower bound $\Lambda^{(2)}$ which is equal either to 0 or to the eigenvalue of a bound state $\varphi_{(1)}(\boldsymbol{x}_1)$. In the latter case the choice $H_a = H_0(\boldsymbol{x}_2) + \Lambda^{(2)}$, corresponding to the scattering of the third particle by the bound fragment, tells us that eq. (2.4.38) is fulfilled. In case $\Lambda^{(2)} = 0$ we write $\Lambda^{(2)} = \Lambda^{(1)} + \Lambda^{(1)}$, and by considering the scattering of three unbound particles, $H_a = H_0(\boldsymbol{x}_1, \boldsymbol{x}_2)$, we obtain eq. (2.4.38) again.

Let us now assume that relations of the form (2.4.38) have been proved for $2,3,\ldots,n-1$ particles. To establish the desired result for n particles, we consider again a minimum-splitting into n_1 and n_2 particles. If $n_1 \geq 2$ and $\Lambda^{(n_1)}$ is not the eigenvalue of a bound state, $\Lambda^{(n_1)}$ must belong to the continuous spectrum of $H^{(n_1)}$. As a matter of fact, it must then be equal to $M^{(n_1)}$, since by definition it is the lower bound of the spectrum of $H^{(n_1)}$. Hence, by our assumption, there is a minimum-splitting

$$\Lambda^{(n_1)} = \Lambda^{(n_{11})} + \Lambda^{(n_{12})} \qquad (n_{11} + n_{12} = n_1). \tag{2.4.39}$$

If $n_{1i} \geq 2$ and the quantity $\Lambda^{(n_{1i})}$ is not the eigenvalue of a bound state, the fragment consisting of n_{1i} particles is split further. And so on. In this way we finally obtain a decomposition of the form

$$\Lambda^{(n_1)} + \Lambda^{(n_2)} = \sum_{j=1}^{m'} \Lambda^{(n'_j)} + (m-m')\Lambda^{(1)} \qquad \left(m - m' = n - \sum_{j=1}^{m'} n'_j\right), \tag{2.4.40}$$

each $\Lambda^{(n'_j)}$ being the eigenvalue of a bound state $\varphi_{(j)}(\boldsymbol{x}_j)$. If we now consider the scattering problem in which in the distant past the system was split into m' bound fragments in eigenstates $\varphi_{(j)}(\boldsymbol{x}_j)$, plus $m-m'$ single unbound particles, hence

$$H_a = H_0(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}) + \sum_{j=1}^{m'} \Lambda^{(n'_j)}, \tag{2.4.41}$$

we see that

$$M^{(n)} = \sum_{j=1}^{m'} \Lambda^{(n'_j)} = \Lambda^{(n_1)} + \Lambda^{(n_2)}, \tag{2.4.42}$$

as we wished to prove.

2.5. The wave-operators and the resolvent

2.5.1. The spectral resolution

Under the assumption that the interaction is such that there exist wave-operators $\Omega_{a\pm}$, we proceed to express the quantities $(g, \Omega_{a\pm} f_a)$ in terms of the resolvent of the Hamiltonian H, which is denoted by R. The resolvent corresponding to H_a is denoted by R_a, the resolution of the identity by E_a. In the following g may be any function in $\mathfrak{L}^2$, the function f_a is restricted to the form (2.3.4).

Since $E_a(K^2)f_a$ belongs to $\mathfrak{D}(H_0)$, it is convenient to consider the relation

$$f_a(\boldsymbol{x}) = \underset{K\to\infty}{\text{l.i.m.}} E_a(K^2)f_a(\boldsymbol{x}) = \prod_{j=1}^{m'} \varphi_{(j)}(\boldsymbol{x}_j) \underset{K\to\infty}{\text{l.i.m.}} E_a(K^2)f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}). \tag{2.5.1}$$

Corresponding to this we have

$$(g, \Omega_{a\pm} f_a) = \lim_{K\to\infty} (g, \Omega_{a\pm} E_a(K^2)f_a). \tag{2.5.2}$$

Remembering eq. (2.2.37), we now write

$$(g, \Omega_{a\pm} f_a) = \mp \{\lim_{K\to\infty} \lim_{\varepsilon\to 0}\} \varepsilon \int_0^{\mp\infty} e^{-\varepsilon|t|}(g, e^{iHt} e^{-iH_a t} E_a(K^2) f_a) dt, \tag{2.5.3}$$

where the limit-symbol means that

$$\lim_{K\to\infty} \lim_{\varepsilon\to 0} = \lim_{\varepsilon\to 0} \lim_{K\to\infty}. \tag{2.5.4}$$

Since $E_a(K^2)f_a$ belongs to $\mathfrak{D}(H_0)$, it follows from arguments such as used in section 2.4.1 that in eq. (2.5.3) we may integrate by parts, with the result that

$$(g, [\Omega_{a\pm} - 1] f_a) = i\{\lim_{K\to\infty} \lim_{\varepsilon\to 0}\} \int_0^{\mp\infty} e^{-\varepsilon t}(g, e^{iHt}[H - H_a] e^{-iH_a t} E_a(K^2) f_a) dt. \tag{2.5.5}$$

For convenience we now define

$$V_a = H - \sum_{j=1}^{m'} H_{(j)}(\boldsymbol{x}_j) - H_a(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}) + \lambda_a = \sum_{p,q} V_{pq}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{2m-1}) \tag{2.5.6}$$

(cf. eq. (2.4.7)). Acting on functions $E_a(K^2)f_a$, the operator V_a has the same effect as the operator $H - H_a$.

For the following it is slightly inconvenient that the quantity $V_a \exp(-iHt)g$ need not belong to $\mathfrak{L}^2$. However, if λ is any non-real number, we may write

$$\left.\begin{aligned}(g, e^{iHt} V_a e^{-iH_a t} E_a(K^2) f_a) &= (g, e^{iHt} V_a [H - V_a - \lambda]^{-1} [H - V_a - \lambda] e^{-iH_a t} E_a(K^2) f_a) \\ &= (g, e^{iHt} V_a [H - V_a - \lambda]^{-1} e^{-iH_a t} [H_a - \lambda] E_a(K^2) f_a).\end{aligned}\right\} \tag{2.5.7}$$

Here $[H - V_a - \lambda]^{-1}$ stands for the resolvent of $H - V_a$. According to eq. (2.1.5), its range is $\mathfrak{D}(H_0)$. Hence $V_a[H - V_a - \lambda]^{-1}$ is a bounded operator, again by eq. (2.1.5). Denoting its adjoint by $\{[H - V_a - \bar{\lambda}]^{-1} V_a\}$, we obtain

$$(g, e^{iHt} V_a e^{-iH_a t} E_a(K^2) f_a) = (\{[H - V_a - \bar{\lambda}]^{-1} V_a\} e^{-iHt} g, e^{-iH_a t} [H_a - \lambda] E_a(K^2) f_a). \tag{2.5.8}$$

We can now apply the spectral-resolution formula (1.4.28) to $\exp(-iH_a t)$. This yields

$$\left.\begin{aligned} i \int_0^{\mp\infty} e^{-\varepsilon|t|}(g, e^{iHt} V_a e^{-iH_a t} E_a(K^2) f_a) dt &= \frac{1}{2\pi} \int_0^{\mp\infty} dt \lim_{U_\pm \to \pm\infty} \lim_{\zeta\to 0} \int_{U_-}^{U_+} A\, du, \\ A = e^{-\varepsilon|t| - iut}(\{[H - V_a - \bar{\lambda}]^{-1} V_a\} e^{-iHt} g, &[R_a(u + i\zeta) - R_a(u - i\zeta)][H_a - \lambda] E_a(K^2) f_a).\end{aligned}\right\} \tag{2.5.9}$$

It follows from eq. (1.4.9) that in the above expression the integral with respect to u is a bounded function of t, uniformly with respect to $U_\pm$ and ζ. In virtue of this, we have

$$\int_0^{\mp\infty} dt \lim_{U_\pm\to\pm\infty} \lim_{\zeta\to 0} \int_{U_-}^{U_+} du = \lim_{U_\pm\to\pm\infty} \lim_{\zeta\to 0} \int_0^{\mp\infty} dt \int_{U_-}^{U_+} du = \lim_{U_\pm\to\pm\infty} \lim_{\zeta\to 0} \int_{U_-}^{U_+} du \int_0^{\mp\infty} dt. \quad (2.5.10)$$

The shortest, if not the most subtle way of justifying this uses first the theorem of dominated convergence, next Fubini's theorem (BURKILL (22) sections 3.10, 5.4). This implies that the integrals are considered as Lebesgue integrals. A justification entirely within the framework of Riemann integration requires several continuity arguments. These can also be carried through without too much difficulty.

Now that we have eq. (2.5.9), we may skip the factors $[H - V_a - \lambda]^{-1}$ and $H_a - \lambda$. Next we can apply the spectral-resolution formula to $\exp(iHt)$. In virtue of a relation analogous to eq. (2.5.10), this yields the expression

$$\left.\begin{aligned} &\frac{1}{4\pi^2 i} \lim_{U_\pm\to\pm\infty} \lim_{\zeta\to 0} \int_{U_-}^{U_+} du \lim_{V_\pm\to\pm\infty} \lim_{\eta\to 0} \int_{V_-}^{V_+} dv \int_0^{\mp\infty} B dt, \\ &B = e^{-\varepsilon|t| - iut + ivt}(g, [R(v + i\eta) - R(v - i\eta)] V_a [R_a(u + i\zeta) - R_a(u - i\zeta)] E_a(K^2) f_a). \end{aligned}\right\} \quad (2.5.11)$$

The integration with respect to t can now be performed. Using the integral representation of the resolvent $R(v \pm i\eta)$, eq. (1.4.11), we finally obtain

$$\left.\begin{aligned} &(g, [\Omega_{a\pm} - 1] f_a) \\ &= -\frac{1}{2\pi i} \{\lim_{K\to\infty} \lim_{\varepsilon\to 0}\} \lim_{U_\pm\to\pm\infty} \lim_{\zeta\to 0} \int_{U_-}^{U_+} (g, R(u \pm i\varepsilon) V_a [R_a(u + i\zeta) - R_a(u - i\zeta)] E_a(K^2) f_a) du. \end{aligned}\right\} \quad (2.5.12)$$

It is shown in the next section that in this expression the integration with respect to u may in fact be restricted to the interval $\lambda_a \leq u \leq K^2$.

2.5.2. Auxiliary formulas

In the final formula of the previous section, it is often convenient to go over to the Fourier transform of the function $f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$. To show why this is so, we first consider, in the notation of section 1.4.2,

$$\left.\begin{aligned} &(g, e^{iH_0 t} E_0(K^2) f) = \int_{-\infty}^{\infty} e^{iut} dE_0(u; g, E_0(K^2) f) \equiv \int_{-\infty}^{\infty} e^{iut} d_u(g, E_0(u) E_0(K^2) f) \\ &= \int_{-\infty}^{K^2} e^{iut} d(g, E_0(u) f) \equiv \int_{-\infty}^{K^2} e^{iut} dE_0(u; g, f) = \frac{1}{2\pi i} \lim_{\zeta\to 0} \int_0^{K^2} e^{iut} (g, [R_0(u + i\zeta) - R_0(u - i\zeta)] f) du \\ &= \frac{1}{\pi} \lim_{\zeta\to 0} \int_0^{K^2} e^{iut} du \int \bar{g}(\boldsymbol{x}) d\boldsymbol{x} \int [\mathrm{Im} G_0^{(m)}(\boldsymbol{x}, \boldsymbol{y}; u + i\zeta)] f(\boldsymbol{y}) d\boldsymbol{y}. \end{aligned}\right\} \quad (2.5.13)$$

According to eq. (1.2.17), the Green function has the form

$$G_0^{(m)}(\boldsymbol{x},\boldsymbol{y};\lambda) = \frac{i}{4}\left[\frac{\sqrt{\lambda}}{2\pi|\boldsymbol{x}-\boldsymbol{y}|}\right]^{\frac{3}{2}m-\frac{5}{2}} H^{(1)}_{\frac{3}{2}m-\frac{5}{2}}\left(\sqrt{\lambda}\,|\boldsymbol{x}-\boldsymbol{y}|\right). \tag{2.5.14}$$

It refers to $(3m-3)$-dimensional $\boldsymbol{x}$ and $\boldsymbol{y}$.

For the Fourier transform of $f(\boldsymbol{x})$ we use the notation

$$\hat{f}(\boldsymbol{k}) = (2\pi)^{-\frac{3}{2}m+\frac{3}{2}}\int e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} f(\boldsymbol{x})d\boldsymbol{x}. \tag{2.5.15}$$

The quantity $|\boldsymbol{k}|$ is denoted by k, and similarly for other vectors.

It is explained below that

$$(2\pi)^{-\frac{3}{2}m+\frac{3}{2}}\int e^{i\boldsymbol{k}\cdot\boldsymbol{y}} G_0^{(m)}(\boldsymbol{x},\boldsymbol{y};\lambda)d\boldsymbol{y} = (2\pi)^{-\frac{3}{2}m+\frac{3}{2}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \frac{1}{k^2-\lambda}. \tag{2.5.16}$$

Now $G_0^{(m)}(\boldsymbol{x},\boldsymbol{y};\lambda)$ depends only on $\boldsymbol{x}-\boldsymbol{y}$, and it belongs to $\mathfrak{L}(\boldsymbol{x}-\boldsymbol{y})$. Hence, by Parseval's formula and a theorem on resultants (TITCHMARSH (24) theorem 65),

$$\int \bar{g}(\boldsymbol{x})d\boldsymbol{x}\int G_0^{(m)}(\boldsymbol{x},\boldsymbol{y};\lambda)f(\boldsymbol{y})d\boldsymbol{y} = \int \bar{\hat{g}}(\boldsymbol{k})\frac{1}{k^2-\lambda}\hat{f}(\boldsymbol{k})d\boldsymbol{k}. \tag{2.5.17}$$

Equation (2.5.13) can therefore be simplified to

$$(g, e^{iH_0t}E_0(K^2)f) = \frac{1}{\pi}\lim_{\zeta\to 0}\int_0^{K^2} e^{iut}du\int \bar{\hat{g}}(\boldsymbol{k})\frac{\zeta}{(k^2-u)^2+\zeta^2}\hat{f}(\boldsymbol{k})d\boldsymbol{k}. \tag{2.5.18}$$

Here $\int d\boldsymbol{k}$ is a Lebesgue integral. On the other hand, $\int du$ was originally meant to be a Riemann integral. It is convenient to consider it as a Lebesgue integral henceforth. This does not change its value. It makes it possible to use Fubini's theorem and the theorem of dominated convergence to justify that

$$\lim_{\zeta\to 0}\int_0^{K^2} du\int d\boldsymbol{k} = \int d\boldsymbol{k}\lim_{\zeta\to 0}\int_0^{K^2} du. \tag{2.5.19}$$

The limit with respect to ζ can now be performed. By the theory of Cauchy's singular integral (TITCHMARSH (24) section 1.17), we have

$$\left.\begin{aligned} \frac{1}{\pi}\lim_{\zeta\to 0}\int_0^{K^2} e^{iut}\frac{\zeta}{(k^2-u)^2+\zeta^2}du &= e^{ik^2t} \qquad (0<k<K),\\ &= 0 \qquad (k>K). \end{aligned}\right\} \tag{2.5.20}$$

Hence we finally obtain

$$(g, e^{iH_0 t} E_0(K^2) f) = \int_{k<K} e^{ik^2 t}\, \bar{\hat{g}}(\boldsymbol{k}) \hat{f}(\boldsymbol{k}) d\boldsymbol{k}. \tag{2.5.21}$$

This shows that the Fourier transform of $E_0(K^2)f(\boldsymbol{x})$ is equal to $\hat{f}(\boldsymbol{k})$ if $0 < k < K$ and vanishes if $k > K$. Since $E_a(K^2)$ is nothing but $E_0(K^2 - \lambda_a)$ acting in the space $\mathfrak{L}^2(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$, the Fourier transform of $E_a(K^2)f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$ is equal to $\hat{f}(\boldsymbol{k}_{m+1}, \ldots, \boldsymbol{k}_{2m-1})$ if $0 < k < (K^2 - \lambda_a)^{\frac{1}{2}}$ and vanishes if $k > (K^2 - \lambda_a)^{\frac{1}{2}}$. If the argument of eq. (2.5.13) is applied to eq. (2.5.9), it follows that in eqs. (2.5.9) to (2.5.12) the integration can be restricted to the interval $\lambda_a \leq u \leq K^2$.

It still remains to show that the Fourier transform of the Green function satisfies eq. (2.5.16). If $m = 2$, this is easily checked directly. Let us now assume that it has been proved for $m = m_1$ and $m = m_2$. We know from eq. (1.5.27) that

$$\left.\begin{aligned} Q &\equiv \int \exp[i\boldsymbol{k}_1 \cdot (\boldsymbol{y}_1 - \boldsymbol{x}_1) + i\boldsymbol{k}_2 \cdot (\boldsymbol{y}_2 - \boldsymbol{x}_2)] G_0^{(m_1 + m_2 - 1)}(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_1, \boldsymbol{y}_2; \lambda) d\boldsymbol{y}_1 d\boldsymbol{y}_2 \\ &= \frac{1}{2\pi i} \int \exp[i\boldsymbol{k}_1 \cdot (\boldsymbol{y}_1 - \boldsymbol{x}_1) + i\boldsymbol{k}_2 \cdot (\boldsymbol{y}_2 - \boldsymbol{x}_2)] d\boldsymbol{y}_1 d\boldsymbol{y}_2 \int_C G_0^{(m_2)}(\boldsymbol{x}_2, \boldsymbol{y}_2; \lambda - \sigma) G_0^{(m_1)}(\boldsymbol{x}_1, \boldsymbol{y}_1; \sigma) d\sigma, \end{aligned}\right\} \tag{2.5.22}$$

where C is a contour in the σ-plane such that the singularities of $G_0(\sigma)$ are on the right of it, and those of $G_0(\lambda - \sigma)$ on the left of it. Now $G_0(\boldsymbol{x}, \boldsymbol{y}; \lambda)$ is an integrable function of $\boldsymbol{y}$, by eq. (1.7.83). More generally, it follows from the estimate given in eq. (1.7.83) that, if C is chosen in a suitable way, the repeated integral in eq. (2.5.22) converges absolutely. It is again convenient to consider it as a Lebesgue integral. Then it follows immediately from Fubini's theorem that the order of integration may be inverted. Our assumption concerning the transforms for $m = m_1$ and $m = m_2$ thus yields

$$Q = \frac{1}{2\pi i} \int_C \frac{1}{(k_2^2 - \lambda + \sigma)(k_1^2 - \sigma)} d\sigma. \tag{2.5.23}$$

Integration with respect to σ now gives the desired transform for $m = m_1 + m_2 - 1$. Hence eq. (2.5.16) is satisfied generally, as we wished to show.

2.5.3. The wave-operators in momentum space

We now extend the use of Fourier transforms to eq. (2.5.12). In doing so, it is convenient to combine the coordinates $\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}$ into a $(3m-3)$-dimensional coordinate $\boldsymbol{x}_a$, the coordinates $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{m'}$ into a coordinate $\boldsymbol{x}'_a$, and to write

$$\prod_{j=1}^{m'} \varphi_{(j)}(\boldsymbol{x}_j) = \varphi_a(\boldsymbol{x}'_a). \tag{2.5.24}$$

To be explicit, we henceforth write m_a instead of m. We use the operator $P_a(X_a)$ defined by

$$\left.\begin{aligned} P_a(X_a)f(\boldsymbol{x}'_a,\boldsymbol{x}_a) &= f(\boldsymbol{x}'_a,\boldsymbol{x}_a) \qquad (x_a < X_a),\\ &= 0 \qquad\qquad\quad (x_a > X_a). \end{aligned}\right\} \tag{2.5.25}$$

In terms of the operator $P_a(X_a)$, we have

$$\left.\begin{aligned} &\int_0^{\mp\infty} e^{-\varepsilon|t|}(g, e^{iHt}[H - H_a]e^{-iH_at}E_a(K^2)f_a)dt\\ &= \lim_{X_a\to\infty}\int_0^{\mp\infty} e^{-\varepsilon|t|}(g, e^{iHt}P_a(X_a)[H - H_a]e^{-iH_at}E_a(K^2)f_a)dt. \end{aligned}\right\} \tag{2.5.26}$$

If this relation is used in eq. (2.5.5), the reasoning of section 2.5.1 can be carried through essentially unchanged to show that in eq. (2.5.12) we may replace V_a by $V_aP_a(X_a)$, provided we take

$$\{\lim_{K\to\infty}\lim_{\varepsilon\to 0}\}\lim_{X_a\to\infty}\lim_{\zeta\to 0}\int_{\lambda_a}^{K^2} du. \tag{2.5.27}$$

We now recall that f_a is of the product-form (2.5.1). The operator $R_a(u \pm i\zeta)$ is nothing but $R_0(u - \lambda_a \pm i\zeta)$ acting only in $\mathfrak{L}^2(\boldsymbol{x}_a)$. The function $P_a(X_a)V_aR(u \mp i\varepsilon)g$ belongs to $\mathfrak{L}^2(\boldsymbol{x}'_a,\boldsymbol{x}_a)$. If we denote it by $h(\boldsymbol{x}'_a,\boldsymbol{x}_a)$, the quantity

$$\int \bar{\varphi}_a(\boldsymbol{x}'_a)h(\boldsymbol{x}'_a,\boldsymbol{x}_a)d\boldsymbol{x}'_a \tag{2.5.28}$$

is analogous to the function $\exp(-iut)g(\boldsymbol{x})$ in eq. (2.5.13). It is appropriate to denote the complex conjugate of its Fourier transform by

$$(2\pi)^{-\frac{3}{2}m_a+\frac{3}{2}}(g, R(u \pm i\varepsilon)V_aP_a(X_a)\varphi_a e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a}). \tag{2.5.29}$$

This is analogous to the function $\exp(iut)\bar{\hat{g}}(\boldsymbol{k})$ in eq. (2.5.18). Owing to the operator P_a, it does not exceed a constant depending on X_a, times the norm $||V_aR(u \mp i\varepsilon)g||$. Now it follows from eqs. (1.7.18) and (1.7.19) that, if each function V_{ij} satisfies eq. (2.1.5), the norm in question is bounded uniformly in u in the interval $\lambda_a \le u \le K^2$. Hence we may repeat the step (2.5.19). With the resolvent equation (1.2.11) it is now easily checked that the Fourier transform (2.5.29) is a continuous function of u. This makes it possible to perform the limit with respect to ζ as in eq. (2.5.20). The final result takes the form

$$\left.\begin{aligned} &(g, [\Omega_{a\pm} - 1]f_a)\\ &= -(2\pi)^{-\frac{3}{2}m_a+\frac{3}{2}}\{\lim_{K\to\infty}\lim_{\varepsilon\to 0}\}\lim_{X_a\to\infty}\int_{k_a<K}(g, R(k_a^2 + \lambda_a \pm i\varepsilon)V_aP_a(X_a)\varphi_a e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a})\hat{f}(\boldsymbol{k}_a)d\boldsymbol{k}_a. \end{aligned}\right\} \tag{2.5.30}$$

2.6. The scattering operators and the resolvent

2.6.1. General formulas

If both f_a and g_b are of the product-form (2.3.4), it is obvious that with the help of eq. (2.5.12) we can express $(g_b, \Omega^*_{b-}\Omega_{a+}f_a)$ in terms of the resolvent. A straightforward way of doing this yields a repeated integral, say $\int du \int dv$. A more interesting expression, with a single integral $\int du$, arises in the following way.

According to eq. (2.5.5) and the intertwining property (2.3.11), we have

$$\left.\begin{aligned}
&(g_b, \Omega^*_{b-}[\Omega_{a+} - 1]f_a) \\
&= -i\{\lim_{K_a\to\infty}\lim_{\delta\to 0}\}\int_{-\infty}^{0} e^{\delta t}(g_b, e^{iH_b t}\Omega^*_{b-}V_a e^{-iH_a t}E_a(K_a^2)f_a)dt \\
&= -i\{\lim_{K_a\to\infty}\lim_{\delta\to 0}\}\int_{-\infty}^{0} e^{\delta t}dt\Big[(g_b, e^{iH_b t}V_a e^{-iH_a t}E_a(K_a^2)f_a) \\
&-i\{\lim_{K_b\to\infty}\lim_{\varepsilon\to 0}\}\int_{0}^{\infty} e^{-\varepsilon s}(E_b(K_b^2)g_b, e^{iH_b(s+t)}V_b e^{-iHs}V_a e^{-iH_a t}E_a(K_a^2)f_a)ds\Big].
\end{aligned}\right\} \tag{2.6.1}$$

Now in eq. (2.5.3) the integral $\int dt$ is bounded uniformly in K and ε. Hence so is the integral $\int dt$ in eq. (2.5.5). Likewise, the integral $\int ds$ in the last term of eq. (2.6.1) is bounded uniformly in K_b and ε. Hence $\int dt$ and $\{\lim_{K_b}\lim_{\varepsilon}\}$ may be interchanged. With the techniques of sections 2.5.1 and 2.5.2 we thus obtain

$$(g_b, \Omega^*_{b-}[\Omega_{a+} - 1]f_a) = \{\lim_{K_a\to\infty}\lim_{\delta\to 0}\}[A + \{\lim_{K_b\to\infty}\lim_{\varepsilon\to 0}\}B], \tag{2.6.2}$$

where A and B are given by

$$\left.\begin{aligned}
A &= -\frac{1}{2\pi i}\lim_{\zeta\to 0}\int_{\lambda_a}^{K_a^2}(g_b, R_b(u+i\delta)V_a[R_a(u+i\zeta) - R_a(u-i\zeta)]f_a)du \\
&= \frac{1}{2\pi i}\lim_{K_b\to\infty}\lim_{\zeta\to 0}\int_{\lambda_b}^{K_b^2}(g_b, [R_b(u+i\zeta) - R_b(u-i\zeta)]V_a R_a(u-i\delta)E_a(K_a^2)f_a)du, \\
B &= -\frac{1}{2\pi i}\lim_{\zeta\to 0}\int_{\lambda_b}^{K_b^2}(g_b, [R_b(u+i\zeta) - R_b(u-i\zeta)]V_b R(u+i\varepsilon)V_a R_a(u-i\delta)E_a(K_a^2)f_a)du.
\end{aligned}\right\} \tag{2.6.3}$$

To obtain an expression which is more symmetric in a and b, we now consider $(g_b, \Omega^*_{b-}\Omega_{a-}f_a)$. According to eq. (2.3.23), this is equal to $\delta_{ba}(g_b, f_a)$. To express $(g_b, \Omega^*_{b-}\Omega_{a-}f_a)$ in terms of the resolvent, we merely have to replace $\int_{-\infty}^{0}\exp(\delta t)dt$ in

eq. (2.6.1) by $-\int_0^\infty \exp(-\delta t)dt$. Corresponding to eq. (2.6.3), this yields relations with $-\delta$ instead of δ. Hence from the expression for $(g_b, \Omega_{b-}^{\ddagger}[\Omega_{a+} - \Omega_{a-}]f_a)$ it follows that

$$\left.\begin{aligned}
(g_b, S_{ba} f_a) &= \delta_{ba}(g_b, f_a) + \Big\{\lim_{K_a\to\infty} \lim_{\delta\to 0}\Big\}[C + \Big\{\lim_{K_b\to\infty} \lim_{\varepsilon\to 0}\Big\}D], \\
C &= -\frac{1}{2\pi i}\lim_{K_b\to\infty}\lim_{\zeta\to 0}\int_{\lambda_{1b}}^{K_b^2}(g_b, [R_b(u+i\zeta) - R_b(u-i\zeta)]V_a[R_a(u+i\delta) - R_a(u-i\delta)]E_a(K_a^2)f_a)du, \\
D &= \frac{1}{2\pi i}\lim_{\zeta\to 0}\int_{\lambda_{1b}}^{K_b^2}(g_b, [R_b(u+i\zeta) - R_b(u-i\zeta)]V_b R(u+i\varepsilon)V_a[R_a(u+i\delta) - R_a(u-i\delta)]E_a(K_a^2)f_a)du.
\end{aligned}\right\} \tag{2.6.4}$$

As regards the quantity C, we observe that, owing to eqs. (2.3.17) and (2.3.20),

$$\mp\lim_{\delta\to 0}\delta\int_0^{\mp\infty} e^{-\delta|t|}(g_b, e^{iH_b t}e^{-iH_a t}f_a)dt = \delta_{ba}(g_b, f_a). \tag{2.6.5}$$

Upon integrating by parts, this yields

$$(\delta_{ba} - 1)(g_b, f_a) = i\Big\{\lim_{K_a\to\infty}\lim_{\delta\to 0}\Big\}\int_0^{\mp\infty} e^{-\delta|t|}(g_b, e^{iH_b t}[H_b - H_a]e^{-iH_a t}E_a(K_a^2)f_a)dt. \tag{2.6.6}$$

In this expression the operator $H_b - H_a$ may be replaced by $V_a - V_b$, by eq. (2.5.6). Hence

$$\left.\begin{aligned}
&(\delta_{ba} - 1)(g_b, f_a) \\
&= \frac{1}{2\pi i}\Big\{\lim_{K_a\to\infty}\lim_{\delta\to 0}\Big\}\lim_{K_b\to\infty}\lim_{\zeta\to 0}\int_{\lambda_{1b}}^{K_b^2}(g_b, [R_b(u+i\zeta) - R_b(u-i\zeta)][V_a - V_b]R_a(u\mp i\delta)E_a(K_a^2)f_a)du,
\end{aligned}\right\} \tag{2.6.7}$$

from which it follows that

$$\left.\begin{aligned}
&\Big\{\lim_{K_a\to\infty}\lim_{\delta\to 0}\Big\}\lim_{K_b\to\infty}\lim_{\zeta\to 0}\int_{\lambda_{1b}}^{K_b^2}(g_b, [R_b(u+i\zeta) - R_b(u-i\zeta)] \\
&\times [V_a - V_b][R_a(u+i\delta) - R_a(u-i\delta)]E_a(K_a^2)f_a)du = 0.
\end{aligned}\right\} \tag{2.6.8}$$

Combining this with eq. (2.6.4), we see that in the expression for C the operator V_a may be replaced by $(V_a + V_b)/2$. This increases the symmetry between a and b. However, as for the quantity D, there is still a fundamental asymmetry owing to the fact that $\lim_\varepsilon$ must be performed before $\lim_\delta$. This prevents us from going over to the

Fourier transform of f_a. It seems that this cannot be changed unless we make additional assumptions on the function f_a and on the interaction V_a. This point is the subject of the following sections.

2.6.2. The repeated limit

Equation (2.6.4) essentially results from evaluating

$$\left.\begin{aligned} &\lim_{\delta\to 0}\int_{-\infty}^{\infty} e^{-\delta|t|}(g_b, e^{iH_bt}\Omega_{b-}^{\ddagger}V_a e^{-iH_at}E_a(K_a^2)f_a)dt \\ &= \lim_{\delta\to 0}\lim_{\varepsilon\to 0}\int_{-\infty}^{\infty} e^{-\delta|t|}(g_b, e^{iH_bt}\Omega_{b-,\varepsilon}^{\ddagger}V_a e^{-iH_at}E_a(K_a^2)f_a)dt, \end{aligned}\right\} \tag{2.6.9}$$

where $\Omega_{b-,\varepsilon}$ is an obvious notation for an operator analogous to the quantity (2.2.39). Now we should like to interchange the two limits in eq. (2.6.9). Going over to the Fourier transform of f_a, we could then perform the limit with respect to δ by the method of section 2.5.3. Interchanging the limits is permitted if and only if

$$\lim_{\varepsilon\to 0}\lim_{\delta\to 0}\int_{-\infty}^{\infty} e^{-\delta|t|}([\Omega_{b-,\varepsilon}-\Omega_{b-}]e^{-iH_bt}g_b, V_a e^{-iH_at}E_a(K_a^2)f_a)dt = 0. \tag{2.6.10}$$

Since $E_a(K_a^2)f_a$ belongs to $\mathfrak{D}(H_0)$, it is not difficult to see that the inner product in eq. (2.6.10) is a bounded and continuous function of t. Hence, if $\delta > 0$, the integral certainly exists. But it is not at all obvious that it tends to a limit as δ tends to 0. However, let us for a moment drop the operator $E_a(K_a^2)$, let us assume that V_a satisfies the sufficient condition (2.4.16), and let us consider the special set of functions f_a introduced in section 2.4.2. Denoting this set by $\mathfrak{E}_a$, we see from eq. (2.4.17) that, if f_a is any particular function in $\mathfrak{E}_a$, there exist numbers $N(f_a)$ and ζ, with $0 < \zeta < 1$, such that

$$||V_a e^{-iH_at}f_a|| < N(f_a)(1+t^2)^{-\frac{1}{2}-\frac{1}{4}\zeta}. \tag{2.6.11}$$

Hence the integrand in eq. (2.6.10) does not exceed an integrable function of t. As a result $\lim_\delta$ and $\int dt$ may be interchanged, by the theorem of dominated convergence. Also,

$$\left.\begin{aligned} &\int_{-\infty}^{\infty}||(\Omega_{b-,\varepsilon}-\Omega_{b-})e^{-iH_bt}g_b||\;||V_a e^{-iH_at}f_a||dt \\ &< N(f_a)\int_{-T}^{T}||(\Omega_{b-,\varepsilon}-\Omega_{b-})e^{-iH_bt}g_b||dt + 2N(f_a)||g_b||\left(\int_{-\infty}^{-T}+\int_{T}^{\infty}\right)(1+t^2)^{-\frac{1}{2}-\frac{1}{4}\zeta}dt. \end{aligned}\right\} \tag{2.6.12}$$

As T tends to ∞, the second term on the right clearly tends to 0. Given T, it follows from an analogue of eq. (2.2.39) that

$$
\begin{aligned}
I &\equiv \int_{-T}^{T} ||(\Omega_{b-,\varepsilon} - \Omega_{b-})e^{-iH_b t} g_b||dt \\
&\leq \int_{-T}^{T} ||e^{\varepsilon t} e^{-iHt}\Omega_{b-,\varepsilon} g_b + \varepsilon e^{\varepsilon t} e^{-iHt} \int_{t}^{0} e^{-\varepsilon s}\Omega_b(s)ds g_b - e^{-iHt}\Omega_{b-} g_b||dt \\
&\leq \int_{-T}^{T} [||(\Omega_{b-,\varepsilon} - \Omega_{b-})g_b|| + ||g_b||\,|e^{\varepsilon t} - 1| + \varepsilon||g_b||e^{\varepsilon t}|\int_{t}^{0} e^{-\varepsilon s}ds|]dt \\
&\leq 2T||(\Omega_{b-,\varepsilon} - \Omega_{b-})g_b|| + 4(\cosh \varepsilon T - 1)||g_b||/\varepsilon.
\end{aligned}
\tag{2.6.13}
$$

Hence, if given T and a positive η, we choose ε so small that

$$
2T||(\Omega_{b-,\varepsilon} - \Omega_{b-})g_b|| < \eta, \qquad 4(\cosh \varepsilon T - 1)||g_b||/\varepsilon < \eta, \tag{2.6.14}
$$

the quantity I does not exceed 2η. From this it follows that by choosing first T sufficiently large, next ε sufficiently small, the right-hand side of eq. (2.6.12) can be made arbitrarily close to 0. Hence eq. (2.6.10) is satisfied if we drop the operator $E_a(K_a^2)$ and for f_a take a function in $\mathfrak{F}_a$. For future reference we note that this result is simply due to $||V_a \exp(-iH_a t)f_a||$ being a bounded and integrable function of t.

Unfortunately, it does not follow from the foregoing that eq. (2.6.10) holds true generally. A conclusion to that effect could be drawn if it were known, for instance, that the limit with respect to δ existed and were bounded by a constant times $||f_a||$, uniformly in ε. But a result of this sort is not available. There is another difficulty, which is related to the operator $E_a(K_a^2)$. Throughout this investigation, we find it convenient to have functions of the form $E_a(K_a^2)f_a$, i. e. functions whose Fourier transforms with respect to $\boldsymbol{x}_a$ vanish outside bounded regions. Now the functions in $\mathfrak{F}_a$ are not of the desired form. Hence they cannot really be used in the present context. We have not succeeded in deciding whether there is a suitable set of functions $E_a(K_a^2)f_a$ such that eq. (2.6.10) holds true whenever V_a satisfies the relation (2.4.16). What we do know is that eq. (2.6.10) is valid for fairly large classes of interactions V_a and functions $E_a(K_a^2)f_a$. We now pass on to discussing this.

2.6.3. Restrictions on the interaction and on the relative motion

In the present section we formulate sufficient conditions on the interaction V_a and on the wave-function f_a to guarantee that in eqs. (2.6.1) and (2.6.4) the limits with respect to ε and δ may be interchanged. The functions f_a we consider all have Fourier transforms with respect to $\boldsymbol{x}_a$ which vanish outside bounded regions. Hence, if K_a is large enough, $E_a(K_a^2)f_a$ is nothing but f_a, and we need not distinguish between the two quantities.

If the limits are interchangeable for any particular combination V_a,f_a, we say that this combination is admissible. It is clear from eq. (2.6.1) that, if both V_{a1},f_a and V_{a2},f_a are admissible, so is $V_{a1} + V_{a2}$,f_a. Hence we may restrict the discussion

to certain standard forms of the interaction V_a, it being understood that a linear combination of these can be considered without additional difficulties.

As in previous sections, the function f_a will be of the form

$$f_a(\boldsymbol{x}) = \prod_{j=1}^{m'} \varphi_{(j)}(\boldsymbol{x}_j) f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}). \tag{2.6.15}$$

Now let $\mathfrak{F}$ denote the set of all functions $f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$ in $\mathfrak{L}^2$ the Fourier transforms of which have bounded first-order partial derivatives with respect to $\boldsymbol{k}_{m+1}, \ldots, \boldsymbol{k}_{2m-1}$ and vanish if $k_{m+1}^2 + \ldots + k_{2m-1}^2 > K^2$, the parameter K running through all finite values. Then we assume in the following that f belongs to $\mathfrak{F}$. If f belongs to $\mathfrak{F}$ and f_a is of the form (2.6.15), we say that f_a belongs to $\mathfrak{F}_a$.

It is not difficult to see that $\mathfrak{F}$ is dense in $\mathfrak{L}^2(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$. Indeed, the Fourier transform of any function in $\mathfrak{L}^2(\boldsymbol{x})$ belongs to $\mathfrak{L}^2(\boldsymbol{k})$. It can be approximated in mean square by a continuous function which vanishes outside a bounded region (McShane (25) section 42.4s). Such a continuous function can be approximated uniformly by a function which vanishes outside a bounded region and has continuous partial derivatives of all orders (Schwartz (26) ch. I, theorem I). Hence the set of Fourier transforms of functions in $\mathfrak{F}$ is dense in $\mathfrak{L}^2(\boldsymbol{k}_{m+1}, \ldots, \boldsymbol{k}_{2m-1})$. As a result $\mathfrak{F}$ is dense in $\mathfrak{L}^2(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1})$. The set $\mathfrak{F}_a$ is dense in the set of functions (2.6.15).

We now turn to the function V_a. This is a sum of two-body interactions V_{pq}, by eq. (2.5.6). We saw in eq. (2.4.8) that each V_{pq} depends on the internal coordinates $\boldsymbol{x}_{j(p)}$ of the fragment to which particle p belongs, similarly on the coordinates $\boldsymbol{x}_{j(q)}$ ($j(p) \neq j(q); j(p), j(q) = 1, 2, \ldots, m'$), and on one or more coordinates $\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}$. For the major part of the following sections, we concentrate on one particular V_{pq}. Given p and q, we choose the coordinates $\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}$ in such a way that there is a certain $\boldsymbol{x}_h$ ($h = m+1, \ldots, 2m-1$) proportional to the distance between the centres of mass of the fragments $j(p)$ and $j(q)$. This yields

$$V_{pq}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{2m-1}) = V_{pq}(\sum_r d_r \boldsymbol{x}_{j(p),r} + \sum_s d_s \boldsymbol{x}_{j(q),s} + c\boldsymbol{x}_h) \tag{2.6.16}$$

(cf. eq. (2.4.8)).

The restrictions we want to impose upon V_{pq} are most easily expressed in terms of the function

$$W_{pq}(\boldsymbol{x}_h) = \int\int |V_{pq}(\sum_r d_r \boldsymbol{x}_{j(p),r} + \sum_s d_s \boldsymbol{x}_{j(q),s} + c\boldsymbol{x}_h) \varphi_{(j(p))}(\boldsymbol{x}_{j(p)}) \varphi_{(j(q))}(\boldsymbol{x}_{j(q)})|^2 d\boldsymbol{x}_{j(p)}\, d\boldsymbol{x}_{j(q)}, \tag{2.6.17}$$

appropriate modifications being understood in case the fragments $j(p)$ and $j(q)$ consist of only one particle. We assume that W_{pq} is integrable, hence that V_{pq} is a square-integrable function of $\boldsymbol{x}_h$. Then the general sufficient condition of section 2.4.2 is certainly fulfilled. For the time being we further restrict ourselves to the case that

$$\int [W_{pq}(\boldsymbol{x}_h) x_h^2]^{\mu} d\boldsymbol{x}_h < \infty \tag{2.6.18}$$

for some μ with $1 < \mu < 2$. Slightly more general classes of functions W_{pq} are considered in section 2.6.5.

2.6.4. A convergence problem

It follows from section 2.6.2 that for V_a, f_a to be admissible, it is sufficient if $||V_a \exp(-iH_a t) f_a||$ is a bounded and integrable function of t. Assuming that f_a belongs to $\mathfrak{F}_a$, we now show that the particular function V_{pq} we are considering satisfies

$$\int_{-\infty}^{\infty} ||V_{pq} e^{-iH_a t} f_a|| dt < \infty. \tag{2.6.19}$$

Since $\mathfrak{F}_a$ is contained in $\mathfrak{D}(H_0)$, the integrand in eq. (2.6.19) is a bounded and continuous function of t. Hence the integration over the interval $-1 < t < 1$ does not present difficulties. To cope with the case $|t| > 1$, we write

$$\left.\begin{aligned} &\exp\left[i \sum_{j=m+1}^{2m-1} \Delta(\boldsymbol{x}_j) t\right] f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}) \\ = (2\pi)^{-\frac{3}{2}m+\frac{3}{2}} &\int \exp\left[i \sum_{j=m+1}^{2m-1} (-k_j^2 t + \boldsymbol{k}_j \cdot \boldsymbol{x}_j)\right] \hat{f}(\boldsymbol{k}_{m+1}, \ldots, \boldsymbol{k}_{2m-1}) d\boldsymbol{k}_{m+1} \ldots d\boldsymbol{k}_{2m-1}. \end{aligned}\right\} \tag{2.6.20}$$

Integration by parts with respect to k_h yields

$$\left.\begin{aligned} &\exp\left[i \sum_{j=m+1}^{2m-1} \Delta(\boldsymbol{x}_j) t\right] f(\boldsymbol{x}_{m+1}, \ldots, \boldsymbol{x}_{2m-1}) \\ &= \frac{(2\pi)^{-\frac{3}{2}m+\frac{3}{2}}}{2it} \int \exp\left[i \sum_{j=m+1}^{2m-1} (-k_j^2 t + \boldsymbol{k}_j \cdot \boldsymbol{x}_j)\right] \\ &\times (i\boldsymbol{k}_h \cdot \boldsymbol{x}_h + 1 + \boldsymbol{k}_h \cdot \operatorname{grad}_h) \hat{f}(\boldsymbol{k}_{m+1}, \ldots, \boldsymbol{k}_{2m-1}) k_h^{-2} d\boldsymbol{k}_{m+1} \ldots d\boldsymbol{k}_{2m-1}, \end{aligned}\right\} \tag{2.6.21}$$

the integrated term vanishing since $\hat{f}$ vanishes if $k_h > K$.

We first consider the term proportional to $i\boldsymbol{k}_h \cdot \boldsymbol{x}_h$. Owing to our special choice of coordinates, we have

$$\left.\begin{aligned} I_1(t) &\equiv ||V_{pq}(\boldsymbol{x}) \prod_{j=1}^{m'} \varphi_{(j)}(\boldsymbol{x}_j) \int \exp\left[i \sum_{j=m+1}^{2m-1} (-k_j^2 t + \boldsymbol{k}_j \cdot \boldsymbol{x}_j)\right] \\ &\times \boldsymbol{k}_h \cdot \boldsymbol{x}_h \hat{f}(\boldsymbol{k}_{m+1}, \ldots, \boldsymbol{k}_{2m-1}) k_h^{-2} d\boldsymbol{k}_{m+1} \ldots d\boldsymbol{k}_{2m-1}||^2 \\ &= \int W_{pq}(\boldsymbol{x}_h) |\int \exp[i(-k_h^2 t + \boldsymbol{k}_h \cdot \boldsymbol{x}_h)] \boldsymbol{k}_h \cdot \boldsymbol{x}_h F(\boldsymbol{k}_h) k_h^{-2} d\boldsymbol{k}_h|^2 d\boldsymbol{x}_h, \end{aligned}\right\} \tag{2.6.22}$$

where F is a bounded function of $\boldsymbol{k}_h$ which vanishes if $k_h > K$. It is an essential point that F does not depend on t.

In the rest of the analysis, we drop the subscript h. On the other hand, we consider separately the three components of $\boldsymbol{k}_h$ and $\boldsymbol{x}_h$, which we denote by k_γ and x_γ ($\gamma = 1,2,3$).

If in eq. (2.6.18) $\mu = 1$, the function

$$Z_{\beta\gamma}(\boldsymbol{k}-\boldsymbol{k}') = (2\pi)^{-\frac{3}{2}}\int W_{pq}(\boldsymbol{x})\exp[i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{x}]x_\beta x_\gamma d\boldsymbol{x} \tag{2.6.23}$$

is bounded. If $1 < \mu \leq 2$, it satisfies

$$\left.\begin{aligned}&\left[(2\pi)^{-\frac{3}{2}}\int |Z_{\beta\gamma}(\boldsymbol{k}-\boldsymbol{k}')|^{\mu/(\mu-1)}d(\boldsymbol{k}-\boldsymbol{k}')\right]^{(\mu-1)/\mu}\\ &\quad < \left[(2\pi)^{-\frac{3}{2}}\int |W_{pq}(\boldsymbol{x})x_\beta x_\gamma|^\mu d\boldsymbol{x}\right]^{1/\mu}.\end{aligned}\right\} \tag{2.6.24}$$

The corresponding relation for Fourier transforms depending on one-dimensional variables k and x was proved by TITCHMARSH (24) (sections 4.1–4.5) and, by a different method, by ZYGMUND (27) (ch. XVI, section 3). Zygmund's proof, which is based on the Riesz-Thorin convexity theorem (ZYGMUND (27) ch. XII, section 1), applies to functions of several variables essentially unchanged.

With the help of eq. (2.6.24) it is easily shown that in eq. (2.6.22) the integration with respect to $\boldsymbol{x}_h$ may be performed first. Hence

$$I_1(t) = (2\pi)^{\frac{3}{2}}\sum_{\beta,\gamma}\int\int Z_{\beta\gamma}(\boldsymbol{k}-\boldsymbol{k}')\exp[-i(k^2-k'^2)t]k_\beta k'_\gamma F(\boldsymbol{k})\bar{F}(\boldsymbol{k}')k^{-2}k'^{-2}d\boldsymbol{k}d\boldsymbol{k}'. \tag{2.6.25}$$

We now go over to new variables as follows. First we write

$$\boldsymbol{k}-\boldsymbol{k}' = \boldsymbol{w}, \qquad \boldsymbol{k}+\boldsymbol{k}' = \boldsymbol{v}. \tag{2.6.26}$$

Next we consider $\boldsymbol{v}$ in a coordinate frame fixed to $\boldsymbol{w}$. In this frame we introduce polar coordinates v,ϑ,φ, choosing the direction of $\boldsymbol{w}$ as the polar axis. Finally we go over from $\boldsymbol{w},v,\vartheta,\varphi$ to $\boldsymbol{w},v,\varphi$, $r = vw\cos\vartheta$, where w stands for $|\boldsymbol{w}|$. With this choice of coordinates we have

$$\left.\begin{aligned}k^2-k'^2 = \boldsymbol{v}.\boldsymbol{w} = r, \qquad 2k &= |\boldsymbol{v}+\boldsymbol{w}| = (v^2+w^2+2r)^{\frac{1}{2}},\\ 2k' &= |\boldsymbol{v}-\boldsymbol{w}| = (v^2+w^2-2r)^{\frac{1}{2}}.\end{aligned}\right\} \tag{2.6.27}$$

The quantity I_1 therefore takes the form

$$I_1(t) = \sum_{\beta,\gamma}\int_{-K^2}^{K^2} dr \int_{w=\frac{|r|}{2K}}^{w=2K} d\boldsymbol{w}\int_{\frac{|r|}{w}}^{2K} dv\int_0^{2\pi} d\varphi\, e^{-irt}Z_{\beta\gamma}(\boldsymbol{w})w^{-1}v[(v^2+w^2)^2-4r^2]^{-\frac{1}{2}}G_{\beta\gamma}(\boldsymbol{w},v,\varphi,r), \tag{2.6.28}$$

$G_{\beta\gamma}$ being some bounded function. Now if $w < 2K$,

$$\left.\begin{aligned}&\int_{\frac{|r|}{w}}^{2K} v[(v^2+w^2)^2-4r^2]^{-\frac{1}{2}}dv = \tfrac{1}{2}\log(4K^2+w^2+[(4K^2+w^2)^2-4r^2]^{\frac{1}{2}})\\ &-\tfrac{1}{2}\log\left(\frac{r^2}{w^2}+w^2+\left|\frac{r^2}{w^2}-w^2\right|\right) \leq \log 4K - \tfrac{1}{4}\log\frac{2r^2}{w^2} - \tfrac{1}{4}\log 2w^2 = \tfrac{1}{2}\log\frac{8K^2}{|r|}.\end{aligned}\right\} \tag{2.6.29}$$

Hence

$$I_1(t) = \sum_{\beta,\gamma} \int_{-K^2}^{K^2} dr \int_{w=\frac{|r|}{2K}}^{w=2K} d\boldsymbol{w}\, e^{-irt} \log\frac{8K^2}{|r|} Z_{\beta\gamma}(\boldsymbol{w}) w^{-1} H_{\beta\gamma}(\boldsymbol{w}, r), \tag{2.6.30}$$

with some bounded function $H_{\beta\gamma}$.

It follows from eq. (2.6.24) that, if $1 < \mu < 2$,

$$\int_{w=\frac{|r|}{2K}}^{w=2K} |Z_{\beta\gamma}(\boldsymbol{w})|\, w^{-1} d\boldsymbol{w} < \left[\int |Z_{\beta\gamma}(\boldsymbol{w})|^{\mu/(\mu-1)} d\boldsymbol{w}\right]^{(\mu-1)/\mu} \left[\int_{w=\frac{r}{2K}}^{w=2K} w^{-\mu} d\boldsymbol{w}\right]^{1/\mu} < \infty. \tag{2.6.31}$$

If $\mu = 1$, the left-hand side of eq. (2.6.31) is likewise finite. Hence $I_1(t)$ is bounded. Also, $I_1(t)$ is the Fourier transform of a function of r which belongs to $\mathfrak{L}^{\nu}(r)$ $(1 < \nu \leq 2)$. As a result $I_1(t)$ belongs to $\mathfrak{L}^{\nu/(\nu-1)}(t)$. Hence $[I_1(t)]^{\frac{1}{2}}/t$ is integrable over $-\infty < t \leq -1$ and $1 \leq t < \infty$, by Hölder's inequality. In view of eq. (2.6.22), this shows that in eq. (2.6.21) the term proportional to $i\boldsymbol{k}_\hbar . \boldsymbol{x}_\hbar$ is compatible with eq. (2.6.19).

The term proportional to $\boldsymbol{k}_\hbar . \mathrm{grad}_\hbar$ can be discussed along the same lines. Instead of eq. (2.6.18) we merely need the fact that W_{pq} is integrable. For the term proportional to 1 we have to consider

$$\left.\begin{aligned} \int_{\frac{|r|}{2K}}^{2K} dw \int_{\frac{|r|}{w}}^{2K} wv[(v^2+w^2)^2 - 4r^2]^{-1} dv &= \frac{1}{8r} \int_{\frac{|r|}{2K}}^{2K} w \log\frac{(4K^2+w^2-2r)(w^2+r)^2}{(4K^2+w^2+2r)(w^2-r)^2} dw \\ &= \frac{1}{8r}[(4K^2+r)\log|4K^2+r| - (4K^2-r)\log|4K^2-r| - 2r\log 2|r|]. \end{aligned}\right\} \tag{2.6.32}$$

Now since

$$\lim_{r\to 0} \frac{1}{r}(\log|4K^2+r| - \log|4K^2-r|) = \frac{1}{2K^2}, \tag{2.6.33}$$

the right-hand side of eq. (2.6.32) has only logarithmic singularities. Hence, by analogy with the function $I_1(t)$, the term proportional to 1 yields a bounded function $I_2(t)$ which again belongs to $\mathfrak{L}^{\nu/(\nu-1)}(t)$ and has the property that $[I_2(t)]^{\frac{1}{2}}/t$ is integrable over $-\infty < t \leq -1$ and $1 \leq t < \infty$.

According to the results obtained thus far,

$$e^{-iH_a t} f_a = \sum_{i=1}^{3} f_i(t). \tag{2.6.34}$$

If W_{pq} is integrable and satisfies eq. (2.6.18),

$$\int_{|t|>1} ||V_{pq} f_i(t)||\, dt = \text{const.} \int_{|t|>1} [I_i(t)]^{\frac{1}{2}} \frac{1}{t} dt < \infty \qquad (i = 1,2,3). \tag{2.6.35}$$

Now given eqs. (2.6.34) and (2.6.35), it follows from Minkowski's inequality that $||V_{pq}\exp(-iH_at)f_a||$ is integrable over $-\infty < t \leq -1$ and $1 \leq t < \infty$. Combining this with our previous result for $-1 < t < 1$, we see that eq. (2.6.19) is fulfilled, as we wished to show.

In proving eq. (2.6.19), essential use has been made of the fact that the coordinates $\boldsymbol{x}_{m+1},\ldots,\boldsymbol{x}_{2m-1}$ were adapted to the particular function V_{pq} under discussion. Hence, this equation has thus far only been established for one single pair p,q. To extend it to all the interactions contained in V_a, we consider a term V_{rs} with $r,s \neq p,q$. By an orthogonal transformation among the coordinates $\boldsymbol{x}_{m+1},\ldots,\boldsymbol{x}_{2m-1}$, we go over to coordinates adapted to V_{rs}. This will entail a transformation among $\boldsymbol{k}_{m+1},\ldots,\boldsymbol{k}_{2m-1}$. However, if $\hat{f}(\boldsymbol{k}_{m+1},\ldots,\boldsymbol{k}_{2m-1})$ has bounded first-order partial derivatives with respect to the original coordinates, so it has with respect to the new ones. If it vanishes outside a bounded region before the transformation, then the same applies afterwards. Hence, after the transformation the methods developed for V_{pq} can be used for V_{rs} without alteration. From this it follows with Minkowski's inequality that $||V_a\exp(-iH_at)f_a||$ is an integrable function of t. This function is also bounded, since f_a belongs to $\mathfrak{D}(H_0)$. Hence, if f_a belongs to $\mathfrak{F}_a$ and each function W_{pq} is integrable and satisfies eq. (2.6.18), the combination V_a,f_a is admissible.

2.6.5. Alternative restrictions on the interaction

If in eq. (2.6.18) μ is small, W_{pq} may be fairly singular, but at large distances it must tend to 0 rather fast. If μ is large, W_{pq} must not have serious singularities, except possibly at the origin. In this case W_{pq} need not tend to 0 very fast as x_h tends to ∞, a decrease faster than $x_h^{-\frac{7}{2}}$ being sufficient if $\mu = 2$. Our general arguments do not apply beyond $1 \leq \mu \leq 2$ because it is only in this interval that we can draw a conclusion of the form (2.6.24). However, the condition at infinity can be relaxed in a special case. For let us consider a function W_{pq} which is integrable and satisfies

$$W_{pq}(\boldsymbol{x}_h) < \text{const.}\, x_h^{-3-\eta} \qquad (x_h > R) \tag{2.6.36}$$

for some positive η. This function is conveniently written in the form

$$\left.\begin{aligned} W_{pq}(\boldsymbol{x}_h) &= W_<(\boldsymbol{x}_h) + W_>(\boldsymbol{x}_h), \\ W_<(\boldsymbol{x}_h) &= W_{pq}(\boldsymbol{x}_h), \quad W_>(\boldsymbol{x}_h) = 0 \qquad (0 < x_h < R), \\ W_<(\boldsymbol{x}_h) &= 0, \quad W_>(\boldsymbol{x}_h) = W_{pq}(\boldsymbol{x}_h) \qquad (x_h > R). \end{aligned}\right\} \tag{2.6.37}$$

Since $W_<$ is integrable and satisfies eq. (2.6.18) with $\mu = 1$, it can be discussed with the methods outlined above. In an obvious notation, it gives rise to functions $I_{i<}(t)$ $(i = 1,2,3)$ belonging to $\mathfrak{L}^{\nu/(\nu-1)}(t)$. Our previous methods also apply to the functions $I_{2>}$ and $I_{3>}$ associated with $W_>$. For these derive from the terms in eq. (2.6.21) proportional to 1 and $\boldsymbol{k}_h \cdot \text{grad}_h$, respectively. In analysing these terms, it was assumed only that W_{pq} is integrable.

To investigate the term proportional to $i\boldsymbol{k}_h.\boldsymbol{x}_h$, we assume for simplicity that $\eta_j \leq 1/2$. There is no loss of generality in doing so. We drop the subscript h again and we use the variables $\boldsymbol{w},v,\varphi,r$ described in eqs. (2.6.26) and (2.6.27). Expressing $\boldsymbol{x}$ in terms of polar coordinates x,χ,ψ in a frame of reference which has its polar axis in the direction of $\boldsymbol{w}$, we obtain

$$\left.\begin{aligned} (\boldsymbol{k}-\boldsymbol{k}').\boldsymbol{x} &= wx\cos\chi, \\ (\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{x} &= vx\left[\frac{r}{vw}\cos\chi+\left(1-\frac{r^2}{v^2w^2}\right)^{\frac{1}{2}}\sin\chi(\cos\varphi\cos\psi+\sin\varphi\sin\psi)\right]. \end{aligned}\right\} \tag{2.6.38}$$

From this it follows that $(\boldsymbol{k}.\boldsymbol{x})(\boldsymbol{k}'.\boldsymbol{x})$ can be written as a linear combination of terms proportional to v^2x^2, vwx^2 and w^2x^2, respectively, the coefficients depending on $r/vw,\varphi,\chi,\psi$ and being expressible in terms of low-order spherical harmonics $Y_{lm}(\chi,\psi)$. Hence, in view of eq. (2.6.22),

$$\left.\begin{aligned} I_{1>}(t) &< \lim_{X\to\infty}\int_0^X dx\int_{-1}^{1} d\cos\chi\int_0^{2\pi} d\psi\int_{-K^2}^{K^2} dr\int_{w=\frac{|r|}{2K}}^{w=2K} d\boldsymbol{w}\int_{\frac{|r|}{w}}^{2K} dv\int_0^{2\pi} d\varphi A, \\ A &= x^{1-\eta}\exp[i(-rt+\boldsymbol{w}\cdot\boldsymbol{x})]\sum_{l=0}^{L}\sum_m Y_{lm}(\chi,\psi)w^{-1}v[(v^2+w^2)^2-4r^2]^{-1} \\ &\quad\times[v^2C_{lm1}(\boldsymbol{w},v,\varphi,r)+vwC_{lm2}(\boldsymbol{w},v,\varphi,r)+w^2C_{lm3}(\boldsymbol{w},v,\varphi,r)] \end{aligned}\right\} \tag{2.6.39}$$

with some set of bounded functions C. Integration with respect to $\cos\chi,\psi$, and φ yields

$$\left.\begin{aligned} I_{1>}(t) &< \lim_{X\to\infty}\int_0^X dx\int_{-K^2}^{K^2} dr\int_{w=\frac{|r|}{2K}}^{w=2K} d\boldsymbol{w}\int_{\frac{|r|}{w}}^{2K} dv\,x^{\frac{1}{2}-\eta}e^{-irt}\sum_{l=0}^{L} J_{l+\frac{1}{2}}(wx)w^{-\frac{3}{2}}v[(v^2+w^2)^2-4r^2]^{-1} \\ &\quad\times[v^2D_{l1}(\boldsymbol{w},v,r)+vwD_{l2}(\boldsymbol{w},v,r)+w^2D_{l3}(\boldsymbol{w},v,r)], \end{aligned}\right\} \tag{2.6.40}$$

the functions D being bounded. The integration with respect to x may be performed next, by Fubini's theorem. Also,

$$\int_0^X x^{\frac{1}{2}-\eta}J_{l+\frac{1}{2}}(wx)dx = w^{-\frac{3}{2}+\eta}G_X(w), \tag{2.6.41}$$

where $G_X(w)$ is bounded uniformly in X. Hence,

$$\lim_{X\to\infty}\int dr\int d\boldsymbol{w}\int dv\int_0^X dx = \int dr\int d\boldsymbol{w}\int dv\lim_{X\to\infty}\int_0^X dx, \tag{2.6.42}$$

by the theorem of dominated convergence. As a result,

$$\left.\begin{aligned} I_{1>}(t) < \int_{-K^2}^{K^2} dr \int_{w=\frac{|r|}{2K}}^{w=2K} d\boldsymbol{w} \int_{w}^{2K} dv\, e^{-irt} w^{-3+\eta} v[(v^2+w^2)^2 - 4r^2]^{-1} \\ \times [v^2 E_1(\boldsymbol{w},v,r) + vw E_2(\boldsymbol{w},v,r) + w^2 E_3(\boldsymbol{w},v,r)]. \end{aligned}\right\} \quad (2.6.43)$$

We now consider separately the terms E_1, E_2, and E_3. In an obvious notation, we write

$$I_{1>}(t) < I_{11>}(t) + I_{12>}(t) + I_{13>}(t). \quad (2.6.44)$$

Owing to eqs. (2.6.32) and (2.6.33),

$$I_{13>}(t) = \int_{-K^2}^{K^2} e^{-irt} \log|r| F_3(r) dr, \quad (2.6.45)$$

where F_3 is a bounded function. Hence $I_{13>}(t)$ belongs to $\mathfrak{L}^{\nu/(\nu-1)}(t) (1 < \nu < 2)$, by previous arguments.

For the term $I_{11>}$ we consider

$$\left.\begin{aligned} &\int_{\frac{|r|}{2K}}^{2K} dw \int_{\frac{|r|}{w}}^{2K} dv\, w^{-1+\eta} v^3 [(v^2+w^2)^2 - 4r^2]^{-1} \\ &= \frac{1}{8r} \int_{\frac{|r|}{2K}}^{2K} w^{1+\eta} \log \frac{(4K^2+w^2+2r)(w^2-r)^2}{(4K^2+w^2-2r)(w^2+r)^2} dw \\ &+ \tfrac{1}{4} \int_{\frac{|r|}{2K}}^{2K} w^{-1+\eta} \log \frac{(4K^2+w^2+2r)(4K^2+w^2-2r)w^4}{(w^2+r)^2(w^2-r)^2} dw. \end{aligned}\right\} \quad (2.6.46)$$

Here the first term on the right equals $\log|r|$ times a bounded function of r, again by eqs. (2.6.32) and (2.6.33). Since $0 < \eta \leq 1/2$ by assumption, $w^{-1+\eta} \leq (|r|/2K)^{-1+\eta}$. Also, the logarithm in the second term on the right is integrable. Hence, the second term on the right is equal to $r^{-1+\eta}$ times a bounded function of r. Summarizing,

$$I_{11>}(t) = \int_{-K^2}^{K^2} e^{-irt} r^{-1+\eta} F_1(r) dr, \quad (2.6.47)$$

with some bounded function F_1. This shows that, if ν satisfies $1 < \nu < (1-\eta)^{-1} \leq 2$, the function $I_{11>}(t)$ is the Fourier transform of a function in $\mathfrak{L}^{\nu}(r)$. Hence $I_{11>}(t)$ belongs to $\mathfrak{L}^{\nu/(\nu-1)}(t)$.

It is now obvious that $I_{12>}(t)$ also belongs to $\mathfrak{L}^{\nu/(\nu-1)}(t)$, for some suitable set

of numbers ν. For, given eqs. (2.6.45) and (2.6.47), it follows from Schwarz's inequality that

$$I_{12>}(t) = \int_{-K^2}^{K^2} e^{-irt}(r^{-1+\eta}\log|r|)^{\frac{1}{2}} F_2(r)dr, \tag{2.6.48}$$

and the argument can be completed as before. Summarizing, each function $I_{1i>}(t)$ ($i = 1,2,3$) belongs to $\mathfrak{L}^{\nu/(\nu-1)}(t)$. Hence so does $I_{1>}(t)$, by eq. (2.6.44).

Since W_{pq} is the sum of $W_<$ and $W_>$, the function $I_i(t)$ is the sum of $I_{i<}(t)$ and $I_{i>}(t)$. Hence $I_i(t)$ belongs to $\mathfrak{L}^{\nu/(\nu-1)}(t)$. Equation (2.6.35) is therefore satisfied also in the present case. From this it follows as before that $||V_{pq}\exp(-iH_at)f_a||$ is integrable over $-\infty < t \leq -1$ and $1 \leq t < \infty$, next that the same applies to $||V_a\exp(-iH_at)f_a||$. Since either norm is a bounded function of t, the final conclusion is that the quantity $||V_a\exp(-iH_at)f_a||$ is bounded and belongs to $\mathfrak{L}(t)$. Hence the combination V_a,f_a is admissible, as we wished to show.

According to the results obtained thus far, V_a,f_a is admissible (i.e. in eqs. (2.6.1) and (2.6.4) the limits with respect to ε and δ may be interchanged) whenever f_a belongs to $\mathfrak{F}_a$ and each W_{pq} is an integrable function satisfying either eq. (2.6.18) or eq. (2.6.36). This is due to certain functions $I(t)$ belonging to $\mathfrak{L}^{\nu/(\nu-1)}(t)$. Now the functions $I(t)$ depend linearly on W_{pq}, by eq. (2.6.22). Hence, if f_a belongs to $\mathfrak{F}_a$ and each W_{pq} is integrable, for V_a,f_a to be admissible it is already sufficient if W_{pq} is some linear combination of functions satisfying eq. (2.6.18) or (2.6.36), possibly with different exponents μ. This is the most general result we have obtained in this connection.

2.6.6. Examples of admissible interactions

It does not seem easy to translate the conditions on W_{pq} into conditions on V_{pq}, unless something is known about the asymptotic behaviour of the functions $\varphi_{(j)}(\boldsymbol{x}_j)$. We recall here that in eq. (2.6.16) the quantity $\sum_r d_r\boldsymbol{x}_{j(p),r}$ stands for the distance between particle p and the centre of mass of fragment $j(p)$. Now given this interpretation, it will be shown in a separate paper that, if all the interactions V_{ij} within the fragment $j(p)$ are square-integrable and the eigenvalue $\lambda_{(j(p))}$ does not belong to the continuous spectrum of the Hamiltonian $H_{(j(p))}(\boldsymbol{x}_{j(p)})$,

$$N_{p\alpha} \equiv \int |(\sum_r d_r\boldsymbol{x}_{j(p),r})^{\alpha}\varphi_{(j(p))}(\boldsymbol{x}_{j(p)})|^2 d\boldsymbol{x}_{j(p)} < \infty \tag{2.6.49}$$

for every $\alpha \geq 0$. This result ensues from a study of the analytic properties of scattering amplitudes, which is beyond the scope of the present paper. However, let us assume that eq. (2.6.49) holds true. Let us also assume that

$$U_\mu \equiv \int [V_{pq}(\boldsymbol{X})X]^{2\mu} d^3\boldsymbol{X} < \infty, \qquad V_\mu \equiv \int [V_{pq}(\boldsymbol{X})]^{2\mu} d^3\boldsymbol{X} < \infty, \tag{2.6.50}$$

with $\mu = 1$. The inequality

$$x_h^\beta \leq (3/c)^\beta \big(|\boldsymbol{y}_p + \boldsymbol{y}_q + c\boldsymbol{x}_h|^\beta + y_p^\beta + y_q^\beta\big) \qquad (\beta \geq 0), \tag{2.6.51}$$

applied with $\beta = 2$, then yields

$$\int W_{pq}(\boldsymbol{x}_h) x_h^2 \, d\boldsymbol{x}_h < \text{const.}\,(U_1 N_{p0} N_{q0} + V_1 N_{p1} N_{q0} + V_1 N_{p0} N_{q1}) \tag{2.6.52}$$

(cf. eqs. (2.6.16) and (2.6.17)). Hence eq. (2.6.18) is satisfied with $\mu = 1$. Similarly, if eq. (2.6.50) is true for $\mu = 2$, so is eq. (2.6.18). Both for $\mu = 1$ and for $\mu = 2$, it also follows from eq. (2.6.50) that V_{pq} is square-integrable, hence that W_{pq} is integrable. This shows that, if f_a belongs to $\mathfrak{F}_a$, if eq. (2.6.49) holds true for $\alpha = 1$, and if each V_{pq} satisfies eq. (2.6.50) with either $\mu = 1$ or $\mu = 2$, the combination V_a, f_a is admissible.

Again, let us consider the case that each V_{pq} is square-integrable and such that

$$|V_{pq}(\boldsymbol{X})| < \text{const.}\, X^{-\frac{3}{2} - \frac{1}{2}\eta} \qquad (X > R) \tag{2.6.53}$$

for some positive η. In this case it is convenient to write

$$\left.\begin{aligned} V_{pq}(\boldsymbol{X}) &= V_<(\boldsymbol{X}) + V_>(\boldsymbol{X}), \\ [V_{pq}(\boldsymbol{X})]^2 &= [V_<(\boldsymbol{X})]^2 + [V_>(\boldsymbol{X})]^2, \end{aligned}\right\} \tag{2.6.54}$$

the functions $V_<$ and $V_>$ being defined as in eq. (2.6.37). Since $V_<$ satisfies eq. (2.6.50) with $\mu = 1$, it yields a function W with $\mu = 1$. Also, $V_>$ yields a function W of the form (2.6.36). For if in eq. (2.6.51) we take $\beta = 3 + \eta$, we obtain

$$\left.\begin{aligned} &\int |V_>(\sum_r d_r \boldsymbol{x}_{j(p),r} + \sum_s d_s \boldsymbol{x}_{j(q),s} + c\boldsymbol{x}_h) \varphi_{(j(p))}(\boldsymbol{x}_{j(p)}) \varphi_{(j(q))}(\boldsymbol{x}_{j(q)})|^2 d\boldsymbol{x}_{j(p)} d\boldsymbol{x}_{j(q)} \\ &< \text{const.}\, x_h^{-3-\eta} \big(N_{p0} N_{q0} + N_{p,\frac{3}{2}+\frac{1}{2}\eta} N_{q0} + N_{p0} N_{q,\frac{3}{2}+\frac{1}{2}\eta}\big) \qquad \big(x_h > R\big). \end{aligned}\right\} \tag{2.6.55}$$

Hence, if eq. (2.6.49) holds true for $\alpha = (3+\eta)/2$ and if each V_{pq} is a square-integrable function satisfying eq. (2.6.53), each W_{pq} is the sum of two suitable functions. If f_a belongs to $\mathfrak{F}_a$, the combination V_a, f_a is admissible.

2.6.7. The scattering operators in momentum space

If f_a belongs to $\mathfrak{F}_a$ and each function W_{pq} satisfies the sufficient conditions summarized at the end of section 2.6.5, in eqs. (2.6.1) and (2.6.4) the limits with respect to ε and δ may be interchanged. Going over to the Fourier transform of f_a, we can then perform the limit with respect to δ. This yields an expression for the operator S_{ba} in momentum space which is the subject of the present section.

In discussing the quantity $(g_b, S_{ba} f_a)$, we obviously have to assume that V_b is such that the operator Ω_{b-} exists. Also, g_b must belong to $\mathfrak{G}_b$. Thus far no further

restrictions were imposed upon g_b. From now on we assume explicitly that g_b is of the product-form (2.3.4).

In applying the results of the last few sections, it is convenient to start with a function $E_b(K_b^2)g_b$ the Fourier transform of which vanishes outside a region characterized by K_b, and to perform the limit with respect to K_b as the last step. Obviously this is always permitted. In this way we are led to consider

$$\lim_{K_b\to\infty}\lim_{\varepsilon\to 0}\lim_{\delta\to 0}. \tag{2.6.56}$$

Since, under the present assumptions, the quantity $||V_a\exp(-iH_at)f_a||$ is bounded and integrable, the integral

$$\int_{-\infty}^{\infty} e^{-\delta|t|}(E_b(K_b^2)g_b, e^{iH_bt}V_a e^{-iH_at}f_a)dt \tag{2.6.57}$$

tends to a limit as δ tends to 0. Hence, in eq. (2.6.4) the quantities C and D each have a limit with respect to δ.

For the transition to Fourier transforms it is convenient to use the operators $P_a(X_a)$ and $P_b(X_b)$ defined in eq. (2.5.25). Replacing in eq. (2.6.4) $R_a(u\pm i\delta)$ by $P_a(X_a)R_a(u\pm i\delta)$ and $R_b(u\pm i\zeta)$ by $R_b(u\pm i\zeta)P_b(X_b)$, we have to evaluate

$$\lim_{K_b\to\infty}\lim_{\varepsilon\to 0}\lim_{\delta\to 0}\Big\{\lim_{X_b\to\infty}\lim_{X_a\to\infty}\Big\}\lim_{\zeta\to 0}, \tag{2.6.58}$$

by analogy with eq. (2.5.27). We now show first that in eq. (2.6.4)

$$\lim_{\delta\to 0}\Big\{\lim_{X_b\to\infty}\lim_{X_a\to\infty}\Big\}\lim_{\zeta\to 0} = \Big\{\lim_{X_b\to\infty}\lim_{X_a\to\infty}\Big\}\lim_{\delta\to 0}\lim_{\zeta\to 0}. \tag{2.6.59}$$

This is most easily proved with the help of eq. (2.6.1). For we have

$$\left.\begin{aligned} e^{-\delta|t|}|(E_b(K_b^2)g_b, e^{iH_b(s+t)}P_b(X_b)V_b e^{-iHs}V_a P_a(X_a)e^{-iH_at}f_a)| \\ < ||V_b e^{-iH_b(s+t)}E_b(K_b^2)g_b||\ ||V_a e^{-iH_at}f_a|| \\ < (\alpha||H_0E_b(K_b^2)g_b|| + \beta||E_b(K_b^2)g_b||)||V_a e^{-iH_at}f_a||, \end{aligned}\right\} \tag{2.6.60}$$

the second inequality following from eq. (2.1.4). According to eq. (2.6.60), in the last integral in eq. (2.6.1) the integrand does not exceed an integrable function of t which does not depend on X_a, X_b, and δ. Hence, if $\varepsilon > 0$,

$$\left.\begin{aligned} \lim_{\delta\to 0}\int dt\int ds\Big\{\lim_{X_b\to\infty}\lim_{X_a\to\infty}\Big\} &= \int dt\int ds\Big\{\lim_{\delta\to 0}\lim_{X_b\to\infty}\lim_{X_a\to\infty}\Big\} \\ &= \Big\{\lim_{\delta\to 0}\lim_{X_b\to\infty}\lim_{X_a\to\infty}\Big\}\int dt\int ds, \end{aligned}\right\} \tag{2.6.61}$$

by the theorem of bounded convergence. And similarly for the first integral on the right in eq. (2.6.1). If from eq. (2.6.1) we now deduce eq. (2.6.4), the limit-property (2.6.59) follows as an obvious consequence.

The limit with respect to ζ can now be performed with the methods of section 2.5.3. In writing it down, we use the notation in terms of $\boldsymbol{x}'_a,\boldsymbol{x}_a$ introduced in section 2.5.3. Since $\boldsymbol{x}'_a$ stands for the internal coordinates, $\boldsymbol{x}_a$ for the relative coordinates of the m_a fragments into which the system is split when it is in channel a, it is appropriate to express f_a in terms of $\boldsymbol{x}'_a,\boldsymbol{x}_a$. For convenience we express g_b in terms of $\boldsymbol{x}'_b,\boldsymbol{x}_b$, this being a set of coordinates which is related to $\boldsymbol{x}'_a,\boldsymbol{x}_a$ through an orthogonal transformation.

In the new notation, taking the limit with respect to ζ yields

$$\left.\begin{aligned}(g_b,S_{ba}f_a) &= \delta_{ba}(g_b,f_a) + (2\pi)^{-\frac{3}{2}m_b+\frac{3}{2}} \lim_{K_b\to\infty}\lim_{\varepsilon\to 0}\Big\{\lim_{X_b\to\infty}\lim_{X_a\to\infty}\Big\}\lim_{\delta\to 0}\int\limits_{k_b\le K_b} I\,d\boldsymbol{k}_b,\\ I &= \bar{\tilde{g}}(\boldsymbol{k}_b)(P_b(X_b)\varphi_b e^{i\boldsymbol{k}_b\cdot\boldsymbol{x}_b},[-1+V_bR(k_b^2+\lambda_b+i\varepsilon)]V_aP_a(X_a)\\ &\quad\times[R_a(k_b^2+\lambda_b+i\delta)-R_a(k_b^2+\lambda_b-i\delta)]\varphi_a f).\end{aligned}\right\} \tag{2.6.62}$$

In going over to the Fourier transform of f, it is now a question of

$$\lim_{\delta\to 0}\int\limits_{k_b\le K_b} d\boldsymbol{k}_b\int d\boldsymbol{k}_a\,\bar{\tilde{g}}(\boldsymbol{k}_b)M(\boldsymbol{k}_b,\boldsymbol{k}_a)\frac{\delta}{(k_b^2+\lambda_b-k_a^2-\lambda_a)^2+\delta^2}\hat{f}(\boldsymbol{k}_a), \tag{2.6.63}$$

where M can be found from eq. (2.6.62). Since $P_b(X_b)\varphi_b$ and $V_aP_a(X_a)\varphi_a$ belong to $\mathfrak{L}^2$ and $V_bR(k_b^2+\lambda_b+i\varepsilon)$ is a bounded operator, the function M is bounded. Hence, since f belongs to $\mathfrak{F}$ by assumption, the integral $\int d\boldsymbol{k}_a$ does not exceed an integrable function of $\boldsymbol{k}_b$, uniformly in δ. As a result

$$\lim_{\delta\to 0}\int d\boldsymbol{k}_b\int d\boldsymbol{k}_a = \int d\boldsymbol{k}_b\lim_{\delta\to 0}\int d\boldsymbol{k}_a. \tag{2.6.64}$$

Performing the limit with respect to δ now shows that in the final result there will be contributions only from the region where

$$k_a^2+\lambda_a = k_b^2+\lambda_b \equiv E. \tag{2.6.65}$$

This brings out the conservation of energy during the scattering process. Since k_b is thereby restricted automatically, the limit with respect to K_b may be omitted from eq. (2.6.62). Expressing $\boldsymbol{k}_i$ $(i = a,b)$ in terms of k_i and various polar angles ω_{k_i}, with

$$\int d\boldsymbol{k}_i = \int k_i^{3m_i-4}\,dk_i\,d\omega_{k_i} \qquad (i = a,b), \tag{2.6.66}$$

we thus obtain

$$\left.\begin{aligned} (g_b, S_{ba} f_a) &= \delta_{ba}(g_b, f_a) \\ &+ \tfrac{1}{4}\, i(2\pi)^{-\frac{3}{2}(m_b+m_a)+4} \lim_{\varepsilon\to 0}\Big\{\lim_{X_b\to\infty}\lim_{X_a\to\infty}\Big\}\int dE \int\int d\omega_{k_b} d\omega_{k_a} k_b^{3m_b-5} k_a^{3m_a-5}\, \bar{g}(\boldsymbol{k}_b) F(\boldsymbol{k}_b,\boldsymbol{k}_a;\varepsilon;X_b,X_a)\hat{f}(\boldsymbol{k}_a), \\ F(\boldsymbol{k}_b,\boldsymbol{k}_a;\varepsilon;X_b,X_a) &= (P_b(X_b)\varphi_b e^{i\boldsymbol{k}_b\cdot\boldsymbol{x}_b}, [-1 + V_b R(E+i\varepsilon)] V_a P_a(X_a)\varphi_a e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a}). \end{aligned}\right\} \quad (2.6.67)$$

It follows from our discussion of eq. (2.2.11) that $S_{ba}f_a$ belongs to $\mathfrak{S}_b$. Let us now assume that the two-body interactions V_{ij} contained in V_b satisfy eq. (2.4.25). Then all functions in $\mathfrak{S}_b$ are of the form $\varphi_b(\boldsymbol{x}_b')h(\boldsymbol{x}_b)$, by section 2.4.3. In particular,

$$\left.\begin{aligned} (S_{ba} - \delta_{ba}) f_a &= \varphi_b(\boldsymbol{x}_b') h(\boldsymbol{x}_b), \\ (g_b, [S_{ba} - \delta_{ba}] f_a) &= \int \bar{\tilde{g}}(\boldsymbol{k}_b)\hat{h}(\boldsymbol{k}_b) d\boldsymbol{k}_b, \end{aligned}\right\} \quad (2.6.68)$$

with some function h in $\mathfrak{Q}^2$.

If in eq. (2.6.67) the integration with respect to ω_{k_a} is performed first, the remaining integral has an integrand which essentially depends only on k_b and ω_{k_b}, the quantities E and k_a being determined by k_b according to eq. (2.6.65). Hence, combining eqs. (2.6.67) and (2.6.68), we obtain a relation of the form

$$\int \bar{\tilde{g}}(\boldsymbol{k}_b)\hat{h}(\boldsymbol{k}_b) d\boldsymbol{k}_b = \lim_N \int \bar{\tilde{g}}(\boldsymbol{k}_b)\hat{h}_N(\boldsymbol{k}_b) d\boldsymbol{k}_b, \quad (2.6.69)$$

where N stands for ε, X_b, X_a. Taking in particular $g = h$ and applying eq. (2.6.69) once more yields

$$\int |\hat{h}(\boldsymbol{k}_b)|^2 d\boldsymbol{k}_b = \lim_N \lim_{N'} \int \bar{\hat{h}}_{N'}(\boldsymbol{k}_b)\hat{h}_N(\boldsymbol{k}_b) d\boldsymbol{k}_b. \quad (2.6.70)$$

The probability of scattering into channel b thus takes the form

$$\left.\begin{aligned} &||(S_{ba} - \delta_{ba}) f_a||^2 \\ &= \tfrac{1}{4}(2\pi)^{-3(m_b+m_a)+8} \lim_{\varepsilon\to 0}\Big\{\lim_{X_b\to\infty}\lim_{X_a\to\infty}\Big\}\lim_{\varepsilon'\to 0}\Big\{\lim_{X_b'\to\infty}\lim_{X_a'\to\infty}\Big\}\int \bar{A}(\boldsymbol{k}_b;\varepsilon';X_b',X_a') A(\boldsymbol{k}_b;\varepsilon;X_b,X_a) d\boldsymbol{k}_b, \\ &A(\boldsymbol{k}_b;\varepsilon;X_b,X_a) = \int k_a^{3m_a-5} F(\boldsymbol{k}_b,\boldsymbol{k}_a;\varepsilon;X_b,X_a)\hat{f}(\boldsymbol{k}_a) d\omega_{k_a}. \end{aligned}\right\} \quad (2.6.71)$$

2.6.8. Discussion

The results of the previous section are subject to the assumption that f_a belongs to $\mathfrak{F}_a$, and that V_a satisfies the sufficient conditions discussed in sections 2.6.4 and 2.6.5. These restrictions are imposed to guarantee that in eq. (2.6.67) the limits with respect to ε and X_b, X_a do in fact exist. In eq. (2.6.1) we have introduced the repeated limit with respect to ε and δ to replace the limits with respect to the time variables s and t. These entered the problem because we have considered transitions from an initial state in the distant past to a final state in the remote future. The condition that there should

be a limit as ε tends to 0 is very closely related to the condition that in a scattering experiment the scattered fragments should become free sufficiently rapidly as the time t goes to ∞. This condition is fulfilled if the interaction between any two fragments tends to 0 sufficiently rapidly as their distance increases. Roughly speaking, we may therefore say that the behaviour of the resolvent in the neighbourhood of the continuous spectrum reflects the asymptotic properties of scattered wave-packets at very large times. These in turn depend on the interaction, and in particular on its behaviour at large distances, according to the foregoing analysis.

By taking ε sufficiently small but different from 0, a good approximation can be obtained to the limit in eq. (2.6.67). Doing so may have advantages owing to the fact that off the real axis the resolvent can be studied much more easily than in the continuous spectrum. As a matter of fact, it was shown in part I of the present investigation that, if all the two-body interactions in the system are square-integrable, there is a systematic procedure for constructing the resolvent for non-real energies. This method breaks down in the continuous spectrum. From the general theory of resolvents and spectra one gets the impression that this is a fundamental difficulty which cannot be solved within the framework of a Hilbert-space formalism. In view of the correspondence between small values of ε and large times, we may say that taking a non-vanishing ε is analogous to extending a scattering experiment over a finite time only. The analogy should not be taken too literally, however, the precise relationship between non-real energies and finite times being fairly complicated.

In eq. (2.6.67) there is also a limit with respect to X_b,X_a. If X_a is finite, the interaction V_a is distorted in so far as it takes place outside a hypersphere of radius X_a in $\boldsymbol{x}_a$-space. Hence, taking X_a large but finite may yield a good approximation, provided the properties of the system are such that, if any two fragments are far apart, all the fragments are effectively free. This is again a condition which refers to the interaction between the fragments decreasing sufficiently rapidly. Accordingly, once it is known that there is a limit as ε tends to 0, the limit with respect to X_b,X_a does not present further difficulties. This we saw in the proof of eq. (2.6.59). Letting X_b,X_a remain finite corresponds to performing a scattering experiment in a finite region of space.

It is a crucial point that in eq. (2.6.67) the integration must be performed before the limits are taken. This equation thus contains a statement concerning a sequence of linear functionals. It is essentially the kind of relation one studies in the theory of distributions, the function $\bar{\hat{g}}\hat{f}$ playing the part of the test-function. From this point of view it is not surprising that $\hat{f}$ must satisfy certain conditions of smoothness. In this connection it may be remarked that, since in measurements there are always errors, one cannot distinguish experimentally between a wave-function f_1 and a wave-function f_2 which is almost equal to f_1 in the sense that $||f_1 - f_2|| < \eta$, where η is a small positive number determined by the accuracy of the experiment in question. Hence, in practice no loss of generality is involved if the initial state of a scattering process is described in terms of a set of functions which is dense in $\mathfrak{C}_a$.

2.7. The scattering of two fragments

2.7.1. Restrictions on the interaction and on the relative motion

If in channel a the system is split into not more than two fragments, it is convenient to develop the function $\hat{f}(\boldsymbol{k}_a)$ in terms of spherical harmonics, $\boldsymbol{k}_a$ now being a three-dimensional vector. In many cases of practical interest we have

$$\hat{f}(\boldsymbol{k}_a) = \sum_{l=0}^{L} \sum_{m} \hat{f}_{lm}(k_a) Y_{lm}(\omega_{k_a}), \tag{2.7.1}$$

where L is finite. In any case the function $\hat{f}$ can be approximated in mean square by a sum of the form (2.7.1).

If $\hat{f}$ is of the form (2.7.1) and each $\hat{f}_{lm}$ is suitably restricted, the combination V_a, f_a is admissible under conditions on V_a which are much less stringent than the ones imposed in sections 2.6.4 and 2.6.5. The present section is devoted to this point.

We assume for the time being that $\hat{f}_{lm}$ belongs to the set $\hat{\mathfrak{S}}_{lm}$ consisting of all functions defined in $0 \leq k_a < \infty$ which have bounded derivatives of the first order and vanish outside bounded intervals. If each $\hat{f}_{lm}$ belongs to $\hat{\mathfrak{S}}_{lm}$ and $\hat{f}$ is of the form (2.7.1), we say that $\hat{f}$ belongs to $\hat{\mathfrak{S}}$. The set of functions f which are Fourier transforms of functions in $\hat{\mathfrak{S}}$ is denoted by $\mathfrak{S}$. The set of functions f_a which are equal to $\varphi_a(\boldsymbol{x}'_a)$ times a function $f(\boldsymbol{x}_a)$ in $\mathfrak{S}$ is denoted by $\mathfrak{S}_a$.

It is not difficult to see that $\mathfrak{S}_a$ is dense in the set of functions (2.3.4). To show that this is so, we merely have to prove that, given a positive ξ and a function $\hat{f}_{lm}(k_a)$ such that

$$\int_0^\infty |\hat{f}_{lm}(k_a)|^2 k_a^2 \, dk_a < \infty, \tag{2.7.2}$$

there is a function $\hat{g}(k_a)$ in $\hat{\mathfrak{S}}_{lm}$ such that

$$\int_0^\infty |\hat{f}_{lm}(k_a) - \hat{g}(k_a)|^2 k_a^2 dk_a < \xi. \tag{2.7.3}$$

Now if eq. (2.7.2) holds true, $\hat{f}_{lm}(k_a)k_a$ can be approximated in mean square by a function which is equal to $\hat{f}_{lm}(k_a)k_a$ in some interval $0 < 3\eta \leq k_a < K - 2\eta$ and vanishes everywhere else. This function can be approximated in mean square by a continuous function which vanishes outside the interval $2\eta \leq k_a \leq K - \eta$ (McShane (25) section 42.4s). Next, the continuous function can be approximated uniformly by a continuously differentiable function which vanishes unless $\eta \leq k_a \leq K$ (Schwartz (26) ch. I, theorem I). Let us denote the last function by $\hat{h}(k_a)$. Since $\hat{h}(k_a)$ vanishes in the neighbourhood of the origin, we can consider the function $\hat{g}(k_a) = \hat{h}(k_a)/k_a$. This clearly belongs to $\hat{\mathfrak{S}}_{lm}$. By the foregoing argument, it can be chosen in such a way that, in the sense of eq. (2.7.3), it approximates $\hat{f}_{lm}(k_a)$ as close as we please.

Hence in this sense $\mathfrak{S}_{lm}$ is dense in the set of functions $\hat{f}_{lm}(k_a)$ which satisfy eq. (2.7.2). From this it follows that $\mathfrak{S}_a$ is dense in the set of functions (2.3.4).

Since in the special case of the present section $\boldsymbol{x}_a$ is proportional to the distance between the centres of mass of the two scattered fragments, it is automatically equal to the coordinate $\boldsymbol{x}_h$ used in section 2.6.3. Expressing $\boldsymbol{x}_a$ in terms of polar coordinates x_a, ω_{x_a}, we define

$$Q_{pq}(x_a) = \int W_{pq}(\boldsymbol{x}_a) d\omega_{x_a}. \tag{2.7.4}$$

Instead of eq. (2.6.18) we now consider the inequality

$$\int [Q_{pq}(x_a) x_a^2]^{\mu} dx_a < \infty, \tag{2.7.5}$$

μ being restricted again to $1 \leq \mu \leq 2$. If eq. (2.7.5) holds true, it follows from Hölder's inequality that

$$\int Q_{pq}(x_a)(1 + x_a)^{-1+\zeta} x_a^2 dx_a < \infty \tag{2.7.6}$$

whenever $\zeta < 1/\mu$. Hence the wave-operator Ω_{a+} certainly exists, the sufficient condition (2.4.18) being fulfilled.

2.7.2. The convergence problem

We proceed to show that, if f_a belongs to $\mathfrak{S}_a$ and each two-body interaction V_{pq} contained in V_a is such that the respective equation (2.7.5) is satisfied, the combination V_a, f_a is admissible. The argument runs in many ways parallel to section 2.6.4, the crucial point being again the proof that $||V_{pq}\exp(-iH_a t)f_a||$ belongs to $\mathfrak{L}(t)$.

Assuming for simplicity that the sum in eq. (2.7.1) consists of only one term and dropping the subscript a, we write

$$\left.\begin{aligned} \exp[i\Delta(\boldsymbol{x})t]f(\boldsymbol{x}) &= (2\pi)^{-\frac{3}{2}} \int \exp[i(-k^2 t + \boldsymbol{k}\cdot\boldsymbol{x})] \hat{f}_{lm}(k) Y_{lm}(\omega_k) d\boldsymbol{k} \\ &= i^l Y_{lm}(\omega_x) \int \exp(-ik^2 t) \frac{1}{\sqrt{kx}} J_{l+\frac{1}{2}}(kx) \hat{f}_{lm}(k) k^2 dk \\ &= \frac{i^{l-1}}{2t} Y_{lm}(\omega_x) \int \exp(-ik^2 t) \left[\frac{l+1}{\sqrt{kx}} J_{l+\frac{1}{2}}(kx) - \sqrt{kx} J_{l+\frac{3}{2}}(kx) + \frac{k}{\sqrt{kx}} J_{l+\frac{1}{2}} \frac{d}{dk} \right] \hat{f}_{lm}(k) dk, \end{aligned}\right\} \tag{2.7.7}$$

the last member following upon integration by parts. Now

$$\sqrt{kx} J_{l+\frac{3}{2}}(kx) = 2(2\pi)^{-\frac{1}{2}} \sin(kx - \tfrac{1}{2} l\pi - \tfrac{1}{2}\pi) + R_{l+\frac{3}{2}}(kx), \tag{2.7.8}$$

where the remainder $R_{l+\frac{3}{2}}(kx)$ does not exceed a constant times $(1+kx)^{-1}$. Also, $(kx)^{-\frac{1}{2}} J_{l+\frac{1}{2}}(kx)$ does not exceed a constant times $(1+kx)^{-1}$. Hence, if we write

$$\left.\begin{aligned} &\exp[i\Delta(\boldsymbol{x})t]f(\boldsymbol{x}) \\ &= \frac{i^{l-1}}{t} Y_{lm}(\omega_x)\int \exp(-ik^2t)[-(2\pi)^{-\frac{1}{2}}\sin(kx-\tfrac{1}{2}l\pi-\tfrac{1}{2}\pi)\hat{f}_{lm}(k)+S(k,x)]dk, \end{aligned}\right\} \tag{2.7.9}$$

the function $S(k,x)$ does not exceed a constant times $(1+kx)^{-1}$. It vanishes if k is larger than some finite K, in virtue of our assumption that $\hat{f}_{lm}$ belongs to $\mathfrak{G}_{lm}$.

Let us now consider the relation

$$\left.\begin{aligned} I_1(t) &\equiv \int W_{pq}(\boldsymbol{x})|Y_{lm}(\omega_x)\int \exp(-ik^2t)\sin(kx-\tfrac{1}{2}l\pi-\tfrac{1}{2}\pi)\hat{f}_{lm}(k)dk|^2d\boldsymbol{x} \\ &< \text{const.}\int Q_{pq}(x)x^2dx\iint \exp[-i(k^2-k'^2)t] \\ &\times[(-1)^l\cos(kx+k'x)+\cos(kx-k'x)]\hat{f}_{lm}(k)\bar{\hat{f}}_{lm}(k')dkdk'. \end{aligned}\right\} \tag{2.7.10}$$

If eq. (2.7.5) holds true for some μ in the interval $1 < \mu \leq 2$, the quantities

$$Z_{X\pm}(k\pm k') = (2\pi)^{-\frac{1}{2}}\int_0^X Q_{pq}(x)x^2\cos(kx\pm k'x)dx \tag{2.7.11}$$

satisfy

$$\left[(2\pi)^{-\frac{1}{2}}\int_{-\infty}^{\infty}|Z_{X\pm}(k\pm k')|^{\mu/(\mu-1)}d(k\pm k')\right]^{(\mu-1)/\mu} \leq \left[(2\pi)^{-\frac{1}{2}}\int_0^X[Q_{pq}(x)x^2]^\mu dx\right]^{1/\mu} \tag{2.7.12}$$

(cf. eq. (2.6.24)). If in eq. (2.7.5) $\mu = 1, Z_{X\pm}$ is bounded uniformly in X. Hence in the third member of eq. (2.7.10)

$$\lim_{X\to\infty}\int_0^X dx\iint dkdk' = \iint dkdk'\lim_{X\to\infty}\int_0^X dx. \tag{2.7.13}$$

Denoting $Z_{\infty\pm}$ by $Z_\pm$, we thus obtain

$$I_1(t) < \iint[(-1)^l Z_+(k+k')+Z_-(k-k')]\exp[-i(k^2-k'^2)t]F(k,k')dkdk', \tag{2.7.14}$$

where F is bounded and vanishes outside a bounded region.

In an obvious notation we now write

$$I_1(t) < I_{1+}(t)+I_{1-}(t). \tag{2.7.15}$$

In terms of the variables

$$k^2-k'^2 = r, \qquad k+k' = v \tag{2.7.16}$$

the function $I_{1+}(t)$ takes the form

$$I_{1+}(t) = \int_{-K^2}^{K^2} dr \int_{|r|}^{2K} dv e^{-irt} Z_+(v) v^{-1} G(v,r), \tag{2.7.17}$$

with some bounded function G. Hence, if $\mu = 1$, $I_{1+}(t)$ is the Fourier transform of $\log|r|$ times a bounded function of r. If $1 < \mu \leq 2$, we have the inequality

$$\int_{|r|}^{2K} |Z_+(v)| v^{-1} dv \leq \left[\int |Z_+(v)|^{\mu/(\mu-1)} dv\right]^{(\mu-1)/\mu} \left[\int_{|r|}^{2K} v^{-\mu} dv\right]^{1/\mu} \leq \text{const.} |r|^{(1-\mu)/\mu}. \tag{2.7.18}$$

In either case $I_{1+}(t)$ is the Fourier transform of a function in $\mathfrak{L}^p(r)$ $(1 < p < 2)$. Hence $I_{1+}(t)$ belongs to $\mathfrak{L}^{p/(p-1)}(t)$. By a similar argument $I_{1-}(t)$ belongs to $\mathfrak{L}^{p/(p-1)}(t)$. Hence so does $I_1(t)$.

We now turn to the term $S(k,x)$ in eq. (2.7.9). This yields a function $I_2(t)$ such that

$$I_2(t) = \iint \exp[-i(k^2 - k'^2)t](kk')^{(1-\mu)/2\mu} H(k,k') dk dk', \tag{2.7.19}$$

where H vanishes outside a bounded region and satisfies

$$\left.\begin{aligned} |H(k,k')| &\leq (kk')^{(\mu-1)/2\mu} \int W_{pq}(\boldsymbol{x}) |Y_{lm}(\omega_x)|^2 |S(k,x) S(k',x)| d\boldsymbol{x} \\ &< \text{const.} (kk')^{(\mu-1)/2\mu} \int Q_{pq}(x) x^2 (1+kx)^{-1} (1+k'x)^{-1} dx \\ < \text{const.} (kk')^{(\mu-1)/2\mu} &\left[\int [Q_{pq}(x) x^2]^\mu dx\right]^{1/\mu} \left[\int [(1+kx)(1+k'x)]^{\mu/(1-\mu)} dx\right]^{(\mu-1)/\mu} < \text{const.} \end{aligned}\right\} \tag{2.7.20}$$

In terms of the variables r and v we have

$$I_2(t) = \int_{-K^2}^{K^2} dr \int_{|r|}^{2K} dv e^{-irt} \left(v^2 - \frac{r^2}{v^2}\right)^{(1-\mu)/2\mu} v^{-1} J(v,r), \tag{2.7.21}$$

with some bounded function J. If $1 < \mu \leq 2$, the substitution $v^4 = r^2 q$ yields

$$\left.\int_{|r|}^{2K} \left|v^2 - \frac{r^2}{v^2}\right|^{(1-\mu)/2\mu} v^{-1} dv \leq \tfrac{1}{4} |r|^{(1-\mu)/2\mu} \int_0^\infty |q-1|^{(1-\mu)/2\mu} q^{-(3\mu+1)/4\mu} dq < \text{const.} |r|^{(1-\mu)/2\mu}.\right\} \tag{2.7.22}$$

From this it follows that $I_2(t)$ is the Fourier transform of a function in $\mathfrak{L}^p(r)$ $(1 < p \leq 2)$. If $\mu = 1$, the same result holds true by a simpler argument. Hence in either case $I_2(t)$ belongs to $\mathfrak{L}^{p/(p-1)}(t)$.

We are now in a situation analogous to the one discussed in section 2.6.4. The function $\exp(-iH_a t)f_a$ can be written in the form $\sum_i f_i(t)$, as in eq. (2.6.34). The functions $||V_{pq}f_i(t)||$ satisfy eq. (2.6.35). Hence $||V_{pq}\exp(-iH_a t)f_a||$ is integrable over $-\infty < t < -1$ and $1 \leq t < \infty$. Also, since f_a belongs to $\mathfrak{D}(H_0)$, $||V_{pq}\exp(-iH_a t)f_a||$ is a bounded function of t. From this it follows as before that $||V_a\exp(-iH_a t)f_a||$ is bounded and belongs to $\mathfrak{L}(t)$. Hence the combination V_a, f_a is admissible, as we wished to show.

Thus far it has been assumed that the sum in eq. (2.7.1) consists of only one term. However, if both V_a, f_{a1} and V_a, f_{a2} are admissible, so is $V_a, f_{a1} + f_{a2}$. Hence in eq. (2.7.1) we may admit any finite number of terms. In other words, V_a, f_a is admissible whenever f_a belongs to $\mathfrak{G}_a$ and each function Q_{pq} satisfies eq. (2.7.5). This result can easily be extended to functions Q_{pq} which satisfy

$$\int_0^R Q_{pq}(x_a)x_a^2 dx_a < \infty, \quad Q_{pq}(x_a) < \text{const.}x_a^{-2-\eta} \quad (x_a > R) \tag{2.7.23}$$

for some positive η. The proof is omitted since, after the foregoing, it is completely straightforward.

2.7.3. Examples of admissible interactions

In the present section we give a short summary of some sufficient conditions on V_{pq} under which eq. (2.7.5) or eq. (2.7.23) is satisfied. It is obvious that, if V_{pq} is square-integrable, eq. (2.7.5) holds true for $\mu = 1$. To obtain a sufficient condition characterized by $\mu = 2$, we observe that

$$[Q_{pq}(x_a)]^2 < 4\pi \int [W_{pq}(\boldsymbol{x}_a)]^2 d\omega_{x_a}. \tag{2.7.24}$$

Hence eq. (2.7.5) holds true for $\mu = 2$ if

$$\int [W_{pq}(\boldsymbol{x}_a)x_a]^2 d\boldsymbol{x}_a < \infty. \tag{2.7.25}$$

To reduce this inequality to a condition on V_{pq}, we require some information as regards the asymptotic behaviour of φ_a. If this is such that eq. (2.6.49) is satisfied for $\alpha = \frac{1}{2}$, eq. (2.7.25) holds true whenever

$$\int [V_{pq}(\boldsymbol{X})]^4 X^2 d^3\boldsymbol{X} < \infty, \qquad \int [V_{pq}(\boldsymbol{X})]^4 d^3\boldsymbol{X} < \infty. \tag{2.7.26}$$

If it is known that in eq. (2.6.49) α may be as large as $\frac{1}{2} + \frac{1}{2}\eta$, with some positive η, the condition V_{pq} has to satisfy at infinity can further be relaxed. In this case it is sufficient if

$$\int_0^R [V_{pq}(\boldsymbol{X})]^2 d^3\boldsymbol{X} < \infty, \quad |V_{pq}(\boldsymbol{X})| < \text{const.} X^{-1-\frac{1}{2}\eta} \quad (X > R). \tag{2.7.27}$$

These statements are easily checked with the methods given in section 2.6.6.

2.7.4. The scattering operators in momentum space

Under the assumptions that f_a belongs to $\mathfrak{H}_a$ and that the interaction V_a is a linear combination of terms satisfying either eq. (2.7.5) or eq. (2.7.23), we proceed to express the quantity $(g_b, S_{ba} f_a)$ in terms of the Fourier transforms $\hat{f}$ and $\hat{g}$. This is most easily done with the help of section 2.6.7. It is obvious that for section 2.6.7 to be valid, it is essential that Ω_{a+} and Ω_{b-} exist. Apart from this we merely need the fact that $||V_a \exp(-iH_a t) f_a||$ is a bounded and integrable function of t, and, in connection with eq. (2.6.64), that $V_a P_a(X_a)\varphi_a$ belongs to $\mathfrak{L}^2$. Since these conditions are satisfied under the present assumptions, section 2.6.7 can be copied unchanged. In particular, if eq. (2.6.67) is combined with eq. (2.7.1), we obtain

$$\left.\begin{aligned} (g_b, S_{ba} f_a) &= \delta_{ba}(g_b, f_a) \\ &+ \tfrac{1}{4} i^{l+1} (2\pi)^{-\frac{3}{2}m_b + \frac{5}{2}} \lim_{\varepsilon \to 0} \lim_{X_b \to \infty} \sum_{l=0}^{L} \sum_{m} \int dE \int d\omega_{k_b} k_b^{3m_b - 5} k_a^{\frac{1}{2}} \bar{\hat{g}}(\boldsymbol{k}_b) F(\boldsymbol{k}_b, l, m; \varepsilon; X_b) \hat{f}_{lm}(k_a), \\ F(\boldsymbol{k}_b, l, m; \varepsilon; X_b) &= (P_b(X_b)\varphi_b e^{i\boldsymbol{k}_b \cdot \boldsymbol{x}_b}, [-1 + V_b R(E + i\varepsilon)] V_a \varphi_a \frac{1}{\sqrt{x_a}} J_{l+\frac{1}{2}}(k_a x_a) Y_{lm}(\omega_{x_a})). \end{aligned}\right\} \tag{2.7.28}$$

In this expression the limit with respect to X_a has been performed in the integrand. This is permitted since under the present assumptions

$$V_a(\boldsymbol{x}'_a, \boldsymbol{x}_a)\varphi_a(\boldsymbol{x}'_a) \frac{1}{\sqrt{x_a}} J_{l+\frac{1}{2}}(k_a x_a) Y_{lm}(\omega_{x_a}) \tag{2.7.29}$$

belongs to $\mathfrak{L}^2(\boldsymbol{x}'_a, \boldsymbol{x}_a)$.

Thus far eq. (2.7.28) is restricted to functions f_a in $\mathfrak{H}_a$. We now show that, if, given V_a, there is an equation of the form (2.7.28) for any particular f_a, then there is a similar equation for $E_a(K^2) f_a$. Since in general $E_a(K^2) f_a$ does not belong to $\mathfrak{H}_a$, the validity of eq. (2.7.28) is thus extended to a larger class of functions f_a. This is of practical importance in future sections.

The proof of our assertion is based on a straightforward generalization of eq. (2.2.28), according to which

$$E_b(K^2) S_{ba} = S_{ba} E_a(K^2). \tag{2.7.30}$$

Let us now assume that V_a and f_a are such that $(g_b, S_{ba} f_a)$ can be evaluated with the help of eq. (2.7.28). Then $(E_b(K^2) g_b, S_{ba} f_a)$ can also be evaluated with eq. (2.7.28). This is due to the fact that we do not have to impose any special restrictions on $\hat{g}$,

apart from its belonging to $\mathfrak{Q}^2$. Now according to eq. (2.5.21), the operator $E_b(K^2)$ transforms $\hat{g}(\boldsymbol{k}_b)$ into a function which is equal to $\hat{g}(\boldsymbol{k}_b)$ if $0 < k_b < (K^2 - \lambda_b)^{\frac{1}{2}}$ and vanishes if $k_b > (K^2 - \lambda_b)^{\frac{1}{2}}$. Hence, to find $(E_b(K^2)g_b, S_{ba}f_a)$ with the help of eq. (2.7.28), we merely have to restrict the integration with respect to E to the interval $\max(\lambda_a, \lambda_b) < E \leq K^2$ (cf. eq. (2.6.65)). But this restricting the integration is tantamount to replacing f_a by $E_a(K^2)f_a$. Hence we are in effect replacing f_a by $E_a(K^2)f_a$, and we are evaluating $(g_b, S_{ba}E_a(K^2)f_a)$, by eq. (2.7.30). This can thus be done with eq. (2.7.28), as we wished to show.

It is appropriate to call a function defined in $0 \leq k < \infty$ a step-function if it is constant in some interval $0 < k < K$ and vanishes if $k > K$. In this terminology, we may say that, if f_a belongs to $\mathfrak{H}_a$, so that $\hat{f}_{lm}$ belongs to $\hat{\mathfrak{H}}_{lm}$, the operator $E_a(K^2)$ transforms $\hat{f}_{lm}$ into a step-function times a function in $\hat{\mathfrak{H}}_{lm}$. We now denote the set consisting of all linear combinations of step-functions by $\mathfrak{S}$. If $\hat{f}_{lm}$ is the product of a function in $\mathfrak{S}$ times a function in $\hat{\mathfrak{H}}_{lm}$, we say that it belongs to $\mathfrak{S}\hat{\mathfrak{H}}_{lm}$. Likewise, if $\hat{f}$ is of the form (2.7.1) and each $\hat{f}_{lm}$ belongs to $\mathfrak{S}\hat{\mathfrak{H}}_{lm}$, we say that $\hat{f}$ belongs to $\mathfrak{S}\hat{\mathfrak{H}}$, f to $\mathfrak{S}\mathfrak{H}$, and f_a to $\mathfrak{S}\mathfrak{H}_a$. It will be observed that $\mathfrak{S}\mathfrak{H}_a$ contains $\mathfrak{H}_a$ as a subset. It follows from the foregoing that for eq. (2.7.28) to be valid, it is sufficient if f_a belongs to $\mathfrak{S}\mathfrak{H}_a$ and V_a satisfies eq. (2.7.5) or eq. (2.7.23).

2.7.5. Partial waves

Thus far no assumption has been made as regards the behaviour of the interaction under rotations in coordinate space. The remaining part of this investigation is devoted to systems in which each two-body interaction V_{ij} is spherically symmetric. This case permits a number of interesting simplifications owing to the conservation of angular momentum. In discussing these, we make the additional restriction that the system is split into two fragments both in the initial and in the final channel.

If the interaction is spherically symmetric, it can be assumed without loss of generality that the eigenfunctions $\varphi_{(j)}(\boldsymbol{x}_j)$ are also eigenfunctions of angular momentum. For simplicity we even assume in the following that $\varphi_a(\boldsymbol{x}'_a)$ and $\varphi_b(\boldsymbol{x}'_b)$ are eigenfunctions of angular momentum 0. This is a far-reaching restriction, which is, however, not essential. It is made only to separate the subject of the present investigation from problems in the field of Clebsch-Gordan coefficients.

If the eigenfunctions $\varphi_{(j)}(\boldsymbol{x}_j)$ do not correspond to angular momentum 0, a function f_a of the product-form $\varphi_a(\boldsymbol{x}'_a)f(\boldsymbol{x}_a)$ will not be an eigenfunction of the total angular momentum. In this case the eigenvalues $\lambda_{(j)}$ will be degenerate. Hence there will be functions $f_a, f_b, \ldots$ with $\lambda_a = \lambda_b = \ldots$, as in eq. (2.3.5). It may be convenient to use asymptotic wave-functions which are eigenfunctions of angular momentum. This can be achieved if, instead of defining the channels as in eq. (2.3.5), one takes as asymptotic wave-functions suitable linear combinations of functions of the form (2.3.5). This leads to a modification of the formalism which is left to the reader.

Analysing eq. (2.7.28) from the point of view of spherical symmetry, we recall

that in channel a we are using a three-dimensional coordinate $\boldsymbol{x}_a$ plus a coordinate $\boldsymbol{x}'_a$ which, in fact, is a set of $n-2$ three-dimensional coordinates $\boldsymbol{x}_j$, where n is the total number of particles. Let us now imagine that there is a three-dimensional coordinate frame in which both $\boldsymbol{x}_j$ ($j = 1,\ldots,n-2$) and $\boldsymbol{x}_a$ are measured, and let us rotate this frame through Euler angles ω. This changes $\boldsymbol{x}_j,\boldsymbol{x}_a$ into $D(\omega)\boldsymbol{x}_j, D(\omega)\boldsymbol{x}_a$. Combining $\boldsymbol{x}_j,\boldsymbol{x}_a$ into a $(3n-3)$-dimensional coordinate $\boldsymbol{x}$, it is convenient to write

$$f(D(\omega)\boldsymbol{x}_j,D(\omega)\boldsymbol{x}_a) = f(D(\omega)\boldsymbol{x}) = D(\omega)f(\boldsymbol{x}).$$

In this notation the assumption of spherical symmetry implies

$$D(\omega)V_{ij} = V_{ij}D(\omega), \qquad D(\omega)R(\lambda) = R(\lambda)D(\omega).$$

If φ_a is an eigenfunction of angular momentum with eigenvalue 0,

$$D(\omega)\varphi_a = \varphi_a, \tag{2.7.31}$$

and similarly for φ_b. Also,

$$\left.\begin{aligned} D(\omega)Y_{lm}(\omega_{x_a}) &= \sum_{m'} D^l_{m'm}(\omega)\,Y_{lm'}(\omega_{x_a}),\\ D(\omega)e^{i\boldsymbol{k}_b\cdot\boldsymbol{x}_b} &= (2\pi)^{\frac{3}{2}}\sum_{l=0}^{\infty}\sum_{m,m'}\frac{i^l}{\sqrt{k_b x_b}}J_{l+\frac{1}{2}}(k_b x_b)\,\overline{Y}_{lm}(\omega_{k_b})D^l_{m'm}(\omega)\,Y_{lm'}(\omega_{x_b}),\end{aligned}\right\} \tag{2.7.32}$$

the functions $D^l_{m'm}$ being orthogonal and having norm $2\pi\sqrt{2}(2l+1)^{-\frac{1}{2}}$ (Rose (28) sections 14,16). Now obviously

$$(g,f) = (D(\omega)g,D(\omega)f) = (8\pi^2)^{-1}\int (D(\omega)g,D(\omega)f)\,d\omega. \tag{2.7.33}$$

Hence, with eq. (2.7.28),

$$\left.\begin{aligned} F(\boldsymbol{k}_b,l,m;\varepsilon;X_b) &= \frac{(-i)^l(2\pi)^{\frac{3}{2}}}{2l+1}\frac{1}{\sqrt{k_b}}Y_{lm}(\omega_{k_b})\\ \times\sum_{m'}(P_b(X_b)\varphi_b\frac{1}{\sqrt{x_b}}J_{l+\frac{1}{2}}(k_b x_b)\,Y_{lm'}(\omega_{x_b}),&[-1+V_bR(E+i\varepsilon)]V_a\varphi_a\frac{1}{\sqrt{x_a}}J_{l+\frac{1}{2}}(k_a x_a)\,Y_{lm'}(\omega_{x_a})).\end{aligned}\right\} \tag{2.7.34}$$

A second application of eq. (2.7.33) shows that the inner product in eq. (2.7.34) does not depend on m'. Developing $\hat{g}(\boldsymbol{k}_b)$ in spherical harmonics, we thus obtain

$$\left.\begin{aligned} (g_b,S_{ba}f_a) &= \tfrac{1}{2}\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\sum_{l=0}^{L}\sum_{m}\int \bar{\hat{g}}_{lm}(k_b)S_{ba}(E,l;\varepsilon;X_b)\hat{f}_{lm}(k_a)\sqrt{k_b k_a}\,dE,\\ S_{ba}(E,l;\varepsilon;X_b) &= \delta_{ba}\\ +\pi i(P_b(X_b)\varphi_b\frac{1}{\sqrt{x_b}}J_{l+\frac{1}{2}}(k_b x_b)\,Y_{l0}(\omega_{x_b}),&[-1+V_bR(E+i\varepsilon)]V_a\varphi_a\frac{1}{\sqrt{x_a}}J_{l+\frac{1}{2}}(k_a x_a)\,Y_{l0}(\omega_{x_a})).\end{aligned}\right\} \tag{2.7.35}$$

This equation holds true whenever f_a belongs to $\mathfrak{S}\mathfrak{B}_a$ and V_a satisfies eq. (2.7.5) or eq. (2.7.23). It is obvious that V_b must be such that the operator Ω_{b-} exists. Defining

$$\chi_{bl} = \varphi_b(\boldsymbol{x}_b') \frac{1}{\sqrt{x_b}} J_{l+\frac{1}{2}}(k_b x_b) Y_{l0}(\omega_{x_b}), \tag{2.7.36}$$

we can say that in many cases of practical interest the quantity $V_b\chi_{bl}$ belongs to $\mathfrak{L}^2$. This is particularly so if the sufficient condition (2.4.18) is satisfied. If $V_{bl}\chi_{bl}$ belongs to $\mathfrak{L}^2$, we may write

$$\left.\begin{aligned} (g_b,S_{ba}f_a) &= \tfrac{1}{2}\{\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\}\sum_{l=0}^{L}\sum_{m}\int \bar{\hat{g}}_{lm}(k_b)\tilde{S}_{ba}(E,l;\varepsilon;X_b)\hat{f}_{lm}(k_a)\sqrt{k_b k_a}\,dE, \\ \tilde{S}_{ba}(E,l;\varepsilon;X_b) &= \delta_{ba} - \pi i(P_b(X_b)\chi_{bl}, V_a\chi_{al}) + \pi i(V_b\chi_{bl}, R(E+i\varepsilon)V_a\chi_{al}), \end{aligned}\right\} \tag{2.7.37}$$

χ_{al} being defined by a relation similar to eq. (2.7.36).

If V_b satisfies eq. (2.7.5) or eq. (2.7.23) and g_b belongs to $\mathfrak{S}\mathfrak{B}_b$, it only requires a slight modification of the argument from eq. (2.6.1) onwards to show that in eq. (2.7.35) the function $S_{ba}(E,l;\varepsilon;X_b)$ may be replaced by

$$S_{ba}(E,l;\varepsilon;X_a) = \delta_{ba} + \pi i(V_b\chi_{bl}, [-1 + R(E+i\varepsilon)V_a]P_a(X_a)\chi_{al}). \tag{2.7.38}$$

The limit with respect to X_b has now already been performed in the integrand, but there appears a limit with respect to X_a. The fact that this replacement yields the same limit as before is directly connected with eq. (2.6.8). If both V_a and V_b satisfy eq. (2.7.5) or eq. (2.7.23) and f_a and g_b belong to $\mathfrak{S}\mathfrak{B}_a$ and $\mathfrak{S}\mathfrak{B}_b$, respectively, we have

$$\left.\begin{aligned} (g_b,S_{ba}f_a) &= \tfrac{1}{2}\{\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\lim_{X_a\to\infty}\}\sum_{l=0}^{L}\sum_{m}\int \bar{\hat{g}}_{lm}(k_b)\tilde{\tilde{S}}_{ba}(E,l;\varepsilon;X_b,X_a)\hat{f}_{lm}(k_a)\sqrt{k_b k_a}\,dE, \\ \tilde{\tilde{S}}_{ba}(E,l;\varepsilon;X_b,X_a) &= \delta_{ba} - \tfrac{1}{2}\pi i(P_b(X_b)\chi_{bl}, V_a\chi_{al}) - \tfrac{1}{2}\pi i(V_b\chi_{bl}, P_a(X_a)\chi_{al}) \\ &\quad + \pi i(V_b\chi_{bl}, R(E+i\varepsilon)V_a\chi_{al}). \end{aligned}\right\} \tag{2.7.39}$$

2.7.6. The scattering matrix

Let us consider eq. (2.7.35) for the special case

$$\left.\begin{aligned} \hat{f}_{lm}(k_a) &= 1, \qquad \hat{g}_{lm}(k_b) = \sqrt{k_a/k_b} \qquad (\max(\lambda_a,\lambda_b) \le E_1 < E < E_2), \\ \hat{f}_{lm}(k_a) &= 0, \qquad \hat{g}_{lm}(k_b) = 0 \qquad (E < E_1, \quad E > E_2). \end{aligned}\right\} \tag{2.7.40}$$

This is compatible with the condition that $\hat{f}_{lm}$ must belong to $\mathfrak{S}\hat{\mathfrak{B}}_{lm}$. In view of the inequality

$$|(g_b,S_{ba}f_a)| \le ||g_b||\,||f_a|| \tag{2.7.41}$$

it yields

$$|\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\int_{E_1}^{E_2} S_{ba}(E,l;\varepsilon;X_b)k_a dE| \leq \int_{E_1}^{E_2} k_a dE. \tag{2.7.42}$$

If we now define

$$\Sigma_{ba}(E,l) = \lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\int_{\max(\lambda_a,\lambda_b)}^{E} S_{ba}(E',l;\varepsilon;X_b)k'_a dE', \tag{2.7.43}$$

eq. (2.7.42) shows that $\Sigma_{ba}(E,l)$ is an absolutely continuous function of E. Hence there exists a function $S_{ba}(E,l)k_a$ such that

$$\Sigma_{ba}(E,l) = \int_{\max(\lambda_a,\lambda_b)}^{E} S_{ba}(E',l)k'_a dE', \tag{2.7.44}$$

$S_{ba}(E,l)k_a$ being the derivative of $\Sigma_{ba}(E,l)$ for almost every E in the interval

$$\max(\lambda_a,\lambda_b) \leq E < \infty. \tag{2.7.45}$$

According to eq. (2.7.42)

$$\left|\int_{E_1}^{E_2} S_{ba}(E,l)k_a dE\right| \leq \int_{E_1}^{E_2} k_a dE. \tag{2.7.46}$$

It is shown in section 2.7.8 that from this it follows that

$$|\mathrm{Re}S_{ba}(E,l)| \leq 1, \qquad |\mathrm{Im}S_{ba}(E,l)| \leq 1 \tag{2.7.47}$$

almost everywhere in the interval (2.7.45).

Let us now consider a function $\hat{f}_{lm}(k_a)$ which takes the value 1 in $E_1 < E < E_2$ and is sufficiently smooth to belong to $\mathfrak{H}_{lm}$. If f_a stands for φ_a times the Fourier transform of $\hat{f}_{lm}(k_a)Y_{lm}(\omega_{k_a})$ and V_a satisfies eq. (2.7.5) or (2.7.23), then $||V_a\exp(-iH_at)f_a||$ is bounded and belongs to $\mathfrak{L}(t)$. If g_b is equal to φ_b times the Fourier transform of $\hat{g}_{lm}(k_b)Y_{lm}(\omega_{k_b})$, where $\hat{g}_{lm}$ is the same function as in eq. (2.7.40), we have

$$\left.\begin{aligned} \tfrac{1}{2}\int_{E_1}^{E_2} S_{ba}(E,l;\varepsilon;X_b)k_a dE &= \delta_{ba}(g_b,f_a) \\ -\int_{-\infty}^{\infty}\left[i(g_b,e^{iH_bt}P_b(X_b)V_ae^{-iH_at}f_a) + \int_0^{\infty} e^{-\varepsilon s}(g_b,e^{iH_b(s+t)}P_b(X_b)V_be^{-iHs}V_ae^{-iH_at}f_a)ds\right]dt. \end{aligned}\right\} \tag{2.7.48}$$

This follows from eq. (2.6.1) and the beginning of section 2.6.7.

As long as ε is positive, either side of eq. (2.7.48) is bounded uniformly in X_b, by the argument of eq. (2.6.60). If E_2 is held fixed, $||H_0g_b||$ does not exceed $||g_b||$

times a constant determined by E_2. Hence, in view of eq. (2.6.60), either side of eq. (2.7.48) is less than

$$\text{const.}||g_b||/\varepsilon = \text{const.}\Big[\int_{E_1}^{E_2} k_a dE\Big]^{\frac{1}{2}}/\varepsilon. \tag{2.7.49}$$

If X_b tends to ∞, the second term in the square brackets in eq. (2.7.48) tends to

$$i(g_b, e^{iH_b t}[\Omega^{*}_{b-,\varepsilon} - 1]V_a e^{-iH_a t} f_a). \tag{2.7.50}$$

Hence, since $||\Omega_{b-,\varepsilon}||$ is bounded uniformly in ε,

$$|\lim_{X_b\to\infty}\int_{E_1}^{E_2} S_{ba}(E,l;\varepsilon;X_b)k_a dE| < \text{const.}\Big[\int_{E_1}^{E_2} k_a dE\Big]^{\frac{1}{2}}. \tag{2.7.51}$$

We want to use these estimates to study the relation

$$\left.\begin{aligned}\int_{E_1}^{E_2} S_{ba}(E,l;\varepsilon;X_b)\sqrt{k_b k_a}\,dE &= \frac{\sqrt{k_b}}{\sqrt{k_a}}\Big|_{E_2}\int_{E_1}^{E_2} S_{ba}(E,l;\varepsilon;X_b)k_a dE \\ &+ \tfrac{1}{4}\int_{E_1}^{E_2}\frac{\sqrt{k_b}}{\sqrt{k_a}}\Big(\frac{1}{k_b^2}-\frac{1}{k_a^2}\Big)\Big[\int_{E_1}^{E} S_{ba}(E',l;\varepsilon;X_b)k'_a dE'\Big]dE.\end{aligned}\right\} \tag{2.7.52}$$

If $k_a > 0$ at the point $E = E_1$, eq. (2.7.52) is straightforward. If $E_1 = \lambda_a$, there might be convergence difficulties. However, let ε be positive. The estimate (2.7.49) then shows that, even if $E_1 = \lambda_a$, eq. (2.7.52) is completely correct. In the second term on the right the integrand is less than an integrable function of E which does not depend on X_b. Hence in this particular term

$$\lim_{X_b\to\infty}\int_{E_1}^{E_2}\Big[\int_{E_1}^{E} dE'\Big]dE = \int_{E_1}^{E_2}\lim_{X_b\to\infty}\Big[\int_{E_1}^{E} dE'\Big]dE, \tag{2.7.53}$$

by the theorem of dominated convergence. With the help of eq. (2.7.51) the argument can now be extended to show that in fact

$$\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\int_{E_1}^{E_2}\Big[\int_{E_1}^{E} dE'\Big]dE = \int_{E_1}^{E_2}\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\Big[\int_{E_1}^{E} dE'\Big]dE. \tag{2.7.54}$$

Combing this result with eq. (2.7.52) yields

$$\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\int_{E_1}^{E_2} S_{ba}(E,l;\varepsilon;X_b)\sqrt{k_b k_a}\,dE = \int_{E_1}^{E_2} S_{ba}(E,l)\sqrt{k_b k_a}\,dE. \tag{2.7.55}$$

Now let $\hat{f}_{lmM}$ and $\hat{g}_{lmN}$ be any two functions in $\mathfrak{S}\hat{\mathfrak{G}}_{lm}$. Integration by parts as in eq. (2.7.52) shows that

$$\left.\begin{aligned}\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\int \bar{\hat{g}}_{lmN}(k_b)S_{ba}(E,l;\varepsilon;X_b)\bar{\hat{f}}_{lmM}(k_a)\sqrt{k_bk_a}\,dE \\ = \int \bar{\hat{g}}_{lmN}(k_b)S_{ba}(E,l)\hat{f}_{lmM}(k_a)\sqrt{k_bk_a}\,dE.\end{aligned}\right\} \quad (2.7.56)$$

Hence, in view of eq. (2.7.35),

$$(g_{bN},S_{ba}f_{aM}) = \tfrac{1}{2}\int \bar{\hat{g}}_{lmN}(k_b)S_{ba}(E,l)\hat{f}_{lmM}(k_a)\sqrt{k_bk_a}\,dE. \quad (2.7.57)$$

If $\hat{f}_{lm}$ is any function satisfying eq. (2.7.2), there is a sequence $\hat{f}_{lmM}$ in $\mathfrak{S}\hat{\mathfrak{G}}_{lm}$ such that

$$\lim_{M\to\infty}\int_0^\infty |\hat{f}_{lm}(k_a)-\hat{f}_{lmM}(k_a)|^2k_a^2dk_a = 0, \quad (2.7.58)$$

and similarly for $\hat{g}_{lm}$. Now S_{ba} is a bounded operator. Also, $S_{ba}(E,l)$ is a bounded function, by eq. (2.7.47). Letting M and N tend to ∞, we thus obtain

$$\lim_{N,M\to\infty}(g_{bN},S_{ba}f_{aM}) = (g_b,S_{ba}f_a) = \tfrac{1}{2}\int \bar{\hat{g}}_{lm}(k_b)S_{ba}(E,l)\hat{f}_{lm}(k_a)\sqrt{k_bk_a}\,dE, \quad (2.7.59)$$

even for the most general functions $\hat{f}_{lm}$ and $\hat{g}_{lm}$ we may want to consider.

With eq. (2.7.35) it follows that

$$\left.\begin{aligned}\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\int \bar{\hat{g}}_{lm}(k_b)S_{ba}(E,l;\varepsilon;X_b)\hat{f}_{lm}(k_a)\sqrt{k_bk_a}\,dE \\ = \int \bar{\hat{g}}_{lm}(k_b)S_{ba}(E,l)\hat{f}_{lm}(k_a)\sqrt{k_bk_a}\,dE\end{aligned}\right\} \quad (2.7.60)$$

whenever $\hat{f}_{lm}$ belongs to $\mathfrak{S}\hat{\mathfrak{G}}_{lm}$ and $\hat{g}_{lm}$ satisfies a relation of the form (2.7.2). Here it is understood that V_a satisfies eq. (2.7.5) or eq. (2.7.23). If, in addition, V_b is such that $V_b\chi_{bl}$ belongs to $\mathfrak{L}^2$, the function $S_{ba}(E,l;\varepsilon;X_b)$ may be replaced by the function $\tilde{S}_{ba}(E,l;\varepsilon;X_b)$ defined in eq. (2.7.37).

If in eq. (2.7.59) we choose in particular

$$\left.\begin{aligned}\hat{g}_{lm}(k_b) = \hat{f}_{lm}(k_a) = 0 \qquad (E < \max(\lambda_a,\lambda_b)), \\ \hat{g}_{lm}(k_b) = S_{ba}(E,l)\hat{f}_{lm}(k_a)\sqrt{k_a/k_b} \qquad (E > \max(\lambda_a,\lambda_b)),\end{aligned}\right\} \quad (2.7.61)$$

the inequality (2.7.41) gives

$$\int_{\max(\lambda_a,\lambda_b)} |S_{ba}(E,l)\hat{f}_{lm}(k_a)|^2k_adE \leq \int_{\max(\lambda_a,\lambda_b)} |\hat{f}_{lm}(k_a)|^2k_adE. \quad (2.7.62)$$

Since this must hold true whenever the right-hand side is finite, it follows that

$$|S_{ba}(E,l)| \leq 1 \tag{2.7.63}$$

almost everywhere in the interval (2.7.45).

2.7.7. Properties of the scattering matrix

In the present section we assume that V_b satisfies eq. (2.4.25), so that all functions in $\mathfrak{S}_b$ are of the form $\varphi_b(\boldsymbol{x}'_b)h(\boldsymbol{x}_b)$. Then

$$S_{ba}\varphi_a(\boldsymbol{x}'_a)\int e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a}\hat{f}_{lm}(k_a)Y_{lm}(\omega_{k_a})d\boldsymbol{k}_a = \varphi_b(\boldsymbol{x}'_b)\int e^{i\boldsymbol{k}_b\cdot\boldsymbol{x}_b}\hat{h}_{lm}(k_b)Y_{lm}(\omega_{k_b})d\boldsymbol{k}_b, \tag{2.7.64}$$

where $\hat{h}_{lm}$ satisfies

$$\int \bar{\hat{g}}_{lm}(k_b)\hat{h}_{lm}(k_b)k_b dE = \int \bar{\hat{g}}_{lm}(k_b)S_{ba}(E,l)\hat{f}_{lm}(k_a)\sqrt{k_b k_a}\,dE, \tag{2.7.65}$$

by eq. (2.7.59). Hence

$$\left.\begin{aligned} &S_{ba}\varphi_a(\boldsymbol{x}'_a)\int e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a}\hat{f}_{lm}(k_a)Y_{lm}(\omega_{k_a})d\boldsymbol{k}_a \\ &= \varphi_b(\boldsymbol{x}'_b)\int e^{i\boldsymbol{k}_b\cdot\boldsymbol{x}_b}S_{ba}(E,l)\hat{f}_{lm}(k_a)Y_{lm}(\omega_{k_b})\sqrt{k_a/k_b}\,d\boldsymbol{k}_b. \end{aligned}\right\} \tag{2.7.66}$$

If $\lambda_a < \lambda_b$ and $\hat{f}_{lm}(k_a)$ vanishes except in the interval $\lambda_a \leq E \leq \lambda_b$, the right-hand side of eq. (2.7.65) vanishes. This means that $S_{ba}f_a = 0$. It is obvious from eq. (2.6.67) that this situation arises whenever $\hat{f}(k_a)$ vanishes outside $\lambda_a \leq E \leq \lambda_b$. It does not matter whether in channels a and b the system is split into only two fragments. It is therefore appropriate to call λ_b the threshold for scattering into channel b, channel b being open or closed according as $E > \lambda_b$ or $E < \lambda_b$.

Now let $\hat{f}_{lm}(k_a)$ be zero except in an interval I in which there are no thresholds. Let the channels which are open in I all refer to splittings into two fragments, the respective functions φ_b all having angular momentum 0. The scattering with initial state f_a can then be described completely in terms of a set of scattering functions $S_{ba}(E,l)$, the parameter b running through all open channels. Let us now assume that there is unitarity in the sense of section 2.3.5. If eq. (2.3.33) holds true we have

$$\sum_b (S_{bc}g_c, S_{ba}f_a) = \delta_{ca}(g_c, f_a). \tag{2.7.67}$$

With eq. (2.7.66) this yields

$$\sum_b \int_I \bar{\hat{g}}_{lm}(k_c)\bar{S}_{bc}(E,l)S_{ba}(E,l)\hat{f}_{lm}(k_a)\sqrt{k_c k_a}\,dE = \delta_{ca}\int_I \bar{\hat{g}}_{lm}(k_c)\hat{f}_{lm}(k_a)\sqrt{k_c k_a}\,dE. \tag{2.7.68}$$

Hence, since $\hat{f}_{lm}$ and $\hat{g}_{lm}$ are arbitrary,

$$\sum_b \bar{S}_{bc}(E,l)S_{ba}(E,l) = \delta_{ca}, \tag{2.7.69}$$

it being understood that E is restricted to a certain interval I in which the channels a and c are open, the summation including all open channels and no closed ones.

In the present problem it is useful to consider the conjugation C which transforms f_a into $\bar{f}_a$. This can be discussed along the lines of section 2.3.6. Since φ_a refers to angular momentum 0, it may be assumed without loss of generality that φ_a is real. Hence in eq. (2.3.54) $a' = a$. Therefore,

$$(g_b, \Omega^*_{b+}\Omega_{a-}f_a) = (C\Omega_{a-}f_a, C\Omega_{b+}g_b) = (\Omega_{a+}\bar{f}_a, \Omega_{b-}\bar{g}_b) = (S_{ba}\bar{f}_a, \bar{g}_b). \tag{2.7.70}$$

Equation (2.7.59) now gives

$$(g_b,\Omega^*_{b+}\Omega_{a-}f_a) = \tfrac{1}{2}\int \bar{\hat{g}}_{lm}(k_b)\bar{S}_{ba}(E,l)\hat{f}_{lm}(k_a)\sqrt{k_b k_a}\,dE. \tag{2.7.71}$$

This shows that, if $S_{ba}(E,l)$ corresponds to $\Omega^*_{b-}\Omega_{a+}$, the function $\bar{S}_{ba}(E,l)$ corresponds to $\Omega^*_{b+}\Omega_{a-}$. Also, since the left-hand side of eq. (2.7.71) is nothing but $(S_{ab}g_b,f_a)$,

$$S_{ab}(E,l) = S_{ba}(E,l) \tag{2.7.72}$$

almost everywhere in the interval (2.7.45). Combining this result with eq. (2.7.69), we see that, if in the interval I the functions $S_{ba}(E,l)$ are considered as the elements of a matrix $\mathcal{S}(E,l)$, this matrix is unitary and symmetric.

The symmetry of $\mathcal{S}(E,l)$ is simply due to the Hamiltonian commuting with the conjugation C. It must be stressed that, to obtain the unitarity, we had to assume that eq. (2.3.33) holds true. Now it was remarked already at the end of section 2.3.4 that we do not know what conditions on the interaction are sufficient for eq. (2.3.33) to be satisfied. Hence we do not really have any insight into the question of unitarity.

2.7.8. An auxiliary formula

We must still justify eq. (2.7.47). This has been used to obtain eq. (2.7.59) and is thus an essential step in the argument. Simplifying the notation of eq. (2.7.46), we consider a function $S(E)$ which is defined in an interval I_0 and satisfies

$$\left|\int_I S(E)dE\right| < m(I), \tag{2.7.73}$$

I denoting any particular interval contained in I_0, and $m(I)$ its measure. Decomposing S into its real and imaginary parts, $S = A + iB$, we want to show that $|A| \leq 1$, $|B| \leq 1$ almost everywhere in I_0.

Let us now suppose that $|A| > 1$ in a set U of positive measure. Let us suppose in particular that $A > 1$ in U. Then

$$\int_U A(E)dE > m(U) > 0. \tag{2.7.74}$$

From this it follows that there is a positive number η such that

$$\int_U A(E)dE > m(U) + 2\eta. \tag{2.7.75}$$

The set U is not necessarily an interval, hence there is not yet a contradiction with eq. (2.7.73). However, we can choose a sequence O_n of open sets all containing U such that $m(O_n)$ tends to $m(U)$ as n tends to ∞. If n exceeds some N, the set O_n satisfies

$$m(O_n) < m(U) + \eta. \tag{2.7.76}$$

An open set being the sum of a denumerable set of open intervals, it follows from eq. (2.7.73) that, if $n > N$,

$$|\int_{O_n} A(E)dE| < m(O_n) < m(U) + \eta. \tag{2.7.77}$$

Also, since A is integrable,

$$|\int_{O_n - U} A(E)dE| < \eta, \tag{2.7.78}$$

provided n exceeds some M. Hence, if $n > M$,

$$|\int_{O_n} A(E)dE| \geq \int_U A(E)dE - |\int_{O_n - U} A(E)dE| > m(U) + \eta. \tag{2.7.79}$$

Since this is incompatible with eq. (2.7.77), it follows that A cannot exceed 1 in a set of positive measure. By a similar argument, it cannot be less than -1 in a set of positive measure. Hence $|A| \leq 1$ almost everywhere in I_0, and similarly for B. This completes the proof of eq. (2.7.47).

2.8. The scattering of a beam

2.8.1. Sums of partial waves

We conclude the present investigation with a discussion of the function

$$\left.\begin{aligned} &F_{ba}(\boldsymbol{k}_b, \boldsymbol{k}_a; \varepsilon; X_b) \\ &= -(P_b(X_b)\varphi_b e^{i\boldsymbol{k}_b\cdot\boldsymbol{x}_b}, V_a\varphi_a e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a}) + (V_b\varphi_b e^{i\boldsymbol{k}_b\cdot\boldsymbol{x}_b}, R(E+i\varepsilon)V_a\varphi_a e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a}), \end{aligned}\right\} \tag{2.8.1}$$

it being assumed that both $V_a\varphi_a$ and $V_b\varphi_b$ belong to $\mathfrak{L}^2$. It follows from eq. (2.6.67) that the function F_{ba} is an intermediate step in evaluating $(g_b, S_{ba}f_a)$. It also occurs in the expression for $||(S_{ba} - \delta_{ba})f_a||$, according to eq. (2.6.71). In view of this, we want to study the limiting behaviour of certain integrals which have F_{ba} in their integrands. This is done first from a formal point of view. In section 2.8.4 our results

on the mathematical properties of F_{ba} will make it possible to define the scattering amplitude. The physical interpretation of this quantity is discussed in sections 2.8.6 to 2.8.8, where it is shown to describe the scattering through fixed angles of beams of projectiles.

In the following it is assumed throughout that in channels a and b the system is split into two fragments. Each interaction V_{ij} is spherically symmetric, both φ_a and φ_b are eigenfunctions of angular momentum 0. The functions $V_a\varphi_a$ and $V_b\varphi_b$ belong to $\mathfrak{L}^2$, a further restriction being imposed in eq. (2.8.18).

Under the present assumptions we have

$$V_a\varphi_a e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a} = \underset{N\to\infty}{\text{l.i.m.}}\,(2\pi)^{\frac{3}{2}} V_a\varphi_a \sum_{l=0}^{N}\sum_m \frac{i^l}{\sqrt{k_a x_a}} J_{l+\frac{1}{2}}(k_a x_a)\,\bar{Y}_{lm}(\omega_{k_a})\,Y_{lm}(\omega_{x_a}), \tag{2.8.2}$$

and similarly for channel b. If we write

$$\cos\vartheta = (\boldsymbol{k}_b\cdot\boldsymbol{k}_a)/k_b k_a, \tag{2.8.3}$$

it follows with the methods of section 2.7.5 that

$$\left.\begin{aligned} &F_{ba}(\boldsymbol{k}_b,\boldsymbol{k}_a;\varepsilon;X_b) = \\ &\frac{2\pi^2}{\sqrt{k_b k_a}}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)[-(P_b(X_b)\chi_{bl},V_a\chi_{al})+(V_b\chi_{bl},R(E+i\varepsilon)V_a\chi_{al})]. \end{aligned}\right\} \tag{2.8.4}$$

In obtaining this result, use was made of the relation

$$\sum_m Y_{lm}(\omega_{k_b})\,\bar{Y}_{lm}(\omega_{k_a}) = \frac{2l+1}{4\pi}P_l(\cos\vartheta). \tag{2.8.5}$$

For future reference we note that the sum in eq. (2.8.4) converges absolutely.

It is obvious from eq. (2.8.4) that, apart from ε and X_b, F_{ba} depends only on the angle ϑ between $\boldsymbol{k}_a$ and $\boldsymbol{k}_b$, and on the variable E, which is related to k_a and k_b according to eq. (2.6.65). We therefore define

$$F_{ba}(E,\vartheta;\varepsilon;X_b) = F_{ba}(\boldsymbol{k}_b,\boldsymbol{k}_a;\varepsilon;X_b). \tag{2.8.6}$$

In view of eq. (2.7.37) we may write

$$F_{ba}(E,\vartheta;\varepsilon;X_b) = \frac{2\pi i}{\sqrt{k_b k_a}}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)[\delta_{ba}-\tilde{S}_{ba}(E,l;\varepsilon;X_b)], \tag{2.8.7}$$

this series being absolutely convergent.

Now let $\hat{f}(k_a)$ and $\hat{g}(k_b)$ be any two functions in $\hat{\mathfrak{H}}_{lm}$. Let us define

$$\left.\begin{aligned} \hat{f}_l(\boldsymbol{k}_a) &= \hat{f}(k_a) Y_{l0}(\omega_{k_a}), \\ f_l(\boldsymbol{x}_a) &= (2\pi)^{-\frac{3}{2}} \int e^{i\boldsymbol{k}_a \cdot \boldsymbol{x}_a} \hat{f}_l(\boldsymbol{k}_a) d\boldsymbol{k}_a, \\ f_{al}(\boldsymbol{x}'_a, \boldsymbol{x}_a) &= \varphi_a(\boldsymbol{x}'_a) f_l(\boldsymbol{x}_a), \end{aligned}\right\} \quad (2.8.8)$$

and let us define $g_{bl}(\boldsymbol{x}'_b, \boldsymbol{x}_b)$ in a similar way. Then it is clear that f_{al} belongs to $\mathfrak{H}_a$. Hence, since V_a is square-integrable by assumption, the combination V_a, f_{al} is admissible in the sense of section 2.7.1. Since V_b is also square-integrable, the quantity $(g_{bl}, S_{ba} f_{al})$ can be evaluated with the help of eq. (2.7.37).

Under suitable restrictions on V_a and V_b, we first study the integral

$$J(\varepsilon) = \int \bar{\hat{g}}(k_b)(V_b \varphi_b e^{i\boldsymbol{k}_b \cdot \boldsymbol{x}_b}, R(E + i\varepsilon) V_a \varphi_a e^{i\boldsymbol{k}_a \cdot \boldsymbol{x}_a}) \hat{f}(k_a) k_b k_a dE. \quad (2.8.9)$$

This can be decomposed into angular-momentum components with the help of eq. (2.8.4). From eq. (2.8.7) it is clear that the component l is fairly closely related to $(g_{bl}, S_{ba} f_{al})$. If the way is remembered in which the expression (2.7.37) for $(g_{bl}, S_{ba} f_{al})$ was derived from eq. (2.6.1) plus a similar equation for $(g_{bl}, \Omega^*_{b-} \Omega_{a-} f_{al})$, it follows that

$$\left.\begin{aligned} J(\varepsilon) &= 2\pi^2 \sum_{l=0}^{\infty} (2l+1) P_l(\cos\vartheta) \int \bar{\hat{g}}(k_b)(V_b \chi_{bl}, R(E + i\varepsilon) V_a \chi_{al}) \hat{f}(k_a) \sqrt{k_b k_a}\, dE \\ &= 4\pi i \sum_{l=0}^{\infty} (2l+1) P_l(\cos\vartheta) \int_{-\infty}^{\infty} dt \int_0^{\infty} ds e^{-\varepsilon s} (g_{bl}, e^{iH_b(s+t)} V_b e^{-iHs} V_a e^{-iH_a t} f_{al}). \end{aligned}\right\} \quad (2.8.10)$$

Hence

$$|J(\varepsilon)| \leq 4\pi \sum_{l=0}^{\infty} (2l+1) \int_{-\infty}^{\infty} ||V_b e^{-iH_b s} g_{bl}|| ds \int_{-\infty}^{\infty} ||V_a e^{-iH_a t} f_{al}|| dt, \quad (2.8.11)$$

assuming the series on the right to be convergent.

2.8.2. A convergence problem

The function $J(\varepsilon)$ is the sum of a series each term of which is known to have a limit as ε tends to 0. If we can show that the series converges uniformly with respect to ε, it follows that we have

$$\lim_{\varepsilon \to 0} J(\varepsilon) = \lim_{\varepsilon \to 0} \sum_{l=0}^{\infty} = \sum_{l=0}^{\infty} \lim_{\varepsilon \to 0}. \quad (2.8.12)$$

A sufficient condition for this relation to be valid is the convergence of the series on the right-hand side of eq. (2.8.11). We therefore proceed to investigate this.

According to eq. (2.7.7)

$$\left.\begin{aligned}&\sum_{l=0}^{\infty}(2l+1)||V_{pq}e^{-iH_a t}f_{al}||^2\\ &=\text{const.}\sum_{l=0}^{\infty}(2l+1)\int Q_{pq}(x)x^2dx\Big|\int\exp(-ik^2t)\frac{1}{\sqrt{kx}}J_{l+\frac{1}{2}}(kx)\hat{f}(k)k^2dk\Big|^2.\end{aligned}\right\}\quad(2.8.13)$$

In this expression the sum with respect to l can be performed explicitly with the help of the addition theorem

$$\pi\sum_{l=0}^{\infty}(l+\tfrac{1}{2})\frac{1}{\sqrt{kk'}}J_{l+\frac{1}{2}}(kx)J_{l+\frac{1}{2}}(k'x)=\frac{\sin|k-k'|x}{|k-k'|}\quad(2.8.14)$$

(WATSON (29) section 11.41 eq. (9)). Indeed, since V_{pq} is square-integrable, the function $Q_{pq}(x)x^2$ is integrable. On the right-hand side of eq. (2.8.13) the summation and the integrations may therefore be interchanged. This yields

$$\left.\begin{aligned}&\sum_{l=0}^{\infty}(2l+1)||V_{pq}e^{-iH_a t}f_{al}||^2\\ &=\text{const.}\int Q_{pq}(x)x^2dx\int\int\exp[-i(k^2-k'^2)t]\frac{\sin|k-k'|x}{|k-k'|x}\hat{f}(k)\bar{\hat{f}}(k')k^2k'^2dkdk'.\end{aligned}\right\}\quad(2.8.15)$$

Taking into account that $\hat{f}$ vanishes outside a bounded interval, it is now obvious that

$$\sum_{l=0}^{\infty}(2l+1)||V_{pq}e^{-iH_a t}f_{al}||^2<\text{const.}\quad(2.8.16)$$

uniformly in t. A similar argument applies to channel b. Since V_a is nothing but a sum of two-body interactions V_{pq}, it follows that

$$\sum_{l=0}^{\infty}(2l+1)\left[\int_{-1}^{1}||V_a e^{-iH_a t}f_{al}||dt\right]^2<\infty,\quad(2.8.17)$$

and similarly for channel b.

To extend this result so as to prove that the right-hand side of eq. (2.8.11) is finite, we now assume that the two-body interactions V_{pq} that constitute V_a and V_b are such that there is a positive ζ with

$$\int Q_{pq}(x)(1+x)^{1+\zeta}x^2dx<\infty,\quad(2.8.18)$$

a condition which is fulfilled whenever eq. (2.6.49) holds true for $\alpha=(1+\zeta)/2$ and V_{pq} satisfies

$$\int[V_{pq}(\boldsymbol{X})]^2(1+X)^{1+\zeta}d^3\boldsymbol{X}<\infty.\quad(2.8.19)$$

With eq. (2.7.7) we write

$$\left.\begin{aligned}&\exp[i\Delta(\boldsymbol{x})t]f_l(\boldsymbol{x})\\ &= \frac{i^{l-1}}{4t}Y_{l0}(\omega_x)\int\exp(-ik^2t)\left[\frac{1}{\sqrt{kx}}J_{l+\frac{1}{2}}(kx)+\sqrt{kx}J_{l-\frac{1}{2}}(kx)-\sqrt{kx}J_{l+\frac{3}{2}}(kx)\right.\\ &\qquad\left.+\frac{2k}{\sqrt{kx}}J_{l+\frac{1}{2}}(kx)\frac{d}{dk}\right]\hat{f}(k)dk,\end{aligned}\right\}\tag{2.8.20}$$

hence

$$e^{-iH_at}f_{al} = \sum_{i=1}^{4} f_{li}(t),\tag{2.8.21}$$

say. In connection with the term $f_{l1}(t)$ we first consider

$$\left.\begin{aligned}I_1(t) &\equiv \sum_{l=0}^{\infty}(2l+1)\int Q_{pq}(x)x^2dx\Big|\int\exp(-ik^2t)\frac{1}{\sqrt{kx}}J_{l+\frac{1}{2}}(kx)\hat{f}(k)dk\Big|^2\\ &= \text{const.}\int Q_{pq}(x)x^2dx\iint\exp[-i(k^2-k'^2)t]\frac{\sin|k-k'|x}{|k-k'|x}\hat{f}(k)\bar{\hat{f}}(k')dkdk'.\end{aligned}\right\}\tag{2.8.22}$$

Owing to eq. (2.8.18)

$$\int Q_{pq}(x)x^2\frac{\sin|k-k'|x}{|k-k'|x}dx < \text{const.}\tag{2.8.23}$$

uniformly in $k-k'$. Hence, if we go over to the variables

$$k^2-k'^2 = r, \qquad k-k' = w,\tag{2.8.24}$$

we find

$$I_1(t) = \left[\int_{-K^2}^{0}dr\int_{-K}^{\frac{r}{2K}}dw+\int_{0}^{K^2}dr\int_{\frac{r}{2K}}^{K}dw\right]e^{-irt}w^{-1}G(w,r),\tag{2.8.25}$$

with some bounded function G. From this it follows as before that $I_1(t)$ is the Fourier transform of a function in $\mathfrak{L}^{\nu}(r)$ $(1<\nu\leq 2)$, hence that $I_1(t)$ belongs to $\mathfrak{L}^{\nu/(\nu-1)}(t)$.

We now discuss the function

$$\left.\begin{aligned}I_2(t) &\equiv \sum_{l=0}^{\infty}(2l+1)\int Q_{pq}(x)x^2dx\Big|\int\exp(-ik^2t)\sqrt{kx}J_{l-\frac{1}{2}}(kx)\hat{f}(k)dk\Big|^2\\ &= \text{const.}\int Q_{pq}(x)x^2dx\Big|\int\exp(-ik^2t)\cos\sqrt{kx}\,\hat{f}(k)dk\Big|^2\\ &+\text{const.}\int Q_{pq}(x)x^3dx\iint\exp[-i(k^2-k'^2)t]\frac{\sin|k-k'|x}{|k-k'|}\hat{f}(k)\bar{\hat{f}}(k')kk'dkdk'.\end{aligned}\right\}\tag{2.8.26}$$

After the foregoing it is obvious that the first term on the right belongs to $\mathfrak{L}^{\nu/(\nu-1)}(t)$. Let us denote the second term by $I_{22}(t)$. If in eq. (2.8.18) we choose ζ in the interval $0 < \zeta < 1$, the inequality

$$|\sin x| \leq x^{\zeta}/\zeta \qquad (x \geq 0,\ 0 < \zeta < 1) \tag{2.8.27}$$

yields

$$I_{22}(t) = \int\int \exp[-i(k^2 - k'^2)t] \frac{Z(|k-k'|)}{|k-k'|} \hat{f}(k)\bar{\hat{f}}(k')kk'dkdk', \tag{2.8.28}$$

the function Z satisfying

$$|Z(|k-k'|)| < \text{const.}|k-k'|^{\zeta}. \tag{2.8.29}$$

In terms of the variables w and r we thus obtain

$$I_{22}(t) = \left[\int_{-K^2}^{0} dr \int_{-K}^{\frac{r}{2K}} dw + \int_{0}^{K^2} dr \int_{\frac{r}{2K}}^{K} dw\right] e^{-irt}|w|^{-2+\zeta} H(w,r), \tag{2.8.30}$$

H being a bounded function. This shows that $I_{22}(t)$ is the Fourier transform of a function which belongs to the classes $\mathfrak{L}^{\nu}(r)$ with $\nu < (1-\zeta)^{-1}$. It follows that there is a ν in the interval $0 < \nu < 1$ such that $I_{22}(t)$ belongs to $\mathfrak{L}^{\nu/(\nu-1)}(t)$.

The terms $f_3(t)$ and $f_4(t)$ in eq. (2.8.21) can be discussed along exactly the same lines. The general result is therefore that there is a class $\mathfrak{L}^{\nu/(\nu-1)}(t)$ which contains each of the four functions $I_i(t)$. Also, $[I_i(t)]^{\frac{1}{2}}/t$ is integrable over $-\infty < t \leq -1$ and $1 \leq t < \infty$.

From the inequalities of Schwarz and Minkowski it now follows that

$$\left.\begin{aligned} &\left\{\sum_{l=0}^{\infty}(2l+1)\left[\int_{1}^{\infty}||V_{pq}e^{-iH_a t}f_{al}||dt\right]^2\right\}^{\frac{1}{2}} \leq \int_{1}^{\infty}\left[\sum_{l=0}^{\infty}(2l+1)||V_{pq}e^{-iH_a t}f_{al}||^2\right]^{\frac{1}{2}}dt \\ \leq \int_{1}^{\infty}&\left[\sum_{l=0}^{\infty}(2l+1)\left(\sum_{i=1}^{4}||V_{pq}f_{li}(t)||\right)^2\right]^{\frac{1}{2}}dt \leq \int_{1}^{\infty}\sum_{i=1}^{4}\left[\sum_{l=0}^{\infty}(2l+1)||V_{pq}f_{li}(t)||^2\right]^{\frac{1}{2}}dt \\ &= \text{const.}\int_{1}^{\infty}\sum_{i=1}^{4}[I_i(t)]^{\frac{1}{2}}\frac{1}{t}dt < \infty, \end{aligned}\right\} \tag{2.8.31}$$

and similarly for the interval $-\infty < t < -1$. This relation applies to all the two-body interactions V_{pq} contained in V_a. Hence, with eq. (2.8.17),

$$\sum_{l=0}^{\infty}(2l+1)\left[\int_{-\infty}^{\infty}||V_a e^{-iH_a t}f_{al}||dt\right]^2 < \infty. \tag{2.8.32}$$

There is a similar inequality for channel b. From this it follows with Schwarz's inequality that the right-hand side of eq. (2.8.11) is finite, as we wished to show. We can now use the relation (2.8.12), with the result that

$$\left.\begin{aligned} &\lim_{\varepsilon\to 0}\int \bar{\tilde{g}}(k_b)(V_b\varphi_b e^{i\boldsymbol{k}_b\cdot\boldsymbol{x}_b}, R(E+i\varepsilon)V_a\varphi_a e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a})\hat{f}(k_a)k_b k_a dE \\ &= 2\pi i\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\lim_{X_b\to\infty}\int \bar{\tilde{g}}(k_b)[\delta_{ba}-S_{ba}(E,l)-\pi i(P_b(X_b)\chi_{bl}, V_a\chi_{al})]\hat{f}(k_a)\sqrt{k_b k_a}\,dE, \end{aligned}\right\} \quad (2.8.33)$$

the series on the right being absolutely convergent.

2.8.3. The imaginary part of the scattering amplitude

If it is understood that φ_a and φ_b have been chosen real, there is a much more powerful result for the imaginary part of F_{ba}. Since the Hamiltonian commutes with the conjugation operator which transforms f into $\bar{f}$, it follows with eqs. (2.3.48) and (2.8.4) that

$$\left.\begin{aligned} \operatorname{Im} F_{ba}(E,\vartheta;\varepsilon) &\equiv \lim_{X_b\to\infty}\operatorname{Im} F_{ba}(E,\vartheta;\varepsilon;X_b) \\ &= \frac{1}{2i}(V_b\varphi_b e^{i\boldsymbol{k}_b\cdot\boldsymbol{x}_b}, [R(E+i\varepsilon)-R(E-i\varepsilon)]V_a\varphi_a e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a}). \end{aligned}\right\} \quad (2.8.34)$$

Also, by eq. (2.8.33),

$$\left.\begin{aligned} &\lim_{\varepsilon\to 0}\int \bar{\tilde{g}}(k_b)[\operatorname{Im} F_{ba}(E,\vartheta;\varepsilon)]\hat{f}(k_a)k_b k_a dE \\ &= \lim_{\varepsilon\to 0} 2\pi\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\int \bar{\tilde{g}}(k_b)[\delta_{ba}-\operatorname{Re}\tilde{S}_{ba}(E,l;\varepsilon;X_b)]\hat{f}(k_a)\sqrt{k_b k_a}\,dE \\ &= 2\pi\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\int \bar{\tilde{g}}(k_b)[\delta_{ba}-\operatorname{Re}S_{ba}(E,l)]\hat{f}(k_a)\sqrt{k_b k_a}\,dE. \end{aligned}\right\} \quad (2.8.35)$$

Let us now first concentrate on the case $a = b$, and let us choose $\hat{f}$ and $\hat{g}$ positive. In each term of the series in the third member of eq. (2.8.35) the integrand is then positive, owing to eq. (2.7.63). The series converges absolutely, by our previous analysis. From this it follows that the series

$$2\pi\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\bar{\tilde{g}}(k_a)[1-\operatorname{Re}S_{aa}(E,l)]\hat{f}(k_a)k_a \quad (2.8.36)$$

converges for almost every E, its sum being an integrable function (Burkill (22) section 3.10). Denoting the sum in question by

$$\bar{\tilde{g}}(k_a)[\operatorname{Im} F_{aa}(E,\vartheta)]\hat{f}(k_a)k_a^2 \quad (2.8.37)$$

we have

$$\lim_{\varepsilon\to 0}\int \bar{\tilde{g}}(k_a)[\operatorname{Im} F_{aa}(E,\vartheta;\varepsilon)]\hat{f}(k_a)k_a^2 dE = \int \bar{\tilde{g}}(k_a)[\operatorname{Im} F_{aa}(E,\vartheta)]\hat{f}(k_a)k_a^2 dE. \quad (2.8.38)$$

Now let $\hat{f}$ and $\hat{g}$ take the value 1 in a certain interval I, and let us consider the second member of eq. (2.8.35). This involves $R(E+i\varepsilon)-R(E-i\varepsilon)$, by analogy with eq. (2.8.34). If h is any function in $\mathfrak{L}^2$, we have

$$(h,[R(E+i\varepsilon)-R(E-i\varepsilon)]h) = 2i\varepsilon||R(E+i\varepsilon)h||^2. \tag{2.8.39}$$

As a result

$$1-\mathrm{Re}\tilde{S}_{aa}(E,l;\varepsilon;X_a) \geq 0. \tag{2.8.40}$$

Hence, $\hat{f}$ and $\hat{g}$ being positive,

$$\int_I [1-\mathrm{Re}\tilde{S}_{aa}(E,l;\varepsilon;X_a)]k_a dE \leq \int \bar{\hat{g}}(k_a)[1-\mathrm{Re}\tilde{S}_{aa}(E,l;\varepsilon;X_a)]\hat{f}(k_a)k_a dE. \tag{2.8.41}$$

Since we know from the previous section that the series in eq. (2.8.35) converge uniformly with respect to ε, it now follows that

$$\left.\begin{aligned} &\lim_{\varepsilon\to 0}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\int_I [1-\mathrm{Re}\tilde{S}_{aa}(E,l;\varepsilon;X_a)]k_a dE \\ &=\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\lim_{\varepsilon\to 0}\int_I [1-\mathrm{Re}\tilde{S}_{aa}(E,l;\varepsilon;X_a)]k_a dE, \end{aligned}\right\} \tag{2.8.42}$$

either series in eq. (2.8.42) converging absolutely, uniformly with respect to ε. On the right the limit with respect to ε can be performed with eq. (2.7.60). The argument which led to eq. (2.8.38) then yields

$$\lim_{\varepsilon\to 0}\int_I \mathrm{Im}F_{aa}(E,\vartheta;\varepsilon)k_a^2 dE = \int_I \mathrm{Im}F_{aa}(E,\vartheta)k_a^2 dE. \tag{2.8.43}$$

If E_1 and E_2 are any two points in the interval I, and the integral

$$\int_{E_1}^{E_2} \mathrm{Im}F_{aa}(E,\vartheta;\varepsilon)k_a^2 dE \tag{2.8.44}$$

is considered as a function of E_2, this function is of bounded variation, uniformly with respect to ε. If this result is combined with eq. (2.8.43), it follows from the Helly-Bray theorem on limits of Stieltjes integrals (Widder (30) ch. I, theorem 16.4) that eq. (2.8.38) holds true in all cases in which $\bar{\hat{g}}(k_a)\hat{f}(k_a)$ vanishes outside a bounded interval and is continuous except for a finite number of jumps.

To extend the foregoing to the case $a \neq b$, we observe that

$$|\delta_{ba}-\mathrm{Re}\tilde{S}_{ba}(E,l;\varepsilon;X_b)|^2 \leq [1-\mathrm{Re}\tilde{S}_{bb}(E,l;\varepsilon;X_b)][1-\mathrm{Re}\tilde{S}_{aa}(E,l;\varepsilon;X_b)], \tag{2.8.45}$$

owing to eq. (2.8.39). With the help of this inequality it is readily shown that there exists a function $\mathrm{Im}F_{ba}(E,\vartheta)$ which for almost every E satisfies

$$\operatorname{Im} F_{ba}(E,\vartheta)k_b k_a = 2\pi \sum_{l=0}^{\infty} (2l+1)P_l(\cos\vartheta)[\delta_{ba} - \operatorname{Re} S_{ba}(E,l)]\sqrt{k_b k_a}. \quad (2.8.46)$$

If $\bar{\hat{g}}(k_b)\hat{f}(k_a)$ vanishes outside a bounded region and is continuous except for a finite number of jumps, we have

$$\lim_{\varepsilon\to 0}\int \bar{\hat{g}}(k_b)[\operatorname{Im} F_{ba}(E,\vartheta;\varepsilon)]\hat{f}(k_a)k_b k_a dE = \int \bar{\hat{g}}(k_b)[\operatorname{Im} F_{ba}(E,\vartheta)]\hat{f}(k_a)k_b k_a dE. \quad (2.8.47)$$

The function $\operatorname{Im} F_{ba}(E,\vartheta)/4\pi$ is called the imaginary part of the scattering amplitude.

It is sometimes convenient to consider $\cos\vartheta$ as a function of E and

$$\Delta = |\boldsymbol{k}_a - \boldsymbol{k}_b|, \quad (2.8.48)$$

according to

$$\cos\vartheta = (k_a^2 + k_b^2 - \Delta^2)/2k_a k_b. \quad (2.8.49)$$

In order that $|\cos\vartheta| \leq 1$, it is necessary that

$$|k_a - k_b| \leq \Delta \leq k_a + k_b. \quad (2.8.50)$$

If this condition is fulfilled throughout the interval I, we have

$$\left.\begin{aligned}\lim_{\varepsilon\to 0}\int_I P_l((k_a^2 + k_b^2 - \Delta^2)/2k_a k_b)[\delta_{ba} - \operatorname{Re}\tilde{S}_{ba}(E,l;\varepsilon;X_b)]\sqrt{k_b k_a}\,dE \\ = \int_I P_l((k_a^2 + k_b^2 - \Delta^2)/2k_a k_b)[\delta_{ba} - \operatorname{Re} S_{ba}(E,l)]\sqrt{k_b k_a}\,dE,\end{aligned}\right\} \quad (2.8.51)$$

owing to eq. (2.7.60). The convergence properties of sums of integrals of this form can be discussed with the methods developed above. It can also be shown that both eq. (2.8.46) and eq. (2.8.47) remain valid when $\cos\vartheta$ is considered to be function of E and Δ, provided Δ is such that $|\cos\vartheta| \leq 1$ throughout the energy region considered.

2.8.4. The scattering amplitude

To get some insight into the real part of F_{ba}, a more elaborate analysis is required. For this we assume as before that V_a satisfies the restriction imposed by eq. (2.8.18). It is sufficient if V_b is square-integrable. It is assumed that $\hat{f}(k_a)$ belongs to $\hat{\mathfrak{H}}_{lm}$. The function $\hat{g}(k_b)$ may be any function satisfying

$$\int |\hat{g}(k_b)|^2 k_b^2 dk_b < \infty. \quad (2.8.52)$$

We define f_{al} and g_{bl} as in eq. (2.8.8).

It follows from the method by which an expression for S_{ba} was obtained from eq. (2.6.1) that

$$\left.\begin{aligned} &|\tfrac{1}{2}\int \bar{\hat{g}}(k_b)[\delta_{ba} - \tilde{S}_{ba}(E,l;\varepsilon;X_b)]\hat{f}(k_a)\sqrt{k_b k_a}\,dE| \\ &= |\int_{-\infty}^{\infty}(g_{bl}, e^{iH_b t}[P_b(X_b) - 1 + \Omega^*_{b-,\varepsilon}]V_a e^{-iH_a t}f_{al})dt| \le 2||g_{bl}||\int_{-\infty}^{\infty}||V_a e^{-iH_a t}f_{al}||dt \end{aligned}\right\} \quad (2.8.53)$$

(cf. eqs. (2.7.48) and (2.7.50)). Taking in particular

$$\hat{g}(k_b) = [\delta_{ba} - \tilde{S}_{ba}(E,l;\varepsilon;X_b)]\hat{f}(k_a)\sqrt{k_a/k_b}, \quad (2.8.54)$$

we obtain

$$\tfrac{1}{2}\int |[\delta_{ba} - \tilde{S}_{ba}(E,l;\varepsilon;X_b)]\hat{f}(k_a)|^2 k_a dE \le 4\Big[\int_{-\infty}^{\infty}||V_a e^{-iH_a t}f_{al}||dt\Big]^2. \quad (2.8.55)$$

Now, in virtue of eq. (2.7.60),

$$\left.\begin{aligned} &\{\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\}\{\lim_{\varepsilon'\to 0}\lim_{X_b'\to\infty}\}\int \bar{\hat{f}}(k_a)[\delta_{ba} - \bar{\tilde{S}}_{ba}(E,l;\varepsilon';X_b')][\delta_{ba} - \tilde{S}_{ba}(E,l;\varepsilon;X_b)]\hat{f}(k_a)k_a dE \\ &\qquad = \int |[\delta_{ba} - S_{ba}(E,l)]\hat{f}(k_a)|^2 k_a dE. \end{aligned}\right\} \quad (2.8.56)$$

Hence, with eq. (2.8.55),

$$\tfrac{1}{2}\int |[\delta_{ba} - S_{ba}(E,l)]\hat{f}(k_a)|^2 k_a dE \le 4\Big[\int_{-\infty}^{\infty}||V_a e^{-iH_a t}f_{al}||dt\Big]^2. \quad (2.8.57)$$

Owing to eq. (2.8.32) it now follows that

$$\int_{-1}^{1} d\cos\vartheta \int |\sum_{l=N}^{\infty}(2l+1)P_l(\cos\vartheta)[\delta_{ba} - \tilde{S}_{ba}(E,l;\varepsilon;X_b)]\hat{f}(k_a)|^2 k_a dE \quad (2.8.58)$$

tends to 0 as N tends to ∞, uniformly in ε, X_b. In view of eq. (2.8.7) this means that, given a positive ξ, we can determine N in such a way that

$$\int_{-1}^{1} d\cos\vartheta \int \left|\left\{\frac{\sqrt{k_b k_a}}{2\pi i}F_{ba}(E,\vartheta;\varepsilon;X_b) - \sum_{l=0}^{N}(2l+1)P_l(\cos\vartheta)[\delta_{ba} - \tilde{S}_{ba}(E,l;\varepsilon;X_b)]\right\}\hat{f}(k_a)\right|^2 k_a dE < \xi \quad (2.8.59)$$

for every ε, X_b. There also exists a function $F_{ba}(E,\vartheta)$ such that

$$\int_{-1}^{1} d\cos\vartheta \int \left|\left\{\frac{\sqrt{k_b k_a}}{2\pi i}F_{ba}(E,\vartheta) - \sum_{l=0}^{N}(2l+1)P_l(\cos\vartheta)[\delta_{ba} - S_{ba}(E,l)]\right\}\hat{f}(k_a)\right|^2 k_a dE < \xi, \quad (2.8.60)$$

by eqs. (2.8.32), (2.8.57) and the Riesz-Fischer theorem (Riesz and Sz.-Nagy (11) section 28). This function is square-integrable in the sense that

$$\int_{-1}^{1} d\cos\vartheta \int_I |F_{ba}(E,\vartheta)|^2 k_b k_a^2 dE < \infty, \quad (2.8.61)$$

where I may be any bounded interval contained in the interval (2.7.45). In the space of all functions satisfying eq. (2.8.61) we can say that

$$F_{ba}(E,\vartheta) = \underset{N\to\infty}{\text{l.i.m.}} \frac{2\pi i}{\sqrt{k_b k_a}} \sum_{l=0}^{N} (2l+1) P_l(\cos\vartheta)[\delta_{ba} - S_{ba}(E,l)]. \tag{2.8.62}$$

In the following $F_{ba}(E,\vartheta)/4\pi$ is called the scattering amplitude. If a function $\mathrm{Im}F_{ba}(E,\vartheta)$ can be defined according to eq. (2.8.46), it is clear that this is the imaginary part of the present function $F_{ba}(E,\vartheta)$. We recall in this connection that in the previous section we obtained the result that the series in eq. (2.8.46) converges for almost every E. For this we had to assume that V_b satisfies eq. (2.8.18). In the present section we merely consider convergence in mean, which is established under the much weaker condition that V_b be square-integrable. In either section V_a is assumed to satisfy eq. (2.8.18).

In an obvious notation we can write eqs. (2.8.59) and (2.8.60) in the form

$$\left.\begin{aligned} \int_{-1}^{1} d\cos\vartheta \int |[F(E,\vartheta;\varepsilon;X_b) - F_N(E,\vartheta;\varepsilon;X_b)]\hat{f}(k_a)|^2 k_b k_a^2 dE < 2\pi\xi, \\ \int_{-1}^{1} d\cos\vartheta \int |[F(E,\vartheta) - F_N(E,\vartheta)]\hat{f}(k_a)|^2 k_b k_a^2 dE < 2\pi\xi. \end{aligned}\right\} \tag{2.8.63}$$

Let us now consider the integral

$$\int_{-1}^{1} d\cos\vartheta \int \bar{B}(E,\vartheta) F_{ba}(E,\vartheta;\varepsilon;X_b)\hat{f}(k_a)\sqrt{k_b k_a}\, k_a dE, \tag{2.8.64}$$

where B satisfies

$$\int_{-1}^{1} d\cos\vartheta \int |B(E,\vartheta)|^2 k_a dE < \infty. \tag{2.8.65}$$

According to eq. (2.8.63) and Schwarz's inequality, there exists an integer N such that, given ξ,

$$\left.\begin{aligned} \left| \int_{-1}^{1} d\cos\vartheta \int \bar{B}(E,\vartheta)[F(E,\vartheta;\varepsilon;X_b) - F_N(E,\vartheta;\varepsilon;X_b)]\hat{f}(k_a)\sqrt{k_b k_a}\, k_a dE \right| < \xi, \\ \left| \int_{-1}^{1} d\cos\vartheta \int \bar{B}(E,\vartheta)[F(E,\vartheta) - F_N(E,\vartheta)]\hat{f}(k_a)\sqrt{k_b k_a}\, k_a dE \right| < \xi, \end{aligned}\right\} \tag{2.8.66}$$

for every ε, X_b. Now it is not difficult to see that

$$\int_{-1}^{1} P_l(\cos\vartheta) B(E,\vartheta)\sqrt{k_a/k_b}\, d\cos\vartheta \tag{2.8.67}$$

can be considered as a function $\hat{g}(k_b)$ satisfying eq. (2.8.52). Hence, given N, we can choose ε, X_b in such a way that

$$\left| \int_{-1}^{1} d\cos\vartheta \int \bar{B}(E,\vartheta)[F_N(E,\vartheta) - F_N(E,\vartheta;\varepsilon;X_b)]\hat{f}(k_a)\sqrt{k_b k_a}\, k_a dE \right| < \xi, \tag{2.8.68}$$

owing to eq. (2.7.60). If this result is combined with eq. (2.8.66), it follows that

$$\left.\begin{aligned} \left\{\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\right\} \int_{-1}^{1} d\cos\vartheta \int \bar{B}(E,\vartheta) F_{ba}(E,\vartheta;\varepsilon;X_b)\hat{f}(k_a)\sqrt{k_b k_a}\, k_a dE \\ = \int_{-1}^{1} d\cos\vartheta \int \bar{B}(E,\vartheta) F_{ba}(E,\vartheta)\hat{f}(k_a)\sqrt{k_b k_a}\, k_a dE. \end{aligned}\right\} \tag{2.8.69}$$

In particular, since F satisfies eq. (2.8.61),

$$\left.\begin{aligned} \left\{\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\right\}\left\{\lim_{\varepsilon'\to 0}\lim_{X_b'\to\infty}\right\} \int_{-1}^{1} d\cos\vartheta \int \bar{\hat{f}}(k_a)\bar{F}_{ba}(E,\vartheta;\varepsilon';X_b') F_{ba}(E,\vartheta;\varepsilon;X_b)\hat{f}(k_a) k_b k_a^2 dE \\ = \int_{-1}^{1} d\cos\vartheta \int |F_{ba}(E,\vartheta)\hat{f}(k_a)|^2 k_b k_a^2 dE. \end{aligned}\right\} \tag{2.8.70}$$

In the present section it has been assumed thus far that $\hat{f}$ belongs to $\hat{\mathfrak{G}}_{lm}$. However, given the fact that eqs. (2.8.63) and (2.8.66) hold true for functions $\hat{f}$ in $\hat{\mathfrak{G}}_{lm}$, it is clear that these equations are satisfied for every $\hat{f}$ which is bounded and vanishes outside a bounded region, it being understood that the integer N depends on the particular $\hat{f}$ considered. Also, since for eq. (2.7.60) to hold true it is sufficient if $\hat{f}$ belongs to $\mathfrak{S}\hat{\mathfrak{G}}_{lm}$, eq. (2.8.68) is valid for every $\hat{f}$ in $\mathfrak{S}\hat{\mathfrak{G}}_{lm}$. Hence so are eqs. (2.8.69) and (2.8.70).

Now let E_1 and E_2 be two points in some bounded interval I contained in the interval (2.7.45). If E_1 is held fixed and the integral

$$\int_{-1}^{1} d\cos\vartheta \int_{E_1}^{E_2} \bar{B}(E,\vartheta) F_{ba}(E,\vartheta;\varepsilon;X_b)\sqrt{k_b k_a}\, k_a dE \tag{2.8.71}$$

is considered as a function of E_2, this function is of bounded variation, uniformly with respect to ε, X_b. This can be shown with Schwarz's inequality and the methods used in connection with eqs. (2.8.41) to (2.8.44). It follows with the Helly–Bray theorem that eqs. (2.8.69) and (2.8.70) hold true for every $\hat{f}$ which vanishes outside a bounded interval and is continuous except for a finite number of jumps.

It is easily checked that throughout this section $\cos\vartheta$ can be considered as a function of E and Δ, according to eq. (2.8.49).

2.8.5. Beams of projectiles

Let us consider a system which in the distant past was in channel a and behaved according to some wave-function $\exp(-iH_at)\varphi_a(\boldsymbol{x}'_a)f(\boldsymbol{x}_a)$. If the wave-function is decomposed into an incident wave plus a scattered wave, and it is assumed that V_a and V_b are square-integrable, the probability that in the remote future the scattered wave will be in channel b is given by

$$\left.\begin{aligned} ||(S_{ba}-\delta_{ba})f_a||^2 &= \tfrac{1}{4}(2\pi)^{-4}\Big\{\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\Big\}\Big\{\lim_{\varepsilon'\to 0}\lim_{X'_b\to\infty}\Big\}\int \bar{A}_{ba}(\boldsymbol{k}_b;\varepsilon';X'_b)A_{ba}(\boldsymbol{k}_b;\varepsilon;X_b)d\boldsymbol{k}_b, \\ A_{ba}(\boldsymbol{k}_b;\varepsilon;X_b) &= \int k_a F_{ba}(\boldsymbol{k}_b,\boldsymbol{k}_a;\varepsilon;X_b)\hat{f}(\boldsymbol{k}_a)d\omega_{k_a}. \end{aligned}\right\} \quad (2.8.72)$$

This is a simplified form to which eq. (2.6.71) can be reduced if $m_a = m_b = 2$ and V_a and V_b are square-integrable.

In the initial wave-function as well as in the function F_{ba}, there occurs a vector $\boldsymbol{x}_a$. This denotes the distance between the two fragments which are scattered at each other. For the following it is convenient to consider the scattering in a coordinate frame in which one of the fragments, the target, is fixed at the origin. Obviously $\boldsymbol{x}_a$ then stands for the distance between the origin and the projectile. The motion of the projectile is determined by $f(\boldsymbol{x}_a)$.

We now compare the event considered in eq. (2.8.72) with the scattering from an initial state

$$e^{-iH_at}f_a(\boldsymbol{r}) \equiv e^{-iH_at}\varphi_a(\boldsymbol{x}'_a)f(\boldsymbol{x}_a+\boldsymbol{r}). \quad (2.8.73)$$

In this state the motion of the projectile is determined by $f(\boldsymbol{x}_a+\boldsymbol{r})$, hence in the distant past the projectile behaved like the original one, except for a translation over $\boldsymbol{r}$. By analogy with eq. (2.8.72), we get

$$\left.\begin{aligned} ||(S_{ba}-\delta_{ba})f_a(\boldsymbol{r})||^2 &= \tfrac{1}{4}(2\pi)^{-4}\Big\{\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\Big\}\Big\{\lim_{\varepsilon'\to 0}\lim_{X'_b\to\infty}\Big\}\int \bar{A}_{ba}(\boldsymbol{k}_b;\boldsymbol{r};\varepsilon';X'_b)A_{ba}(\boldsymbol{k}_b;\boldsymbol{r};\varepsilon;X_b)d\boldsymbol{k}_b, \\ A_{ba}(\boldsymbol{k}_b;\boldsymbol{r};\varepsilon;X_b) &= \int k_a F_{ba}(\boldsymbol{k}_b,\boldsymbol{k}_a;\varepsilon;X_b)e^{i\boldsymbol{k}_a\cdot\boldsymbol{r}}\hat{f}(\boldsymbol{k}_a)d\omega_{k_a}. \end{aligned}\right\} \quad (2.8.74)$$

Now let $\boldsymbol{r}$ be a two-component vector which varies over some plane ϱ. Let us consider a statistical mixture of projectiles $f(\boldsymbol{x}_a+\boldsymbol{r})$ in which the number of projectiles with $\boldsymbol{r}$-vector in $d\boldsymbol{r}$ is equal to $d\boldsymbol{r}$. In the following such a mixture is called a beam. We shall see below that within the framework of Hilbert space it provides a good description of what one usually tries to discuss in terms of plane waves. It will be understood that, if a beam is scattered, all the projectiles are scattered independently, i. e. the total scattering intensity is the integral over $\boldsymbol{r}$ of the intensities due to the separate projectiles. In channel b the beam $f(\boldsymbol{x}_a+\boldsymbol{r})$ thus yields a scattering intensity

$$I_{ba} = \int_{\varrho} ||(S_{ba}-\delta_{ba})f_a(\boldsymbol{r})||^2 d\boldsymbol{r}. \quad (2.8.75)$$

This quantity is now discussed under the assumption that V_b is square-integrable and that V_a satisfies the restriction imposed by eq. (2.8.18).

2.8.6. The scattering intensity

In virtue of eqs. (2.8.5) and (2.8.7)

$$\left.\begin{aligned} &\tfrac{1}{4}(2\pi)^{-4}\int \bar{A}_{ba}(\boldsymbol{k}_b;\boldsymbol{r};\varepsilon';X_b')A_{ba}(\boldsymbol{k}_b;\boldsymbol{r};\varepsilon;X_b)d\boldsymbol{k}_b \\ =\ &\tfrac{1}{2}\sum_{l'=0}^{\infty}\sum_{m'}\sum_{l=0}^{\infty}\sum_{m}\int \bar{Y}_{l'm'}(\omega_{k_b})Y_{lm}(\omega_{k_b})d\omega_{k_b}\int[\delta_{ba}-\bar{\tilde{S}}_{ba}(E,l';\varepsilon';X_b')][\delta_{ba}-\hat{S}_{ba}(E,l;\varepsilon;X_b)]k_a dE \\ &\times\int Y_{l'm'}(\omega_{k_a'})e^{-i\boldsymbol{k}_a'\cdot\boldsymbol{r}}\bar{\hat{f}}(\boldsymbol{k}_a')d\omega_{k_a'}\int \bar{Y}_{lm}(\omega_{k_a})e^{i\boldsymbol{k}_a\cdot\boldsymbol{r}}\hat{f}(\boldsymbol{k}_a)d\omega_{k_a}. \end{aligned}\right\} \quad (2.8.76)$$

Here ω_{k_a} and $\omega_{k_a'}$ stand for the polar angles of certain vectors $\boldsymbol{k}_a$ and $\boldsymbol{k}_a'$ which are both of length k_a. If

$$\int|\hat{f}(\boldsymbol{k}_a)|^2 d\omega_{k_a} < M < \infty \quad (2.8.77)$$

and $\hat{f}(\boldsymbol{k}_a)$ vanishes if E is outside some bounded interval I, then each term of the series in eq. (2.8.76) tends to a limit as $\varepsilon, X_b, \varepsilon', X_b'$ tend to 0, ∞, 0, ∞, owing to eq. (2.7.60). Taking into account that

$$\int|\bar{Y}_{l'm'}(\omega_{k_b})Y_{lm}(\omega_{k_b})|d\omega_{k_b} \leq 1, \quad (2.8.78)$$

$$\sum_{l=0}^{\infty}\sum_{m}\left|\int \bar{Y}_{lm}(\omega_{k_a})e^{i\boldsymbol{k}_a\cdot\boldsymbol{r}}\hat{f}(\boldsymbol{k}_a)d\omega_{k_a}\right|^2 = \int|\hat{f}(\boldsymbol{k}_a)|^2 d\omega_{k_a} < M, \quad (2.8.79)$$

it follows from Schwarz's inequality that the series in eq. (2.8.76) is dominated by

$$\left.\begin{aligned} &\tfrac{1}{2}M\left[\sum_{l'=0}^{\infty}(2l'+1)\int_I|\delta_{ba}-\tilde{S}_{ba}(E',l';\varepsilon';X_b')|^2 k_a' dE'\right]^{\frac{1}{2}} \\ &\times\left[\sum_{l=0}^{\infty}(2l+1)\int_I|\delta_{ba}-\tilde{S}_{ba}(E,l;\varepsilon;X_b)|^2 k_a dE\right]^{\frac{1}{2}}. \end{aligned}\right\} \quad (2.8.80)$$

In this expression either series converges uniformly with respect to $\varepsilon, X_b, \varepsilon', X_b'$, owing to eqs. (2.8.32) and (2.8.55). As a result the limit with respect to $\varepsilon, X_b, \varepsilon', X_b'$ of the series in eq. (2.8.76) is the sum of the limits of the separate terms. Also,

$$\left.\begin{aligned} &\tfrac{1}{4}(2\pi)^{-4}\Big\{\lim_{\varepsilon\to 0}\lim_{X_b\to\infty}\Big\}\Big\{\lim_{\varepsilon'\to 0}\lim_{X_b'\to\infty}\Big\}\int \bar{A}_{ba}(\boldsymbol{k}_b;\boldsymbol{r};\varepsilon';X_b')A_{ba}(\boldsymbol{k}_b;\boldsymbol{r};\varepsilon;X_b)d\boldsymbol{k}_b \\ =\ &\tfrac{1}{2}\int d\omega_{k_b}\int\Big|\sum_{l=0}^{\infty}\sum_{m}Y_{lm}(\omega_{k_b})[\delta_{ba}-S_{ba}(E,l)]\int \bar{Y}_{lm}(\omega_{k_a})e^{i\boldsymbol{k}_a\cdot\boldsymbol{r}}\hat{f}(\boldsymbol{k}_a)d\omega_{k_a}\Big|^2 k_a dE. \end{aligned}\right\} \quad (2.8.81)$$

Extending the integration with respect to ω_{k_b} over the full angle 4π, we obtain, with eq. (2.8.74),

$$||(S_{ba} - \delta_{ba})f_a(\boldsymbol{r})||^2 = \tfrac{1}{2}\sum_{l=0}^{\infty}\sum_{m}\int|[\delta_{ba} - S_{ba}(E,l)]\int \bar{Y}_{lm}(\omega_{k_a})e^{i\boldsymbol{k}_a\cdot\boldsymbol{r}}\hat{f}(\boldsymbol{k}_a)d\omega_{k_a}|^2 k_a dE. \quad (2.8.82)$$

At this point it is convenient to introduce a rectangular coordinate frame with axes 1 and 2 in the plane ϱ and axis 3 perpendicular to it. Writing

$$\left.\begin{aligned} k_{a1} &= k_a \sin\beta_a \cos\alpha_a, \\ k_{a2} &= k_a \sin\beta_a \sin\alpha_a, \\ k_{a3} &= k_a \cos\beta_a, \end{aligned}\right\} \quad (2.8.83)$$

we obviously have

$$\int d\omega_{k_a} = \int d\cos\beta_a d\alpha_a. \quad (2.8.84)$$

Now let our beam be directed in the sense that $\hat{f}(\boldsymbol{k}_a) = 0$ if $\cos\beta_a < 0$. In the region of integration there is then a one-to-one correspondence between k_a,β_a,α_a and k_a, k_{a1},k_{a2}. Also,

$$\int d\cos\beta_a d\alpha_a = \int k_a^{-1}(k_a^2 - k_{a1}^2 - k_{a2}^2)^{-\frac{1}{2}} dk_{a1}dk_{a2}. \quad (2.8.85)$$

Hence

$$g_{lm}(E,\boldsymbol{r}) = \int \bar{Y}_{lm}(\omega_{k_a})e^{i\boldsymbol{k}_a\cdot\boldsymbol{r}}\hat{f}(\boldsymbol{k}_a)d\omega_{k_a} \quad (2.8.86)$$

is the Fourier transform of

$$\hat{g}_{lm}(E,k_{a1},k_{a2}) = 2\pi\bar{Y}_{lm}(\omega_{k_a})\hat{f}(\boldsymbol{k}_a)k_a^{-1}(k_a^2 - k_{a1}^2 - k_{a2}^2)^{-\frac{1}{2}}. \quad (2.8.87)$$

As a result

$$\left.\begin{aligned} &\int_{\varrho}|g_{lm}(E,\boldsymbol{r})|^2 d\boldsymbol{r} = \int|\hat{g}_{lm}(E,k_{a1},k_{a2})|^2 dk_{a1}dk_{a2} \\ &= 4\pi^2 k_a^{-2}\int|Y_{lm}(\omega_{k_a})\hat{f}(\boldsymbol{k}_a)|^2(\cos\beta_a)^{-1}d\cos\beta_a d\alpha_a. \end{aligned}\right\} \quad (2.8.88)$$

We now assume that

$$k_a^{-2}\int|\hat{f}(\boldsymbol{k}_a)|^2(\cos\beta_a)^{-1}d\cos\beta_a d\alpha_a < \infty, \quad (2.8.89)$$

a condition which implies eq. (2.8.77). If it is satisfied, it follows with eqs. (2.8.5) and (2.8.75) that

$$I_{ba} = \tfrac{1}{2}\pi\sum_{l=0}^{\infty}(2l+1)\int|\delta_{ba} - S_{ba}(E,l)|^2 k_a^{-1}dE\int|\hat{f}(\boldsymbol{k}_a)|^2(\cos\beta_a)^{-1}d\cos\beta_a d\alpha_a. \quad (2.8.90)$$

According to eq. (2.8.62), we may also write

$$I_{ba} = \frac{1}{16\pi}\int_{-1}^{1}d\cos\vartheta\int|F_{ba}(E,\vartheta)|^2 k_b dE\int|\hat{f}(\boldsymbol{k}_a)|^2(\cos\beta_a)^{-1}d\cos\beta_a d\alpha_a. \quad (2.8.91)$$

Alternatively, defining

$$F_{ba}(\boldsymbol{k}_a, \boldsymbol{k}_a) = F_{ba}(E, \vartheta) \tag{2.8.92}$$

we obtain

$$I_{ba} = \int I_{ba}(\omega_{k_b}) d\omega_{k_b} = \frac{1}{16\pi^2} \int d\boldsymbol{k}_b \int |F_{ba}(\boldsymbol{k}_b, \boldsymbol{k}_a) \hat{f}(\boldsymbol{k}_a)|^2 (\cos\beta_a)^{-1} d\cos\beta_a d\alpha_a . \tag{2.8.93}$$

2.8.7. Scattering in a fixed direction

Equation (2.8.93) suggests that $\int_{\delta\omega} I_{ba}(\omega_{k_b}) d\omega_{k_b}$ is the intensity of the scattering into the angle $\delta\omega$. That this is correct can be seen as follows. If in eq. (2.8.81) the integration over ω_{k_b} is restricted to $\delta\omega$, we obtain the probability that the projectile $f(\boldsymbol{x}_a + \boldsymbol{r})$ yields a wave scattered into the angle $\delta\omega$. This is obvious from the proof of eq. (2.6.71). Let us now define

$$\left.\begin{aligned} F_N(\boldsymbol{k}_b, \boldsymbol{k}_a) &= F_N(E, \vartheta), \\ A_N(\boldsymbol{k}_b, \boldsymbol{r}) &= \int k_a F_N(\boldsymbol{k}_b, \boldsymbol{k}_a) e^{i\boldsymbol{k}_a \cdot \boldsymbol{r}} \hat{f}(\boldsymbol{k}_a) d\omega_{k_a}, \end{aligned}\right\} \tag{2.8.94}$$

$F_N(E,\vartheta)$ being the function considered in eq. (2.8.63). Then it follows from eq. (2.8.63) that there is a function $A(\boldsymbol{k}_b,\boldsymbol{r})$ such that

$$\lim_{N\to\infty} \int |A(\boldsymbol{k}_b, \boldsymbol{r}) - A_N(\boldsymbol{k}_b, \boldsymbol{r})|^2 d\boldsymbol{k}_b = 0. \tag{2.8.95}$$

Either side of eq. (2.8.81) is equal to

$$\tfrac{1}{4}(2\pi)^{-4} \int |A(\boldsymbol{k}_b, \boldsymbol{r})|^2 d\boldsymbol{k}_b = \tfrac{1}{4}(2\pi)^{-4} \lim_{N\to\infty} \int |A_N(\boldsymbol{k}_b, \boldsymbol{r})|^2 d\boldsymbol{k}_b . \tag{2.8.96}$$

The intensity scattered into channel b is obtained from this expression by integrating over $\boldsymbol{r}$. Now

$$\left.\begin{aligned} \tfrac{1}{4}(2\pi)^{-4} \int_{\delta\omega} d\omega_{k_b} \int |A_N(\boldsymbol{k}_b, \boldsymbol{r})|^2 k_b^2 dk_b &\le \tfrac{1}{4}(2\pi)^{-4} \int_{4\pi} d\omega_{k_b} \int |A_N(\boldsymbol{k}_b, \boldsymbol{r})|^2 k_b^2 dk_b \\ &\le ||(S_{ba} - \delta_{ba}) f_a(\boldsymbol{r})||^2, \end{aligned}\right\} \tag{2.8.97}$$

the second inequality following with eq. (2.8.82). Since the right-hand side of eq. (2.8.97) is an integrable function of $\boldsymbol{r}$, it follows that, when integrating the expression (2.8.96) over $\boldsymbol{r}$, we have

$$\int d\boldsymbol{r} \lim_{N\to\infty} = \lim_{N\to\infty} \int d\boldsymbol{r}. \tag{2.8.98}$$

By analogy with eq. (2.8.88)

$$\int_{Q} |A_N(\boldsymbol{k}_b,\boldsymbol{r})|^2 d\boldsymbol{r} = 4\pi^2 \int |F_N(\boldsymbol{k}_b,\boldsymbol{k}_a)\hat{f}(\boldsymbol{k}_a)|^2 (\cos\beta_a)^{-1} d\cos\beta_a d\alpha_a . \qquad (2.8.99)$$

Owing to eq. (2.8.98), the scattering intensity in the angle $\delta\omega$ thus takes the form

$$\frac{1}{16\pi^2} \lim_{N\to\infty} \int_{\delta\omega} d\omega_{k_b} \int k_b^2 dk_b \int |F_N(\boldsymbol{k}_b,\boldsymbol{k}_a)\hat{f}(\boldsymbol{k}_a)|^2 (\cos\beta_a)^{-1} d\cos\beta_a d\alpha_a . \qquad (2.8.100)$$

The limit can now be performed with eq. (2.8.63). We simply obtain

$$\lim_{N\to\infty} \int_{\delta\omega} d\omega_{k_b} \int k_b^2 dk_b \int |F_N \hat{f}|^2 (\cos\beta_a)^{-1} d\omega_{k_a} = \int_{\delta\omega} d\omega_{k_b} \int k_b^2 dk_b \int |F\hat{f}|^2 (\cos\beta_a)^{-1} d\omega_{k_a} . \qquad (2.8.101)$$

This shows that $\int_{\delta\omega} I_{ba}(\omega_{k_b}) d\omega_{k_b}$ is the intensity of the scattering into the angle $\delta\omega$, as we wished to prove.

2.8.8. The cross section

To illustrate the physics of eq. (2.8.93), we consider the particular case that $\hat{f}(\boldsymbol{k}_a)$ vanishes except in a small region $d\boldsymbol{k}_a$. Decomposing our wave-functions into incident and scattered waves, we evaluate the total number of projectiles incident upon a surface element δs of a plane perpendicular to $\boldsymbol{k}_a$. This quantity is denoted by $\delta s \int N(\boldsymbol{k}_a) d\boldsymbol{k}_a$.

The incident wave associated with the projectile $f(\boldsymbol{x}_a + \boldsymbol{r})$ contains as a factor the relative motion

$$f(\boldsymbol{x}_a + \boldsymbol{r}, t) = (2\pi)^{-\frac{3}{2}} \int \exp[i(-k_a^2 t + \boldsymbol{k}_a \cdot \boldsymbol{x}_a + \boldsymbol{k}_a \cdot \boldsymbol{r})] \hat{f}(\boldsymbol{k}_a) d\boldsymbol{k}_a . \qquad (2.8.102)$$

This satisfies the Schrödinger equation

$$\left[\Delta(\boldsymbol{x}_a) + i\frac{\partial}{\partial t}\right] f(\boldsymbol{x}_a + \boldsymbol{r}, t) = 0. \qquad (2.8.103)$$

Hence there is a continuity equation of the form

$$\frac{\partial}{\partial t} |f(\boldsymbol{x}_a + \boldsymbol{r}, t)|^2 + \operatorname{div}\{\operatorname{Re}[-2i\bar{f}(\boldsymbol{x}_a + \boldsymbol{r}, t) \operatorname{grad} f(\boldsymbol{x}_a + \boldsymbol{r}, t)]\} = 0, \qquad (2.8.104)$$

the expression in curly brackets being a flux vector. The unconventional factor 2 is due to our normalization of $\boldsymbol{x}_a$ (cf. eq. (2.1.2)). With this factor, the number of projectiles $f(\boldsymbol{x}_a + \boldsymbol{r})$ with $\boldsymbol{r}$-vector in $d\boldsymbol{r}$ that pass through δs in the time interval dt takes the form

$$\left.\begin{aligned} 2(2\pi)^{-3}dtd\boldsymbol{r}\mathrm{Re}\Big[\int\limits_{\delta s} d\boldsymbol{x}_a \int \exp[-i(-k_a'^2 t + \boldsymbol{k}_a'\cdot\boldsymbol{x}_a + \boldsymbol{k}_a'\cdot\boldsymbol{r})]\bar{\hat{f}}(\boldsymbol{k}_a')d\boldsymbol{k}_a' \\ \times \int k_a \exp[i(-k_a^2 t + \boldsymbol{k}_a\cdot\boldsymbol{x}_a + \boldsymbol{k}_a\cdot\boldsymbol{r})]\hat{f}(\boldsymbol{k}_a)d\boldsymbol{k}_a\Big]. \end{aligned}\right\} \quad (2.8.105)$$

The total number of projectiles passing through δs at some time t is obtained from this expression by integrating over t and $\boldsymbol{r}$. If we remember that

$$\int d\boldsymbol{k}_a = \tfrac{1}{2}\int (k_a^2 - k_{a1}^2 - k_{a2}^2)^{-\frac{1}{2}} dk_a^2 dk_{a1} dk_{a2}, \quad (2.8.106)$$

the integration can be performed explicitly with the standard theory of Fourier transforms. The final result is

$$N(\boldsymbol{k}_a) = |\hat{f}(\boldsymbol{k}_a)|^2 (\cos\beta_a)^{-1}. \quad (2.8.107)$$

Hence, according to eq. (2.8.93),

$$I_{ba}(\omega_{k_b}) = (4\pi)^{-2}\int |F_{ba}(\boldsymbol{k}_b, \boldsymbol{k}_a)|^2 N(\boldsymbol{k}_a) k_b k_a^{-1} d\boldsymbol{k}_a. \quad (2.8.108)$$

The function $|F_{ba}/4\pi|^2$ thus transforms the number of projectiles incident per unit area into the number scattered into a unit angle. It is the cross section for scattering from channel a into channel b.

2.8.9. The optical theorem

According to eq. (2.3.65) the total intensity of the scattering from channel a is given by

$$I = 2\int\limits_{\varrho} \mathrm{Re}(f_a(\boldsymbol{r}), [1 - S_{aa}]f_a(\boldsymbol{r}))d\boldsymbol{r}. \quad (2.8.109)$$

With eq. (2.6.67) this reduces to

$$\left.\begin{aligned} I = \frac{1}{8\pi^2}\int d\boldsymbol{r}\,\mathrm{Im}[\lim_{\varepsilon\to 0}\lim_{X_a\to\infty}\int dE \int\int d\omega_{k_a'} d\omega_{k_a} k_a^2 \bar{\hat{f}}(\boldsymbol{k}_a') e^{-i\boldsymbol{k}_a'\cdot\boldsymbol{r}} \\ \times F_{aa}(\boldsymbol{k}_a', \boldsymbol{k}_a; \varepsilon; X_a)\hat{f}(\boldsymbol{k}_a) e^{i\boldsymbol{k}_a\cdot\boldsymbol{r}}], \end{aligned}\right\} \quad (2.8.110)$$

where F_{aa} is the function (2.8.1) and $\boldsymbol{k}_a', \boldsymbol{k}_a$ are two vectors of length k_a. From the form of F_{aa} it is easily seen that

$$\left.\begin{aligned} I = -\frac{i}{16\pi^2}\int\limits_{\varrho} d\boldsymbol{r}\lim_{\varepsilon\to 0}\int dE\int\int d\omega_{k_a'} d\omega_{k_a} k_a^2 \bar{\hat{f}}(\boldsymbol{k}_a') e^{-i\boldsymbol{k}_a'\cdot\boldsymbol{r}} \\ \times (V_a\varphi_a e^{i\boldsymbol{k}_a'\cdot\boldsymbol{x}_a}, [R(E+i\varepsilon) - R(E-i\varepsilon)]V_a\varphi_a e^{i\boldsymbol{k}_a\cdot\boldsymbol{x}_a})\hat{f}(\boldsymbol{k}_a) e^{i\boldsymbol{k}_a\cdot\boldsymbol{r}}. \end{aligned}\right\} \quad (2.8.111)$$

With the help of eqs. (2.8.5) and (2.8.7), I can be developed according to

$$I = \int_{\Omega} d\boldsymbol{r} \lim_{\varepsilon \to 0} \sum_{l=0}^{\infty} \sum_{m} \int [1 - \mathrm{Re}\check{S}_{aa}(E,l;\varepsilon;X_a)] \left| \int \bar{Y}_{lm}(\omega_{k_a}) e^{i\boldsymbol{k}_a \cdot \boldsymbol{r}} \hat{f}(\boldsymbol{k}_a) d\omega_{k_a} \right|^2 k_a dE. \quad (2.8.112)$$

Now let $\hat{f}(\boldsymbol{k}_a)$ satisfy eq. (2.8.77) and let it vanish outside some bounded interval. Then each term of the series in eq. (2.8.112) tends to a limit as ε tends to 0, by eq. (2.7.60). Also, the function $g_{lm}(E,\boldsymbol{r})$ defined in eq. (2.8.86) is bounded uniformly with respect to l,m. The terms of the series in eq. (2.8.112) are all non-negative, by eq. (2.8.40). Therefore, since in eq. (2.8.42) the series on the left converges uniformly with respect to ε, so does the series in eq. (2.8.112). From this it follows that the limit of the sum is the sum of the limits of the separate terms. In other words,

$$I = \int_{\Omega} d\boldsymbol{r} \sum_{l=0}^{\infty} \sum_{m} \int [1 - \mathrm{Re}S_{aa}(E,l)] |g_{lm}(E,\boldsymbol{r})|^2 k_a dE. \quad (2.8.113)$$

If $\hat{f}(\boldsymbol{k}_a)$ satisfies the further restriction (2.8.89), the integration over $\boldsymbol{r}$ can be performed with the help of eq. (2.8.88). With eqs. (2.8.36) and (2.8.37), the result is

$$\left.\begin{aligned} I &= \pi \sum_{l=0}^{\infty} (2l+1) \int [1 - \mathrm{Re}S_{aa}(E,l)] k_a^{-1} dE \int |\hat{f}(\boldsymbol{k}_a)|^2 (\cos\beta_a)^{-1} d\cos\beta_a \, d\alpha_a \\ &= \int \mathrm{Im}\, F_{aa}(E,0) |\hat{f}(\boldsymbol{k}_a)|^2 (k_a \cos\beta_a)^{-1} d\boldsymbol{k}_a . \end{aligned}\right\} \quad (2.8.114)$$

By analogy with eq. (2.8.108) we may write

$$I = \int \mathrm{Im}\, F_{aa}(E,0) k_a^{-1} N(\boldsymbol{k}_a) d\boldsymbol{k}_a . \quad (2.8.115)$$

This shows that $\mathrm{Im}F_{aa}(E,0)k_a^{-1}$ is the total cross section, which is thus equal to $4\pi k_a^{-1}$ times the imaginary part of the forward elastic scattering amplitude. This is a special form of the optical theorem discussed in section 2.3.7.

2.8.10. Discussion

In the standard treatment of one-channel potential scattering, it is shown that an incoming plane wave $\exp(i\boldsymbol{k}_a \cdot \boldsymbol{x}_a)$ yields a radially outgoing wave which for large x_a behaves asymptotically as

$$\frac{1}{x_a} X_{aa}\left(\frac{k_a}{x_a}\boldsymbol{x}_a, \boldsymbol{k}_a\right) \exp(ik_a x_a), \quad (2.8.116)$$

with some function X_{aa} depending only on k_a and on the angle between $\boldsymbol{x}_a$ and $\boldsymbol{k}_a$. From the asymptotic behaviour it follows that $|X_{aa}|^2$ is the cross section for elastic

scattering. If we compare the standard theory with the present formalism, we see that X_{aa} is nothing but $F_{aa}/4\pi$. Hence the name scattering amplitude used in the foregoing.

Since a plane wave is not of finite norm, it cannot easily be incorporated in our Hilbert-space formalism. It is, of course, possible to consider superpositions of plane waves, i. e. wave-packets. However, the expression we found for the scattering intensity due to a single wave-packet is more complicated than a mere integral of the form

$$\int d\boldsymbol{k}_b \int |F_{ba}(\boldsymbol{k}_b, \boldsymbol{k}_a)\hat{h}(\boldsymbol{k}_a)|^2 d\omega_{k_a}. \tag{2.8.117}$$

Indeed, in eqs. (2.6.71) and (2.8.74) we have multiple integrals

$$\int d\boldsymbol{k}_b \int \bar{F}_{ba}(\boldsymbol{k}_b, \boldsymbol{k}'_a)\bar{\hat{h}}(\boldsymbol{k}'_a) d\omega_{k'_a} \int F_{ba}(\boldsymbol{k}_b, \boldsymbol{k}_a)\hat{h}(\boldsymbol{k}_a) d\omega_{k_a}. \tag{2.8.118}$$

These apply to a single scattering event. What one observes experimentally is the cross section. This is the number of fragments emerging per unit angle per unit time, divided by the number incident per unit area per unit time. It thus refers to a stream of projectiles. One usually describes such a stream with the help of a plane wave, but in the present paper we use a statistical mixture of wave-packets called a beam. This procedure leads to the conditions (2.8.89) and (2.8.18) on the wave-function $\hat{f}(\boldsymbol{k}_a)$ and on the interaction, respectively. If these are fulfilled, the intensity scattered from the beam can be evaluated in a completely straightforward manner. It yields an expression of the form (2.8.117). From this it then follows that $|F_{ba}/4\pi|^2$ is the cross section. If the theory is set up in this way, the difficulties of the standard plane-wave theory are avoided completely. In particular, there are no normalization problems, nor is there any ambiguity as regards the channel concept. Also, if $\hat{f}(\boldsymbol{k}_a)$ vanishes except in a small region $d\boldsymbol{k}_a$, the beam $\hat{f}(\boldsymbol{k}_a)$ more closely resembles a collimated stream of projectiles than does the plane wave $\exp(i\boldsymbol{k}_a \cdot \boldsymbol{x}_a)$. To describe a scattering experiment, a beam as defined here is therefore an improvement on a plane wave.

The condition (2.8.89) implies that $\hat{f}(\boldsymbol{k}_a)$ must vanish as $\cos\beta_a = 0$. It thus guarantees that the beam properly passes through the plane ϱ. If $\hat{f}(\boldsymbol{k}_a)$ were different from 0 only in the neighbourhood of $\cos\beta_a = 0$, the beam would propagate almost parallel to the plane ϱ. Since all projectiles would then have almost the same interaction with the target, the total scattering intensity would not remain finite. Similarly, the scattering intensities due to the separate projectiles would add up to infinity if at large distances the interaction did not fall off sufficiently rapidly. It is only if the interaction tends to 0 reasonably fast that projectiles with large $\boldsymbol{r}$-values are not disturbed appreciably. Hence it is only under some suitable condition on V_{pq} that we may expect the integral over $\boldsymbol{r}$ of the separate scattering intensities to be convergent. A sufficient condition is formulated explicitly in eq. (2.8.18).

Throughout the present paper we have tried to keep the formalism mathematically rigorous. It is unfortunate that this has led to tedious considerations, par-

ticularly as regards limits with respect to ε. It must be emphasized, however, that every time we prove that there is a limit, the argument can be traced back to the time development in a scattering system, and to the properties of the interaction between scattered fragments. We thus feel that the limiting behaviour as ε tends to 0 reflects in a mathematical form what is the essence of a scattering event.

In eq. (2.7.44) the function $S_{ba}(E,l)$ is defined as the derivative of the limit of a sequence of integrals,

$$S_{ba}(E,l)k_a = \frac{d}{dE} \lim_{\varepsilon \to 0} \lim_{X_b \to \infty} \int^{E} S_{ba}(E',l;\varepsilon;X_b)k'_a dE'. \tag{2.8.119}$$

There is a similar relation for the imaginary part of the scattering amplitude, the definition of the real part being slightly more complicated. Now it is conceivable that in some, or perhaps even in many, cases we have

$$S_{ba}(E,l) = \lim_{\varepsilon \to 0} \lim_{X_b \to \infty} S_{ba}(E,l;\varepsilon;X_b). \tag{2.8.120}$$

However, thus far we have found no evidence to this effect. On the other hand, there is a much more useful limiting relation. In fact, it will be shown in a sequel to the present paper that for a large class of interactions there exists an analytic function $S_{ba}(E+i\varepsilon,l;X_b)$ such that

$$S_{ba}(E,l) = \lim_{\varepsilon \to 0} \lim_{X_b \to \infty} S_{ba}(E+i\varepsilon,l;X_b) \tag{2.8.121}$$

for almost every E. The scattering amplitude is likewise the boundary value of an analytic function. In the neighbourhood of the real axis this function is sufficiently smooth to satisfy a dispersion relation. Also, in virtue of eq. (2.8.121), there is a parameter expansion for the scattering matrix which brings out the existence of resonances against a smoothly varying background. The present results thus make a starting-point for further work. A sequel to this paper will show again that there is an intimate connection between the limiting behaviour of scattering functions and the qualitative features of scattering events.

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Note added in proof

After the present paper was completed we learned that FADDEEV (31, 32) has shown that in a three-particle system there is unitarity in the sense of eq. (2.3.35) under fairly mild conditions on the interaction. This result gives a partial answer to the problem discussed in sections 2.3.4 and 2.3.5.

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