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DEFORMED EXCITED STATES IN CLOSED SHELL NUCLEI

BY

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Synopsis

A systematic theory of treating the complex ground-state correlations for 2particle-2hole excitations is proposed. It is shown that these new ground-state correlations describe the collective predisposition of the *spherical* ground state in closed-shell nuclei to produce *deformed* excited states. The resulting deformation of the excited states incorporates the deformation of the core. These features are made evident by a self-consistent method. Formal properties of the solutions and their influence on various electromagnetic transitions are discussed.

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1. Introduction

For a long time it has been difficult to understand the position of low lying even parity states in closed-shell nuclei. Several years ago a clue to the solution was suggested by BOHR and MOTTELSON in connection with the "mysterious zero plus states". The suggestion (pointing out the special importance of seeing the low lying states from the stand-point of deformed excited states⁽¹⁾) has been confirmed by recent experiments⁽²⁾ which show that many of the low lying excited states in O^{16} and Ca^{40} can be fitted into rotational bands. Along this line, several investigations^(3, 4) have been made, in particular in the interesting work of G. E. BROWN^(5, 6), how to interpret the rotational band structure and in connection with it the low excitation energy of the even parity states.

As a first step, Brown considers in his model unperturbed excited states with a definite number of particles and holes. These states may be obtained⁽³⁾ from a Hartree-Fock approximation*. They turn out to be deformed in a body-fixed system and thus account for the occurrence of rotational bands. The deformation then is regarded as the main reason for the low excitation energy of the first excited 0^+ state in O^{16} . However, excitations consisting of pure 2particle-2hole (2p-2h) or 4particle-4hole (4p-4h) configurations would not be able to account for the observed strong electromagnetic transitions between the rotational band and the ground state. Therefore, Brown^(5, 6) introduces, in a second step, a considerable mixing between a few specific unperturbed excited states and the spherical shell-model ground state. Of course, this procedure will in general destroy the rotational band structure obtained in the first step. The problem then is to find a reasonable mixing of unperturbed states, which explains both the electromagnetic transitions and at the same time preserves the rotational band structure. Because of this restriction, and in spite of the striking success of the model, it appears to us that the account for ground-state correlations is somewhat artificial and insufficient, and a refined treatment is desirable.

* Actually, in Brown's model the core deformation is taken into account phenomenologically as an important correction.

Such a refinement should be based on ground-state correlations which are known to be particularly important for collective phenomena in nuclei. We may expect that the correct ground state has a collective predisposition for collective excitations. In other words, the collective correlation which is responsible for collective excited states will also be present in the ground state as a ground-state correlation. In the phenomenological theory, the collective predisposition clearly manifests itself in the zero-point motion. Correspondingly, the success of the new Tamm-Dancoff method (NTD) or random-phase approximation (RPA) in describing collective phenomena is essentially due to the *symmetrical* treatment of correlations for both the excited states and the ground state. In this way the collective predisposition is properly incorporated in the theory. This is certainly an improvement over the Tamm-Dancoff method (TD) which asymmetrically attributes all the collectiveness exclusively to the excited states. For instance, if we just consider configurations with a definite number of particles and holes and treat them in the TD⁽⁷⁾ or (in order to obtain a more clear-cut notion of "intrinsic deformation") in the Hartree-Fock approximation⁽³⁾, the resulting collectiveness which produces the deformation is entirely ascribed to the excited states. But we have seen above that *the collectiveness should be incorporated in the ground state as a collective predisposition to produce deformed excited states*. This collective point of view has been especially stressed by BOHR and MOTTELSON*, and is the essential stand-point of the present theory. Once the corresponding ground-state correlations have been taken into account properly, the excited states will become much more "collective", and both the deformations and the level positions of the excited states will be quite different from those obtained by the TD or Hartree-Fock method. The importance of such changes for explaining the actual deformations and actual level positions has long been recognized⁽⁸⁾; the effect is often referred to as the "deformation of the core by the excited particle". This cooperation effect of the core is usually discussed in the single-particle picture, where it is reflected in the change of the energy difference between the highest occupied and the lowest unoccupied Nilsson level as a function of the deformation^(5, 6). Quantitatively this effect can be seen in the Volkov⁽⁹⁾ type calculations. In O¹⁶, for example, the energy necessary to excite a particle pair has a minimum for large prolate deformations. From our collective point of view, this precisely corresponds to the collective predisposition of the *spherical* ground state to produce *deformed* excited states.

* See, for instance, the discussion in Congrès International de Physique Nucléaire, Vol. I (Paris, 1964) 129.

The main purpose of this paper is to propose a theory which takes into account such a collective predisposition in the spherical ground state and to treat the cooperation effect of the core for deformations in the excited states in a self-consistent way. Of course, one might try to solve the problem by diagonalizing the Hamiltonian in a space which includes enough configurations to describe core deformation effects. However, the straightforward approach has two essential defects: (a) the rank of the matrix to be diagonalized is too large to get solutions without serious approximations; (b) even if we have the exact solution we do not gain any physical insight into the nature of excitation. In order to reach a better understanding we are forced to extract the basic physical elements from our problem. To this end it is useful to invoke the well-known notions of the *field-producing force* and the *residual interaction* as a guide. The field-producing force generates a (deformed) self-consistent field and is well accounted for in a Hartree-Fock approximation. By definition, the residual interaction cannot be incorporated in a self-consistent field. It is responsible for the pairing correlations in the superconducting state and for two-particle (or two-hole) scattering correlations in the normal (non-superconducting) state. Usually the residual interaction is considered to be unimportant for closed-shell nuclei because of the large energy spacing between occupied and unoccupied levels. However, we have discussed above that for large prolate deformations (due to the field-producing force) the occupied and unoccupied levels come quite close to each other. This means that even if the residual interaction is small, *the interplay between the residual interaction and the field-producing force will be of decisive importance.* (This is also reflected in Brown's model where the residual interaction gives rise to mixing effects). We may reformulate the statement in another way: If, for simplicity, we adopt the "pairing plus quadrupole force model", then the difference in parity between major shells prevents the quadrupole force from exciting particles from an occupied shell to the nearest unoccupied shell even if the force is strong. In fact, particles can only be excited by the *pairing force* even if its strength is weak. Once particles are excited, however, the quadrupole force will act strongly among the excited configurations and efficiently lead to deformations.

Both this picture and the aim of investigating the important interplay between field-producing forces and the residual interaction suggest the following two-step procedure: In a first step we diagonalize the residual interaction including ground-state correlations, and in a second step we diagonalize the field-producing forces. This gives rise to a new type of ground-state correlations which will be shown to exhibit the collective predisposition of

the spherical ground state for deformed excited states. The outline of this two-step method is presented in section 2 and the details of both steps in sections 3 and 4, respectively. In section 5, we extract the basic element, which produces deformations in the excited states, from the general solution of sect. 4. We show, in a succession of generalizations of the customary Hartree-Fock approximation⁽³⁾ (which leads to deformed excited states), how we can get a self-consistent method which contains the core deformation effect explicitly and is an approximation for the method given in section 4. In section 6, the theory is applied to electromagnetic transitions in which the interplay between the field-producing force and the residual interaction plays a decisive role. In section 7, finally, we indicate the application of our theory to other problems and summarize our results.

2. Outline of the Theory

It is the purpose of the present section to give a first understanding of and additional motivation for our theory. For clarity, we will not use here a decomposition of the interaction into a field-producing force and a residual interaction, as discussed in the introduction, but rather use a closely related subdivision which characterizes various parts of the Hamiltonian by Feynman diagrams. The original point of view will be taken up in section 5.

2.1. Notation and Hamiltonian

Let us consider a closed-shell nucleus and assume its ground state to be spherical and normal (i.e., non-superconducting). Adopting the j - j coupling shell model for the zero-order states, we can define the particle- and hole creation and annihilation operators as

$$\left. \begin{aligned} c_{\alpha}^{+} &= (1 - \theta_{\alpha})c_{\alpha}^{+} + \theta_{\alpha}c_{\alpha}^{+} = a_{\alpha}^{+} + b_{\alpha} \\ c_{\alpha} &= (1 - \theta_{\alpha})c_{\alpha} + \theta_{\alpha}c_{\alpha} = a_{\alpha} + b_{\alpha}^{+} \end{aligned} \right\} \quad (2.1)$$

where α denotes the complete set of quantum numbers $\alpha \equiv \{n, l, j, m, \tau\}$, and $a = \{n, l, j\}$ denotes the same set except for the projection quantum numbers.

Furthermore,

$$\theta_{\alpha} = \left. \begin{aligned} &1 \text{ for levels occupied in the free ground state} \\ &0 \text{ for levels unoccupied in the free ground state} \end{aligned} \right\} \quad (2.2)$$

where the free (unperturbed) ground state $|\Phi_0\rangle$ is defined by $a_\alpha|\Phi_0\rangle = b_\alpha|\Phi_0\rangle = 0$. For a basis of stationary states it is possible to build the entire treatment on real quantities if the phase convention is suitably chosen. In the following, we always assume this to be the case. The Hamiltonian can be written as

$$\left. \begin{aligned} H &= H_0 + H_{\text{int}} \\ H_0 &= \sum_{\alpha} (\varepsilon_{\alpha}^{(0)} - \lambda) : c_{\alpha}^{\dagger} c_{\alpha} : = \sum_{\alpha} \varepsilon_{\alpha} : c_{\alpha}^{\dagger} c_{\alpha} : \\ &= \sum_{\alpha} \varepsilon_{\alpha} (a_{\alpha}^{\dagger} a_{\alpha} - b_{\alpha}^{\dagger} b_{\alpha}) \\ H_{\text{int}} &= \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} : c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma} : \end{aligned} \right\} \quad (2.3)$$

where the symbol $: :$ denotes the normal product with respect to particles and holes, and λ is the chemical potential. The potential matrix element has the symmetry properties

$$v_{\alpha\beta\gamma\delta} = -v_{\beta\alpha\gamma\delta} = -v_{\alpha\beta\delta\gamma} = v_{\gamma\delta\alpha\beta}. \quad (2.4)$$

2.2 The Matrix Elements of the Interaction

In order to discuss the various parts of the interaction H_{int} we divide the Hamiltonian (2.3) in the following way:

$$H = H_0 + H_{pp} + H_{hh} + H_{ph} + H_V + H_Y, \quad (2.5)$$

where

$$\left. \begin{aligned} H_{pp} &= \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \\ H_{hh} &= \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} b_{\alpha}^{\dagger} b_{\beta}^{\dagger} b_{\delta} b_{\gamma} \\ H_{ph} &= 4 \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} b_{\delta}^{\dagger} a_{\gamma} b_{\beta} \\ H_V &= \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} (a_{\alpha}^{\dagger} a_{\beta}^{\dagger} b_{\delta}^{\dagger} b_{\gamma}^{\dagger} + a_{\alpha} a_{\beta} b_{\delta} b_{\gamma}) \\ H_Y &= 2 \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} (a_{\alpha}^{\dagger} a_{\beta}^{\dagger} b_{\delta}^{\dagger} a_{\gamma} + a_{\alpha}^{\dagger} b_{\beta} a_{\delta} a_{\gamma} \\ &\quad + a_{\alpha}^{\dagger} b_{\delta}^{\dagger} b_{\gamma}^{\dagger} b_{\beta} + b_{\delta}^{\dagger} b_{\alpha} b_{\beta} a_{\gamma}). \end{aligned} \right\} \quad (2.6)$$

Each matrix element is represented by one of the diagrams in fig. 1. The first three parts, H_{pp} , H_{hh} and H_{ph} , conserve the number of particles and holes and therefore are the only ones considered in the Tamm-Dancoff

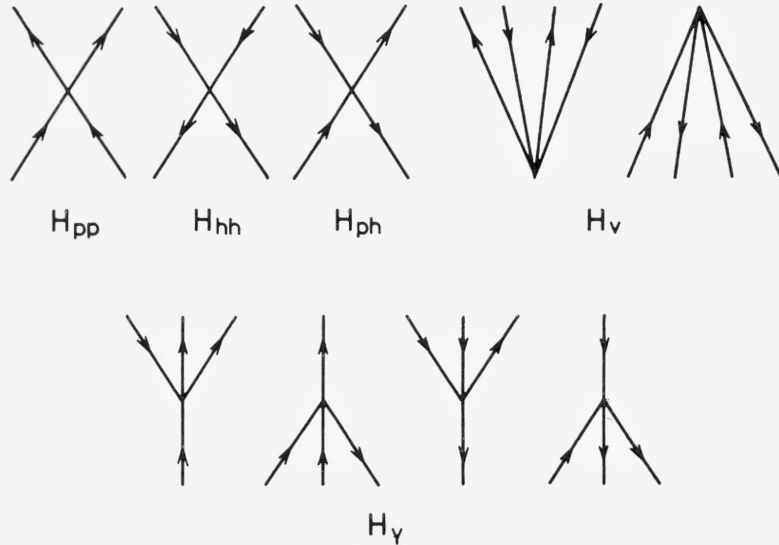


Fig. 1. Graphic representation of the matrix elements of the interaction. Lines with arrows pointing upwards indicate particles, lines with arrows pointing downwards indicate holes. Each diagram includes both the “direct” term and the “exchange” term.

calculation or the Hartree-Fock approximation⁽³⁾ for a fixed number of particles and holes. The part, H_v , introduces ground-state correlations and is discussed in the following subsection. Finally, the part H_Y will be neglected in our treatment. This is equivalent to the assumption that *only the excitations with an even number of particles and even number of holes are important for a description of low lying even parity states in closed-shell nuclei*. The assumption may be justified by the following arguments. (a) Among the $2\hbar\omega$ excitations the 2p-2h configurations offer by far more coupling possibilities than the 1p-1h configurations. Since a strong collectiveness is necessary to produce the deformed excited states, the space of all 2p-2h configurations will be of main importance. (b) Calculations^(7, 10) for O^{16} , using the Tamm-Dancoff approximation for 1p-1h and 2p-2h configurations, have failed to explain the electromagnetic transitions between the lowest excited states of even parity and the ground state. The calculated transition probabilities are by orders of magnitude too small. This means that the effect of 1p-1h configurations would be of less importance compared with the effect of ground-state correlations for the low lying even parity states in O^{16} .

2.3 A Two-Step Method

As has been indicated in the introduction, it is our aim to take the ground-state correlations properly into account and to investigate the important interplay between the field-producing force and the residual interaction. This has to be done in two distinct steps. G. E. Brown, in his model^(5,6), *first* treats the effects of the field-producing force on the excited states and afterwards incorporates, to some extent, effects of the residual interaction in the mixing of the deformed states. Such a procedure deals with the effects in the order of their importance; however, it encounters two intrinsic difficulties. (a) The unperturbed states obtained in the first step by a Hartree-Fock method will belong to different deformations. Thus (unless one uses the SU_3 model instead of the Hartree-Fock procedure), the unperturbed (deformed) states will not form an orthogonal set which, however, is required in order to treat the collective ground-state correlations properly. (b) Even if the problem of orthogonality did not arise, the incorporation of the residual interaction would destroy the rotational band structure obtained previously. To avoid such difficulties, we start from the excitation mechanism and treat the effects of the *residual interaction* in the *first step*. For a normal ground state in closed-shell nuclei, these effects will lead to 2-particle (or 2-hole) scattering correlations described by the following linearized relations:

$$[H, a_\alpha^+ a_\beta^+] = \sum_{\gamma\delta} (M_{\alpha\beta\gamma\delta} a_\gamma^+ a_\delta^+ + M'_{\alpha\beta\gamma\delta} b_\delta b_\gamma) \quad (2.7a)$$

$$[H, b_\alpha^+ b_\beta^+] = \sum_{\gamma\delta} (M_{\alpha\beta\gamma\delta} b_\gamma^+ b_\delta^+ + M'_{\alpha\beta\gamma\delta} a_\delta a_\gamma), \quad (2.7b)$$

where the coefficients M and M' depend only on the part $H_0 + H_{pp} + H_{hh} + H_V$ of the Hamiltonian (2.5). The equation of motion corresponding to the approximation (2.7) is solved by introducing certain eigenmodes (or elementary excitations) which consist of a correlated particle pair, A^+ , or a correlated hole pair B^+ . The correlated pairs (virtual Cooper pairs if $J = 0$) are represented schematically in fig. 2 together with the corresponding ground-state correlations. It is important to note that in constructing the pair scattering modes we have taken into account the interaction H_V at a stage where it is still easy to handle without severely reducing the dimension of the space in which the interaction is diagonalized as it is done in Brown's model.

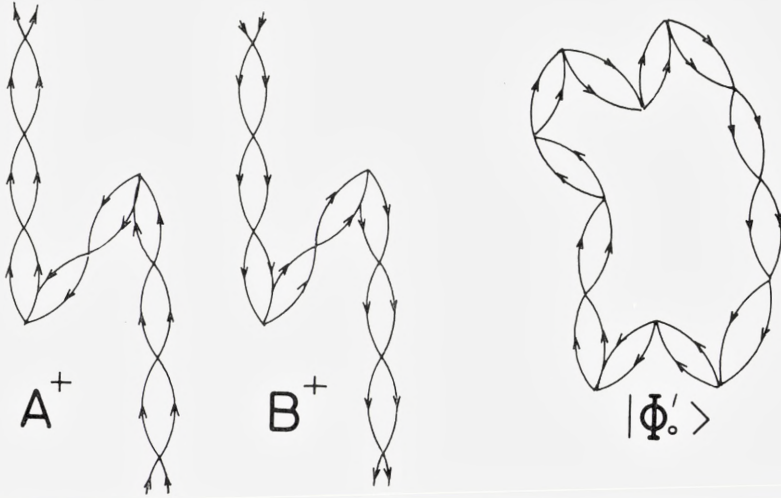


Fig. 2. Schematic representation of pair scattering modes for a particle pair A^+ and a hole pair B^+ . To the right: the corresponding ground-state correlations for the ground state $|\Phi'_0\rangle$. The states $A^+ B^+ |\Phi'_0\rangle$ will, in the following, often be called "2p-2h" states where the quotation marks indicate that also 4p-4h, 6p-6h, ... amplitudes (in the sense of the TD method) are admitted. The correlations will be called "pair scattering ground-state correlations" due to the residual interaction.

In the *second step* we diagonalize the particle-hole interaction* H_{ph} by using another linearized relation

$$[H, A_\mu^+ B_\nu^+] = \sum_{\rho\sigma} (N_{\mu\nu\rho\sigma} A_\rho^+ B_\sigma^+ + N'_{\mu\nu\rho\sigma} A_\rho B_\sigma) \quad (2.8)$$

which gives us new and very complex correlations. They are indicated in fig. 3 with broken lines symbolizing correlated pairs of the type shown in fig. 2. The formal resemblance with the correlations known from the ordinary RPA for the "1p-1h" problem suggests the appearance of new collective effects. The new ground-state correlations may be called *ground-state correlations due to the field producing force*. They exhibit the collective pre-disposition of the ground state for deformed excited states.

It should not be concealed here that these results can be derived only

* The main source of deformation in the excited states of closed-shell nuclei will be the repulsive particle-hole interaction (corresponding to an attractive particle-core interaction). This interaction forces, for example, the particles to the poles of the core if the holes are concentrated in the equatorial plane, so that particles and holes contribute to the deformation with equal sign. In the SU_3 model, this corresponds to the fact that the lowest 2p-2h states in O^{16} are those with maximum weight, namely with the SU_3 representation (42). These states have the particles along one axis and the holes in the plane vertical to this axis. For details, see the discussion at the end of sect. 4.1.

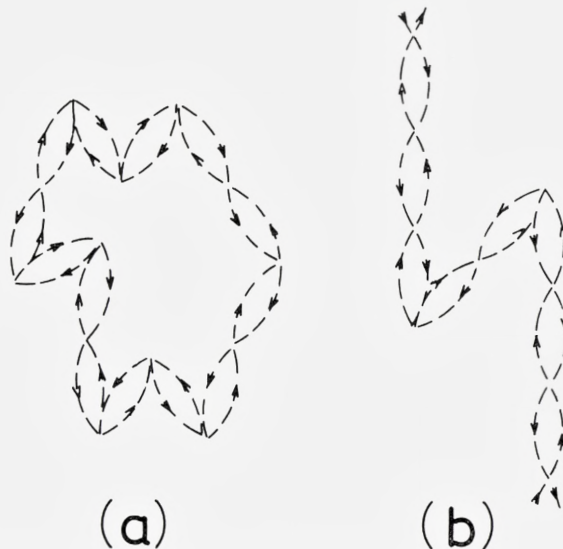


Fig. 3. Correlations introduced by the particle-hole interaction H_{ph} or by the field-producing force. The broken lines represent pair scattering modes: for a "particle pair" A^+ if the arrow points upwards, for a "hole pair" B^+ if the arrow points downwards. The diagram (a) is a typical graph taken into account in the ground state, the diagram (b) is typical of the graphs included in the description of a "dressed 2p-2h" system.

at the expense of giving up the Pauli principle between particles and holes belonging to different correlated pairs. Still, the Pauli principle is accurately taken into account as long as we are dealing with a 2p-2h system in the sense of the TD method. (For details, see section 3.3). In this respect our approximation is superior to the case in which the "particle-hole" pair is coupled to a *unit*, so that the Pauli principle is neglected even for a 2p-2h system in the sense of the TD method.

2.4 A Self-Consistent Approximation

In order to show that the solutions of our two-step procedure describe indeed deformed excited states, we propose a new self-consistent approximation which treats the cooperation effect of the core deformation in a self-consistent way. The conventional Hartree-Fock approximation for the excited states⁽³⁾ is obtained as a special case of our generalized self-consistent method if we neglect ground-state correlations and thus the effect of the core deformation.

3. Pair Scattering Correlations

In the preceding section we have shown that it is convenient to treat the particle pair (and hole pair) scattering correlation before entering the full complexity of “2p-2h” (in the NTD sense) or even higher excitations. In the present section we turn to the construction of these pair scattering modes and to the discussion of their properties.

3.1 The Equation of Motion

We define the operators for pair scattering eigenmodes by

$$C_\mu^+ = \sum_{\alpha\beta} (\psi_\mu(\alpha\beta) a_\alpha^+ a_\beta^+ + \varphi_\mu(\alpha\beta) b_\alpha b_\beta) \quad (3.1)$$

with

$$\psi_\mu(\alpha\beta) = -\psi_\mu(\beta\alpha) \quad \text{and} \quad \varphi_\mu(\alpha\beta) = -\varphi_\mu(\beta\alpha), \quad (3.2)$$

where

$$\mu = \{N, JM, TZ\}, \quad m = \{N, J, T\}$$

characterize the pair by the angular momentum J and its projection M , the isospin T and its projection Z , and a set of additional quantum numbers N . We start with the following linearized relation in the NTD approximation:

$$\left. \begin{aligned} [H, a_\alpha^+ a_\beta^+] &= \sum_{\gamma\delta} (M_{\alpha\beta\gamma\delta} a_\gamma^+ a_\delta^+ + M'_{\alpha\beta\gamma\delta} b_\delta b_\gamma) \\ [H, b_\alpha^+ b_\beta^+] &= \sum_{\gamma\delta} (M_{\alpha\beta\gamma\delta} b_\gamma^+ b_\delta^+ + M'_{\alpha\beta\gamma\delta} a_\delta a_\gamma). \end{aligned} \right\} \quad (3.3)$$

The matrices M and M' are obtained by taking the appropriate matrix elements of eq. (3.3) with respect to the unperturbed ground state and 2p-2h states. It is clear that only H_0 , H_{pp} , H_{hh} and H_V out of the Hamiltonian (2.5) contribute to the matrix elements M and M' . The correlation amplitudes $\psi_\mu(\alpha\beta)$ and $\varphi_\mu(\alpha\beta)$ (taken as real) are now determined as the solutions of the equation of motion

$$[H, C_\mu^+] = \omega_m C_\mu^+. \quad (3.4)$$

Using eq. (3.3) one obtains two coupled eigenvalue equations for ψ and φ which can be written in the compact form

$$\omega_m \Psi_\mu(\alpha\beta) = \sum_{\gamma\delta} \{ (|\varepsilon_a| + |\varepsilon_b|) \delta_{\alpha\gamma} \delta_{\beta\delta} + 2v_{\alpha\beta\gamma\delta} \} (1 - \theta_c - \theta_a) \Psi_\mu(\gamma\delta) \quad (3.5)$$

by using the convenient notation

$$\left. \begin{aligned} \psi_\mu(\alpha\beta) &= (1 - \theta_a)(1 - \theta_b)\Psi_\mu(\alpha\beta) \\ \psi_\mu(\alpha\beta) &= \theta_a\theta_b \Psi_\mu(\alpha\beta), \end{aligned} \right\} (3.6)$$

where θ_a is defined in eq. (2.2).

The vanishing of one of the eigenvalues ω_m would indicate an instability* of the normal ground state⁽¹¹⁾, but according to our assumption of a normal ground state we neglect this possibility. Equations of the structure (3.5) have been discussed previously in connection with the "independent pair model including the hole motion"⁽¹²⁾ and (for the special case of $J = 0$) in connection with the "pairing vibration"^(13, 14).

3.2 Properties of the Pair Scattering Modes

The secular matrix of eq. (3.5) can formally be considered as Hermitian provided we adopt an indefinite metric expressed by the following orthogonality relation^(12, 13):

$$\sum_{\alpha\beta} \Psi_\mu(\alpha\beta)(1 - \theta_a - \theta_b)\Psi_\nu(\alpha\beta) = \frac{1}{2}s_\mu \cdot \delta_{\mu\nu}, \quad (3.7)$$

where the sign function s_μ is defined by

$$s_\mu = \left\{ \begin{array}{ll} 1 & \text{if } \omega_m > 0 \\ -1 & \text{if } \omega_m < 0. \end{array} \right\} (3.8)$$

If none of the eigenvalues ω_m vanishes we also have the completeness relation

$$\sum_{\mu} \Psi_\mu(\alpha\beta)s_\mu\Psi(\gamma\delta) = \frac{1}{4}(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})(1 - \theta_a - \theta_b). \quad (3.9)$$

It is now convenient to distinguish the operators of the pair scattering eigenmodes according to the sign s_μ of the corresponding energy eigenvalue. Therefore we define, in formal analogy to eq. (2.1) for the fermion operators, the pair operators

* In that case we have a superconducting ground state so that we should make the Bogoliubov transformation.

$$\left. \begin{aligned} C_{\mu}^{+} &= \begin{cases} A_{\mu}^{+} & \text{if } \omega_m > 0 \\ B_{\mu} & \text{if } \omega_m < 0 \end{cases} \\ C_{\mu} &= \begin{cases} A_{\mu} & \text{if } \omega_m > 0 \\ B_{\mu}^{+} & \text{if } \omega_m < 0. \end{cases} \end{aligned} \right\} \quad (3.10)$$

The physical interpretation of the operators defined in eq. (3.10) is the following. The operator A_{μ}^{+} is the creation operator for a correlated particle pair: This means A_{μ}^{+} creates two particles with the large amplitudes $\varphi_{\mu}(\alpha\beta)$ {for $\omega_m > 0$ } and annihilates two holes with the small amplitudes $\varphi_{\mu}(\alpha\beta)$ {for $\omega_m > 0$ }. The operator B_{μ}^{+} is the creation operator for a correlated hole pair. This means that B_{μ}^{+} creates two holes with the large amplitudes $\varphi_{\mu}(\alpha\beta)$ {for $\omega_m < 0$ } and annihilates two particles with the small amplitudes $\varphi_{\mu}(\alpha\beta)$ {for $\omega_m < 0$ }. In the absence of ground-state correlations, A_{μ}^{+} and B_{μ}^{+} are identical with the operators which create an exact 2-particle eigenstate and 2-hole eigenstate in the TD method.

The definition and physical interpretation of the creation (annihilation) operators $A_{\mu}^{+}(A_{\mu})$ and $B_{\mu}^{+}(B_{\mu})$ for correlated pairs enable us to define a new ground state $|\Phi'_0\rangle$ by requiring

$$A_{\mu}|\Phi'_0\rangle = B_{\mu}|\Phi'_0\rangle = 0. \quad (3.11)$$

Clearly the new ground state now contains correlations due to the interactions H_{pp} , H_{hh} and H_V . It is a mixture of 0p-0h, 2p-2h, 4p-4h, etc. excitations in the sense of the TD method. Thus the diagrams considered in the ground state and the "2p-2h" excited states (in the NTD sense) are all diagrams of the type given in fig. 2.

3.3 The Physical Meaning of the Approximation

We want to use the pair scattering modes as a new basis of the theory and so it is necessary to discuss the physical implications of our approximations. For definiteness, we restrict ourselves in the following to a "2p-2h" problem* (in the sense of the NTD method, thus including 4p-4h, 6p-6h excitations, etc). The New Tamm-Dancoff method on which the present theory is built and which allows to describe the collective predisposition of the ground state has two important consequences.

* It is in principle possible⁽¹⁵⁾, however, to extend the theory to a "4p-4h" problem if it should turn out that a simple "2p-2h" description is not adequate for O¹⁶.

(a) The Pauli principle is violated between identical fermions belonging to different 2p-2h pairs. Writing down the linearized relation (3.3) implies, for consistency, that the commutation relations for fermion pairs reduce to Bose commutation rules. In other words, the 2-particle pairs $a_\alpha^+ a_\beta^+$ and 2-hole pairs $b_\gamma^+ b_\delta^+$ are approximated by quasi-boson operators

$$\left. \begin{aligned} a_\alpha^+ a_\beta^+ &\rightarrow \mathfrak{A}_{\alpha\beta}^+ & \text{with} & \quad \mathfrak{A}_{\alpha\beta}^+ = -\mathfrak{A}_{\beta\alpha}^+ \\ b_\gamma^+ b_\delta^+ &\rightarrow \mathfrak{B}_{\gamma\delta}^+ & \text{with} & \quad \mathfrak{B}_{\gamma\delta}^+ = -\mathfrak{B}_{\delta\gamma}^+ \end{aligned} \right\} \quad (3.12)$$

which satisfy the boson commutation relations

$$\left. \begin{aligned} [\mathfrak{A}_{\alpha_1\beta_1}^+, \mathfrak{A}_{\alpha_2\beta_2}^+] &= \delta_{\alpha_1\alpha_2} \delta_{\beta_1\beta_2} - \delta_{\alpha_1\beta_2} \delta_{\alpha_2\beta_1} \\ [\mathfrak{B}_{\gamma_1\delta_1}^+, \mathfrak{B}_{\gamma_2\delta_2}^+] &= \delta_{\gamma_1\gamma_2} \delta_{\delta_1\delta_2} - \delta_{\gamma_1\delta_2} \delta_{\gamma_2\delta_1} \\ [\mathfrak{A}_{\alpha\beta}^+, \mathfrak{B}_{\gamma\delta}^+] &= [\mathfrak{A}_{\alpha\beta}^+, \mathfrak{B}_{\gamma\delta}] = 0. \end{aligned} \right\} \quad (3.13 \text{ a})$$

Due to eqs. (3.1) and (3.10) these relations are equivalent to the well-known boson commutation relation for the correlated pair operators A_μ^+ and B_μ^+

$$\left. \begin{aligned} [A_\mu, A_\nu^+] &= \delta_{\mu\nu}, \quad [B_\mu, B_\nu^+] = \delta_{\mu\nu} \\ [A_\mu^+, B_\nu^+] &= [A_\mu^+, B_\nu] = 0. \end{aligned} \right\} \quad (3.13 \text{ b})$$

Now it is clear that, within the subspace S composed of the unperturbed ground state and all unperturbed 2p-2h excited states in the TD sense, there exists the following one-to-one correspondence between the fermion space and the boson space:

$$|\Phi_0\rangle \leftrightarrow |\Phi_0\rangle\rangle$$

and

$$a_\alpha^+ a_\beta^+ b_\gamma^+ b_\delta^+ |\Phi_0\rangle \equiv |\alpha\beta\gamma\delta\rangle \leftrightarrow \mathfrak{A}_{\alpha\beta}^+ \mathfrak{B}_{\gamma\delta}^+ |\Phi_0\rangle\rangle \equiv |\alpha\beta\gamma\delta\rangle\rangle,$$

where $|\Phi_0\rangle\rangle$ is the unperturbed ground state in the boson space defined by $\mathfrak{A}_{\alpha\beta}^+ |\Phi_0\rangle\rangle = \mathfrak{B}_{\gamma\delta}^+ |\Phi_0\rangle\rangle = 0$. Thus it is easily seen from eq. (3.12) that the Pauli principle is rigorously satisfied in a 2particle-2hole system even though it is treated in the boson space.

(b) As a second consequence of our NTD method (to keep the consistency with the determination of the matrix elements M and M' in (3.3)), we observe that all occurring matrix elements of physical one-body or two-body operators T are entirely restricted to matrix elements taken within a subspace composed of the unperturbed ground state and the unperturbed 2p-2h states. This, however, is just the subspace S in which the Pauli principle is *not* violated by the use of eqs. (3.13).

Thus it is possible to give a rule how to transcribe any physical operator T given in the fermion space into an operator \hat{T} defined in the boson space⁽¹⁵⁾. The new operator \hat{T} has to be constructed such that within the subspace S

$$\left. \begin{aligned} \langle\langle \alpha_1 \beta_1 \gamma_1 \delta_1 | \hat{T} | \alpha_2 \beta_2 \gamma_2 \delta_2 \rangle\rangle &= \langle \alpha_1 \beta_1 \gamma_1 \delta_1 | T | \alpha_2 \beta_2 \gamma_2 \delta_2 \rangle \\ \langle\langle \Phi_0 | \hat{T} | \alpha \beta \gamma \delta \rangle\rangle &= \langle \Phi_0 | T | \alpha \beta \gamma \delta \rangle \\ \langle\langle \alpha \beta \gamma \delta | \hat{T} | \Phi_0 \rangle\rangle &= \langle \alpha \beta \gamma \delta | T | \Phi_0 \rangle. \end{aligned} \right\} \quad (3.14)$$

Since all matrix elements which occur in the NTD method are taken with respect to states belonging to the subspace S , we can regard the operators \hat{T} as the *effective physical operators* in our NTD method. Clearly, if we neglect ground-state correlations, then, according to construction, all results obtained with the operator \hat{T} in the NTD method are identical to the results obtained with the operator T in the TD method.

3.4 The Expansion of Physical Operators

The preceding subsection provides us with a firm basis for expanding various physical operators in terms of pair scattering modes. The first task is to express the creation operator for two uncorrelated particles or holes in terms of pair scattering modes. This is easily achieved with the help of the completeness relation (3.9), and the result is

$$\left. \begin{aligned} a_\alpha^+ a_\beta^+ &\rightarrow \mathfrak{A}_{\alpha\beta}^+ \\ b_\alpha b_\beta &\rightarrow \mathfrak{B}_{\beta\alpha} \end{aligned} \right\} = \begin{cases} 2(1 - \theta_a - \theta_b) \sum_\mu \Psi_\mu(\alpha\beta)(A_\mu^+ - B_\mu) \\ 2(1 - \theta_a - \theta_b) \sum_\mu \Psi_\mu(\alpha\beta) s_\mu C_\mu^+ \end{cases} \quad (3.15)$$

The next problem is to find the effective physical operators which are consistent with our NTD approximation. As an example, let us consider a physical one-body operator \mathfrak{D} :

$$\mathfrak{D} = \sum_{\alpha\beta} \mathfrak{D}_{\alpha\beta} : c_\alpha^+ c_\beta : = \sum_{\alpha\beta} \mathfrak{D}_{\alpha\beta} (a_\alpha^+ a_\beta - b_\beta^+ b_\alpha + a_\alpha^+ b_\beta^+ - a_\beta b_\alpha). \quad (3.16)$$

Then, the rule (3.14) easily gives us the transcribed operator

$$\hat{\mathfrak{D}} = \sum_{\alpha\beta\gamma} \mathfrak{D}_{\alpha\beta} \{ \mathfrak{A}_{\alpha\gamma}^+ \mathfrak{A}_{\beta\gamma} - \mathfrak{B}_{\beta\gamma}^+ \mathfrak{B}_{\alpha\gamma} \}, \quad (3.17)$$

which is equivalent to the replacement

$$a_\alpha^+ a_\beta \rightarrow \sum_\gamma \mathfrak{A}_{\alpha\gamma}^+ \mathfrak{A}_{\beta\gamma} \quad \text{and} \quad b_\beta^+ b_\alpha \rightarrow \sum_\gamma \mathfrak{B}_{\beta\gamma}^+ \mathfrak{B}_{\alpha\gamma}. \quad (3.18)$$

In order to get the expansion of one-body operators (3.16) in terms of pair scattering modes C^+ and C , we have now only to insert (3.15) into (3.17). As an application of the resulting expansion, one can easily find that the total number operator of our system

$$\mathfrak{N} = \sum_{\alpha} c_{\alpha}^{\dagger} c_{\alpha} = \sum_{\alpha} (a_{\alpha}^{\dagger} a_{\alpha} - b_{\alpha}^{\dagger} b_{\alpha}) + \text{total number of particles in the system} \quad (3.19)$$

is expanded as

$$\mathfrak{N} = 2 \sum_{\mu} (A_{\mu}^{\dagger} A_{\mu} - B_{\mu}^{\dagger} B_{\mu}) + \text{total number of particles in the system.} \quad (3.20)$$

Similarly, the μ -component of the angular momentum operator

$$J_{\mu} = \sum_{\alpha\beta} \langle \alpha | J_{\mu} | \beta \rangle \delta_{ab} \delta_{\tau_{\alpha} \tau_{\beta}} : c_{\alpha}^{\dagger} c_{\beta} : \quad (3.21)$$

with

$$\langle \alpha | J_{\mu} | \beta \rangle \delta_{ab} = \langle j_b 1 m_{\beta} \mu | j_a m_{\alpha} \rangle \sqrt{j_a(j_a + 1)} \delta_{ab}$$

is expanded as

$$\hat{J}_{\mu} = \sum_{\varrho\sigma} \langle \varrho | J_{\mu} | \sigma \rangle \delta_{rs} \delta_{z_{\varrho} z_{\sigma}} (A_{\varrho}^{\dagger} A_{\sigma} - B_{\varrho}^{\dagger} B_{\sigma}) \quad (3.22)$$

with

$$\langle \varrho | J_{\mu} | \sigma \rangle \delta_{rs} = \langle J_s 1 M_{\sigma} \mu | J_r M_{\varrho} \rangle \sqrt{J_r(J_r + 1)} \delta_{rs}.$$

The formal analogy to the usual expressions in the fermion space indicates the usefulness and, in fact, the simplicity of the expansion in terms of pair scattering modes.

3.5 The Expansion of the Hamiltonian

The rule (3.14) also enables us to expand the Hamiltonian in terms of pair scattering modes. Each term (2.6) in the decomposition (2.5) of the Hamiltonian can be transcribed into the boson space. The result is

$$H_0 \rightarrow \hat{H}_0 = \frac{1}{2} \sum_{\alpha\beta} (\varepsilon_a + \varepsilon_b) (\mathfrak{A}_{\alpha\beta}^{\dagger} \mathfrak{A}_{\alpha\beta} - \mathfrak{B}_{\alpha\beta}^{\dagger} \mathfrak{B}_{\alpha\beta}) \quad (3.23 a)$$

$$H_{pp} \rightarrow \hat{H}_{pp} = \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} \mathfrak{A}_{\alpha\beta}^{\dagger} \mathfrak{A}_{\gamma\delta} \quad (3.23 b)$$

$$H_{hh} \rightarrow \hat{H}_{hh} = \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} \mathfrak{B}_{\alpha\beta}^{\dagger} \mathfrak{B}_{\gamma\delta} \quad (3.23 c)$$

$$H_V \rightarrow \hat{H}_V = \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} (\mathfrak{A}_{\alpha\beta}^{\dagger} \mathfrak{B}_{\delta\gamma}^{\dagger} + \mathfrak{A}_{\alpha\beta} \mathfrak{B}_{\delta\gamma}) \quad (3.23 d)$$

$$H_{ph} \rightarrow \mathring{H}_{ph} = -4 \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} \sum_{\varepsilon} \mathfrak{A}_{\alpha\varepsilon}^+ \mathfrak{A}_{\gamma\varepsilon} \sum_{\varphi} \mathfrak{B}_{\delta\varphi}^+ \mathfrak{B}_{\beta\varphi} \quad (3.23\text{e})$$

$$H_Y \rightarrow 0. \quad (3.23\text{f})$$

As has been discussed in section 2.1, the operator H_Y does not contribute in our approximation where only states with an even number of particles and holes are considered. This is shown once more in eq. (3.23f).

Remembering that the pair scattering modes were constructed to take into account the interaction terms H_{pp} , H_{hh} and H_V , we calculate the commutators

$$[\mathfrak{S}_0, \mathfrak{A}_{\alpha\beta}^+] \quad \text{and} \quad [\mathfrak{S}_0, \mathfrak{B}_{\alpha\beta}^+]$$

where

$$\mathfrak{S}_0 = \mathring{H}_0 + \mathring{H}_{pp} + \mathring{H}_{hh} + \mathring{H}_V. \quad (3.24)$$

Using eqs. (3.13) and (3.23) we regain the equations (3.3) which had been the starting point in constructing the pair scattering modes. Correspondingly one obtains for \mathfrak{S}_0 the expansion

$$\mathfrak{S}_0 = \sum_{\mu} \omega_m (A_{\mu}^+ A_{\mu} - B_{\mu}^+ B_{\mu}). \quad (3.25)$$

This confirms once more the internal consistency of the transcription rule (3.14) with the linearization approximation (3.3).

So far the particle-hole interaction has not been considered at all. But, in the following section, it will be of great importance as the source of new ground-state correlations which reflect the collective predisposition of the ground state for deformed excited states. The desired expansion in terms of pair scattering modes is obtained by inserting (3.15) into (3.23e). This leads to

$$\mathring{H}_{ph} = \sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma} C_{\mu}^+ C_{\rho} C_{\sigma} C_{\nu}^+. \quad (3.26)$$

Now it is convenient to rewrite \mathring{H}_{ph} as a normal product (symbolized by $\vdots\vdots$) with respect to the operators A^+ and B^+ . The necessary contractions give us a renormalization of the single-pair energies ω_m which should be determined in a self-consistent way. Here we assume for simplicity that the renormalization is already incorporated in the definition of ω_m . So we can write

$$\mathring{H}_{ph} = \sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma} \vdots C_{\mu}^+ C_{\nu}^+ C_{\sigma} C_{\rho} \vdots \quad (3.27)$$

where the transformed potential matrix element has the symmetry

$$V_{\mu\nu\rho\sigma} = V_{\rho\sigma\mu\nu} \quad (3.28)$$

and is explicitly defined by

$$V_{\mu\nu\rho\sigma} = -64 \left. \begin{array}{l} \sum'_{\alpha\beta\gamma\delta} \sum_{\varepsilon\varphi} v_{\alpha\beta\gamma\delta} s_{\mu} s_{\nu} s_{\rho} s_{\sigma} \Psi_{\mu}(\alpha\varepsilon) \Psi_{\rho}(\gamma\varepsilon) \Psi_{\nu}(\beta\varphi) \Psi_{\sigma}(\delta\varphi) \\ \text{with } \left\{ \begin{array}{l} \theta_a = \theta_c = \theta_e = 0 \\ \theta_b = \theta_d = \theta_f = 1 \end{array} \right\} \end{array} \right\} \quad (3.29)$$

4. Interaction Between Pairs

In the preceding section, a new basis system has been constructed which consists of pair scattering modes for particles and holes. The properties of these modes have been investigated, and it has been shown how to express all operators of physical interest on the new basis. After this preparation we can turn to the proper aim of the present work, namely the collective description of even parity states in closed-shell nuclei. The present section, therefore, is devoted to the formal solution of the problem, whereas the following section will show where the deformations in the excited states come in.

4.1 The Hamiltonian in Terms of Pair Scattering Modes

Using the expansions (3.25) and (3.27), we can write the Hamiltonian of our system in the form

$$\hat{H} = \mathfrak{H}_0 + \hat{H}_{ph} = \sum_{\mu} \omega_{\mu} (A_{\mu}^{+} A_{\mu} - B_{\mu}^{+} B_{\mu}) + \sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma} : C_{\mu}^{+} C_{\nu}^{+} C_{\sigma} C_{\rho} :. \quad (4.1)$$

In analogy to the procedure of section 2.2 we now decompose the Hamiltonian in various terms

$$\hat{H} = \mathfrak{H}_0 + \mathfrak{H}_{pp} + \mathfrak{H}_{hh} + \mathfrak{H}_{ph} + \mathfrak{H}_V + \mathfrak{H}_Y, \quad (4.2)$$

where \mathfrak{H}_0 is given in eq. (3.25) and

$$\mathfrak{H}_{pp} = \sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma} A_{\mu}^{+} A_{\nu}^{+} A_{\sigma} A_{\rho} \quad (4.3a)$$

$$\mathfrak{H}_{hh} = \sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma} B_{\mu}^{+} B_{\nu}^{+} B_{\sigma} B_{\rho} \quad (4.3b)$$

$$\mathfrak{H}_{ph} = \sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma} \{ A_{\mu}^{+} B_{\sigma}^{+} A_{\rho} B_{\nu} + A_{\mu}^{+} B_{\rho}^{+} A_{\sigma} B_{\nu} + A_{\nu}^{+} B_{\sigma}^{+} A_{\rho} B_{\mu} + A_{\nu}^{+} B_{\rho}^{+} A_{\sigma} B_{\mu} \} \quad (4.3c)$$

$$\mathfrak{H}_V = \sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma} \{ A_{\mu}^{+} A_{\nu}^{+} B_{\sigma}^{+} B_{\rho}^{+} + A_{\mu} A_{\nu} B_{\sigma} B_{\rho} \}. \quad (4.3d)$$

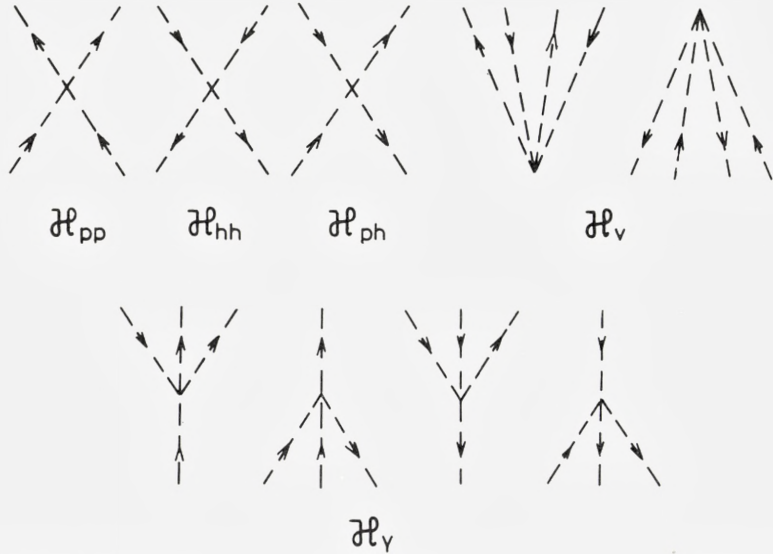


Fig. 4. Graphic representation of the matrix elements arising from the particle-hole interaction or the field-producing force. The broken lines indicate pair scattering modes, for a "particle pair" if the arrow points upwards, for a "hole pair", if the arrow points downwards.

Finally, \mathfrak{S}_V contains all possible matrix elements analogous to H_V in (2.6). If we graphically symbolize a correlated pair by a broken line, we can depict in fig. 4 the matrix elements of each part of the particle-hole interaction \hat{H}_{ph} by diagrams which are formally similar to those of fig. 1. In order to illustrate the physical meaning of these new diagrams, typical graphs contributing to \mathfrak{S}_{ph} and \mathfrak{S}_V are shown in fig. 5 in the conventional representation. From the structure of $V_{\mu\nu\rho\sigma}$ defined in eq. (3.29) it is seen that, in the absence of ground-state correlations due to pair scattering (see fig. 2), only the first term in (4.3c) survives among all the terms occurring in (4.3). This term is represented in fig. 5(a). Its significance will be discussed in section 5 in connection with deformations for the excited states. The appearance of diagrams of the type \mathfrak{S}_V indicates that the interaction between pairs introduces a new kind of ground-state correlations, which will be shown later to describe the collective predisposition of the ground state for deformed excited states.

Here, it should be pointed out that the interplay between the effect of the field-producing force and the effect of the residual interaction is especially important in producing this new type of ground-state correlations. This

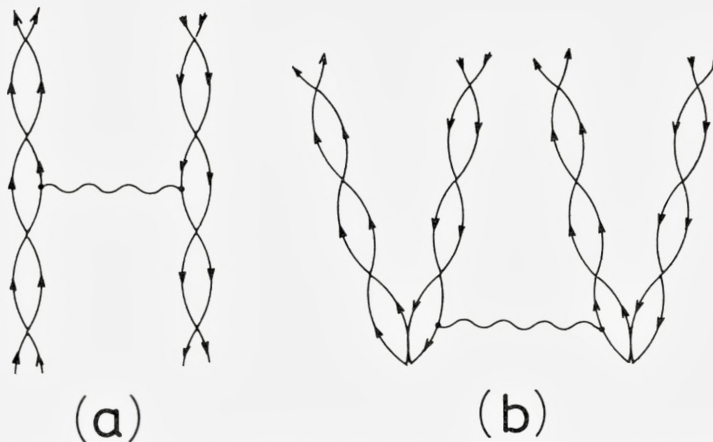


Fig. 5. Typical diagrams in the conventional fermion representation which contribute to the term H_{ph} decomposed in fig. 4. The diagram (a) occurs, for example, in \mathfrak{S}_{ph} , and (b), for example, in \mathfrak{S}_V .

is most obvious in the limit where the pair scattering ground-state correlation due to the residual interaction vanishes. Then the new correlations due to the field-producing force, H_{ph} , vanish as well.

At this point it might be appropriate to discuss a shortcoming of the present treatment in the two-step method. With the aim of taking into account the “residual interaction effect” in the first step, we have split the Hamiltonian into $H_{pp} + H_{hh} + H_V$ and H_{ph} , and then have diagonalized $H_{pp} + H_{hh} + H_V$ only in the subspace of two particles and in the subspace of two holes (including pair scattering ground-state correlations). In the second step, H_{ph} was taken as the field-producing part of the interaction, which acts between *different* pairs. As a result, those parts of H_{pp} and H_{hh} which act between *different* pairs have been neglected. Physically, this means that the neglected field-producing (i.e., long range) parts of H_{pp} and H_{hh} are assumed to be unimportant compared to H_{ph} . Indeed, if we considered a “2particle-2hole” system (in the NTD sense), the parts discarded in H_{pp} and H_{hh} would enter only via *ground-state correlations*, in contrast to H_{ph} . Thus, their influence* would presumably be very small compared with the influence of H_{ph} . Moreover, the main source of deformations in the excited states of closed-shell nuclei will be the repulsive particle-hole interaction (corresponding to an attractive particle-core interaction). This interaction forces, for example,

* In model calculations it turned out that the interaction $H_{pp}(H_{hh})$ between particles (holes) belonging to different pairs was not at all important for the deformation obtained. See also the arguments at the end of sect. 5.3.

the particles to the poles of the core if the holes are concentrated in the equatorial plane, so that particles and holes contribute with equal sign to the deformation.

To avoid the above shortcoming of our treatment, it is useful to divide the interaction into the residual interaction (with a short range) and the field-producing part (with a long range). In this case, the first step of our treatment corresponds to the diagonalization of the short range force, and the long range force then gives rise to the deformations in the excited states and, at the same time, to the collective ground-state correlations discussed above. The only formal change which results from this decomposition of the Hamiltonian is to modify the definition of the interaction matrix elements $V_{\mu\nu\rho\sigma}$ in (3.29) by dropping the restriction on the summation, i.e.,

$$V_{\mu\nu\rho\sigma} = -64 \sum_{\alpha\beta\gamma\delta} \sum_{\varepsilon\varphi} v_{\alpha\beta\gamma\delta} s_{\mu} s_{\nu} s_{\rho} s_{\sigma} \Psi_{\mu}(\alpha\varepsilon) \Psi_{\rho}(\gamma\varepsilon) \Psi_{\nu}(\beta\varphi) \Psi_{\sigma}(\delta\varphi). \quad (4.4)$$

Thus, the field-producing parts of H_{pp} and H_{hh} are fully included in the Hamiltonian (4.2). It is unnecessary to say that the original division (2.5) of the Hamiltonian has been chosen simply because it is more clear-cut from the formal point of view.

4.2 Collective Modes in the Excitation of Closed Shells

In order to investigate the collective modes due to the field-producing force we start from the following linearized relation:

$$[\hat{H}, A_{\mu}^{+} B_{\nu}^{+}] = \sum_{\rho\sigma} (N_{\mu\nu\rho\sigma} A_{\rho}^{+} B_{\sigma}^{+} + N'_{\mu\nu\rho\sigma} A_{\rho} B_{\sigma}). \quad (4.5)$$

By taking the appropriate matrix elements of eq. (4.5) with respect to the (unperturbed) eigenstates of \mathfrak{S}_0 , it is seen that the coefficients N and N' contain only matrix elements of \mathfrak{S}_0 , \mathfrak{S}_{ph} and \mathfrak{S}_V . In this approximation we can define the creation operators of eigenmodes (or "phonons") for even parity excited states of closed-shell nuclei as solutions of the following equation of motion:

$$[\hat{H}, X_{\lambda}^{+}] = \Omega_l X_{\lambda}^{+} \quad \text{with} \quad \Omega_l > 0, \quad (4.6)$$

where

$$X_{\lambda}^{+} = \sum_{\mu\nu} \{ \xi_{\lambda}(\mu\nu) A_{\mu}^{+} B_{\nu}^{+} + \eta_{\lambda}(\mu\nu) A_{\mu} B_{\nu} \} \quad (4.7)$$

with

$$\lambda = \{L, IM, TZ\}, \quad l = \{L, I, T\}. \quad (4.8)$$

Here, λ means the set of quantum numbers composed of the angular momentum I and its projection M , the isospin T and its projection Z and, finally, a set of additional quantum numbers L necessary for a complete specification of the "phonon". Correspondingly, l stands for the set λ with the exclusion of the projection quantum numbers M and Z . From eq. (4.5) one obtains the eigenvalue equation for the functions $\xi_\lambda(\mu\nu)$ and $\eta_\lambda(\mu\nu)$ (taken as real):

$$\left. \begin{aligned} \Omega_l \xi_\lambda(\mu\nu) &= \sum_{\rho\sigma} \{ N_{\rho\sigma\mu\nu} \xi_\lambda(\rho\sigma) - N'_{\rho\sigma\mu\nu} \eta_\lambda(\rho\sigma) \} \\ \Omega_l \eta_\lambda(\mu\nu) &= - \sum_{\rho\sigma} \{ N_{\rho\sigma\mu\nu} \eta_\lambda(\rho\sigma) - N'_{\rho\sigma\mu\nu} \xi_\lambda(\rho\sigma) \}. \end{aligned} \right\} \quad (4.9)$$

Eq. (4.9) has the same structure as the well-known equations for "1 particle-1 hole" excited states in the RPA, and thus we have the usual orthogonality and completeness relations

$$\sum_{\mu\nu} \{ \xi_{\lambda_1}(\mu\nu) \xi_{\lambda_2}(\mu\nu) - \eta_{\lambda_1}(\mu\nu) \eta_{\lambda_2}(\mu\nu) \} = \delta_{\lambda_1 \lambda_2} \quad (4.10a)$$

$$\left. \begin{aligned} \sum_{\lambda} \{ \xi_\lambda(\mu\nu) \xi_\lambda(\rho\sigma) - \eta_\lambda(\mu\nu) \eta_\lambda(\rho\sigma) \} &= \delta_{\mu\rho} \delta_{\nu\sigma} \\ \sum_{\lambda} \{ \xi_\lambda(\mu\nu) \eta_\lambda(\rho\sigma) - \eta_\lambda(\mu\nu) \xi_\lambda(\rho\sigma) \} &= 0 \end{aligned} \right\} \quad (4.10b)$$

with

$$\Omega_l > 0.$$

From these relations we get immediately the inverse expansion to eq. (4.7)

$$A_\mu^+ B_\nu^+ = \sum_{\lambda} (\xi_\lambda(\mu\nu) X_\lambda^+ - \eta_\lambda(\mu\nu) X_\lambda). \quad (4.11)$$

We are now in a position to define the new ground state $|\Psi_0\rangle$ for closed-shell nuclei by

$$X_\lambda |\Psi_0\rangle = 0 \quad (4.12)$$

and similarly the excited even parity states $|\Psi_\lambda\rangle$ of closed-shell nuclei by

$$|\Psi_\lambda\rangle = X_\lambda^+ |\Psi_0\rangle. \quad (4.13)$$

It is clear from these definitions that both ground state and excited states contain very complex correlations, namely all diagrams of the type indicated in figs. (3a) and (3b).

In order to understand the physical significance of these ground-state correlations, let us first see what happens if we neglect them. (This also means that we neglect the ground-state correlations due to the residual interaction). In that case the linearized equation (4.5) reduces to the equation of the TD method for a 2p-2h system. As an approximation to the TD method one may use the Hartree-Fock approach⁽³⁾ which is known to yield intrinsically deformed 2p-2h states and a spherical ground state. Let us now gradually switch on the ground-state correlations and correspondingly treat the problem in our NTD method. This procedure will gradually decrease the energy of the excited states. At the same time it will leave the excited states deformed and the ground state spherical, until, with increasing interaction strength, the smallest excitation energy (i.e., the lowest Ω_l) passes through zero. Then the spherical ground state becomes unstable and undergoes a phase transition into a deformed state.

Although the physical ground state is spherical, it has a collective predisposition to produce deformed excited states due to the symmetrical treatment of ground state and excited states in our NTD method. This is in contrast to the “1p-1h” problem in the usual RPA, where a spherical (deformed) ground state is always associated with a spherical (deformed) excited state. The difference is that a pure 2p-2h excitation is intrinsically deformed by itself. The bare deformation of the 2p-2h excitation has a further consequence: Due to the ground-state correlations the “dressed 2p-2h” excited states defined by (4.13) possess a “dressed” deformation which includes, and is amplified by, the cooperation effect of the core deformation.

5. Deformation of the Excited States

In the preceding section, general solutions were obtained in a spherical representation, so that the deformation of the excited states would only manifest itself in a rotational band structure. In this section, however, we want to set the deformation into evidence more directly, using a sequence of successively generalized self-consistent field methods. For simplicity, we adopt a separable field-producing force. Starting from the conventional Hartree-Fock approximation⁽³⁾, we easily see how to generalize the method in order to take into account the residual interaction. A final generalization treats the full core polarization due to the collective ground-state correlations in a self-consistent way. This turns out to be an approximation to the general solutions of section 4, thus explicitly demonstrating their deformed nature.

5.1 A Separable Field-Producing Force

In order to see the origin of the deformation in the excited state more clearly, it is convenient to divide the interaction into the field-producing (long-range) part and the residual interaction (short-range part). For simplicity, we furthermore assume the field-producing force to be separable:

$$H_f = -\frac{1}{2} \sum_{LM} \chi_L : Q_{LM} Q_{LM}^+ : , \quad (5.1)$$

where Q_{LM} is given by

$$Q_{LM} = \sum_{\alpha\beta} r \langle \alpha | r^L Y_{LM}(\theta\varphi) | \beta \rangle : c_\alpha^+ c_\beta : . \quad (5.2)$$

With the aid of the rule (3.14) and eq. (3.15), the operator Q_{LM} is expanded in terms of pair scattering modes as

$$\mathring{Q}_{LM} = \sum_{\mu\nu} (\mu | Q_{LM} | \nu) : C_\mu^+ C_\nu : , \quad (5.3)$$

where

$$(\mu | Q_{LM} | r) = 4 \sum_{\alpha\beta\gamma} \langle \alpha | r^L Y_{LM}(\theta\varphi) | \beta \rangle s_\mu \Psi_\mu(\alpha\gamma) (1 - \theta_a - \theta_c) s_\nu \Psi_\nu(\beta\gamma). \quad (5.4)$$

Thus, one may write down the field-producing force in terms of the pair-scattering modes in the following form:

$$\mathring{H}_f = -\frac{1}{2} \sum_{LM} \chi_L : \mathring{Q}_{LM} \mathring{Q}_{LM}^+ : . \quad (5.5)$$

For later discussions it is convenient to divide \mathring{Q}_{LM} and \mathring{H}_f into the following parts:

$$\mathring{Q}_{LM} = \mathring{Q}_{LM}^{(1)} + \mathring{Q}_{LM}^{(2)}, \quad (5.6)$$

$$\left. \begin{aligned} \mathring{H}_f &= \mathfrak{H}^{(1)} + \mathfrak{H}^{(2)} + \mathfrak{H}^{(3)}, \\ \mathfrak{H}^{(1)} &= -\frac{1}{2} \sum_{LM} \chi_L : \mathring{Q}_{LM}^{(1)} \mathring{Q}_{LM}^{(1)+} : \\ \mathfrak{H}^{(2)} &= -\frac{1}{2} \sum_{LM} \chi_L : \mathring{Q}_{LM}^{(2)} \mathring{Q}_{LM}^{(2)+} : \\ \mathfrak{H}^{(3)} &= -\sum_{LM} \chi_L : \mathring{Q}_{LM}^{(1)} \mathring{Q}_{LM}^{(2)+} : \end{aligned} \right\} (5.7)$$

where

$$\left. \begin{aligned} \mathring{Q}_{LM}^{(1)} &= \sum_{\mu\nu} (\mu | Q_{LM} | \nu) (A_\mu^+ A_\nu + B_\nu^+ B_\mu) \\ \mathring{Q}_{LM}^{(2)} &= \sum_{\mu\nu} (\mu | Q_{LM} | \nu) (A_\mu^+ B_\nu^+ + A_\nu B_\mu). \end{aligned} \right\} (5.8)$$

The term $\mathfrak{S}^{(3)}$ in eq. (5.7) corresponds to \mathfrak{S}_Y in eq. (4.2) which has played no role in constructing the collective excited states discussed in sec. 4. For consistency, we therefore discard $\mathfrak{S}^{(3)}$ in the following. It should be noted that, in the absence of pair-scattering ground-state correlations, only $\hat{Q}_{LM}^{(1)}$ and $\mathfrak{S}^{(1)}$ survive. This is easily seen from the structure of $(\mu|Q_{LM}|\nu)$ in eq. (5.4).

5.2 An Extension of the Hartree-Fock Approximation

The origin of the deformation in the excited states can be traced most clearly using the self-consistent field method which leads to the notion of an *intrinsic deformation* in a natural way. In this subsection we investigate the mechanism which leads to intrinsic deformations in the excited states in the case without ground-state correlations.

In this case, the exact 2p-2h eigenstates are given by

$$|\Phi_\lambda\rangle = X_\lambda^{(TD)+}|\Phi_0\rangle, \quad (a_\alpha|\Phi_0\rangle = b_\alpha|\Phi_0\rangle = 0) \quad (5.9)$$

with their creation operators

$$X_\lambda^{(TD)+} = \sum_{\alpha\beta\gamma\delta} f_\lambda(\alpha\beta\gamma\delta) a_\alpha^+ a_\beta^+ b_\gamma^+ b_\delta^+. \quad (5.10)$$

The function f_λ (taken as real) satisfies the eigenvalue equation

$$\Omega_l^{(TD)} f_\lambda(\alpha_1\beta_1\gamma_1\delta_1) = \sum_{\alpha_2\beta_2\gamma_2\delta_2} L_{\alpha_1\beta_1\gamma_1\delta_1, \alpha_2\beta_2\gamma_2\delta_2} f_\lambda(\alpha_2\beta_2\gamma_2\delta_2), \quad (5.11)$$

where the coefficients L are defined by the usual linearized relation characterizing the TD method:

$$[H, a_{\alpha_1}^+ a_{\beta_1}^+ b_{\gamma_1}^+ b_{\delta_1}^+] = \sum_{\alpha_2\beta_2\gamma_2\delta_2} L_{\alpha_1\beta_1\gamma_1\delta_1, \alpha_2\beta_2\gamma_2\delta_2} a_{\alpha_2}^+ a_{\beta_2}^+ b_{\gamma_2}^+ b_{\delta_2}^+. \quad (5.12)$$

It is known that the eigenvalue equation eq. (5.11) can also be obtained from the variational principle

$$\delta\{\langle\Phi_0|X_\lambda^{(TD)}, HX_\lambda^{(TD)+}|\Phi_0\rangle - \Omega_l^{(TD)}\langle\Phi_0|X_\lambda^{(TD)}, X_\lambda^{(TD)+}|\Phi_0\rangle\} = 0. \quad (5.13)$$

The intrinsic deformation of a state $|\Phi_{\lambda_0}\rangle$ in eq. (5.9) with $J = 0$ will manifest itself in a Hartree-Fock approximation^(3, 4) in which the trial function for $f_{\lambda_0}(\alpha\beta\gamma\delta)$ is taken as

$$f_{\lambda_0}(\alpha\beta\gamma\delta) \approx f_{k_0 l_0 m_0 n_0}(\alpha\beta\gamma\delta) = \frac{1}{4} \mathfrak{A}\{\psi_{k_0}(\alpha)\psi_{l_0}(\beta)\}\mathfrak{A}\{\varphi_{m_0}(\gamma)\varphi_{n_0}(\delta)\}. \quad (5.14)$$

(\mathfrak{A} : the antisymmetrization operator)

with separate orthonormality conditions among the ψ and φ . The variational principle leads to the well-known single-particle problem in a self-consistent field, whose deviation from the spherical shape defines the intrinsic deformation of the state $|\Phi_{\lambda_0}\rangle$ with $J = 0$.

In the above Hartree-Fock approximation, the residual interaction is completely discarded, as is clear from its definition, and only the field-producing force is taken into account. To overcome this shortcoming we can use the following procedure:

(a) In a first step we diagonalize the residual interaction. The operators of pair scattering eigenmodes are then of the form

$$\hat{A}_\mu^+ = \sum_{\alpha\beta} \psi_\mu^{(TD)}(\alpha\beta) a_\alpha^+ a_\beta^+, \quad \hat{B}_\nu^+ = \sum_{\gamma\delta} \varphi_\nu^{(TD)}(\gamma\delta) b_\delta^+ b_\gamma^+ \quad (5.15)$$

to which the operators of the pair scattering eigenmodes defined in eq. (3.1) are reduced when the ground-state correlations are neglected. Within the subspace of 2p-2h excitations the Hamiltonian can thus be written

$$H^{(TD)} = \sum_\mu \omega_m^{(TD)} \hat{A}_\mu^+ \hat{A}_\mu - \sum_\nu \omega_n^{(TD)} B_\nu^+ \hat{B}_\nu - \frac{1}{2} \sum_{LM} \chi_L : Q_{LM}^{(1)(TD)} Q_{LM}^{(1)(TD)} + : \quad (5.16)$$

Here, $Q_{LM}^{(1)(TD)}$ is given by

$$Q_{LM}^{(1)(TD)} = \sum_{\mu_1\mu_2} (\mu_1 | Q_{LM} | \mu_2)_{TD} \hat{A}_{\mu_1}^+ \hat{A}_{\mu_2} + \sum_{\nu_1\nu_2} (\nu_1 | Q_{LM} | \nu_2)_{TD} \hat{B}_{\nu_2}^+ \hat{B}_{\nu_1}, \quad (5.17)$$

to which \hat{Q}_{LM} defined by eq. (5.6) is reduced in the absence of ground-state correlations.

(b) In the next step, we use a variational approach, taking a trial state vector for $|\Phi_{\lambda_0}\rangle$ with $J = 0$ as follows:

$$|\Phi_{\lambda_0}\rangle \approx |\Phi_{i_0 j_0}\rangle = \hat{A}_{i_0}^+ \hat{B}_{j_0}^+ |\Phi_0\rangle, \quad (\hat{A}_\mu |\Phi_0\rangle = \hat{B}_\nu |\Phi_0\rangle = 0) \quad (5.18)$$

with

$$\left. \begin{aligned} \hat{A}_{i_0}^+ &= \sum_\mu u_{i_0}(\mu) \hat{A}_\mu^+, & \hat{B}_{j_0}^+ &= \sum_\nu v_{j_0}(\nu) \hat{B}_\nu^+, \\ \sum_\mu u_{i_0}^2(\mu) &= 1, & \sum_\nu v_{j_0}^2(\nu) &= 1. \end{aligned} \right\} \quad (5.19)$$

The variational principle for the Hamiltonian (5.16) gives the following self-consistent eigenvalue equations with $\Omega_{i_0}^{(TD)} = W_{i_0}^{(TD)} - W_{j_0}^{(TD)}$:

$$\left. \begin{aligned} W_{i_0}^{(TD)} u_{i_0}(\mu_1) &= \omega_{m_1}^{(TD)} u_{i_0}(\mu_1) + \sum_{\mu_2} U_{\mu_1\mu_2}^{[h]} u_{i_0}(\mu_2), \\ W_{j_0}^{(TD)} v_{j_0}(\nu_1) &= \omega_{n_1}^{(TD)} v_{j_0}(\nu_1) - \sum_{\nu_2} U_{\nu_1\nu_2}^{[p]} v_{j_0}(\nu_2) \end{aligned} \right\} \quad (5.20)$$

where

$$\left. \begin{aligned} U_{\mu_1\mu_2}^{[h]} &= - \sum_{LM} \chi_L(-)^M (\mu_1 | Q_{L-M} | \mu_2)_{TD} \cdot \alpha_{LM}^{(h)} \\ U_{\nu_1\nu_2}^{[p]} &= - \sum_{LM} \chi_L(-)^M (\nu_1 | Q_{L-M} | \nu_2)_{TD} \cdot \alpha_{LM}^{(p)}, \end{aligned} \right\} \quad (5.21 \text{ a})$$

$$\left. \begin{aligned} \alpha_{LM}^{(h)} &= \sum_{\nu_1\nu_2} (\nu_1 | Q_{LM} | \nu_2)_{TD} v_{j_0}(\nu_1) v_{j_0}(\nu_2) \\ \alpha_{LM}^{(p)} &= \sum_{\mu_1\mu_2} (\mu_1 | Q_{LM} | \mu_2)_{TD} u_{i_0}(\mu_1) u_{i_0}(\mu_2). \end{aligned} \right\} \quad (5.21 \text{ b})$$

The eqs. (5.20) constitute a self-consistent field problem for a single pair of two particles or two holes. The particle pair is moving in the field $U^{[h]}$ generated by the hole pair, and vice versa. Thus, the intrinsic deformation of the state $|\Phi_{\lambda_0}\rangle$ with $J = 0$ is given by

$$\langle \Phi_{i_0j_0} | Q_{LM} | \Phi_{i_0j_0} \rangle = \alpha_{LM}^{(p)} + \alpha_{LM}^{(h)} \equiv \alpha_{LM}. \quad (5.22)$$

The situation obtained by solving (5.20) is illustrated in fig. 6 for a simple model.

In order to see the connection with the Hartree-Fock approximation (5.14), it is noted that the derivation of eqs. (5.20) is essentially equivalent to a variational approach with the following choice of the trial function for $f_{\lambda_0}(\alpha\beta\gamma\delta)$ in eq. (5.10):

$$f_{\lambda_0}(\alpha\beta\gamma\delta) \approx f_{i_0j_0}(\alpha\beta\gamma\delta) = f_{i_0}(\alpha\beta) f_{j_0}(\gamma\delta) \quad (5.23)$$

with

$$f_{i_0}(\alpha\beta) = -f_{i_0}(\beta\alpha), \quad f_{j_0}(\gamma\delta) = -f_{j_0}(\delta\gamma).$$

In this procedure the Pauli principle is taken properly into account, as was pointed out in section 3.3. The two steps used in deriving eqs. (5.20) are just a convenient but unessential decomposition of f_{i_0} and f_{j_0} into

$$f_{i_0}(\alpha\beta) = \sum_{\mu} u_{i_0}(\mu) \psi_{\mu}^{(TD)}(\alpha\beta) \quad \text{and} \quad f_{j_0}(\gamma\delta) = \sum_{\nu} v_{j_0}(\nu) \varphi_{\nu}^{(TD)}(\delta\gamma).$$

From the variational point of view, therefore, the procedure is simply a generalization of the Hartree-Fock approximation with the purpose of taking the residual interaction properly into account.

5.3 The Origin of the Intrinsic Deformation

So far we have considered the simplified case in which the ground-state correlations are completely discarded. However, the formal extension of

the treatment given in the previous subsection to the case in which the pair scattering ground-state correlations are taken into account is straightforward. We only have to consider the Hamiltonian

$$\hat{H}' = \sum_{\mu} \omega_m A_{\mu}^{\dagger} A_{\mu} - \sum_{\nu} \omega_n B_{\nu}^{\dagger} B_{\nu} + \mathfrak{H}^{(1)}. \quad (5.24)$$

where $\mathfrak{H}^{(1)}$ is defined in (5.7). Then we construct the eigenstates of correlated ‘‘2p-2h’’ excitations

$$|\Phi'_{\lambda}\rangle = \sum_{\mu\nu} \tilde{\xi}_{\lambda}(\mu\nu) A_{\mu}^{\dagger} B_{\nu}^{\dagger} |\Phi'_0\rangle, \quad (A_{\mu} |\Phi'_0\rangle = B_{\nu} |\Phi'_0\rangle = 0), \quad (5.25)$$

with the aim of diagonalizing the Hamiltonian (5.24) within the subspace composed of the unperturbed states $A_{\mu}^{\dagger} B_{\nu}^{\dagger} |\Phi'_0\rangle$. Instead of solving the eigenvalue equation for $\tilde{\xi}_{\lambda}(\mu\nu)$ directly, we use a similar variational approach as in section 5.2. To this end we assume for an eigenstate (5.25), $|\Phi'_{\lambda_0}\rangle$ with $J = 0$, the following trial form

$$|\Phi'_{\lambda_0}\rangle \approx |\Phi'_{i_0 j_0}\rangle = A_{i_0}^{\dagger} B_{j_0}^{\dagger} |\Phi'_0\rangle \quad (5.26)$$

with

$$\left. \begin{aligned} A_{i_0}^{\dagger} &= \sum_{\mu} u_{i_0}(\mu) A_{\mu}^{\dagger}, & B_{j_0}^{\dagger} &= \sum_{\nu} v_{j_0}(\nu) B_{\nu}^{\dagger} \\ \sum_{\mu} u_{i_0}^2(\mu) &= 1, & \sum_{\nu} v_{j_0}^2(\nu) &= 1. \end{aligned} \right\} \quad (5.27)$$

The variational principle with the Hamiltonian (5.24) leads to self-consistent eigenvalue equations which are identical with eqs. (5.20), except that the label (TD) has to be dropped everywhere. For the sake of later reference, we just write down the coupled equations

$$\left. \begin{aligned} W_{i_0} u_{i_0}(\mu_1) &= \omega_{m_1} u_{i_0}(\mu_1) + \sum_{\mu_2} U_{\mu_1 \mu_2}^{[h]} u_{i_0}(\mu_2) \\ W_{j_0} v_{j_0}(\nu_1) &= \omega_{n_1} v_{j_0}(\nu_1) - \sum_{\nu_2} U_{\nu_1 \nu_2}^{[p]} v_{j_0}(\nu_2). \end{aligned} \right\} \quad (5.28)$$

All quantities here are defined by eqs. (5.21) if the index (TD) is disregarded. The intrinsic deformation for the state $|\Phi'_{\lambda_0}\rangle$ with $J = 0$ is given by

$$\langle \Phi'_{i_0 j_0} | \overset{\circ}{Q}_{LM} | \Phi'_{i_0 j_0} \rangle = \langle \Phi'_{i_0 j_0} | \overset{\circ}{Q}_{LM}^{(1)} | \Phi'_{i_0 j_0} \rangle \equiv \alpha_{LM}, \quad (5.29)$$

where $\overset{\circ}{Q}_{LM}$ is defined by eq. (5.6) and we have used the result $\langle \Phi'_{i_0 j_0} | \overset{\circ}{Q}_{LM}^{(2)} | \Phi'_{i_0 j_0} \rangle = 0$. In contrast to eq. (5.22) the new equation (5.29) now defines an intrinsic deformation α_{LM} which contains the core polarization

effect due to the pair scattering ground-state correlations. This situation is illustrated in fig. 7 for a simplified model.

Now the origin of the intrinsic deformation in the excited states is obvious. The essential part of the field-producing force responsible for the deformations in the excited states is just the interaction $\mathfrak{S}^{(1)}$. The interaction $\mathfrak{S}^{(1)}$ survives in the absence of ground-state correlations, and can be visualized physically as the repulsive particle-hole interaction as follows: Let us decompose $\mathfrak{S}^{(1)}$ into

$$\mathfrak{S}^{(1)} = \mathfrak{S}_{ph}^{(1)} + \mathfrak{S}_{pp}^{(1)} + \mathfrak{S}_{hh}^{(1)} \quad (5.30)$$

where $\mathfrak{S}_{pp}^{(1)}$ and $\mathfrak{S}_{hh}^{(1)}$ have the same structure as eqs. (4.3a) and (4.3b), respectively, and

$$\mathfrak{S}_{ph}^{(1)} = - \sum_{LM} \chi_L(-)^M \sum_{\mu_1 \nu_1} \sum_{\mu_2 \nu_2} (\mu_1 | Q_{LM} | \nu_1) (\mu_2 | Q_{L-M} | \nu_2) \{ A_{\mu_1}^+ A_{\nu_1} B_{\nu_2}^+ B_{\mu_2} \}. \quad (5.31)$$

We can see that only $\mathfrak{S}_{ph}^{(1)}$, which arises mainly* from the particle-hole interaction, contributes in the ‘‘2p-2h’’ problem since the expectation values of $\mathfrak{S}_{pp}^{(1)}$ and $\mathfrak{S}_{hh}^{(1)}$ with respect to $|\Phi'_{\lambda_0}\rangle$ are zero.

On the other hand, the interaction $\mathfrak{S}^{(2)}$ vanishes in the absence of ground-state correlations and will become important for constructing collective ground-state correlations due to the field-producing force. This will be elucidated in section 5.4.

Numerical Calculations for a Simple Model

The coupled self-consistent equations (5.28) describe a correlated particle pair moving in the field produced by a correlated hole pair, and vice versa. In order to investigate the deformation-producing mechanism, we adopted a simplified model and solved eqs. (5.28) self-consistently. In zeroth order, the model consisted in one occupied level with angular momentum j_h and one unoccupied level with angular momentum j_p . The spacing of these levels was taken to be $2\varepsilon_0$, with ε_0 serving as an energy unit. The interaction was taken to be composed of the conventional pairing force with the strength G_0 and the conventional quadrupole force with the strength χ (both measured in units of ε_0). This system was found to have the following properties:

* This is easily seen by neglecting the pair scattering ground-state correlations. In this case, only the particle-hole interaction H_{ph} contributes to $\mathfrak{S}_{ph}^{(1)}$. Correspondingly, $\mathfrak{S}_{pp}^{(1)}$ and $\mathfrak{S}_{hh}^{(1)}$ are just reduced to the field-producing (i.e., long range) parts of H_{pp} and H_{hh} that have been discussed in section 4.1.

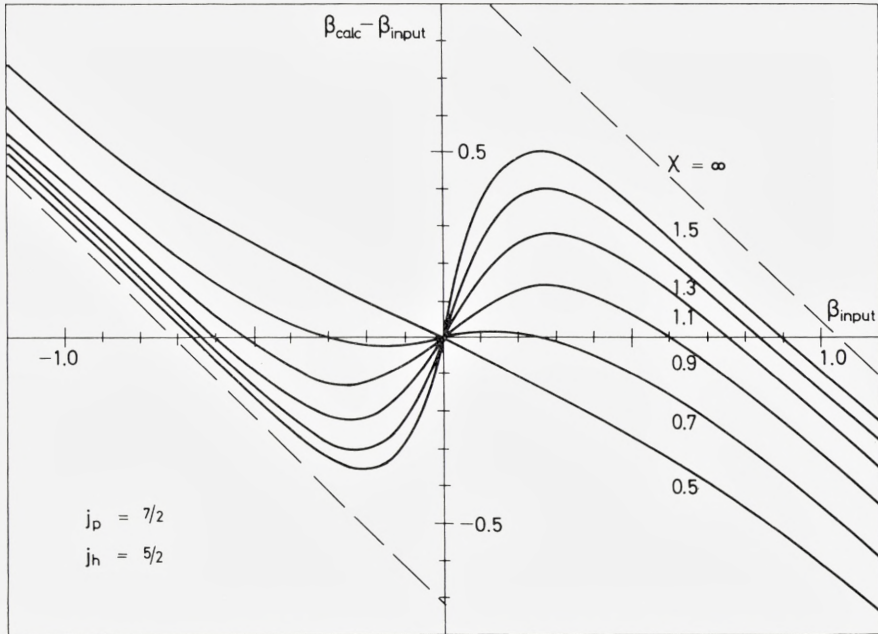


Fig. 6. Illustration showing the instability of a spherical 2p-2h excitation with respect to deformation. Details are explained in the text.

(a) Defining the deformation $\beta = \beta_p + \beta_h$ as the dimensionless *angular* part of α_{20} in eq. (5.29), the following dependence on the parameters χ and G_0 was obtained. For a fixed strength of the pairing force, the spherical shape, $\beta = 0$, is stable as long as the quadrupole force is sufficiently weak. For increasing χ the spherical shape becomes unstable, and two stable deformed solutions emerge, one with a positive and the other with a negative deformation. For large χ the deformation tends to a saturation value. The energy is lowered roughly linearly with χ , starting from the point at which the system becomes deformed. For reasonably weak pairing forces ($G_0 < 0.15$) the results are not very sensitive to G_0 . Therefore we illustrate the stability situation in fig. 6 for $G_0 = 0$, choosing $j_p = 7/2$ and $j_h = 5/2$. For simplicity, we restrict ourselves in fig. 6 to particle pairs and hole pairs with $J = 0$ and $J = 2$, measuring χ in units of the arbitrarily fixed energy splitting between these levels. Inclusion of all possible values of J changes the result by less than 10 percent. In fig. 6 we use $\beta_h = \beta_{input}$ as an input parameter and plot the difference ($\beta_{calc} - \beta_{input}$) of the hole deformation (calculated according to eq. (5.28)) and the input deformation as a function of β_{input} .

Evidently, self-consistency is obtained for $(\beta_{\text{calc}} - \beta_{\text{input}}) = 0$, but the solution is stable only if the derivative $d(\beta_{\text{calc}} - \beta_{\text{input}})/d\beta_{\text{input}} < 0$. It is seen that the spherical solution becomes unstable between $\chi = 0.6$ and $\chi = 0.7$.

(b) In all calculations with an attractive quadrupole force ($\chi > 0$) the particle deformation, β_p , turned out to have the same sign as the hole deformation β_h . This feature is decisive for obtaining stable deformations and is due to the mutual repulsion of particles and holes for $\chi = 0$ (see also footnote on p. 12).

(c) For a fixed value of χ the deformation decreases with increasing G_0 , for small G_0 slowly, for large G_0 more rapidly. The reason is the following: Increasing G_0 enlarges the energy splitting between the particle (hole) pair states with $J = 0$ and $J \neq 0$, thus diminishing the ability of the quadrupole force to mix the levels and to produce deformations.

(d) In our model the pairing force introduces ground-state correlations and consequently an admixture of 4p-4h, 6p-6h, . . . to the dominant 2p-2h configurations. That is, the pairing force leads in a natural way to core excitations. In order to investigate the effect of continuously increasing core excitations we used in fig. 7 a fixed spectrum for the pair scattering modes, unaffected by the pairing force and simulating an ‘‘experimental’’ spectrum. The energies of the particle (hole) pair scattering modes were arbitrarily assumed to be $E_J/\varepsilon_0 = \pm(1.5 + 0.1 \cdot J)$ for $J = 0, 2, \dots, 8$. Fig. 7 shows how the pairing force in this case *increases* the deformation, and decreases the energy by admixing 4p-4h, 6p-6h, . . . configurations. The vertical line indicates the phase transition to superconductivity. When approaching this point, the deformation becomes much larger than the limiting deformation which can be obtained for a pure 2p-2h excitation. Thus the pairing force, by introducing ground-state correlations, softens the core so that the quadrupole force can efficiently produce deformations. However, since we disregarded the effect of the pairing force which *stabilizes the spherical shape* as discussed under (c), the deformation plotted in fig. 7 gives us only a measure of the ‘‘triggering effect’’ for deformations. The actual deformations are mainly due to the core deformation effect which enters through the collective ground-state correlations discussed in sect. 4. *Thus, the core deformation effect due to the field-producing force is triggered by the core softening effect due to the pairing force.*

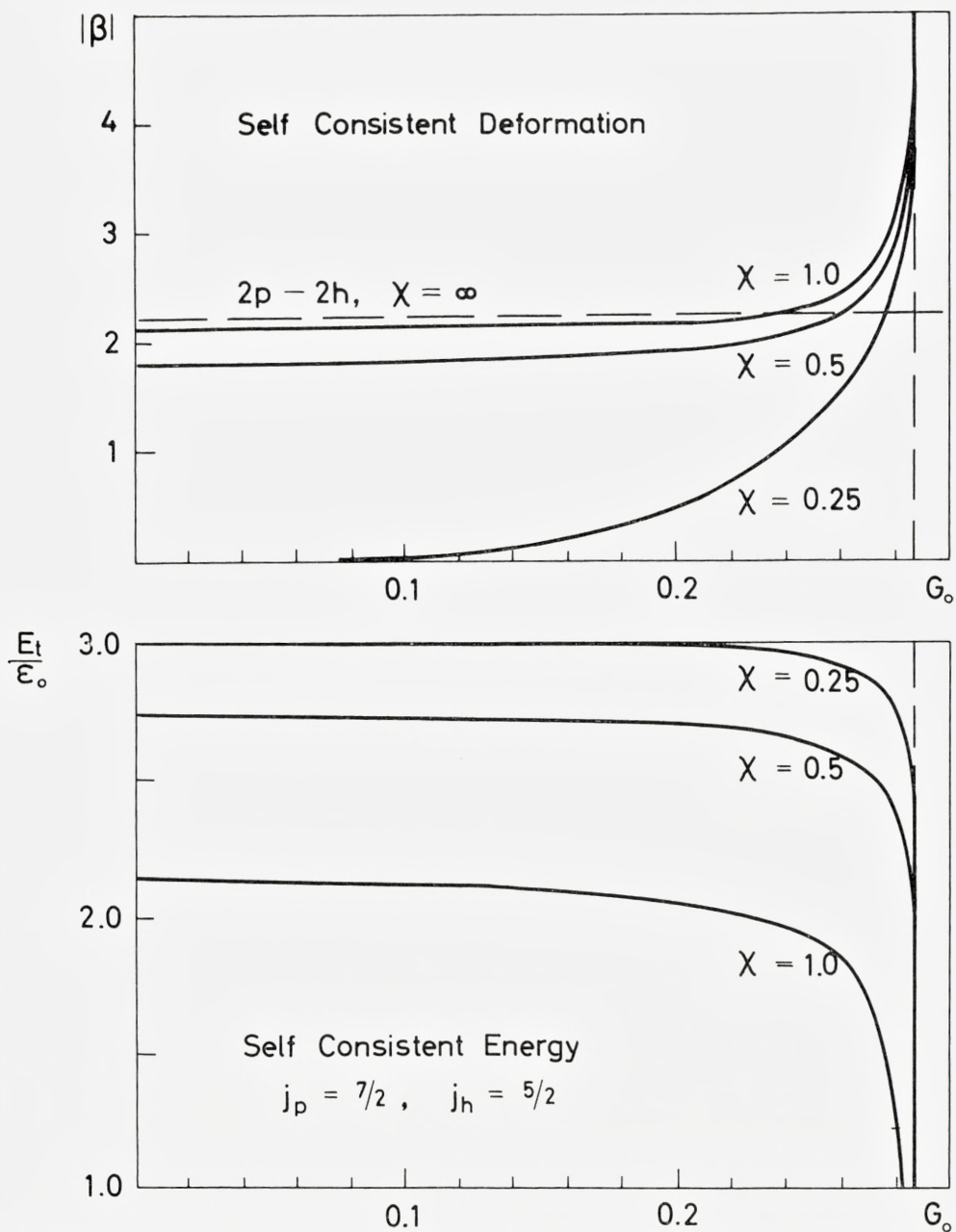


Fig. 7. Self-consistent deformation and self-consistent energy as functions of the strength G_0 of the pairing force for various strength parameters χ of the quadrupole force. Details are explained in the text.

5.4. A Self-Consistent Method Including the Core Deformation

In the preceding subsection we have traced the origin of the intrinsic deformation in excited states. Now we are in a position to present a method which demonstrates explicitly the intrinsic deformation of a ‘‘dressed 2p-2h’’ state containing the collective ground-state correlations. To do this, it is useful to note that the eigenvalue equation (5.28) can also be obtained from the following procedure.

(a) In a first step we introduce the approximation

$$\left. \begin{aligned} \mathfrak{S}_{ph}^{(1)} &\approx - \sum_{LM} \chi_L(-)^M \sum_{\mu\nu} (\mu | Q_{L-M} | \nu) B_\nu^+ B_\mu \cdot \alpha_{LM}^{(p)} \\ &\quad - \sum_{LM} \chi_L(-)^M \sum_{\mu\nu} (\mu | Q_{L-M} | \nu) A_\mu^+ A_\nu \cdot \alpha_{LM}^{(h)} \\ &\quad + \text{const} \left(\sum_{LM} \chi_L(-)^M \alpha_{LM}^{(p)} \alpha_{L-M}^{(h)} \right) \equiv \mathfrak{S}_{ph}^{(1)}(\alpha) \end{aligned} \right\} \quad (5.32)$$

with

$$\left. \begin{aligned} \alpha_{LM}^{(p)} &= \sum_{\mu\nu} (\mu | Q_{LM} | \nu) \langle A_\mu^+ A_\nu \rangle \\ \alpha_{LM}^{(h)} &= \sum_{\mu\nu} (\mu | Q_{LM} | \nu) \langle B_\nu^+ B_\mu \rangle \end{aligned} \right\} \quad (5.33)$$

where $\langle A_\mu^+ A_\nu \rangle$ and $\langle B_\nu^+ B_\mu \rangle$ are expectation values which will be determined later in a self-consistent way.

(b) As the next step we construct the eigenstate

$$|\Phi'_{ij}\rangle = \sum_{\mu\nu} \tilde{\xi}_{ij}(\mu\nu) A_\mu^+ B_\nu^+ |\Phi'_0\rangle \quad (5.34)$$

with the aim of diagonalizing the following Hamiltonian within the subspace composed of the unperturbed states $A_\mu^+ B_\nu^+ |\Phi'_0\rangle$:

$$\hat{H}'(\alpha) = \sum_{\mu} \omega_m A_\mu^+ A_\mu - \sum_{\nu} \omega_n B_\nu^+ B_\nu + \mathfrak{S}_{ph}^{(1)}(\alpha). \quad (5.35)$$

(c) The expectation values $\langle A_\mu^+ A_\nu \rangle$ and $\langle B_\nu^+ B_\mu \rangle$ are determined self-consistently by the condition

$$\left. \begin{aligned} \langle \Phi'_{ij} | A_\mu^+ A_\nu | \Phi'_{ij} \rangle &= \langle A_\mu^+ A_\nu \rangle \\ \langle \Phi'_{ij} | B_\nu^+ B_\mu | \Phi'_{ij} \rangle &= \langle B_\nu^+ B_\mu \rangle. \end{aligned} \right\} \quad (5.36)$$

We can easily see that the eigenvalue equation for $\tilde{\xi}_{ij}(\mu\nu)$ defined by eq. (5.34) is identical to the equation obtained by the variational approach which is described by eqs. (5.26) and (5.27) and yields $\tilde{\xi}_{ij}(\mu\nu) = u_i(\mu) v_j(\nu)$.

This equivalence leads immediately to a self-consistent method which demonstrates explicitly the intrinsic deformation in the ‘‘dressed 2p-2h’’

states subject to the cooperation effect of the core deformation. This method consists of the following operations: With the Hamiltonian

$$\hat{H}(\alpha) = \sum_{\mu} \omega_m A_{\mu}^{+} A_{\mu} - \sum_{\nu} \omega_n B_{\nu}^{+} B_{\nu} + \{\mathfrak{S}_{ph}^{(1)}(\alpha) + \mathfrak{S}_{hh}^{(1)} + \mathfrak{S}_{pp}^{(1)}\} + \mathfrak{S}^{(2)}, \quad (5.37)$$

we start from a linearized relation similar to eq. (4.5)

$$[\hat{H}(\alpha), A_{\mu}^{+} B_{\nu}^{+}] = \sum_{\varrho\sigma} \{N_{\mu\nu\varrho\sigma}(\alpha) A_{\varrho}^{+} B_{\sigma}^{+} + N'_{\mu\nu\varrho\sigma} A_{\varrho} B_{\sigma}\}, \quad (5.38)$$

where the coefficients $N(\alpha)$ are now functions of all $\alpha_{LM}^{(p)}$ and $\alpha_{LM}^{(h)}$. The creation operator of the eigenmode, which satisfies the relation

$$[\hat{H}(\alpha), X_{\gamma}^{+}] = \Omega_{\gamma} X_{\gamma}^{+} \quad \text{with} \quad \Omega_{\gamma} > 0, \quad (5.39)$$

is then given by

$$X_{\gamma}^{+} = \sum_{\mu\nu} \{\xi_{\gamma}(\mu\nu) A_{\mu}^{+} B_{\nu}^{+} + \eta_{\gamma}(\mu\nu) A_{\mu} B_{\nu}\}. \quad (5.40)$$

Here, γ is a set of quantum numbers specifying the excited state under consideration

$$|\Psi_{\gamma}\rangle = X_{\gamma}^{+} |\Psi_0\rangle, \quad (X_{\gamma} |\Psi_0\rangle = 0). \quad (5.41)$$

With the aid of eq. (5.38) the functions $\xi_{\gamma}(\mu\nu)$ and $\eta_{\gamma}(\mu\nu)$ are seen to obey the eigenvalue equations

$$\left. \begin{aligned} \Omega_{\gamma} \xi_{\gamma}(\mu\nu) &= \sum_{\varrho\sigma} \{N_{\varrho\sigma\mu\nu}(\alpha) \xi_{\gamma}(\varrho\sigma) - N'_{\varrho\sigma\mu\nu} \eta_{\gamma}(\varrho\sigma)\} \\ \Omega_{\gamma} \eta_{\gamma}(\mu\nu) &= - \sum_{\varrho\sigma} \{N_{\varrho\sigma\mu\nu}(\alpha) \eta_{\gamma}(\varrho\sigma) - N'_{\varrho\sigma\mu\nu} \xi_{\gamma}(\varrho\sigma)\}. \end{aligned} \right\} \quad (5.42)$$

The orthogonality and completeness relations of $\xi_{\gamma}(\mu\nu)$ and $\eta_{\gamma}(\mu\nu)$ are of the same form as eq. (4.10).

The quantities $\alpha_{LM}^{(p)}$ and $\alpha_{LM}^{(h)}$ are determined self-consistently by

$$\left. \begin{aligned} \alpha_{LM}^{(p)} &= \sum_{\mu\nu} (\mu | Q_{LM} | \nu) \langle \Psi_{\gamma} | A_{\mu}^{+} A_{\nu} | \Psi_{\gamma} \rangle \\ \alpha_{LM}^{(h)} &= \sum_{\mu\nu} (\mu | Q_{LM} | \nu) \langle \Psi_{\gamma} | B_{\nu}^{+} B_{\mu} | \Psi_{\gamma} \rangle. \end{aligned} \right\} \quad (5.43)$$

Now it is clear that the eigenvalue equation (5.42) with the self-consistency condition (5.43) is simply a generalization of eq. (5.20) with eq. (5.21) for the purpose of taking the cooperation effect of the core deformation into

account. The intrinsic deformation of the ‘‘dressed 2p-2h’’ states associated with the core deformation is now given by

$$\alpha_{LM} = \langle \Psi_\gamma | \hat{Q}_{LM} | \Psi_\gamma \rangle = \langle \Psi_\gamma | \hat{Q}_{LM}^{(1)} | \Psi_\gamma \rangle = \alpha_{LM}^{(p)} + \alpha_{LM}^{(h)}. \quad (5.44)$$

Here we have used the result $\langle \Psi_\gamma | \hat{Q}_{LM}^{(2)} | \Psi_\gamma \rangle = 0$, which follows immediately from eq. (4.11). The operators $\hat{Q}_{LM}^{(1)}$ and $\hat{Q}_{LM}^{(2)}$ are defined by eq. (5.8).

Obviously the eigenvalue equation (5.42) is an approximation to our general equation (4.9), thus demonstrating explicitly the deformed nature of the excited states obtained as solutions of (4.9). The ground state defined by (4.12), however, is spherical, and only if eq. (4.9) had a zero-energy solution, it would be really deformed. This has been discussed in section 4.2. Correspondingly, the ground state defined by eq. (5.41) will be ‘‘spherical’’ unless the eigenvalue equation (5.42) has a zero-energy solution.

We now want to solve the eigenvalue equation (5.42) in a way which explicitly traces the effect of $\mathfrak{S}_{ph}^{(1)}(\alpha)$ responsible for the intrinsic deformation. For this purpose we divide the Hamiltonian (5.37) into two parts:

$$\left. \begin{aligned} \hat{H}(\alpha) &= \hat{H}_0 + \mathfrak{S}_{ph}^{(1)}(\alpha), \\ \hat{H}_0 &= \sum_{\mu} \omega_m A_{\mu}^{\dagger} A_{\mu} - \sum_{\nu} \omega_n B_{\nu}^{\dagger} B_{\nu} + \mathfrak{S}_{pp}^{(1)} + \mathfrak{S}_{hh}^{(1)} + \mathfrak{S}^{(2)}, \end{aligned} \right\} \quad (5.45)$$

and introduce the eigenmode creation operator with respect to \hat{H}_0 :

$$X_{\lambda}^{(0)+} = \sum_{\mu\nu} \{ \xi_{\lambda}^{(0)}(\mu\nu) A_{\mu}^{\dagger} B_{\nu}^{\dagger} + \eta_{\lambda}^{(0)}(\mu\nu) A_{\mu} B_{\nu} \} \quad (5.46)$$

which satisfies

$$[\hat{H}_0, X_{\lambda}^{(0)+}] = \Omega_{\lambda}^{(0)} X_{\lambda}^{(0)+} \quad \text{with} \quad \Omega_{\lambda}^{(0)} > 0. \quad (5.47)$$

The functions $\xi_{\lambda}^{(0)}(\mu\nu)$ and $\eta_{\lambda}^{(0)}(\mu\nu)$ clearly satisfy the eigenvalue equation (5.42) with $\alpha_{LM}^{(p)} = \alpha_{LM}^{(h)} = 0$. Similarly as in the usual RPA for ‘‘1p-1h’’ excitations, we then obtain the well-known formulae*

$$\frac{1}{2\chi_{L=I_l}} = \sum_{\substack{\mu\nu \\ \left(\begin{smallmatrix} s_{\mu} \\ s_{\nu} \end{smallmatrix} = \begin{smallmatrix} +1 \\ -1 \end{smallmatrix} \right)}} \frac{|(\mu | Q_{I_l M_{\lambda}} | \nu)|^2 (\omega_m - \omega_n)}{(\omega_m - \omega_n)^2 - \Omega_l^{(0)2}}, \quad (5.48)$$

* Eqs. (5.48) and (5.49) are valid for $T_l = 0$ only, since Q_{LM} has been taken to be a scalar in isospace. For $T_l \neq 0$, eq. (5.46) becomes simply

$$X_{\lambda}^{(0)+} = \sum_{\mu\nu} (-)^{J_n - M_{\nu}(-)} T_n^{-Z_{\nu}} \langle J_m J_n M_{\mu} M_{\nu} | I_l M_{\lambda} \rangle \langle T_m T_n Z_{\mu} - Z_{\nu} | T_l Z_l \rangle A_{\mu}^{\dagger} B_{\nu}^{\dagger}.$$

$$\xi_{\lambda}^{(0)}(\mu\nu) = \frac{N_l(\mu|Q_{I_l M_{\lambda}}|\nu)}{(\omega_m - \omega_n) - \Omega_l^{(0)}}, \quad \eta_{\lambda}^{(0)}(\mu\nu) = \frac{-N_l(\nu|Q_{I_l M_{\lambda}}|\mu)}{(\omega_m - \omega_n) + \Omega_l^{(0)}}, \quad (5.49)$$

where N_l is the normalization constant determined by eq. (4.10 a). States like those created by the operators $X_{\lambda}^{(0)+}$ are conventionally called spherical, similarly as the "1p-1h" states in spherical nuclei known from the usual RPA. This is consistent with our definition of the intrinsic deformation α_{LM} and reconfirms the conclusion of the preceding subsection that $\mathfrak{S}_{ph}^{(1)}(\alpha)$ is the origin of the intrinsic deformation in the excited states of closed-shell nuclei.

Using $X_{\lambda}^{(0)+}$, we now can write the creation operator X_{λ}^{+} in eq. (5.40) for a deformed excited state as

$$\left. \begin{aligned} X_{\lambda}^{+} &= \sum_{\lambda} U_{\gamma}(\lambda) X_{\lambda}^{(0)+} + \sum_{\lambda} V_{\gamma}(\lambda) X_{\lambda}^{(0)} \\ &= \sum_{\mu\nu} \left\{ \sum_{\lambda} U_{\gamma}(\lambda) \xi_{\lambda}^{(0)}(\mu\nu) + \sum_{\lambda} V_{\gamma}(\lambda) \eta_{\lambda}^{(0)}(\mu\nu) \right\} A_{\mu}^{+} B_{\nu}^{+} \\ &\quad + \sum_{\mu\nu} \left\{ \sum_{\lambda} U_{\gamma}(\lambda) \eta_{\lambda}^{(0)}(\mu\nu) + \sum_{\lambda} V_{\gamma}(\lambda) \xi_{\lambda}^{(0)}(\mu\nu) \right\} A_{\mu} B_{\nu}. \end{aligned} \right\} \quad (5.50)$$

Then eq. (5.42) simply becomes a self-consistent equation for U_{γ} and V_{γ} . The functions U_{γ} and V_{γ} describe the effect of $\mathfrak{S}_{ph}^{(1)}(\alpha)$: if $\alpha_{LM}^{(p)} = \alpha_{LM}^{(h)} = 0$, then $V_{\gamma}(\lambda) = 0$ and $U_{\gamma}(\lambda) = \delta_{\gamma\lambda}$. The requirement that the operators X_{γ}^{+} and $X_{\lambda}^{(0)+}$ each form a set of boson operators entails the orthogonality relations

$$\left. \begin{aligned} \sum_{\lambda} \{U_{\gamma_1}(\lambda) U_{\gamma_2}(\lambda) - V_{\gamma_1}(\lambda) V_{\gamma_2}(\lambda)\} &= \delta_{\gamma_1 \gamma_2} \\ \sum_{\lambda} \{U_{\gamma_1}(\lambda) V_{\gamma_2}(\lambda) - V_{\gamma_1}(\lambda) U_{\gamma_2}(\lambda)\} &= 0, \\ \sum_{\gamma} \{U_{\gamma}(\lambda_1) U_{\gamma}(\lambda_2) - V_{\gamma}(\lambda_1) V_{\gamma}(\lambda_2)\} &= \delta_{\lambda_1 \lambda_2} \\ \sum_{\gamma} \{U_{\gamma}(\lambda_1) V_{\gamma}(\lambda_2) - V_{\gamma}(\lambda_1) U_{\gamma}(\lambda_2)\} &= 0, \end{aligned} \right\} \quad (5.51)$$

and the inverse relation to eq. (5.50)

$$X_{\lambda}^{(0)+} = \sum_{\gamma} U_{\gamma}(\lambda) X_{\gamma}^{+} - \sum_{\gamma} V_{\gamma}(\lambda) X_{\gamma}. \quad (5.52)$$

5.5 Intrinsic Deformations in Excited 0^+ States

In this subsection we restrict ourselves, for simplicity, entirely to quadrupole deformations. This corresponds to taking up only the $L = 2$ part* in the expansion (5.32) of $\mathfrak{S}_{ph}^{(1)}(\alpha)$. If the excited 0^+ state $|\Psi_{\gamma_0}\rangle$ defined by eq. (5.41) has an intrinsic quadrupole deformation (i.e. $\alpha_{2M} \neq 0$), then the solution must have the appropriate degeneracy to contain all possible orientations of the ‘‘excited deformed nucleus’’ in space. Without loss of generality we therefore can choose the axes of the intrinsic deformation as coordinate axes, so that $\alpha_{2,M=1} = \alpha_{2,M=-1} = 0$ and $\alpha_{2,M=2} = \alpha_{2,M=-2}$. Furthermore we assume, for simplicity, that the intrinsic deformation in the excited 0^+ state is axially symmetric, so that $\alpha_{2,M=2} = \alpha_{2,M=-2} = 0$. In this case, the intrinsic deformation is characterized by one quantity

$$\alpha_{2M=0} \equiv \beta. \quad (5.53)$$

The projection K_γ of the intrinsic angular momentum on the symmetry axis now is a constant of the motion, so that $K_{\gamma_0} = 0$ for our excited 0^+ state. We need not say that eq. (5.42) gives us the information about the *intrinsic excitations* in the body-fixed coordinate system and eq. (5.37) provides the *intrinsic* Hamiltonian of our system.

The excited 0^+ state under consideration, $|\Psi_{\gamma_0}\rangle$ with $K_{\gamma_0} = 0$, in eq. (5.41) is given by

$$|\Psi_{\gamma_0}\rangle = X_{\gamma_0}^+ |\Psi_0\rangle$$

with

$$X_{\gamma_0}^+ = \sum_{\lambda} U_{\gamma_0}(\lambda) X_{\lambda}^{(0)+} + \sum_{\lambda} V_{\gamma_0}(\lambda) X_{\lambda}^{(0)}. \quad (5.54)$$

Thus the eigenvalue equation (5.42) for this state becomes a self-consistent eigenvalue equation for U_{γ_0} and V_{γ_0} :

$$\left. \begin{aligned} (\Omega_{\gamma_0} - \Omega_{I_1}^{(0)}) U_{\gamma_0}(\lambda_1) &= -\chi \sum_{\lambda_2} (F_{\lambda_1 \lambda_2}^{(1)} \beta^{(p)} + F_{\lambda_1 \lambda_2}^{(2)} \beta^{(h)}) U_{\gamma_0}(\lambda_2) \\ &\quad - \chi \sum_{\lambda_2} (G_{\lambda_1 \lambda_2}^{(1)} \beta^{(p)} + G_{\lambda_1 \lambda_2}^{(2)} \beta^{(h)}) V_{\gamma_0}(\lambda_2), \\ (\Omega_{\gamma_0} + \Omega_{I_1}^{(0)}) V_{\gamma_0}(\lambda_1) &= +\chi \sum_{\lambda_2} (F_{\lambda_1 \lambda_2}^{(1)} \beta^{(p)} + F_{\lambda_1 \lambda_2}^{(2)} \beta^{(h)}) V_{\gamma_0}(\lambda_2) \\ &\quad + \chi \sum_{\lambda_2} (G_{\lambda_1 \lambda_2}^{(1)} \beta^{(p)} + G_{\lambda_1 \lambda_2}^{(2)} \beta^{(h)}) U_{\gamma_0}(\lambda_2) \end{aligned} \right\} \quad (5.55)$$

* Of course, the $L = 0$ part in $\mathfrak{S}_{ph}^{(1)}(\alpha)$ will contribute even under this restriction. However, the effect of this term is only a renormalization of the single pair energy ω_m for $J_m = 0$. In the following we assume, for simplicity, that the renormalization has already been carried out.

where $\chi = \chi_{L=2}$ and

$$\left. \begin{aligned} F_{\lambda_1 \lambda_2}^{(1)} &= \sum_{(s_\varrho = \frac{\varrho\sigma}{s_\sigma} - 1)} (\varrho | Q_{20} | \sigma) \sum_{(s_\mu = \frac{\mu}{s_\mu} + 1)} \{ \xi_{\lambda_1}^{(0)}(\mu\varrho) \xi_{\lambda_2}^{(0)}(\mu\sigma) + \eta_{\lambda_1}^{(0)}(\mu\sigma) \eta_{\lambda_2}^{(0)}(\mu\varrho) \} \\ F_{\lambda_1 \lambda_2}^{(2)} &= \sum_{(s_\mu = \frac{\mu\nu}{s_\nu} + 1)} (\mu | Q_{20} | \nu) \sum_{(s_\varrho = \frac{\varrho}{s_\varrho} - 1)} \{ \xi_{\lambda_1}^{(0)}(\nu\varrho) \xi_{\lambda_2}^{(0)}(\mu\varrho) + \eta_{\lambda_1}^{(0)}(\mu\varrho) \eta_{\lambda_2}^{(0)}(\nu\varrho) \} \\ G_{\lambda_1 \lambda_2}^{(1)} &= \sum_{(s_\varrho = \frac{\varrho\sigma}{s_\sigma} - 1)} (\varrho | Q_{20} | \sigma) \sum_{(s_\mu = \frac{\mu}{s_\mu} + 1)} \{ \xi_{\lambda_1}^{(0)}(\mu\varrho) \eta_{\lambda_2}^{(0)}(\mu\sigma) + \eta_{\lambda_1}^{(0)}(\mu\sigma) \xi_{\lambda_2}^{(0)}(\mu\varrho) \} \\ G_{\lambda_1 \lambda_2}^{(2)} &= \sum_{(s_\mu = \frac{\mu\nu}{s_\nu} + 1)} (\mu | Q_{20} | \nu) \sum_{(s_\varrho = \frac{\varrho}{s_\varrho} - 1)} \{ \xi_{\lambda_1}^{(0)}(\nu\varrho) \eta_{\lambda_2}^{(0)}(\mu\varrho) + \eta_{\lambda_1}^{(0)}(\mu\varrho) \xi_{\lambda_2}^{(0)}(\nu\varrho) \}. \end{aligned} \right\} \quad (5.56)$$

The quantities $\beta^{(p)}$ and $\beta^{(h)}$ are determined self-consistently by

$$\left. \begin{aligned} \beta^{(p)} &= \sum_{\mu\nu} (\mu | Q_{20} | \nu) \langle \Psi_{\gamma_0} | A_\mu^+ A_\nu | \Psi_{\gamma_0} \rangle \\ \beta^{(h)} &= \sum_{\varrho\sigma} (\varrho | Q_{20} | \sigma) \langle \Psi_{\gamma_0} | B_\sigma^+ B_\varrho | \Psi_{\gamma_0} \rangle. \end{aligned} \right\} \quad (5.57)$$

To evaluate eq. (5.57), we first note that the operators

$$\sum_{\mu\nu} (\mu | Q_{20} | \nu) A_\mu^+ A_\nu \quad \text{and} \quad \sum_{\varrho\sigma} (\varrho | Q_{20} | \sigma) B_\sigma^+ B_\varrho$$

can be expanded in terms of the operators $X_\lambda^{(0)+}$ as follows:

$$\left. \begin{aligned} \sum_{\mu\nu} (\mu | Q_{20} | \nu) A_\mu^+ A_\nu &= \sum_{\lambda_1 \lambda_2} F_{\lambda_2 \lambda_1}^{(2)} \cdot X_{\lambda_1}^{(0)} + X_{\lambda_2}^{(0)} \\ - \sum_{\lambda_1 \lambda_2} \sum_{\mu\nu} (\mu | Q_{20} | \nu) & \left[\sum_{\varrho} \xi_{\lambda_1}^{(0)}(\mu\varrho) \eta_{\lambda_2}^{(0)}(\nu\varrho) X_{\lambda_1}^{(0)} + X_{\lambda_2}^{(0)+} + \sum_{\varrho} \eta_{\lambda_1}^{(0)}(\mu\varrho) \xi_{\lambda_2}^{(0)}(\nu\varrho) X_{\lambda_1}^{(0)} X_{\lambda_2}^{(0)} \right], \\ \sum_{\varrho\sigma} (\varrho | Q_{20} | \sigma) B_\sigma^+ B_\varrho &= \sum_{\lambda_1 \lambda_2} F_{\lambda_2 \lambda_1}^{(1)} \cdot X_{\lambda_1}^{(0)} + X_{\lambda_2}^{(0)} \\ - \sum_{\lambda_1 \lambda_2} \sum_{\varrho\sigma} (\varrho | Q_{20} | \sigma) & \left[\sum_{\mu} \xi_{\lambda_1}^{(0)}(\mu\sigma) \eta_{\lambda_2}^{(0)}(\mu\varrho) X_{\lambda_1}^{(0)} + X_{\lambda_2}^{(0)+} + \sum_{\mu} \eta_{\lambda_1}^{(0)}(\mu\sigma) \xi_{\lambda_2}^{(0)}(\mu\varrho) X_{\lambda_1}^{(0)} X_{\lambda_2}^{(0)} \right]. \end{aligned} \right\} \quad (5.58)$$

In obtaining eq. (5.58), we have used a transcription rule similar to eq. (3.14), and then have employed the relation (4.11) with respect to $X_\lambda^{(0)+}$. Finally, by inserting eq. (5.52) into eq. (5.58), we get the deformations

$$\left. \begin{aligned} \beta^{(p)} &= \sum_{\lambda_1 \lambda_2} F_{\lambda_2 \lambda_1}^{(2)} \{ U_{\gamma_0}(\lambda_1) U_{\gamma_0}(\lambda_2) + V_{\gamma_0}(\lambda_1) V_{\gamma_0}(\lambda_2) \} \\ &+ \sum_{\lambda_1 \lambda_2} G_{\lambda_2 \lambda_1}^{(2)} \{ U_{\gamma_0}(\lambda_1) V_{\gamma_0}(\lambda_2) + V_{\gamma_0}(\lambda_1) U_{\gamma_0}(\lambda_2) \}, \end{aligned} \right\} \quad (5.59a)$$

$$\beta^{(h)} = \left. \begin{aligned} & \sum_{\lambda_1 \lambda_2} F_{\lambda_1 \lambda_2}^{(1)} \{U_{\gamma_0}(\lambda_1)U_{\gamma_0}(\lambda_2) + V_{\gamma_0}(\lambda_1)V_{\gamma_0}(\lambda_2)\} \\ & + \sum_{\lambda_1 \lambda_2} G_{\lambda_1 \lambda_2}^{(1)} \{U_{\gamma_0}(\lambda_1)V_{\gamma_0}(\lambda_2) + V_{\gamma_0}(\lambda_1)U_{\gamma_0}(\lambda_2)\}. \end{aligned} \right\} (5.59b)$$

In the expressions (5.59a) and (5.59b) we have already dropped the following terms, respectively:

$$\left. \begin{aligned} & \sum_{\lambda_1 \lambda_2} F_{\lambda_1 \lambda_2}^{(2)} \cdot \sum_{\gamma} V_{\gamma}(\lambda_1)V_{\gamma}(\lambda_2) + \sum_{\lambda_1 \lambda_2} G_{\lambda_1 \lambda_2}^{(2)} \cdot \sum_{\gamma} U_{\gamma}(\lambda_1)V_{\gamma}(\lambda_2) \quad (\text{from (5.59a)}), \\ & \sum_{\lambda_1 \lambda_2} F_{\lambda_1 \lambda_2}^{(1)} \cdot \sum_{\gamma} V_{\gamma}(\lambda_1)V_{\gamma}(\lambda_2) + \sum_{\lambda_1 \lambda_2} G_{\lambda_1 \lambda_2}^{(1)} \cdot \sum_{\gamma} U_{\gamma}(\lambda_1)V_{\gamma}(\lambda_2) \quad (\text{from (5.59b)}). \end{aligned} \right\} (5.60)$$

These terms occur not only in the excited 0^+ states $|\Psi_{\gamma_0}\rangle$ in which we are interested, but they are also common to all other excited states $|\Psi_{\gamma}\rangle$. The sum of both terms can thus be interpreted as an ‘‘unphysical deformation’’ of the spherical ground state $|\Psi_0\rangle$ (defined by eq. (5.41)) given by

$$\left. \begin{aligned} \langle \Psi_0 | \hat{Q}_{20} | \Psi_0 \rangle &= \sum_{\lambda_1 \lambda_2} (F_{\lambda_1 \lambda_2}^{(1)} + F_{\lambda_1 \lambda_2}^{(2)}) \cdot \sum_{\gamma} V_{\gamma}(\lambda_1)V_{\gamma}(\lambda_2) \\ &+ \sum_{\lambda_1 \lambda_2} (G_{\lambda_1 \lambda_2}^{(1)} + G_{\lambda_1 \lambda_2}^{(2)}) \cdot \sum_{\gamma} U_{\gamma}(\lambda_1)V_{\gamma}(\lambda_2). \end{aligned} \right\} (5.61)$$

We are now in a position to write down the final result for the intrinsic deformation β of the excited 0^+ state. The result is

$$\left. \begin{aligned} \beta &= \langle \Psi_{\gamma_0} | \hat{Q}_{20} | \Psi_{\gamma_0} \rangle = \langle \Psi_{\gamma_0} | \hat{Q}_{20}^{(1)} | \Psi_{\gamma_0} \rangle = \beta^{(p)} + \beta^{(h)} \\ &= \sum_{\lambda_1 \lambda_2} (F_{\lambda_1 \lambda_2}^{(1)} + F_{\lambda_1 \lambda_2}^{(2)}) \{U_{\gamma_0}(\lambda_1)U_{\gamma_0}(\lambda_2) + V_{\gamma_0}(\lambda_1)V_{\gamma_0}(\lambda_2)\} \\ &+ \sum_{\lambda_1 \lambda_2} (G_{\lambda_1 \lambda_2}^{(1)} + G_{\lambda_1 \lambda_2}^{(2)}) \{U_{\gamma_0}(\lambda_1)V_{\gamma_0}(\lambda_2) + V_{\gamma_0}(\lambda_1)U_{\gamma_0}(\lambda_2)\}. \end{aligned} \right\} (5.62)$$

Here we have used the fact that $\langle \Psi_{\gamma_0} | \hat{Q}_{20}^{(2)} | \Psi_{\gamma_0} \rangle = 0$, which follows from a relation analogous to eq. (4.11). The operators $\hat{Q}_{20}^{(1)}$ and $\hat{Q}_{20}^{(2)}$ are defined by eq. (5.8). From the definition (5.56) of F and G , it is obvious that in the absence of ground-state correlations due to the field-producing force (that is, if $\eta_{\lambda}^{(0)}(\mu\nu) = 0$ and $V_{\gamma_0}(\lambda) = 0$, (see eq. (5.50)) only the first term in eq. (5.62) contributes to the deformation. Thus the expression (5.62) allows us to identify clearly that part of the deformation in the excited state which arises from the cooperation effect of the core deformation.

5.6 Rotational Bands Built on Excited States

The basic equation (5.42) of our self-consistent method describes the intrinsic excitation in the body-fixed coordinate system associated with the intrinsic deformation of each excited state. Thus the state vector $|\Psi_\gamma\rangle$ in eq. (5.41), describing the intrinsic excited state, has no definite angular momentum. The proper eigenfunctions with definite angular momenta are then obtained by the usual projection operation⁽¹⁶⁾, which also yields the rotational band structure belonging to the intrinsic excited state $|\Psi_\gamma\rangle$.

To avoid the problem of computing overlap integrals in this method, we may apply the conventional Bohr-Mottelson description to our problem. Then our system is described by the following effective Hamiltonian:

$$\mathbf{H} = \sum_{\kappa=1}^3 \frac{\hbar^2}{2\mathfrak{I}_\kappa(\alpha)} \mathbf{R}_\kappa^2 + \hat{H}(\alpha), \tag{5.63}$$

where $\hat{H}(\alpha)$ is given by eq. (5.37) and \mathbf{R}_κ is the component of the “collective” angular momentum in the direction of the κ -axis of the body-fixed coordinate system, and the quantities \mathfrak{I}_κ are the principal moments of inertia.

The physical interpretation of eq. (5.63) is the following: A specific intrinsic excited state $|\Psi_\gamma\rangle$ defined by eq. (5.41) is created by applying the operator X_γ^+ to the spherical ground state of the closed-shell nucleus. Once the state is excited, we can choose the body-fixed coordinate system determined by the axes of the intrinsic quadrupole deformation of this excited state. The corresponding moments of inertia of the state $|\Psi_\gamma\rangle$ can be calculated. With these moments of inertia the intrinsic excited state performs a rotational motion which gives rise to a rotational band belonging to this specific state $|\Psi_\gamma\rangle$. The explicit calculation of the moments of inertia for the state $|\Psi_\gamma\rangle$ is possible by applying the conventional Lagrange multiplier method to our self-consistent approach developed in section 5.4. However, we do not want to go into further details in the present work. With the approximation (5.63), the rotational states belonging to the excited 0^+ state discussed in section 5.5 are of the usual form

$$\left. \begin{aligned} |IM; \gamma_0 K_{\gamma_0} = 0\rangle &= \left[\frac{2I+1}{8\pi} \right]^{1/2} D_{MK_{\gamma_0}=0}^I(\theta_i) |\Psi_{\gamma_0}\rangle \\ I^\pi &= 0^+, 2^+, 4^+, 6^+, \dots \end{aligned} \right\} \tag{5.64}$$

with

Here $|\Psi_{\gamma_0}\rangle$ is defined by eq. (5.54), and the effect of the well-known symmetry restrictions are taken into account in limiting the allowed values of I .

6. Electromagnetic Transitions

In this section we discuss various electromagnetic transitions involving even parity states (with $T = 0$) in closed-shell nuclei. Electromagnetic transitions are a crucial test of the theory, more than energies, in particular they are shown to be decisively influenced by the interplay between the residual interaction and the field-producing force. The essential differences between G. E. Brown's and our theory are pointed out.

6.1 Energy-Weighted Sum Rule

As a preparation we wish to show that, for a general one-body boson operator defined by

$$\hat{\mathfrak{D}} = \sum_{\mu\nu} (\mu|\hat{\mathfrak{D}}|\nu) : C_{\mu}^{+} C_{\nu} :, \quad (6.1)$$

the following sum rule holds within our approximation (4.5)

$$\sum_{\lambda} |\langle \Psi_0 | \hat{\mathfrak{D}} | \Psi_{\lambda} \rangle|^2 (E_{\lambda} - E_0) = \frac{1}{2} \langle \Phi'_0 | [\hat{\mathfrak{D}}[\hat{H}, \hat{\mathfrak{D}}]] | \Phi'_0 \rangle. \quad (6.2)$$

Here the unperturbed ground state $|\Phi'_0\rangle$ is defined by eq. (3.11), $|\Psi_0\rangle$ and $|\Psi_{\lambda}\rangle$ are defined by eqs. (4.12) and (4.13), respectively, and $(E_{\lambda} - E_0) \equiv \Omega_{\lambda}$ are the eigenvalues of eq. (4.9).

With the aid of eqs. (4.11), (4, 9) and the completeness relation (4.10b) we can rewrite the left hand side of (6.2) as

$$\left. \begin{aligned} \sum_{\lambda} |\langle \Psi_0 | \hat{\mathfrak{D}} | \Psi_{\lambda} \rangle|^2 (E_{\lambda} - E_0) &= \sum_{\lambda} \left[\sum_{\mu\nu} (\mu|\hat{\mathfrak{D}}|\nu) \{ \xi_{\lambda}(\mu\nu) - \eta_{\lambda}(\mu\nu) \} \right]^2 \Omega_{\lambda} \\ &= \sum_{\mu\nu\rho\sigma} (\mu|\hat{\mathfrak{D}}|\nu) (\rho|\hat{\mathfrak{D}}|\sigma) (N_{\mu\nu\rho\sigma} - N'_{\mu\nu\rho\sigma}). \end{aligned} \right\} \quad (6.3)$$

On the other hand, we obtain directly

$$\frac{1}{2} \langle \Phi'_0 | [\hat{\mathfrak{D}}[\hat{H}, \hat{\mathfrak{D}}]] | \Phi'_0 \rangle = \sum_{\mu\nu\rho\sigma} (\mu|\hat{\mathfrak{D}}|\nu) (\rho|\hat{\mathfrak{D}}|\sigma) (N_{\mu\nu\rho\sigma} - N'_{\mu\nu\rho\sigma}). \quad (6.4)$$

Comparison of eq. (6.3) and eq. (6.4) proves the sum rule (6.2). An analogous rule is known⁽¹⁷⁾ for "1p-1h" excitations described by the conventional RPA.

Now we observe that in our theory all operators for electromagnetic transitions can be written as one-body boson operators of the form (6.1) by inserting (3.15) into eq. (3.17). Consequently, the usual energy-weighted sum rule for electromagnetic transitions holds in our approximation. This is in contrast to the mixing model^(5, 6) in which there is no guarantee that the sum rule might not be violated.

6.2 Transitions Within Rotational Bands

For simplicity we confine ourselves to the rotational band belonging to the excited 0^+ state discussed in sect. 5.5; in the following we work with the wave functions (5.64). Furthermore it is convenient to refer the mass quadrupole moment operator \mathring{Q}_{2M} (defined by eq. (5.3) with $L = 2$) to the body-fixed coordinate axes which are chosen to be the axes of the intrinsic quadrupole deformation of the excited 0^+ state. This is achieved in the usual way by writing

$$\mathring{Q}_{2M} = \sum_K D_{MK}^{I=2}(\theta_i) \mathring{Q}_{2K}, \quad (K = 0, \pm 2). \quad (6.5)$$

Now the $E2$ transition matrix element between an initial state $|I_i, M_i; \gamma_0 K_{\gamma_0} = 0\rangle$ and a final state $|I_f M_f; \gamma_0 K_{\gamma_0} = 0\rangle$ is given by

$$\left. \begin{aligned} & (I_f M_f; \gamma_0 K_{\gamma_0} = 0 | \mathfrak{M}(E2, M) | I_i M_i; \gamma_0 K_{\gamma_0} = 0) \\ & = \frac{1}{2} e (I_f M_f; \gamma_0 K_{\gamma_0} = 0 | \mathring{Q}_{2M} | I_i M_i; \gamma_0 K_{\gamma_0} = 0). \end{aligned} \right\} \quad (6.6)$$

Here we are considering only $T = 0$ states. With the aid of eqs. (6.5), (5.64) and (5.62), we then obtain the result

$$\left. \begin{aligned} & (I_f M_f; \gamma_0 K_{\gamma_0} = 0 | \mathfrak{M}(E2, M) | I_i M_i; \gamma_0 K_{\gamma_0} = 0) \\ & = \frac{1}{2} e \left[\frac{2I_i + 1}{2I_f + 1} \right]^{1/2} \langle I_i 2 M_i M | I_f M_f \rangle \langle I_i 2 0 0 | I_f 0 \rangle \cdot \beta, \end{aligned} \right\} \quad (6.7)$$

$$B(E2; I_i \rightarrow I_f) = \frac{1}{4} e^2 \langle I_i 2 0 0 | I_f 0 \rangle^2 \cdot \beta^2. \quad (6.8)$$

Eq. (6.8) shows the well-known dependence of the $E2$ transition probabilities within a band on the intrinsic deformation, β , defined by eq. (5.62) characteristic of this specific band.

6.3 E2 Transitions Connecting the Rotational Band with the Ground State

Here we consider the $E2$ transition from the 2^+ state in the rotational band belonging to the excited 0^+ state discussed in sect. 5.5 to the ground state. In this case, the $E2$ transition matrix element connecting the 2^+ state ($I_i = 2, M_i; \gamma_0 K_{\gamma_0} = 0$) and the ground state, $|0_1\rangle$, is given by

$$\left. \begin{aligned} & \langle 0_1, \mathfrak{M}(E2, M) | I_i = 2, M_i; \gamma_0 K_{\gamma_0} = 0 \rangle \\ & = \frac{1}{2} e \langle 22 M_i M | 00 \rangle \langle \Psi_0 | \hat{Q}_{2, K=0}^{\circ} | \Psi_{\gamma_0} \rangle \end{aligned} \right\} \quad (6.9)$$

and so we have

$$B(E2, 2_1^+ \rightarrow 0_1^+) = \frac{1}{20} e^2 |\langle \Psi_0 | \hat{Q}_{2K=0}^{\circ} | \Psi_{\gamma_0} \rangle|^2, \quad (6.10)$$

where $|\Psi_0\rangle$ and $|\Psi_{\gamma_0}\rangle$ are given in eq. (5.54) or eq. (5.40).

In evaluating $\langle \Psi_0 | \hat{Q}_{2, K=0}^{\circ} | \Psi_{\gamma_0} \rangle$ we first observe that $\langle \Psi_0 | \hat{Q}_{2, K=0}^{\circ(1)} | \Psi_{\gamma_0} \rangle = 0$. This result is obtained with the use of the definition (5.8) of $\hat{Q}_{2, K=0}^{\circ(1)}$ and by inserting eq. (5.52) into eq. (5.58). Then, using eq. (4.11) with respect to X_{γ}^+ , we have

$$\left. \begin{aligned} & \langle \Psi_0 | \hat{Q}_{2, K=0}^{\circ} | \Psi_{\gamma_0} \rangle = \langle \Psi_0 | \hat{Q}_{2, K=0}^{\circ(2)} | \Psi_{\gamma_0} \rangle \\ & = \sum_{\mu\nu} (\mu | Q_{20} | \nu) \{ \xi_{\gamma_0}(\mu\nu) - \eta_{\gamma_0}(\mu\nu) \}, \end{aligned} \right\} \quad (6.11)$$

where $\xi_{\gamma_0}(\mu\nu)$ and $\eta_{\gamma_0}(\mu\nu)$ are defined through eq. (5.40) and are written with the help of eq. (5.50) as

$$\left. \begin{aligned} \xi_{\gamma_0}(\mu\nu) &= \sum_{\lambda} \{ U_{\gamma_0}(\lambda) \xi_{\lambda}^{(0)}(\mu\nu) + V_{\gamma_0}(\lambda) \eta_{\lambda}^{(0)}(\mu\nu) \} \\ \eta_{\gamma_0}(\mu\nu) &= \sum_{\lambda} \{ U_{\gamma_0}(\lambda) \eta_{\lambda}^{(0)}(\mu\nu) + V_{\gamma_0}(\lambda) \xi_{\lambda}^{(0)}(\mu\nu) \}. \end{aligned} \right\} \quad (6.12)$$

With eq. (6.11), eq. (6.10) becomes

$$B(E2; 2_1^+ \rightarrow 0_1^+) = \frac{1}{20} e^2 \left[\sum_{\mu\nu} (\mu | Q_{20} | \nu) \{ \xi_{\gamma_0}(\mu\nu) - \eta_{\gamma_0}(\mu\nu) \} \right]^2. \quad (6.13)$$

It is interesting to observe that formally eq. (6.13) has precisely the same structure as the corresponding equation obtained by the conventional RPA for “1p-1h” problems. For the $E2$ transition from the “dressed 2p-2h” excited 2^+ state to the ground state, we will therefore expect the well-known enhancement associated with the structure of eq. (6.13). In particular we will have the usual relation: the stronger the field-producing force, the larger the $B(E2)$ value. Such an enhancement, caused by the collective ground-state correlations due to the field-producing force, is a direct and natural

consequence of the present theory. The enhancement is needed to explain the large measured transition rate in O^{16} namely $B(E2; 2_1^+ \rightarrow 0_1^+) = 5e^2 \text{fm}^4$. An interesting feature of the electromagnetic transitions is the importance of the interplay between the residual interaction and the field-producing force. It becomes most obvious if we neglect altogether the ground-state correlations due to the residual interaction. Then, from the definition (5.4) we have

$$(\mu | Q_{20} | \nu)_{TD} = 0 \quad \text{for} \quad s_\mu = 1, \quad s_\nu = -1,$$

and thus there are no E2 transitions from the 2^+ state to the ground state. But the residual interaction need not be strong either. Even a weak residual interaction may provide a sufficient basis for strong collective ground-state correlations (due to the field-producing force).

6.4 E0 Transitions from Excited 0^+ States to the Ground State

Throughout this subsection we are again considering the excited 0^+ state, $|0_2^+\rangle \equiv |I = 0, M = 0; \gamma_0 K_{\gamma_0} = 0\rangle$, discussed in sect. 5.5. The effective operator for the decay of the state $|0_2^+\rangle$ to the ground state $|0_1^+\rangle$ by electron-positron pair emission or internal conversion is given by

$$P_0 = e \sum_{\alpha\beta} \langle \alpha | \frac{1 + \tau_3}{2} r^2 | \beta \rangle : c_\alpha^+ c_\beta :. \quad (6.14)$$

With the help of the rule (3.14) and eq. (3.13), we can expand the operator in terms of pair scattering modes as

$$\mathring{P}_0 = \sum_{\mu\nu} (\mu | P_0 | \nu) : C_\mu^+ C_\nu : , \quad (6.15)$$

where

$$(\mu | P_0 | \nu) = 4e \sum_{\alpha\beta\gamma} \langle \alpha | \frac{1 + \tau_3}{2} r^2 | \beta \rangle s_\mu \Psi_\mu(\alpha\gamma) (1 - \theta_a - \theta_c) s_\nu \Psi_\nu(\beta\gamma). \quad (6.16)$$

Thus, in the same way as in the preceding subsection, we obtain the matrix element for pair emission as

$$(0_1^+ | P_0 | 0_2^+) = \sum_{\mu\nu} (\mu | P_0 | \nu) \{ \xi_{\gamma_0}(\mu\nu) - \eta_{\gamma_0}(\mu\nu) \}. \quad (6.17)$$

As in the preceding subsection, we may expect from the structure of eq. (6.17) an enhancement of the pair emission rate, possibly sufficient to account for the large experimental value in O^{16} , namely $(0_2^+ | P_0 | 0_1^+) \approx 0.4eR_0^2$

(R_0 = nuclear radius). Furthermore, the arguments given in the preceding subsection for the importance of the interplay between residual interactions and the field-producing force are equally applicable here. The influence of the intrinsic deformation of the state $|0_2^+\rangle$ on the pair emission rate becomes evident if we insert eq. (6.12) into eq. (6.17) and then trace the role of the functions U_{γ_0} and V_{γ_0} .

6.5 Hindrance of Double Gamma Decay of the First Excited 0^+ State

In discussions of the properties of the first excited 0^+ states in closed-shell nuclei, an instructive piece of data has often been neglected, namely the absence of observed $\gamma\gamma$ -decays of these states. Usually the first excited 0^+ state $|0_2^+\rangle \equiv |\Psi_{\lambda_0}\rangle$ decays to the ground state $|0_1^+\rangle \equiv |\Psi_0\rangle$ by the E0 transition discussed in the preceding subsection. However, the two-photon emission^(18, 19) may also contribute to the decay. In this case, the total energy $E_{\lambda_0} - E_0 \equiv \Omega_{i_0} = \hbar(\omega + \omega')$ is split up between two photons with energies $\hbar\omega$ and $\hbar\omega'$. The most probable decay mode will consist in the emission of two dipole quanta. Then the total transition probability is given by^(18, 19)

$$W_{\gamma\gamma} = \frac{2}{105\pi} \frac{1}{(\hbar c)^6} (E_{\lambda_0} - E_0)^7 \left(\frac{4\pi}{3}\right)^2 \times \left| \sum_n \frac{(0_1^+ | \mathfrak{M}(E1, 0) | n)(n | \mathfrak{M}(E1, 0) | 0_2^+)}{E_n - E_0} \right|^2 \quad (6.18)$$

where

$$\mathfrak{M}(E1, 0) = e \sum_{\alpha\beta} \langle \alpha | \frac{1+\tau_3}{2} r Y_{10}(\theta\varphi) | \beta \rangle : c_\alpha^+ c_\beta :$$

is the electric dipole operator. In the sum over the intermediate states $|n\rangle$ in eq. (6.18), the most important contribution will come from the giant dipole resonance, so that $E_n - E_{\lambda_0} \gg \hbar\omega$ or $\hbar\omega'$. This fact has been used to drop the terms $\hbar\omega$ and $\hbar\omega'$ in the energy denominator of eq. (6.18).

In trying to evaluate eq. (6.18) it is necessary to relate $W_{\gamma\gamma}$ to other independent observable quantities in an unambiguous way. This is best done by introducing⁽¹⁹⁾ a parameter η through the definition

$$\sum_n \frac{1}{E_n - E_0} (0_1^+ | \mathfrak{M}(E1, 0) | n)(n | \mathfrak{M}(E1, 0) | 0_2^+) \equiv \eta \sum_n \frac{1}{E_n - E_0} (0_1^+ | \mathfrak{M}(E1, 0) | n)(n | \mathfrak{M}(E1, 0) | 0_1^+). \quad (6.19)$$

The sum of the right-hand side is closely related to the (-2) -moment of the photonuclear absorption cross section⁽²⁰⁾

$$\left. \begin{aligned} \sigma_{-2} &\equiv \int \frac{\sigma(E)}{E^2} dE \\ &= \frac{16 \pi^3}{3 \hbar c} \sum_n \frac{1}{E_n - E_0} (0_1^+ | \mathfrak{M}(E1, 0) | n) (n | \mathfrak{M}(E1, 0) | 0_1^+) \end{aligned} \right\} \quad (6.20)$$

which is known to be a smooth function of the mass number A for most nuclei. The parameter η is a well-defined quantity and can be obtained from the experimental upper limits for $W_{\gamma\gamma}/W(E0)$, from $W(E0)$, and eqs. (6.18) to (6.20). The result of such an evaluation is presented in table I.

TABLE I. Hindrance of Double Gamma Decays

	E [MeV]	$W_{\text{exp}}(E0)^{\text{a}}$ [sec ⁻¹]	$W_{\gamma\gamma}/W_{\text{exp}}(E0)$	$\sigma_{-2}^{\text{used}^{\text{d}}}$ [$\mu\text{b}/\text{MeV}$]	$W_{\gamma\gamma}^{\text{(calc)}}$ [sec ⁻¹]	η^2
O ¹⁶	6.05	$1.4 \cdot 10^{10}$	$< 1.1 \cdot 10^{-4\text{b}}$	$7 A^{5/3}$	$5.8 \cdot 10^9 \eta^2$	$< 2.6 \cdot 10^{-4}$
Ca ⁴⁰	3.35	$2.9 \cdot 10^8$	$\leq 4 \cdot 10^{-4\text{c}}$	$(2.6 \pm 0.5) \cdot 10^3$	$1.2 \cdot 10^8 \eta^2$	$< 0.95 \cdot 10^{-4}$
Ge ⁷²	0.69	$3.4 \cdot 10^6$		$3.5 A^{5/3}$	$5.6 \cdot 10^4 \eta^2$	
Zr ⁹⁰	1.75	$1.1 \cdot 10^7$	$\leq 1.8 \cdot 10^{-4\text{c}}$	$3.5 A^{5/3}$	$8.1 \cdot 10^7 \eta^2$	$< 0.25 \cdot 10^{-4}$

a) see the first of refs. 19.

b) see ref. 23.

c) see ref. 24 and compare the still lower limit given in ref. 25.

d) for Ca⁴⁰, see ref. 26, for the other nuclei ref. 20.

Replacing in eq. (6.19) the main resonance region by a single representative state $|n_0\rangle$, the ‘‘dipole state’’, we may take* η as a measure for the ratio of matrix elements

$$|\eta| \approx \left| \frac{\langle 0_2^+ | \mathfrak{M}(E1, 0) | n_0 \rangle}{\langle 0_1^+ | \mathfrak{M}(E1, 0) | n_0 \rangle} \right|. \quad (6.21)$$

If the two states $|0_1^+\rangle$ and $|0_2^+\rangle$ were of a very similar structure then η should be of the order one. Table I shows, however, that in all measured cases η must be a very small quantity, indicating, quite systematically, that the first excited 0^+ states seem to have no appreciable coupling to the giant dipole resonance.

* This replacement is possible unless there are considerable cancellations in the left hand sum of eq. (6.19) due to fluctuations in the sign of $(n | \mathfrak{M}(E1, 0) | 0_2^+) / (n | \mathfrak{M}(E1, 0) | 0_1^+)$. It is known, however, that the giant dipole resonance behaves like a single coherent state, the dipole state, so that strong cancellations are not to be expected.

Similarly the coupling of the first excited O^+ state in O^{16} with other 1^- states which are normally described as "1p-1h" excitations seems also to be small ^(21, 22)

$$\left. \begin{aligned} B(E1; 1^-(7.12) \rightarrow 0_2^+)/B(E1, 1^-(7.12) \rightarrow 0_1^+) &< 10^{-2} \\ B(E1; 1^-(13.1) \rightarrow 0_2^+)/B(E1, 1^-(13.1) \rightarrow 0_1^+) &< 10^{-2}. \end{aligned} \right\} \quad (6.22)$$

Here, it should be noted that the first transition occurs only through isospin impurities. The limits are not as low as those for η ; on the other hand, the interpretation is unambiguous.

As has been realized long ago ⁽¹⁰⁾, it will be very difficult to explain the experimental limits (6.22) in a model ⁽⁵⁾ in which both $|0_1^+\rangle$ and $|0_2^+\rangle$ are described as a mixture of spherical and deformed states with roughly equal amplitudes. It may be even harder to account for the smallness of $|\eta|$ without simultaneously destroying the strong $E0$ and $E2$ transitions between the rotational band and the ground state of O^{16} . On the other hand, we wish to show that the present theory does not encounter such difficulties.

Suppose that the states $|n\rangle$ are well described as "1p-1h" states in the conventional RPA:

$$|n\rangle = D_n^+ |0_1^+\rangle \quad (6.23)$$

with the creation operators

$$D_n^+ = \sum_{\alpha\beta} (R_n(\alpha\beta) a_\alpha^+ b_\beta^+ + S_n(\alpha\beta) b_\beta a_\alpha). \quad (6.24)$$

Then, with the aid of the inverse relation to eq. (6.24),

$$a_\alpha^+ b_\beta^+ = \sum_n (R_n(\alpha\beta) D_n^+ - S_n(\alpha\beta) D_n), \quad (6.25)$$

the denominator of eq. (6.21) is written in the usual form

$$(0_1^+ | \mathfrak{M}(E1, 0) | n_0) = e \sum_{\alpha\beta} \langle \alpha | \frac{1 + \tau_3}{2} r Y_{10}(\theta\varphi) | \beta \rangle \{ R_n(\alpha\beta) - S_n(\alpha\beta) \}. \quad (6.26)$$

In the same approximation in which eq. (6.26) has been obtained, the numerator in eq. (6.21) becomes

$$\left. \begin{aligned} (0_2^+ | \mathfrak{M}(E1, 0) | n_0) &= e \sum_n \sum_{\alpha\beta} \langle \alpha | \frac{1 + \tau_3}{2} r Y_{10}(\theta\varphi) | \beta \rangle \{ R_n(\alpha\beta) - S_n(\alpha\beta) \} \\ &\quad \times (0_2^+ | \tilde{\mathfrak{S}}_{nn_0} | 0_1^+) \\ &\equiv \sum_n (0_1^+ | \mathfrak{M}(E1, 0) | n) (0_2^+ | \tilde{\mathfrak{S}}_{nn_0} | 0_1^+), \end{aligned} \right\} \quad (6.27)$$

where the operator $\tilde{\mathfrak{D}}_{nn_0}$ is defined by

$$\left. \begin{aligned} \tilde{\mathfrak{D}}_{nn_0} = & - \sum_{\alpha_1\beta_1} \sum_{\alpha_2\beta_2} R_n(\alpha_1\beta_1)R_{n_0}(\alpha_2\beta_2)a_{\alpha_1}^+a_{\alpha_2}^+b_{\beta_1}^+b_{\beta_2}^+ \\ & - \sum_{\alpha_1\beta_1} \sum_{\alpha_2\beta_2} S_n(\alpha_1\beta_1)S_{n_0}(\alpha_2\beta_2)a_{\alpha_1}a_{\alpha_2}b_{\beta_1}b_{\beta_2}. \end{aligned} \right\} \quad (6.28)$$

To get a rough estimate for the order of $|\eta|$, we assume that we can replace the sum over intermediate states by the ‘‘dipole state’’ $|n_0\rangle$. From eq. (6.26) and eq. (6.27) we get for the order of $|\eta|$ the result

$$O(|\eta|) \approx (0_2^+ | \tilde{\mathfrak{D}}_{n_0n_0} | 0_1^+). \quad (6.29)$$

Expanding the operator $\tilde{\mathfrak{D}}_{n_0n_0}$ in terms of the pair scattering modes with the aid of eqs. (3.15) and (4.11), we have

$$\left. \begin{aligned} O(|\eta|) & \approx |\langle \Psi_{\gamma_0} | \tilde{\mathfrak{D}}_{n_0n_0} | \Psi_0 \rangle| \\ & = \left| 4 \sum_{\alpha_1\alpha_2} \sum_{\beta_1\beta_2} (1 - \theta_{a_1} - \theta_{a_2})(1 - \theta_{b_1} - \theta_{b_2}) R_{n_0}(\alpha_1\beta_1) R_{n_0}(\alpha_2\beta_2) \right. \\ \times \sum_{\substack{\mu\nu \\ s_\mu = 1, s_\nu = -1}} & \left. [\xi_{\lambda_0}(\mu\nu) \Psi_\mu(\alpha_1\alpha_2) \Psi_\nu(\beta_1\beta_2) - \eta_{\lambda_0}(\mu\nu) \Psi_\mu(\beta_1\beta_2) \Psi_\nu(\alpha_1\alpha_2)] \right. \\ & + 4 \sum_{\alpha_1\alpha_2} \sum_{\beta_1\beta_2} (1 - \theta_{a_1} - \theta_{a_2})(1 - \theta_{b_1} - \theta_{b_2}) S_{n_0}(\alpha_1\beta_1) S_{n_0}(\alpha_2\beta_2) \\ \times \sum_{\substack{\mu\nu \\ s_\mu = 1, s_\nu = -1}} & \left. [\xi_{\lambda_0}(\mu\nu) \Psi_\mu(\beta_1\beta_2) \Psi_\nu(\alpha_1\alpha_2) - \eta_{\lambda_0}(\mu\nu) \Psi_\mu(\alpha_1\alpha_2) \Psi_\nu(\beta_2\beta_2)] \right|, \end{aligned} \right\} \quad (6.30)$$

in which the leading terms are

$$\left. \begin{aligned} & \left| 4 \sum_{\alpha_1\alpha_2} \sum_{\beta_1\beta_2} (1 - \theta_{a_1} - \theta_{a_2})(1 - \theta_{b_1} - \theta_{b_2}) R_{n_0}(\alpha_1\beta_1) R_{n_0}(\alpha_2\beta_2) \right. \\ & \quad \times \sum_{\substack{s_\mu = 1 \\ s_\nu = -1}} \xi_{\lambda_0}(\mu\nu) \Psi_\mu(\alpha_1\alpha_2) \Psi_\nu(\beta_1\beta_2) \left. \right| \end{aligned} \right\} \quad (6.31)$$

According to the present theory, the hindrance of the double gamma decay comes from the extreme smallness of the overlap in eq. (6.31) between the ‘‘1p-1h’’ correlation functions $R_{n_0}(\alpha_1\beta_1)$ and $R_{n_0}(\alpha_2\beta_2)$ for the giant resonance and the ‘‘2p-2h’’ correlation function, $\sum_{\mu\nu} \xi_{\lambda_0}(\mu\nu) \Psi_\mu(\alpha_1\alpha_2) \Psi_\nu(\beta_1\beta_2)$, for the first excited 0^+ state. One reason for this smallness is simply the angular momentum recoupling which is sufficient to explain the limits (6.22). In the case of the dipole resonance, we have an additional effect: The largest components of $R_{n_0}(\alpha\beta)$ for the giant resonance state come from the highest

particle levels α and the lowest hole levels β , while the largest components of $\sum_{\mu\nu} \xi_{\lambda_0}(\mu\nu) \Psi_{\mu}(\alpha_1\alpha_2) \Psi_{\nu}(\beta_1\beta_2)$ for the first excited 0^+ state come from the lowest particle levels α and the highest hole level β . A rough estimate with simplifying assumptions seems to be in agreement with the experimental limits on $|\eta|$.

7. Conclusions

In the last few years, the RPA describing “1p-1h” excitations has found a wide field of application, particularly in explaining collective phenomena in nuclei. Essentially, however, this approach is exhausted and its limitations are known. In the present work we have attempted to construct a systematic theory for “2p-2h” excitations. Clearly, this problem is next in simplicity after the “1p-1h” excitations, and yet it yields a wealth of new collective phenomena. In constructing the present theory some approximations are necessary, of course. One of the important approximations is the two-step method and the other is the neglect of interaction matrix elements involving an odd number of fermions or fermion pairs (i.e., HY and $\mathfrak{S}Y$, respectively). This shortcoming may partly be compensated by a proper choice of the effective interaction. Similarly as in the conventional RPA we also were forced to renounce the Pauli principle to some extent. As far as the Pauli principle is concerned, our NTD method is constructed in such a way that, in the limiting case of a pure 2p-2h system (without ground-state correlations), all our results are exact.

The starting point of our work was the problem of O^{16} and Ca^{40} . It was felt that existing theories and models were unsatisfactory and not entirely adequate to cope with the situation. The reason why the collective ground-state correlations introduced in our NTD method should become particularly important for closed shell nuclei is obvious: These ground-state correlations carry the decisive interplay between field-producing forces and the residual interaction. Even a weak residual interaction may provide a sufficient basis for strong collective ground-state correlations (due to the field-producing force).

In a pictorial language, the residual interactions are indispensable for softening the core, so that the strong field-producing forces are able to deform it. All these effects are included in the “collective predisposition” of the *spherical* ground state for *deformed* excited states.

Although in the present work our NTD method was primarily designed for closed-shell nuclei, a wide field of applications suggests itself. The next objects of interest will be nuclei which differ by two nucleons from closed-

shell nuclei, like O^{18} and Ca^{42} . Here, certain excited states will be described by a "2p-2h phonon", X_λ^+ , coupled to a correlated pair A_μ^+ . The presently neglected interaction ξY will become important for the coupling. Similarly it will be possible to describe certain excited states in nuclei like O^{17} and F^{17} by coupling a fermion to a "2p-2h phonon", where HY might be expected to play an important role. Since the excitation from a spherical ground state to a deformed excited state is definitely due to an anharmonic effect, we might also expect our NTD method to be useful in describing anharmonic effects in the second excited states ($J^\pi = 0^+, 2^+, 4^+$) in spherical even nuclei.

Before entering on such problems, we duly turn back our attention to the starting point O^{16} and Ca^{40} . It is true that we are not yet able to present any numbers: a quantitative discussion will be the subject of a later publication. But, fortunately, the measured properties of O^{16} and Ca^{40} are so striking that a natural *simultaneous* explanation of the various phenomena has a certain conclusive value even though it is only qualitative.

We believe that we easily can account for the strong collective lowering (with respect to the unperturbed positions) of first excited even parity states. It is due mainly to the deformation, but "triggered" by the residual interaction. Since the excited state with a definite intrinsic deformation contains the ground-state correlations properly, there is no difficulty in simultaneously understanding both the rotational band structure and the $E2$ transition to the ground state. In other words, although the ground state is *spherical* and the excited states are *deformed*, we may expect strong electromagnetic transitions between the rotational band and the ground state. This is borne out both by the validity of the energy weighted sum rule and the expression given explicitly for the transition probabilities. Formally, the expression has a very close resemblance to the corresponding expression for the strong collective transition probabilities described by the conventional RPA. Finally, the collective nature of the first excited 0^+ state in O^{16} and Ca^{40} makes it easy to understand the strong hindrance of the double gamma decays. Thus, we feel that, in principle, all the striking and not easily unifiable features of O^{16} and Ca^{40} can be well accommodated in our theory without depending on a very critical choice of some parameters.

It is sometimes argued that any theory which tries to describe the lowest excited even parity states in O^{16} as consisting mainly of 2p-2h excitations is doomed to fail from the outset. The arguments are usually based on the fact that Hartree-Fock calculations⁽³⁾ for O^{16} , with certain restrictions and confined to a space of *pure* 2p-2h or alternatively *pure* 4p-4h configurations, might give a lower energy for 4p-4h excitations*. From our point of

view, such arguments are not necessarily conclusive. In spite of the result of reference 3, we still tend towards the orthodox belief that the shell-model configuration with the lowest zero-order energy should be of some importance. Furthermore, we feel that taking into account the collective ground-state correlations might change the ordering of the "2p-2h" and "4p-4h" states. The reason is that only the 2p-2h states couple directly to the shell-model ground state (provided that only conventional two-body interactions are considered). Thus, it seems to us that the question of whether the "2p-2h" or the "4p-4h" configurations win the competition of being mainly responsible for the first excited 0^+ state in O^{16} cannot be decided before quantitative calculations in the framework of the present theory are performed.

Whatever the outcome may be, certainly there *will* be states to which our approach is applicable and there may be use for it in other problems.

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* For Ca^{40} the situation would be different from the situation in O^{16} . The uppermost occupied level is a $d_{3/2}$ level in Ca^{40} , but a $p_{1/2}$ level in O^{16} . Thus, the shell in Ca^{40} is not exhausted with four holes.

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