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STOPPING POWER OF ELECTRON GAS AND EQUIPARTITION RULE

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Synopsis

In a self-consistent perturbation treatment, the stopping power of matter for swift charged particles is conveniently expressed by means of the dielectric constant. In the present paper we have studied the results for degenerate, free electron gases, using an explicit expression for the dielectric constant, as derived previously. Approximate results for the stopping at low and high velocities are obtained. At low velocities the stopping is closely proportional to particle velocity, while at high velocities the corrections to the familiar logarithmic dependence on velocity are analogous to atomic shell corrections. The analytic results are compared with direct numerical computations, the results of which are presented in the form of tables and figures.

We prove, and make extensive use of, an equipartition rule, stating exact equality of the stopping contributions from, respectively, close collisions and distant resonance collisions. Possible applications of the results to stopping in other media are discussed.

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§ 1. Introduction

The stopping power of a free electron gas for swift heavy particles of low charge is of considerable interest to actual slowing-down problems. In point of fact, the free electron gas offers an interesting illustration of properties of atomic systems, and the effect of particle interaction on oscillator strength distribution. The free electron gas also elucidates the important question of deviations from the Bethe-Bloch stopping formula at moderate and low velocities.[1]

A basic approximation in the theory of slowing-down is to consider the effect of the particle as a perturbation, so that the energy loss is proportional to the square of the particle charge. In this case, the theory of slowing-down is simplified to a treatment of properties of the medium only, and a linear description of these properties may be applied. The linear properties of an infinite gas of free electrons can be described by the longitudinal and transverse dielectric constants $\varepsilon^l(k,\omega)$ and $\varepsilon^{tr}(k,\omega)$, which are complex functions of wave number and frequency, and which contain collective as well as individual particle aspects of the gas.

In the following non-relativistic problems we need only consider the longitudinal dielectric constant ε^l, which function gives the connection between the Fourier components of the total potential,

$$\Phi(\vec{r},\, t) = \sum_{k,\omega} \Phi(\vec{k},\omega)\, e^{i\vec{k}\cdot\vec{r} - i\omega t} ,$$

and those of the source charge density ϱ_0 through the relation

$$\varepsilon^l(k,\omega)\, k^2 \Phi(\vec{k},\omega) = 4\pi \varrho_0(\vec{k},\omega). \tag{1}$$

For a heavy particle of charge $Z_1 e$ and velocity $\vec{v}$, the source density is given by $\varrho_0(\vec{r},t) = Z_1 e\, \delta(\vec{r}-\vec{v}t)$, corresponding to rectilinear motion. Introducing this charge density in (1), we immediately obtain the retarding force acting on the particle, i. e. the specific energy loss. For a gas of density n electrons per unit volume it is convenient to write the resulting stopping formula in the form

$$\frac{dE}{dx} = \frac{4\pi Z_1^2 e^4}{mv^2} \cdot n \cdot L, \tag{2}$$

where m is the electron mass, and L the dimensionless quantity

$$L = \frac{i}{\pi \omega_0{}^2} \int_0^\infty \frac{dk}{k} \int_{-kv}^{kv} \omega \, d\omega \left(\frac{1}{\varepsilon^l(k,\omega)} - 1 \right). \tag{3}$$

We have here introduced the plasma frequency ω_0, given by

$$\omega_0{}^2 = \frac{4\pi ne^2}{m}.$$

It may be noted that in the retarded ε^l, as used here, the imaginary part is an odd function of ω, whereas the real part is even in ω. The bounds $|\omega| < kv$ in the integration over ω in (3) is simply due to conservation of total energy and momentum between the heavy particle and the system of electrons.

The formula (2) may be used for any atomic system if n is interpreted as the atomic number times the number of atoms per unit volume. The Bethe-Bloch formula, without relativistic corrections, is then given by (2) with

$$L = \log \frac{2mv^2}{I}, \tag{4}$$

where the average excitation potential I is a constant characteristic of the substance in question.

The present work was commenced as an attempt to get comparatively accurate estimates of stopping by an electron gas for various gas densities, and at any velocity of a heavy penetrating particle. Previous estimates have been more or less qualitative, and we thought it worth-while to make numerical calculations, based on a simple dielectric constant of the gas. In this connection we also utilized the analytic properties of the dielectric constant. Thus, we had recourse to the Bethe sum rule, at moderate and high particle velocities, and to asymptotic expansions at low and high velocities. However, prompted by intricacies of the numerical calculations along the plasma resonance curve, we found that quite other types of summation rules could be useful. In particular, we have applied an equipartition rule, stating equality of stopping contributions from plasma resonance excitation and close collisions with gas electrons. In the equipartition rule, summation is made at constant phase velocity, ω/k, of the emitted waves, corresponding to a definite direction of emission of energy.

By the above means, a comparatively accurate description is obtained

of the energy dissipation by charged particles in a degenerate electron gas. It appears to us that the results for free electron gases, in particular as regards deviations from the Bethe-Bloch formula (4), may be carried over to atoms. Thus, in the whole region of low particle velocities, where the so-called shell corrections have been used, the present corrections to stopping power may be summed over the electron density distribution of atoms. This seems justified already from the circumstance that the first terms in series developments of the correction in both distant and close collisions are the same for the electron gas as in the Bethe-Walske procedure.[4]

In § 2 we discuss main features of slowing-down, based on the simple dielectric constant. We make asymptotic expansions at low and high particle velocities, and utilize summation rules. We briefly mention the connection to slowing-down by atoms. The numerical computations are presented in § 3. In § 4 the equipartition rule is derived.

§ 2. Dielectric Constant and Basic Theoretical Treatment

The stopping of a particle as a function of its velocity may be computed from (3) by analytical or numerical means, if the dielectric constant is known. For a free electron gas, a quantum mechanical perturbation treatment leads to the following general formula for the dielectric constant to first order [2]

$$\varepsilon^l(k,\omega) = 1 + \frac{2m^2\omega_0^2}{\hbar^2 k^2} \sum_n \frac{f(E_n)}{N} \left\{ \frac{1}{k^2 + 2\vec{k}\cdot\vec{k}_n - \frac{2m}{\hbar}(\omega + i\delta)} + \right.$$
$$\left. + \frac{1}{k^2 - 2\vec{k}\cdot\vec{k}_n + \frac{2m}{\hbar}(\omega + i\delta)} \right\}. \qquad (5)$$

Here, E_n is the energy and $\vec{k}_n$ the wave vector of the electron in the n'th state. The distribution function $f(E_n)$ is an even function of $\vec{k}_n$, and normalized so that $N = \sum_n f(E_n)$ is the total number of electrons. In equation (5) we shall consider only the retarded dielectric constant of a system in its ground state, corresponding to a small positive value of δ.

In the case of a degenerate free electron gas with Fermi energy E_F the distribution function is $f(E_n) = 1$ for $E_n < E_F$, and $f(E_n) = 0$ for $E_n > E_F$. The Fermi energy is related to the density n of the gas by the familiar relation

$$E_F = \frac{1}{2} m v_F^2 = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}.$$

The summation in (5) may now be performed and the result is conveniently written in the form

$$\varepsilon^l(u,z) = 1 + \frac{\chi^2}{z^2}\{f_1(u,z) + i f_2(u,z)\}, \tag{6}$$

where

$$\left.\begin{aligned} f_1(u,z) = \frac{1}{2} + \frac{1}{8z}\{1-(z-u)^2\}\log\left|\frac{z-u+1}{z-u-1}\right| + \\ + \frac{1}{8z}\{1-(z+u)^2\}\log\left|\frac{z+u+1}{z+u-1}\right|, \end{aligned}\right\}$$

and

$$f_2(u,z) = \begin{cases} \dfrac{\pi}{2} u, & \text{for } z+u<1, \\ \dfrac{\pi}{8z}\{1-(z-u)^2\}, & \text{for } |z-u|<1<z+u, \\ 0, & \text{for } |z-u|>1. \end{cases} \tag{6'}$$

The variables k and ω are here replaced by dimensionless variables z and u, where

$$z = \frac{k}{2k_F} \quad \text{and} \quad u = \frac{\omega}{k v_F}.$$

Moreover, the parameter χ^2 in (6), defined by

$$\chi^2 = \frac{e^2}{\pi \hbar v_F}, \tag{7}$$

is proportional to $n^{-1/3}$. At the same time, χ^2 is a measure of the ratio between the potential energy of two neighbouring particles and their kinetic energy. This indicates that only for small values of χ^2 can the present free particle picture be used.

It should be noted that our present approximate dielectric constant is based on a first order perturbation procedure starting from free electrons, and with self-consistent fields. In higher order, account can be taken of the circumstance that the electrons are not free; corrections of this type are important mainly when $\chi^2 \gtrsim 1$, i.e. at low gas densities.

When one introduces the dielectric constant (6) of the free gas in (3), the factor L in the specific energy loss takes the form [2]

$$L = \frac{-6}{\pi\chi^2}\int_0^{v/v_F} u\,du \int_0^{\infty} z\,dz\ \mathrm{Im}\ \left(\frac{1}{\varepsilon^l} - 1\right)$$
$$= \frac{6}{\pi}\int_0^{v/v_F} u\,du \int_0^{\infty} dz\ \frac{z^3 f_2(u,z)}{\{z^2 + \chi^2 f_1(u,z)\}^2 + \{\chi^2 f_2(u,z)\}^2}. \tag{8}$$

It is seen from (6) that the integral (8) receives contributions from the domain $|u-z|<1$ where $f_2(u,z) \neq 0$, and also from a curve in the region $u>z+1$, for which $\varepsilon^l = 0$, i.e. $z^2+\chi^2 f_1(u,z) = 0$. In the latter case the double integral degenerates to a line integral. The former contribution

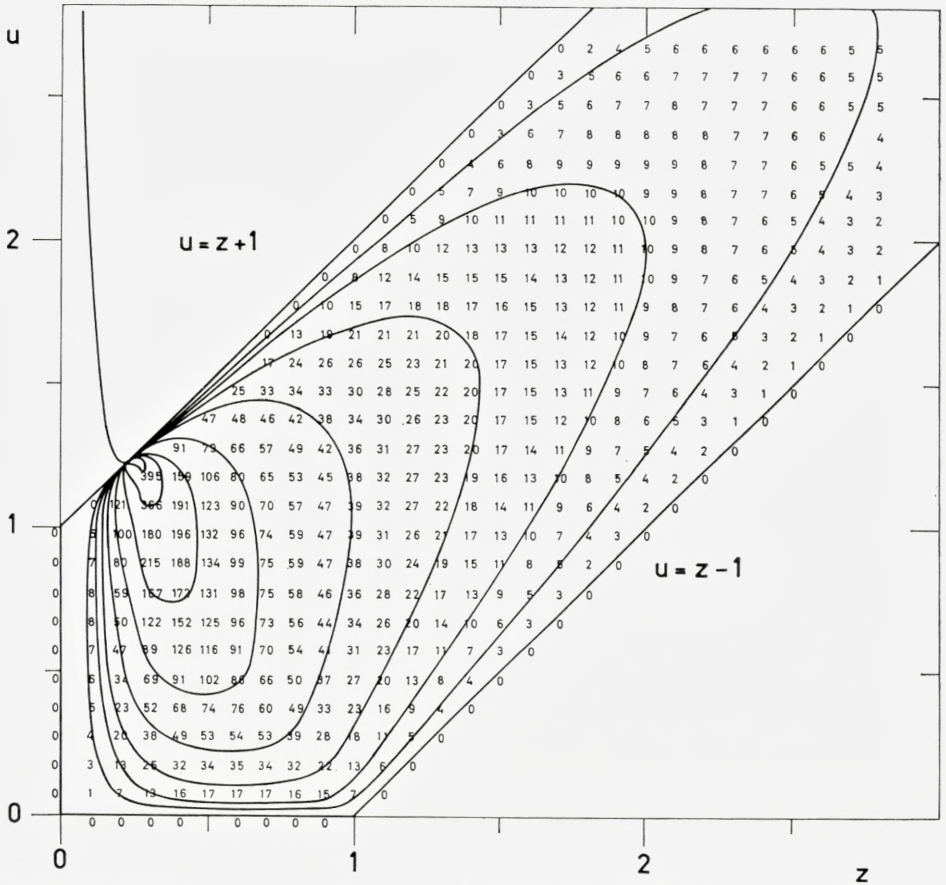

Fig. 1. The quantity $A = -z\ \mathrm{Im}\,(1/\varepsilon^l - 1)$ as a function of the parameters u and z for $\chi^2 = 0.1$. Numbers indicated on the figure give values of A times 10^4, at the points $u = 0,\ 0.1,\ 0.2,\ \ldots$ etc., and $z = 0,\ 0.1,\ 0.2,\ \ldots$ etc. Contour lines are drawn through points where $10^4 \cdot A$ equals respectively 5, 10, 20, 40, 80, 160 and 320. The position of the resonance curve is also indicated. At the point where it joins the domain $|u-z|<1$, it has the line $u = z+1$ as a tangent.

mainly corresponds to close collisions, while the latter arises from plasma resonance at distant collisions.

The behaviour of the integrand in (8) is illustrated in Fig. 1, for the case $\chi^2 = 0.1$. In particular, the figure indicates the magnitude of the absorption in the area between the two parallel lines $u = z+1$ and $u = z-1$. These lines correspond to absorption by electrons at the Fermi surface having, respectively, momentum parallel and antiparallel to the momentum transfer $\vec{k}$. Roughly, there is a maximum of absorption at $u = z$, but for low values of z the behaviour is more complicated. In the neighbourhood of $(z,u) = (0,1)$ the absorption tends quickly to zero, whereas a strong absorption is found as a continuation of the resonance curve. This curve has the line $u = z+1$ as a tangent, in the point $(u_0 - 1, u_0)$ where it joins the domain $|u-z| \leq 1$. For the purpose of an investigation of the behaviour of the resonance curve further apart from this domain, we perform a series expansion of $f_1(u,z)$ in (6′), assuming $|u-z|$ to be large compared to unity:

$$f_1(u,z) = \frac{1}{3(z^2-u^2)} + \frac{z^2+3u^2}{15(z^2-u^2)^3} + \cdots\cdots . \tag{9}$$

The position of the resonance curve is determined by the dispersion relation $\varepsilon^l = 0$, i.e. according to (9)

$$u^2 = \frac{\chi^2}{3z^2} + \frac{3}{5} + \cdots\cdots , \text{ or } \omega = \omega_0 + \frac{3}{10}\frac{{v_F}^2}{\omega_0}k^2 + \cdots\cdots . \tag{10}$$

In the limit of large u, the dispersion relation (10) approaches the hyperbola $u \cdot z = \chi/\sqrt{3}$, or $\omega = \omega_0$.

In § 3 we give the results of numerical evaluation of the double integral (8). Before that we shall discuss on an analytic basis the behaviour of L in the extremes of low and high velocities. In equation (8) the velocity v is measured in units of the Fermi velocity v_F. In the following, however, it turns out that, instead of v/v_F, the parameter

$$y = \frac{2mv^2}{\hbar\omega_0} = \frac{3^{1/2}}{\chi}\left(\frac{v}{v_F}\right)^2 \tag{11}$$

will be useful. The variable y measures the velocity in a unit $(\hbar\omega_0/2m)^{1/2}$, defined by the plasma frequency.

Low velocities.

For extremely low particle velocities we find directly from (8) and (6′) that L is approximately proportional to v^3, i.e.[2]

TABLE 1

The coefficients C_1 and $C_1 \cdot (\chi^2/3)^{3/4}$ as functions of the density parameter χ^2 in (7). These coefficients determine the asymptotic behaviour of L for low particle velocities.

χ^2	0.01	0.02154	0.04642	0.1	0.3163	1.0
C_1	1.823	1.463	1.108	0.787	0.387	0.134
$C_1 \cdot (\chi^2/3)^{3/4}$	0.0253	0.0361	0.0486	0.0614	0.0716	0.0587

$$L = C_1(\chi) \cdot \left(\frac{v}{v_F}\right)^3 = \left(\frac{\chi^2}{3}\right)^{3/4} C_1(\chi) y^{3/2}, \tag{12}$$

where

$$C_1(\chi) = \int_0^1 \frac{z^3 dz}{(z^2 + \chi^2 f_1(0,z))^2}. \tag{13}$$

The function $C_1(\chi)$ has been evaluated numerically for six values of χ^2, and the results are given in Table 1, together with $C_1 \cdot (\chi^2/3)^{3/4}$, which is the coefficient of $y^{3/2}$ in (12). It is seen from Table 1 that this coefficient is nearly independent of the density of the gas, varying by less than a factor of 3, when the density changes by a factor of 10^6. For comparison, it may be mentioned that $\chi^2 = 1$ corresponds to $n = 0.84 \cdot 10^{22}$ cm^{-3}.

We note that the function $C_1(\chi)$ can be approximated quite well by substituting for $f_1(0,z)$ the first two terms in a series expansion in powers of z^2, i.e.

$$f_1(0,z) \simeq 1 - \frac{1}{3} z^2. \tag{14}$$

It then follows from (13) that

$$C_1(\chi) \simeq \frac{1}{2\left(1 + \frac{\chi^2}{3}\right)^2} \left[\log \frac{1 + \frac{2}{3}\chi^2}{\chi^2} - \frac{1 - \frac{1}{3}\chi^2}{1 + \frac{2}{3}\chi^2} \right]. \tag{15}$$

The accuracy of this approximation is illustrated in Fig. 2. The coefficient of $y^{3/2}$ in (12) with $C_1(\chi)$ determined by (15) is here compared with the result of the numerical integration of (13).

The approximation used in (12)–(15) implies that L behaves as v^3, i.e. stopping is proportional to velocity. The velocity region in which this proportionality holds may be inferred from the numerical results in §3. It is seen from Fig. 5 that the approximation remains quite accurate even when v/v_F becomes as large as ~ 1.

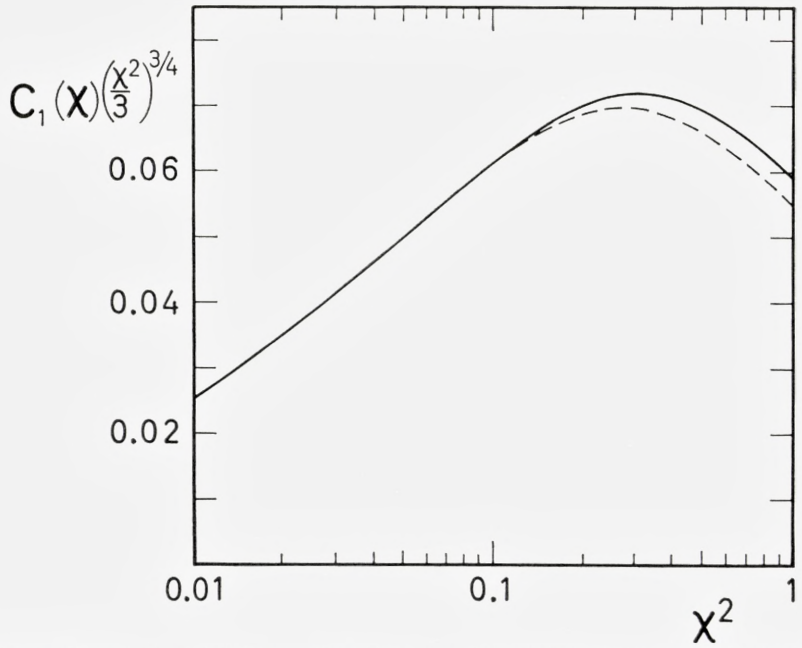

Fig. 2. The coefficient $C_1 \cdot (\chi^2/3)^{3/4}$ as a function of χ^2. The full-drawn curve was obtained from numerical integration of (13). For comparison the approximate formula (15) is also shown (dashed curve). The two curves join when $\chi^2 \sim 0.1$.

High velocities.

Consider next the case of large, but not relativistic, particle velocities. As mentioned in the introduction, in this limit the general formula (2) is reduced to the simple Bethe-Bloch formula (4) for any atomic system. In order to compute the average excitation potential I and stopping at large velocities, one usually has recourse to the Bethe sum rule for generalized oscillator strengths. For a free electron gas, the Bethe sum rule is[3]

$$\int_{-\infty}^{\infty} d\omega \frac{\omega}{i\pi\omega_0^2}\left(\frac{1}{\varepsilon^l(k,\omega)} - 1\right) = 1 . \tag{16}$$

A brief discussion of (16) is given in §4.

The sum rule (16) contains an unbounded integration over ω for fixed k. Now, for some values of k the integration over ω in (3) can in fact be extended to infinity if only ε has no imaginary part and no zeros outside the ω-interval $|\omega| < kv$. If this condition is fulfilled in the k-interval $k_{\min} < k < k_{\max}$, we find immediately from (16) that this k-interval gives the contribution $\log(k_{\max}/k_{\min})$ to L. It is qualitatively clear that for a heavy particle

of high velocity an upper limit, $\hbar k_{\max}$, is given by $2mv$, the maximum momentum transfer to a free electron at rest, while the lower limit, $k_{\min}$, is the adiabatic one, of order of ω_0/v. This simple consideration therefore leads to an estimate of L approximately given by (4) with $I \approx \hbar\omega_0$.

In order to obtain an accurate estimate of I, as well as correction terms to (4) at finite velocities, we may formulate the above consideration in the more convenient u, z-variables. The double integral has the bounds $0 < z < \infty$, $0 < u < v/v_F$. It is seen directly from Fig. 3 that, except for the three shaded

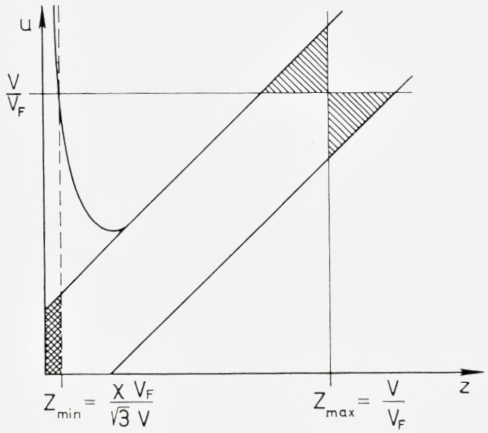

Fig. 3. Illustration of those regions in the u, z-plane, where $\mathrm{Im}\,(1/\varepsilon^l - 1)$ is non-vanishing. In the text is explained the meaning of the shaded areas, and of $z_{\max}$ and $z_{\min}$.

areas, the integral may instead be given the bounds $0 < u < \infty$ and $z_{\min} < z < z_{\max}$. Here, the upper limit is given by $z_{\max} = v/v_F$, while $z_{\min}$ is the value of z at the resonance curve (10) for $u = v/v_F$. For large velocities this leads to $z_{\min} \approx \chi v_F/(v\sqrt{3})$. It is easily shown that the corrections to L from the three shaded areas tend to zero in the limit of high velocities. Firstly, in the two hatched domains the contributions to the integrand (8) tend to zero, while the areas remain constant. Secondly, in the cross-hatched domain ($z < z_{\min} << 1$, $0 < u < z+1$), the integrand as well as the area tend to zero; in fact, the integral vanishes as constant $\cdot\, z^4{}_{\min}$. Applying the sum rule (16) we therefore obtain in the limit of large velocities the formula (4) with

$$I = \hbar\omega_0. \tag{17}$$

Having determined the asymptotic stopping formula, i.e. the constant I in (4), we may next consider deviations from it at lower velocities. The

deviations are analogous to the so-called shell corrections in the atomic case, as treated by BETHE, WALSKE[4], and others. The shell corrections to be added to (4) are normally denoted as $-C/Z$, Z being the atomic number of the medium. In the atomic case, as well as in the present case, several types of estimates of the corrections may be used. Thus, numerical evaluations may be attempted; this has proved rather difficult to carry through completely in the atomic case, whereas the results for an electron gas are easily obtained, cf. §3. Also, at high velocities a series expansion in powers of $1/v^2$ may be attempted. The series expansion is again comparatively simple for the electron gas.

We consider at first accurate formulae for the corrections to (4). As before, for large values of u we are concerned with stopping contributions from the two branches illustrated in Fig. 3, i.e. resonance absorption and close collisions. It would be comparatively easy to make separate computations for each of the two branches. It is simpler, however, to apply the equipartition rule, the use of which renders superfluous one of the two branch computations.

The equipartition rule (cf. §4) states that at particle velocities where resonance occurs, the change in L with velocity receives exactly equal contributions from the resonance curve and from the close collisions. The increase in L between two velocities v_1 and v_2 is thus twice the contribution from the resonance curve, i.e.

$$L(v_1) - L(v_2) = 2\int_{z_r(v_2/v_F)}^{z_r(v_1/v_F)} \frac{dz}{z} F_r(z), \tag{18}$$

where $F_r(z)$ is the oscillator strength of the resonance curve, as a function of z, and $z_r(u)$ denotes the value of z on the resonance curve as a function of the variable u, i.e. $z_r^2(u) = -\chi^2 f_1(u, z_r(u))$. By direct integration over the resonance curve, $F_r(z)$ is easily obtained,

$$F_r(z) = \frac{-6}{\pi\chi^2}\int u du\, z^2 \operatorname{Im}\left(\frac{1}{\varepsilon^l(u,z)} - 1\right) = \frac{6z^4}{\chi^4\left(\dfrac{\partial f_1(u,z)}{u\partial u}\right)_r}, \tag{18'}$$

where the integral over u is from below to above the resonance curve. The quantity $(\partial f_1(u,z)/u\partial u)_r$ is the partial derivative for constant z, taken at the resonance curve. The oscillator strength F_r remains close to unity in the upper part of the resonance curve. In fact, from (18′) we find by series expansion in powers of u^{-2},

$$F_r = 1 - \frac{12}{175u^4} + o\left(\frac{1}{u^6}, \frac{\chi^2}{u^4}\right),$$

where we note the absence of a term proportional to u^{-2}.

In order to obtain a series expansion of L we write (18) as

$$L(v_1) - L(v_2) = \frac{6}{\chi^2} \int_{v_2/v_F}^{v_1/v_F} \frac{z_r^2(u)\, u\, du}{1 + \frac{\chi^2}{2 z_r} \left(\frac{\partial f_1(u,z)}{\partial z} \right)_r}, \tag{19}$$

and neglecting terms of higher order in χ^2 we obtain

$$L(v_1) - L(v_2) = \left\{ u^3 \log \frac{u+1}{u-1} + \log (u^2 - 1) - 2u^2 + o\left(\frac{\chi^2}{u^4} \right) \right\} \Bigg|_{v_2/v_F}^{v_1/v_F}. \tag{19'}$$

Combining (19′) with (17), and taking only the first terms in a series expansion in v_F^2/v^2, the result is

$$\begin{aligned} L &= \log \frac{2mv^2}{\hbar\omega_0} - \frac{3 v_F^2}{5 v^2} - \frac{3 v_F^4}{14 v^4} - \cdots + o\left(\frac{\chi^2 v_F^4}{v^4} \right) = \\ &= \log y - \frac{3^{3/2}}{5\chi} \frac{1}{y} - \frac{9}{14 \chi^2 y^2} - \cdots . \end{aligned} \tag{20}$$

The formula (20) is applicable when v/v_F is above the minimum of the resonance curve. According to the equipartition rule, every term in (20) is contributed equally from the resonance curve and from close collisions, except for the additive constant obtained by integration over the region where u is below the minimum of the resonance curve.

It may be noted that the first correction term in (20) is the average kinetic energy, $\langle mv_i^2/2 \rangle = (3/10)\, m v_F^2$, of an electron in the gas, divided by $mv^2/2$*. This appearance of the average kinetic energy seems to be quite general for an atomic system. At least, FANO and TURNER [5] obtained this result for any atom in the case of resonance collisions, while WALSKE [4] obtained it for both resonance and close collisions in the hydrogen atom. Moreover, the equipartition rule is found to hold for the v^{-2} and v^{-4}-terms in expansions of shell corrections for atomic systems (cf. refs. 5 and 4).

The comparisons made here indicate a wide applicability of the notion of a free gas, in the case of atomic electrons. As we have seen, an average over free electron gases gives asymptotically the same v^{-2}-correction as a direct computation. The picture of the close collisions involving free electrons, with momentum distribution given by their local kinetic energies in the atom, seems appropriate and useful. Having such results in mind, it would seem profitable to estimate stopping in atomic systems on the basis of approximate results for electron gases. If a suitable approximation

* In a more comprehensive manner, and apart from a constant, we may write (20) as the average $\langle \log (v^2 - v_i^2) \rangle$.

is introduced for the electron gas, it may be averaged over the atom in order to obtain, e.g., the shell correction $-C/Z$, which quantity has been notoriously difficult to estimate in other ways. This approach is quite similar to that used previously [1] in a more crude approximation.

§ 3. Numerical Results

In the preceding chapter, the behaviour of the factor L in the specific energy loss was discussed on the basis of sum rules and series developments. In the present chapter we present the results of a direct numerical evaluation of L.

The double integral (8), which constitutes the basis for the numerical computation of L, cannot be evaluated by simple quadrature. When the functions f_1 and f_2 given by (6′) are introduced in the integrand, it is found that in the domain $u > z+1$ the integral degenerates into a line integral.

The integral is thus composed of two different parts. One is the line integral along the curve given implicitly by $\varepsilon^l(u,z) = 0$ in the region $u > z+1$. The other is the double integral over the region of close collisions, $|u-z|<1$, in which region $f_2(u,z)>0$. A direct numerical integration in the latter region is quite straightforward, except for a singularity appearing at the point $(u,z) = (u_0, u_0-1)$, where the resonance curve joins the region of close collisions. Similarly, it is particularly difficult to identify the resonance curve in the neighbourhood of this point.

For numerical evaluations it is important that the line integral along the resonance curve need not at all be performed, since, according to the equipartition rule, it is equal to the corresponding integral over close collisions. Moreover, computations of the double integral in the difficult region around $u = u_0$ may be avoided too. This is because the integral $L(v_1)$ at very high velocities is given accurately by the two first terms in formula (20). Therefore, a numerical calculation of the difference $L(v_1) - L(v_2)$, which is twice the contribution from the region $|z-u|<1$, can give us $L(v_2)$ for all $v_2 > v_F \cdot u_0$.

Numerical computations along these lines were performed by Dr. Peter Naur on the electronic computer DASK. The main results are shown in Table 2. The quantity L is here given as a function of the variable y defined in (11), and for six values of χ^2, as in Table 1.

In the numerical treatment we actually did make computations which are unnecessary according to the above. We evaluated the line integral along the resonance curve, and because of the above-mentioned difficult-

ies near the point $(u_0, u_0 - 1)$, we were led to a closer scrutiny of the integral, which suggested the validity of an equipartition rule. The equipartition rule is thus confirmed by the numerical calculations, as far as they go.

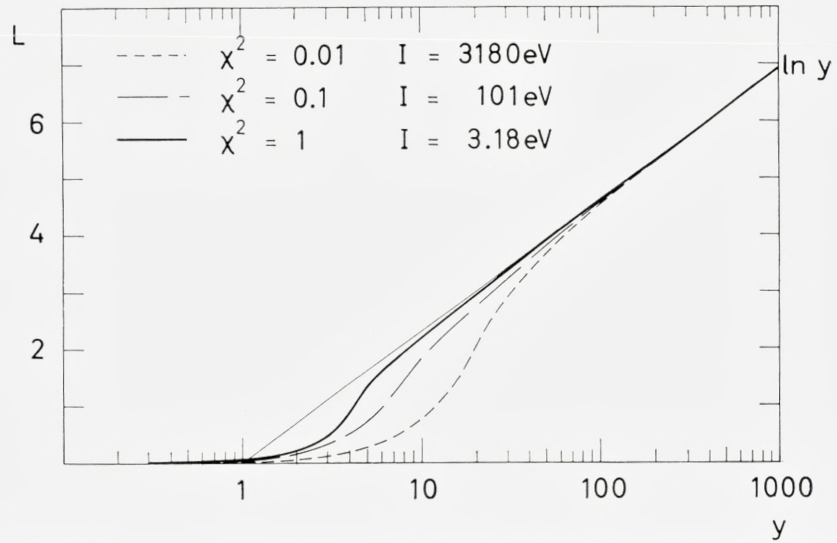

Fig. 4. The factor L as a function of the velocity parameter y from (11), for three gas densities, $\chi^2 = 1$, 0.1 and 0.01, i. e., $I = \hbar\omega_0 = 3.18$, 101 and 3180 eV, respectively. Straight line indicates asymptotic behaviour, $L = \log y$.

The numerical results for $L(y)$ contained in Table 2 are illustrated on the Figs. 4 and 5. In Fig. 4 the results are shown for $\chi^2 = 1$, 0.1 and 0.01, the abscissa y being given in a logarithmic scale. These three values of χ^2 correspond to gas densities $n = 0.84 \cdot 10^{22}$, $0.84 \cdot 10^{25}$ and $0.84 \cdot 10^{28}$ cm^{-3}, or to average excitation potentials $I = \hbar\omega_0 = 3.18$, 101 and 3180 eV, respectively. It is seen that the curves approach the straight line $\log y$, which is the asymptotic limit for large values of y.

A more detailed comparison with asymptotic formulas is shown in Fig. 5, where the full-drawn curves show $L(y)$ as a function of y for $\chi^2 = 0.1$ and 0.01. The dashed curves which join the $L(y)$ curves for small values of y represent formula (12), with the coefficient C_1 taken from Table 1. For large values of y the $L(y)$ curves approach another set of dashed curves. These curves represent the two first terms in the expansion (20), i.e. correction terms of order v^{-2} to the limiting expression, $\log y$, also indicated on the figure. It is noted that the v^{-2} term gives a substantial improvement over the simple expression (4) for low gas densities, and that the two for-

TABLE 2

The factor L in the specific energy loss computed numerically as a function of the particle velocity for six values of the density parameter in (7), $\chi^2 = 1$, $10^{-1/2}$, 10^{-1}, $10^{-4/3}$, $10^{-5/3}$ and 10^{-2}. L is given as a function of the parameter y, defined in (11).

y	log y	$\chi^2 = 0.01$		$\chi^2 = 0.02154$		$\chi^2 = 0.046416$	
		v/v_F	$L\,(y)$	v/v_F	$L\,(y)$	v/v_F	$L\,(y)$
0.10000	–	0.07598	0.0007995	0.09206	0.001145	0.1115	0.001540
0.31623	–	0.13512	0.004491	0.1637	0.006398	0.1983	0.008642
1.0000	0	0.2403	0.02522	0.2909	0.03575	0.3527	0.04839
1.7783	0.5757	0.3204	0.05963	0.3882	0.08459	0.4703	0.1141
3.1623	1.1513	0.4273	0.1407	0.5177	0.1990	0.6272	0.2675
5.6235	1.7269	0.5698	0.3306	0.6903	0.4647	0.8363	0.6220
10.000	2.3026	0.7598	0.7772	0.9206	1.067	1.115	1.420
14.678	2.6864	0.9205	1.341	1.115	1.833	1.351	2.247
21.544	3.0701	1.115	2.280	1.351	2.641	1.637	2.804
31.623	3.4539	1.351	3.029	1.637	3.191	1.983	3.285
56.235	4.0295	1.802	3.820	2.183	3.893	2.645	3.939
100.00	4.6052	2.403	4.496	2.909	4.530	3.527	4.555
316.23	5.7565	4.273	5.724	5.177	5.734	6.272	5.741
1000.0	6.9078	7.598	6.898	9.206	6.901	11.15	6.903

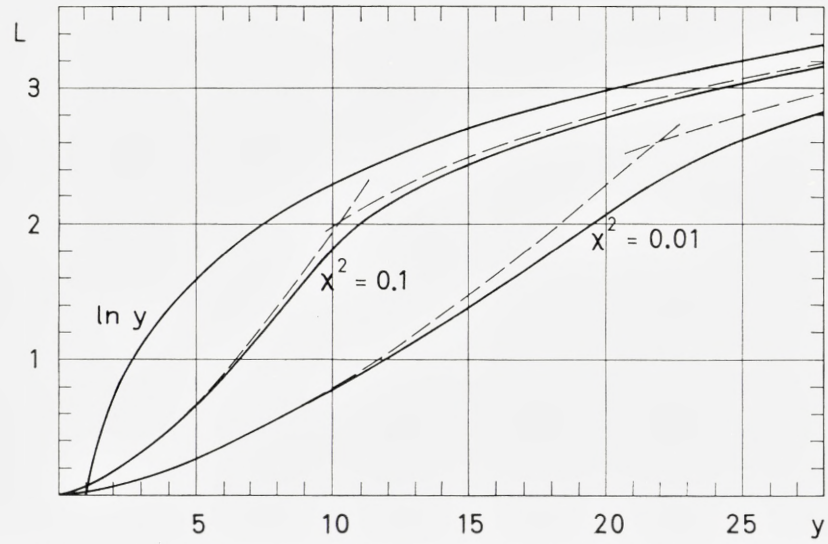

Fig. 5. The factor L as a function of the velocity parameter y from (11), for $y < 25$ and for two gas densities, $\chi^2 = 0.1$ and 0.01. Dashed curves indicate asymptotic formulas (12) and $L = \log y - 3^{3/2}\,(5\,\chi\,y)^{-1}$, valid for small and large y, respectively. The function $\log y$ is also indicated.

TABLE 2 (cont'd)

For large y, L approaches the asymptotic formula $L = \log y$, shown in the second column. For each value of χ^2 the velocity is also given in units of the Fermi velocity v_F.

y	$\log y$	$\chi^2 = 0.1$		$\chi^2 = 0.31623$		$\chi^2 = 1$	
		v/v_F	$L(y)$	v/v_F	$L(y)$	v/v_F	$L(y)$
0.10000	–	0.1351	0.001941	0.1802	0.002282	0.2403	0.001971
0.31623	–	0.2403	0.01091	0.3204	0.01299	0.4273	0.01182
1.0000	0	0.4273	0.06119	0.5698	0.07451	0.7598	0.0743
1.7783	0.5757	0.5698	0.1443	0.7598	0.1791	1.013	0.191
3.1623	1.1513	0.7598	0.3386	1.013	0.4323	1.351	0.502
5.6235	1.7269	1.013	0.7879	1.351	1.078	1.802	1.448
10.000	2.3026	1.351	1.838	1.802	2.074	2.403	2.177
14.678	2.6864	1.637	2.414	2.183	2.542	2.911	2.604
21.544	3.0701	1.983	2.898	2.645	2.976	3.527	3.016
31.623	3.4539	2.403	3.342	3.204	3.392	4.273	3.418
56.235	4.0295	3.204	3.968	4.273	3.996	5.698	4.009
100.00	4.6052	4.273	4.572	5.698	4.586	7.598	4.595
316.23	5.7565	7.598	5.746	10.13	5.751	13.51	5.753
1000.0	6.9078	13.51	6.904	18.02	6.906	24.03	6.907

mulas (12) and (20) taken together essentially reproduce $L(y)$ for $\chi^2 \gtrsim 0.1$. For large densities, higher order terms in (20) are important. They can be of the same order of magnitude as the v^{-2} terms, and they have the same sign.

§ 4. Summation Rules

In this section are treated various properties of integrals over generalized oscillator strengths. These integral properties we call summation rules. In the preceding sections two such rules were used repeatedly, viz. the familiar Bethe sum rule and the equipartition rule. The Bethe sum rule has been previously discussed by several authors.[3] Still, we shall give a derivation of it in the present case, in order to check the properties of the dielectric constant given by (5), and also as an introductory to the equipartition rule, where we utilize the analytic properties of the dielectric constant as a function of momentum, k, and phase velocity, ω/k.

The Bethe sum rule.

In the dielectric formulation, the field equations and the absorption are contained in the dielectric constant. The Bethe sum rule concerns an inte-

gration over ω of $1/\varepsilon^l$, for fixed k. In the integration we have to do with retarded solutions of the equations of motion. This is equivalent to the requirement that an external disturbance of the system, represented by e.g. $\varrho_0(\vec{r},t) = f(\vec{r})\delta(t-t_0)$, never gives rise to a field different from zero prior to the disturbance, i.e. for $t < t_0$. When integrating $1/\varepsilon^l$ over the frequency ω in order to find physical effects, this requirement fixes the path of integration in the complex ω-plane to be above all poles of $1/\varepsilon^l$.

Returning to the Bethe sum rule (16), and using the just mentioned path of integration, we are entitled to change the contour to a large semi-circle, $|\omega| = \text{const.}$, in the upper half of the complex ω-plane, since there are no poles above the original path of integration. However, in the region of large ω and for fixed k, ε^l must always behave as

$$\varepsilon^l(k,\omega) \to 1 - \frac{{\omega_0}^2}{\omega^2}, \quad \text{for } |\omega| \to \infty. \tag{21}$$

We apply (21) to the integration over the semi-circle and obtain (16).

The sum rule is thus directly a consequence of the demand of retardation. In the present description of an electron gas in the ground state, the requirement of retardation is expressed in (5) by the replacement of ω by $\omega + i\delta$, leading to a retarded dielectric constant $\varepsilon^l(k,\omega)$, which is a complex function of k and ω. In this description the path of integration is on the real ω-axis. The path is in fact above all poles of $1/\varepsilon^l$, as can be shown explicitly from (5). In order to prove it, we may note that ε^l in (5) is a real and even function of ω', where $\omega' = \omega + i\delta$. This function has $2N$ zeros, which all lie on the real ω'-axis. For $k > 2k_F$ (or $z > 1$) this is easily seen from the fact that ε^l has $2N$ poles on the real ω'-axis. In between these poles are trapped $2N-2$ zeros of ε^l, and outside the poles are two more zeros, since ε^l has to increase from a negative value to $+1$. The two latter zeros ultimately become the plasma resonance, at low values of k. In order to show that all $2N$ zeros lie on the real ω'-axis also for $k < 2k_F$, one must further take into account that the gas is in its ground state, $f(E_n)$ being the distribution function of a degenerate Fermi gas.

The equipartition rule.

While the Bethe sum rule concerns the integral of $1/\varepsilon^l$ over ω or u for fixed k or z, the equipartition rule has to do with the integral of $1/\varepsilon^l$ over z for fixed u. The rule states that an integral – proportional to that in (8) –

$$\mathfrak{J} = \operatorname{Im} \int_0^\infty 2z\,dz \left(\frac{1}{\varepsilon^l(u,z)} - 1 \right) = \mathfrak{J}_r + \mathfrak{J}_c \tag{22}$$

receives equal contributions, $\mathfrak{J}_r$ and $\mathfrak{J}_c$, respectively, from the plasma resonance and from the region of close collisions, $u-1<z<u+1$ (cf. Fig. 3). In order to prove this, it is important to find the poles of $1/\varepsilon^l$, i.e. the zeros of ε^l, as a function of z for fixed u. It is seen from (5) that whereas ε^l has N zeros as a function of ω'^2 (or $u'^2=\omega'^2/k^2v_F^2$) for fixed z, there must be $N+1$ zeros of ε^l as a function of $x=z^2$ for fixed u'. For a large real value of u', above the value which corresponds to the minimum in the plasma resonance in Fig. 3, all $N+1$ zeros lie on the real x-axis. One zero occurs at a low x-value, and is determined by the intersection with the plasma resonance curve. The remaining N zeros are grouped together in the interval $(u'-1)^2 \lessapprox x<(u'+1)^2$, and may be identified with the N zeros of ε^l as a function of u'^2 for fixed z and $u'>1-z$.

We note that in the retarded dielectric constant used in (22), u' has a small positive imaginary part. Suppose now that ω is positive. It is seen directly from (5) that a small positive imaginary part $i\delta$ added to ω, or to u, is equivalent to a displacement of the zeros of $\varepsilon^l(u,x^{1/2})$ in the complex x-plane in such a way that the zero at plasma resonance lies below the real x-axis, while the zeros in the region $(u-1)^2<x<(u+1)^2$ lie above this axis. The opposite sense of displacement in these two cases appears because the slope du/dz is negative at the plasma curve, but positive at the other zero curves in the u,z-plane, cf. Fig. 3. The integral (22) may thus alternatively be written

$$\mathfrak{J}=-\frac{i}{2}\int_C dx\left(\frac{1}{\varepsilon^l(u',x^{1/2})}-1\right). \tag{23}$$

Here, ε^l is a real function of u' and x, and the path of integration C is indicated on Fig. 6.

In order to complete the proof of the equipartition rule, we merely note that, if we revert the sign of the plasma resonance contribution, $\mathfrak{J}_r$, in (22), we obtain the path of integration C' (cf. Fig. 6), which may be deformed into a large circle, $|x|=$ const., in the complex x-plane. However, for large values of $|x|$ (or $|k|$), the dielectric constant must behave as

$$\varepsilon^l\to 1+\frac{\chi^2}{3x^2},\quad \text{for } |x|\to\infty, \tag{24}$$

according to (5). Since the integral of $1/(1+\chi^2/3x^2)-1$ along a large circle tends to zero, we observe that a change of sign of $\mathfrak{J}_r$ in (23) makes the integral vanish, i.e. $\mathfrak{J}_r=\mathfrak{J}_c$. This is the equipartition rule. It is based on the circumstances that the integral around the plasma resonance in the x-plane is in the opposite sense of the integration around the remaining

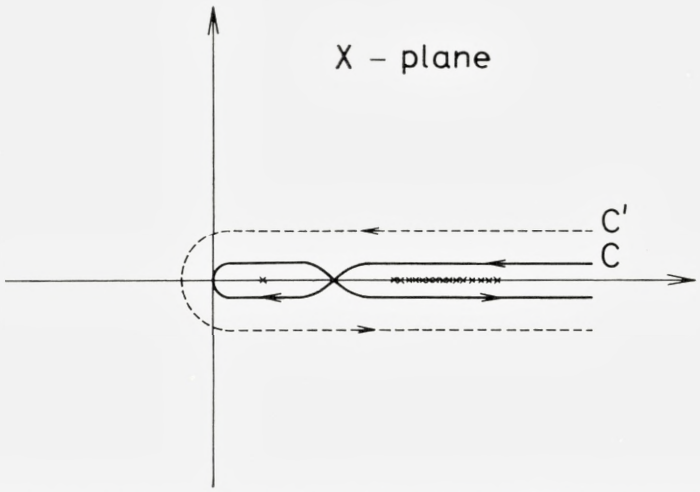

Fig. 6. Illustration of contours C and C', in complex x-plane. Isolated cross on real x-axis indicates plasma pole; group of crosses indicates poles in close collisions. For further explanation cf. text.

resonances, and that the integral of $(1/\varepsilon^l - 1)$ vanishes at large x. Moreover, it can only be used for u-values ($u \gtrsim u_0$, cf. Fig. 3) where plasma resonance occurs. For lower values of u, the plasma resonance splits up in two poles in the complex x-plane.

The contents of the equipartition rule may be stated in a more pictorial way. Thus, a constant value of u implies a constant phase velocity, $v_{ph} = \omega/k = u \cdot v_F$, of the emitted waves. When the creation of waves is due to a heavy particle travelling with constant velocity v, all waves emitted with the phase velocity v_{ph} will have an angle ϑ with the particle motion where $\cos \vartheta = v_{ph}/v$. In this direction two kinds of waves travel, i.e. plasma resonance waves and essentially single electron waves, and according to the equipartition rule the two waves moving in the direction ϑ carry an equal amount of energy. It may be interesting to compare the group velocities of the two wave types. The electron waves have approximately the connection $\omega = \hbar k^2/2m$ between k and ω, if v_{ph} is large compared to v_F. Accordingly, they have a group velocity $v_{gr}^{el} \simeq 2 v_{ph}$, i.e. larger than the phase velocity. The plasma waves, on the other hand, have a rather well-defined group velocity, v_{gr}^{pl}, which according to the dispersion relation (10) is given by

$$v_{gr}^{pl} \simeq \frac{3}{5} v_F^2 / v_{ph} = \langle v_i^2 \rangle / v_{ph} ,$$

and thus much less than v_{ph}, since $v_{ph} > v_F$.

We shall not treat the equipartition rule for an atomic system in general. However, it may be noted that the asymptotic relation (24) always holds in the non-relativistic case, which implies that the sum of residues in the complex k^2-plane is zero. Therefore, if residues are vanishing except on the real, positive k^2-axis, the contributions to energy loss at constant phase velocity, ω/k, may be divided in two parts with equal contribution to energy loss, so that an equipartition rule holds. The two parts are analogous to, respectively, the plasma resonance and the close collisions in Fig. 6; they have the same sequence on the k^2-axis, and the path of integration should be as in Fig. 6.

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