Kinetic theory of particle stopping in a medium with internal motion

Peter Sigmund
*Fysisk Institut, Odense Universitet, DK-5230 Odense M, Denmark**
and IBM Research, Yorktown Heights, New York, 10598
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Expressions have been derived that relate the stopping power and energy-loss straggling in a medium with internal motion for penetrating charged particles to the corresponding quantities applying to the equivalent medium at rest. These expressions have been based on a general binary-encounter picture and apply to nonrelativistic velocities and arbitrary mass ratios. Convenient expansions have been found in the limits of very high and very low projectile velocity. The results are applied to both nuclear and electronic stopping of charged particles. The capability of the scheme is tested upon the degenerate free-electron gas, for which accurate expansions at high and low projectile speed are known, with regard to both stopping and straggling. The scheme allows evaluation of shell corrections to stopping power and straggling of atomic and molecular gases beyond the range of validity of the leading terms in an expansion in inverse powers of electron velocity. A seeming disparity between high-speed straggling parameters calculated for the Fermi gas on the one hand, and an atomic target on the other hand, is attributed to different ground-state properties of the two systems in zero order. An essential difference is pointed out between the predictions of the dielectric theory and the present scheme with regard to the velocity dependence of energy-loss straggling in the low-speed limit.

I. INTRODUCTION

This work deals with the stopping of fast particles such as protons, alpha particles, and heavy ions or atoms in matter. The particular problem addressed is the effect of internal motion in the penetrated medium on the statistics of the stopping process, especially on the magnitude of stopping power and straggling.

Elementary stopping theory (cf. Ref. 1, Chaps. 1−3) deals with the slowing down of a projectile moving faster than all the constituents (atoms, molecules, electrons) of the penetrated medium. In that case, it is a valid starting point to disregard the initial motion of the target particles in the analysis of the stopping process. This applies to the classical theory of electronic and nuclear stopping[1,2] and, with some modification, to the simplest form of the quantum theory of electronic stopping of swift charged particles (Ref. 3 and Sec. 2 of Ref. 4).

We note that if the stopping medium is in thermal equilibrium, a particle slows down until its *kinetic energy* has approached the equilibrium value. This means that if the projectile is heavier than at least part of the constituents of the stopping medium, slowing down may go on at projectile *velocities* well below thermal or zero-point velocities of the target particles. Therefore the neglect of the internal motion of target particles is a severe limitation of elementary stopping theory.

This is particularly important for electronic stopping of ions. Shell corrections to the simple Bethe formula (Refs. 5 and 6 and Sec. 4 of Ref. 4) are known to be significant at all but the highest heavy-particle velocities, in particular for heavy target atoms where inner-shell electron velocities approach the velocity of light. For low-velocity ions, the stopping power is known to show a quite different behavior[7] from that predicted in the high-velocity approximation. For the same reason, the stopping power of a high-temperature plasma becomes temperature dependent.[8]

Internal motion of the stopping medium may also be important for nuclear stopping; this is obvious in case of heavy ions slowing down in light target materials, but must be true more generally at velocities not too far above equilibrium velocities. Note that, due to generation of high-density atomic collision cascades (spikes), heavy ions slowing down in solids may move through regions of particularly high *local* temperature ($kT \lesssim 10$ eV).[9] While thermalization problems have been treated extensively in case of neutrons[10] and electrons,[11] the problem seems to have received little attention with regard to atomic particles, except for small deviations from thermal equilibrium, i.e., in the regime of kinetic theory.[12]

The main purpose of the present paper is to explore the possibility of extending the range of validity of elementary stopping theory to lower velocities by incorporating features of kinetic theory. In the regime of kinetic theory, collisions take place, in general, between *moving* collision partners; the collision dynamics is described in the proper frame of reference, usually the center-of-mass frame. This increase in complexity, as compared with the case of collisions where one partner is initially at rest, may be compensated by the lack of significance of external forces.

There are at least two model systems that have been studied extensively with a similar purpose in mind. One is the stopping of a point charge in a free-electron gas[13,14]; this forms the basis of the dielectric theory of stopping. In view of a considerable amount of rigor in that treatment, its results have served as a very useful tool in electronic stopping of atomic systems[15,16] (for a summary cf. Ref. 17). The other model system, often called the binary-encounter approximation,[18–20] deals with binary collisions between moving *point charges.* There are well-known difficulties inherent in such a model; in addition, it appears that its potential is difficult to assess on the basis of existing treatments[21,22] because of other model assumptions entering simultaneously.

In elementary stopping theory, it is usually sufficient to keep within one or two frames of reference, the laboratory system and, possibly, the center-of-mass system. In case of a moving target, it is convenient to consider four frames of reference, called C_L, C_0, C_M, and C_S, respectively:

(i) C_L is the laboratory frame in which stopping parameters are measured.

(ii) C_0 is a system in which an individual *target particle* is at rest; expressions for stopping parameters from elementary stopping theory apply to this frame.

(iii) C_M is a system in which the *projectile* is momentarily at rest; the frequency of individual collision events is conveniently determined in this frame.

(iv) C_S is the center-of-mass frame in an individual binary collision event; the dynamics of binary elastic collisions is treated readily in this frame

The aim is to derive expressions for stopping parameters in the C_L frame, involving stopping parameters in the C_0 frame and only one additional characteristic of the target material, the velocity spectrum of the target particles. Neither the type of particle nor their mutual interaction are specified in the general treatment.

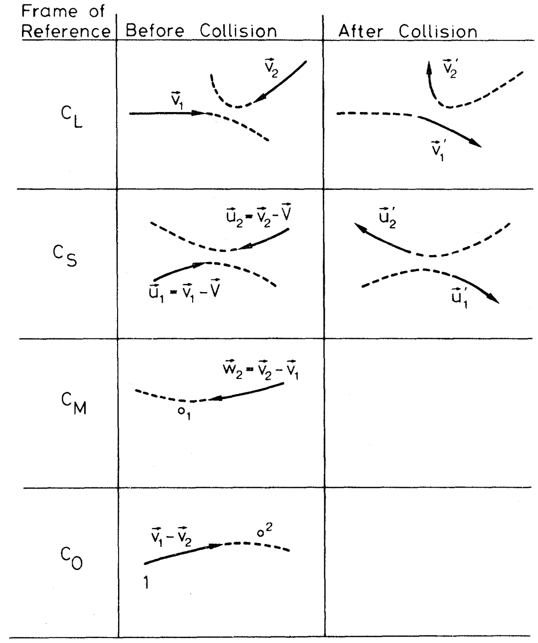

FIG. 1. Illustration of frames of reference used. C_L is the laboratory frame, projectile velocity $\vec{v}_1$ and $\vec{v}_1'$ before and after collision, respectively, $\vec{v}_2$ and $\vec{v}_2'$ corresponding target velocities. C_s is the center-of-mass frame, projectile velocity $\vec{u}_1$ and $\vec{u}_1'$ before and after collision, $\vec{u}_2$ and $\vec{u}_2'$ corresponding target velocities. $\vec{V}$ is the center-of-mass velocity. C_M is the frame of reference moving with $\vec{v}_1$. C_0 is the frame of reference moving with $\vec{v}_2$.

II. GENERAL

A. Differential cross section

Consider a random, infinite stopping medium composed of only one type of particle with mass m_2 and a velocity spectrum $f(\vec{v}_2)$ such that

$$\int d^3v_2 f(\vec{v}_2)=1 \;, \tag{1}$$

and a uniform density of n target particles per unit volume. Consider a projectile with mass m_1 moving with velocity $\vec{v}_1$, and let it interact with the target particles via *binary collisions.* Let the (nonrelativistic) velocities in the laboratory frame C_L after a specific collision be $\vec{v}_1'$ and $\vec{v}_2'$, respectively (Fig. 1).

In the center-of-mass frame C_S, a target particle has the velocities (Fig. 1)

$$\vec{u}_2=\vec{v}_2-\vec{V} \;, \tag{2a}$$

$$\vec{u}_2'=\vec{v}_2'-\vec{V} \tag{2b}$$

before and after a collision, respectively, where

$$\vec{V}=(m_1\vec{v}_1+m_2\vec{v}_2)/(m_1+m_2) \;. \tag{3}$$

Let us assume that the collision is elastic in C_S, i.e.,

$$u_2'^2 = u_2^2 \ . \tag{4}$$

Then the energy loss T of the projectile in the laboratory frame C_L is[19]

$$T = \frac{m_2}{2}(v_2'^2 - v_2^2) = m_2 \vec{V}\cdot(\vec{u}_2' - \vec{u}_2) \ . \tag{5}$$

In the system C_M moving with the projectile, a target particle has the initial velocity (Fig. 1)

$$\vec{w}_2 = \vec{v}_2 - \vec{v}_1 \ . \tag{6}$$

There is a particle flux of

$$n \vec{w}_2 f(\vec{w}_2 + \vec{v}_1) d^3 w_2$$

target particles per unit area and time with velocity $(\vec{w}_2, d^3w_2)$ passing the projectile in this system.

Let $d\sigma_0(w_2,\theta)$ be the differential cross section for a scattering event leading to a scattering angle $(\theta, d\theta)$ in the center-of-mass system C_S. This quantity depends on the *relative speed* w_2 and on the reduced mass m_0,

$$m_0 = m_1 m_2/(m_1+m_2) \ . \tag{7}$$

From the conventional definition of the cross section,[1] one finds the expected number of collision events $(\theta, d\theta)$ undergone by target particles with velocity $(\vec{w}_2, d^3w_2)$ with the projectile in a time interval dt to be given by

$$n w_2 dt f(\vec{w}_2+\vec{v}_1) d^3w_2 d\sigma_0(w_2,\theta) \ . \tag{8}$$

Dividing by nv_1dt, one finds the apparent cross section for a scattering event $(\theta, d\theta)$ involving the projectile and all target particles within $(\vec{w}_2, d^3w_2)$,

$$\frac{w_2}{v_1} f(\vec{w}_2+\vec{v}_1) d^3w_2 d\sigma_0(w_2,\theta) \ , \tag{9}$$

or, in terms of C_L velocities,

$$d\sigma = \frac{|\vec{v}_1-\vec{v}_2|}{v_1} f(\vec{v}_2) d^3v_2 d\sigma_0(|\vec{v}_1-\vec{v}_2|,\theta) \tag{10}$$

by means of Eq. (6).

B. Stopping cross section

The specific energy loss of the projectile is given by[1]

$$\frac{dE}{dx} = -nS \ , \tag{11}$$

where

$$S = \int T\, d\sigma \ , \tag{12}$$

with $d\sigma$ the differential cross section for energy loss (T,dT). [This notation does not by any means exclude *negative* values of the energy loss T, i.e., an energy gain in a particular collision. Indeed, the derivation of Eq. (12)—as well as Eq. (21) below—does not preclude this possibility.]

Combining (12) with (5) and (10) one finds for the total stopping cross section

$$S(v_1) = m_2 \int d^3v_2 f(\vec{v}_2) \frac{|\vec{v}_1-\vec{v}_2|}{v_1} \int d\sigma_0(|\vec{v}_1-\vec{v}_2|,\theta) \vec{V}\cdot(\vec{u}_2'-\vec{u}_2) \ . \tag{13}$$

By definition, the center-of-mass scattering angle is given by

$$\cos\theta = (\vec{u}_2\cdot\vec{u}_2')/u_2^2 \tag{14}$$

for elastic collisions, and therefore, in case of azimuthal symmetry of $d\sigma_0$ around $\vec{u}_2$,

$$\int d\sigma_0(|\vec{v}_1-\vec{v}_2|,\theta)(\vec{u}_2'-\vec{u}_2) = -\vec{u}_2\cdot\sigma^{(1)}(|\vec{v}_1-\vec{v}_2|) \ , \tag{15}$$

where

$$\sigma^{(1)}(v) \equiv \int d\sigma_0(v,\theta)(1-\cos\theta) \tag{16}$$

is the transport cross section of first order. Inserting (15) into (13) and making use of (2a) and (3) one finds

$$S(v_1) = \int d^3v_2 f(\vec{v}_2) m_0 \vec{V}\cdot(\vec{v}_1-\vec{v}_2) \times \frac{|\vec{v}_1-\vec{v}_2|}{v_1} \sigma^{(1)}(|\vec{v}_1-\vec{v}_2|) \ . \tag{17}$$

This type of connection between stopping and transport cross section is well known.[7,23,24]

Let us consider (17) in the limit of $v_1 \gg v_2$. This defines a function $S_0(v_1)$ given by

$$S_0(v_1) = \int d^3v_2 f(\vec{v}_2) m_0 \frac{m_1 v_1^2}{m_1+m_2} \sigma^{(1)}(v_1) \equiv \frac{m_1 m_2}{(m_1+m_2)^2} m_1 v_1^2 \sigma^{(1)}(v_1) \ , \tag{18}$$

in view of Eq. (1). Eliminating the transport cross section from (17) and (18), one then finds the relation

$$S(v_1)=\int d^3v_2 f(\vec{v}_2)\times\frac{[\vec{v}_1+(m_2/m_1)\vec{v}_2]\cdot(\vec{v}_1-\vec{v}_2)}{v_1\,|\vec{v}_1-\vec{v}_2|}\times S_0(|\vec{v}_1-\vec{v}_2|) \quad (19)$$

between the effective stopping cross section S in the laboratory frame C_L and the stopping cross section in the system C_0 where the target particle is initially at rest (Fig. 1).

It may be appropriate to stress the main assumptions entering Eq. (17):

(i) nonrelativistic velocities v_1 and v_2,
(ii) binary collisions,
(iii) elastic collisions, and
(iv) azimuthal symmetry of the differential cross section.

No specific assumptions enter concerning the interaction potential between the collision partners, nor is it assumed that the individual collision be classical or semiclassical.

C. Straggling parameter

For a random medium, the energy-loss straggling of the projectile over a path length Δx is known to be given by[1,25]

$$\langle(\Delta E-\langle\Delta E\rangle)^2\rangle=N\Delta x W\,, \quad (20)$$

where W, the straggling parameter, is given by

$$W=\int T^2 d\sigma\,. \quad (21)$$

This expression is evaluated on the basis of Eqs. (5) and (10). Introducing spherical coordinates with the polar axis along $\vec{u}_2$, and noticing again the azimuthal symmetry of the cross section $d\sigma(v,\theta)$, one obtains

$$T^2=m_2^2V^2u_2^2[\cos^2\phi(1-\cos\theta)^2+\tfrac{1}{2}\sin^2\phi\sin^2\theta] \quad (22)$$

in the average over all azimuths, where ϕ is the angle between $\vec{V}$ and $\vec{u}_2$. Thus, (21) takes on the form

$$W(v_1)=m_2^2\int d^3v_2 f(\vec{v}_2)\frac{|\vec{v}_1-\vec{v}_2|}{v_1}u_2^2V^2[(\tfrac{3}{2}\cos^2\phi-\tfrac{1}{2})\sigma^{(2)}(|\vec{v}_1-\vec{v}_2|)+\sin^2\phi\,\sigma^{(1)}(|\vec{v}_1-\vec{v}_2|)]\,, \quad (23)$$

where

$$\sigma^{(2)}(v)=\int d\sigma_0(v,\theta)(1-\cos\theta)^2 \quad (24)$$

is the transport cross section of second order. For a target at rest, (23) reduces to

$$W_0(v_1)=m_2^2u_2^2V^2\sigma^{(2)}(v_1)=\left[\frac{m_1m_2}{(m_1+m_2)^2}\right]^2(m_1v_1^2)^2\sigma^{(2)}(v_1)\,. \quad (25)$$

After eliminating the transport cross sections in (23) by means of (18) and (25) one finds

$$W(v_1)=\int d^3v_2 f(\vec{v}_2)\left[\left[1+\frac{m_2}{m_1}\right]^2\frac{\tfrac{3}{2}[(\vec{v}_1-\vec{v}_2)\cdot\vec{V}]^2-\tfrac{1}{2}(\vec{v}_1-\vec{v}_2)^2V^2}{v_1\,|\vec{v}_1-\vec{v}_2|^3}W_0(|\vec{v}_1-\vec{v}_2|)+m_2\frac{(\vec{v}_1-\vec{v}_2)^2V^2-[(\vec{v}_1-\vec{v}_2)\cdot\vec{V}]^2}{v_1\,|\vec{v}_1-\vec{v}_2|}S_0(|\vec{v}_1-\vec{v}_2|)\right], \quad (26)$$

which is the analog of Eq. (19) for the straggling parameter. Depending on the specific application, the following variant of Eq. (26) may be easier to deal with:

$$W(v_1)=\int d^3v_2 f(\vec{v}_2)\left[\frac{\{(\vec{v}_1-\vec{v}_2)\cdot[\vec{v}_1+(m_2/m_1)\vec{v}_2]\}^2}{v_1\,|\vec{v}_1-\vec{v}_2|^3}W_0(|\vec{v}_1-\vec{v}_2|)+\tfrac{1}{2}\left[1+\frac{m_2}{m_1}\right]^2\frac{(\vec{v}_1\cdot\vec{v}_2)^2-v_1^2v_2^2}{v_1\,|\vec{v}_1-\vec{v}_2|^3}\times W_0(|\vec{v}_1-\vec{v}_2|)-m_2\frac{(\vec{v}_1\cdot\vec{v}_2)^2-v_1^2v_2^2}{v_1\,|\vec{v}_1-\vec{v}_2|}S_0(|\vec{v}_1-\vec{v}_2|)\right]. \quad (26')$$

D. Isotropic velocity distribution

Although Eqs. (19) and (26) could readily be used to determine the *Doppler shift* in stopping parameters for a medium with a *drift velocity,* the most obvious application appears to be the *Doppler broadening* in a medium in random *internal* motion, i.e., with an isotropic velocity spectrum

$$f(\vec{v}_2)\equiv f(v_2)\ . \tag{27}$$

Introducing the variables $v_2=|\vec{v}_2|$ and $v'=|\vec{v}_1-\vec{v}_2|$ in (19) and (26′) one finds

$$S(v_1)=\frac{\pi}{v_1^2}\int_0^\infty f(v_2)v_2dv_2\int_{|v_1-v_2|}^{v_1+v_2}dv'S_0(v')\left[(v_1^2-v_2^2)\left[1+\frac{m_2}{m_1}\right]+v'^2\left[1-\frac{m_2}{m_1}\right]\right] \tag{28}$$

and

$$W(v_1)=\frac{\pi}{2v_1^2}\int_0^\infty f(v_2)v_2dv_2\int_{|v_1-v_2|}^{v_1+v_2}\frac{dv'}{v'^2}\left\{W_0(v')\left[(v_1^2-v_2^2)\left[1+\frac{m_2}{m_1}\right]+v'^2\left[1-\frac{m_2}{m_1}\right]\right]^2\right.$$
$$+\left[\tfrac{1}{2}W_0(v')\left[1+\frac{m_2}{m_1}\right]-m_2v'^2S_0(v')\right]$$
$$\left.\times[(v'^2-v_1^2-v_2^2)^2-4v_1^2v_2^2]\right\}\ . \tag{29}$$

Of particular interest will be the case of small target mass, $m_2\ll m_1$, where (28) and (29) simplify to

$$S(v_1)=\frac{\pi}{v_1^2}\int_0^\infty f(v_2)v_2dv_2\int_{|v_1-v_2|}^{v_1+v_2}dv'S_0(v')(v_1^2-v_2^2+v'^2) \tag{28′}$$

and

$$W(v_1)=\frac{\pi}{2v_1^2}\int_0^\infty f(v_2)v_2dv_2\int_{|v_1-v_2|}^{v_1+v_2}\frac{dv'}{v'^2}\{W_0(v')(v_1^2-v_2^2+v'^2)^2$$
$$+[\tfrac{1}{2}W_0(v')-m_2v'^2S_0(v')][(v'^2-v_1^2-v_2^2)^2-4v_1^2v_2^2]\}\ . \tag{29′}$$

E. Stopping cross section at high projectile speed

Let the projectile speed v_1 exceed the highest target speed v_2. Then, Taylor expansion in terms of the parameter v_2/v_1 up to fourth order of (28) yields

$$S(v_1)=S_0(v_1)+\frac{\langle v_2^2\rangle}{v_1^2}\left[-\frac{1}{3}\left[1+\frac{2m_2}{m_1}\right]S_0+\frac{1}{3}\left[1-\frac{m_2}{m_1}\right]v_1S_0'+\tfrac{1}{6}v_1^2S_0''\right]$$
$$+\frac{\langle v_2^4\rangle}{v_1^4}\left[-\frac{1}{30}\left[1+\frac{4m_2}{m_1}\right]v_1^2S_0''+\frac{1}{30}\left[1-\frac{m_2}{m_1}\right]v_1^3S_0'''+\tfrac{1}{120}v_1^4S_0''''\right]+\cdots\ , \tag{30}$$

where

$$S_0'=\frac{d}{dv_1}S_0(v_1)\ , \tag{31}$$

and similarly for the higher derivatives. In (30), $\langle v_2^2\rangle$ is given by

$$\langle v_2^2\rangle=\int f(v_2)d^3v_2v_2^2\equiv\int_0^\infty 4\pi v_2^4dv_2f(v_2)$$

and $\langle v_2^4\rangle$ correspondingly. In particular, for low target mass, $m_2\ll m_1$, (30) reads

$$S(v_1)=S_0+\frac{\langle v_2^2\rangle}{v_1^2}(-\tfrac{1}{3}S_0+\tfrac{1}{3}v_1S_0'+\tfrac{1}{6}v_1^2S_0'')+\frac{\langle v_2^4\rangle}{v_1^4}(-\tfrac{1}{30}v_1^2S_0''+\tfrac{1}{30}v_1^3S_0'''+\tfrac{1}{120}v_1^4S_0'''')+\cdots\ , \tag{30′}$$

while in the opposite case, $m_1 \ll m_2$,

$$S(v_1)=S_0+\frac{m_2\langle v_2^2\rangle}{m_1 v_1^2}(-\tfrac{2}{3}S_0-\tfrac{1}{3}v_1S_0')+\frac{m_2\langle v_2^4\rangle}{m_1 v_1^4}(-\tfrac{2}{15}v_1^2S_0''-\tfrac{1}{30}v_1^3S_0''')+\cdots \quad (30'')$$

F. Straggling parameter at high projectile speed

The same procedure applied to Eq. (29) yields the straggling parameter

$$W(v_1)=W_0+\frac{\langle v_2^2\rangle}{v_1^2}\left[-\left[1+\frac{4}{3}\frac{m_2}{m_1}\right]W_0-\frac{2}{3}\frac{m_2}{m_1}v_1W_0'+\tfrac{1}{6}v_1^2W_0''+\tfrac{2}{3}m_2v_1^2S_0\right]+\cdots , \quad (32)$$

where terms of higher than first order in $\langle v_2^2\rangle/v_1^2$ have been omitted. For low target mass, $m_2 \ll m_1$, (32) reads

$$W(v_1)=W_0+\frac{\langle v_2^2\rangle}{v_1^2}(-W_0+\tfrac{1}{6}v_1^2W_0''+\tfrac{2}{3}m_2v_1^2S_0)+\cdots . \quad (32')$$

The last term in the square brackets has been kept, since it turns out to become significant for cases of interest.

G. Stopping for cross section at low projectile speed

Let the projectile speed v_1 now be small compared to the typical target speed v_2. This situation is of interest mainly for the case of small target mass, $m_2 \ll m_1$. It is well known that for isotropic distribution of target velocities, the stopping power is linear in v_1 in this limit.[7,13,14,23]

Within the present scheme, this result can be derived either from Eq. (28′) or, slightly more convenient, from Eq. (19) directly, which, for $m_2 \ll m_1$, reads

$$S(v_1)=\int d^3v_2 f(v_2)\frac{\vec{v}_1\cdot(-\vec{v}_2+\vec{v}_1)}{v_1\,|\vec{v}_2-\vec{v}_1|}S_0(|\vec{v}_2-\vec{v}_1|),\quad m_2 \ll, m_1 .$$

Taylor expansion in powers of v_1/v_2 yields

$$S(v_1)\simeq v_1\int_0^\infty 4\pi v_2^2 f(v_2)dv_2 \times\left[\frac{2}{3v_2}S_0(v_2)+\tfrac{1}{3}S_0'(v_2)\right] \quad (33)$$

for the leading term, provided that $f(v_2)$ and $S_0(v_2)$ are well-behaved near $v_2=0$. (In subsequent applications, S_0 will actually be zero below some cutoff velocity.)

H. Straggling parameter at low projectile speed

Similar considerations apply to the straggling parameter (26′) or (29′). Taylor expansion of (26′) in powers of v_1/v_2 yields

$$W(v_1)\simeq\tfrac{2}{3}m_2v_1\int_0^\infty 4\pi v_2^2 f(v_2)dv_2v_2S_0(v_2) \quad (34)$$

for the leading term, provided again that $f(v_2)$ and $S_0(v_2)$ are well-behaved at small values of v_2. Note that W_0 does not enter into Eq. (34).

III. NUCLEAR STOPPING

Let us consider the stopping of an atom or ion of mass M_1 in a monatomic gas with atomic mass M_2. The aim is to estimate the significance of the *thermal motion of gas atoms* on the stopping process.

Equation (30′) indicates that for $M_1 \gg M_2$, the *velocity* ratio $\langle v_2^2\rangle/v_1^2$ is the primary quantity determining whether or not the thermal correction is small, while for $M_1 \ll M_2$, the *energy* ratio $\langle M_2v_2^2\rangle/M_1v_1^2$ appears to be the crucial parameter.

However, the mass-independent correction terms in Eq. (30′) may cancel for specific forms of the stopping cross section $S_0(v)$. In that case, (30″) applies even to the case of $M_1 \gg M_2$.

An important case is that of a frictionlike energy-loss function,

$$S_0(v) = \text{const} \times v \; , \tag{35}$$

where indeed Eq. (30′) would predict $S(v_1) \simeq S_0(v_1)$. Straight evaluation of Eq. (28) yields, however,

$$S(v_1) = S_0(v_1) \left[1 - \frac{M_2 \langle v_2^2 \rangle}{M_1 v_1^2} \right] \tag{36}$$

as an exact result. In terms of energy, this reads

$$S(E) = S_0(E) \left[1 - \frac{3kT}{2E} \right] , \tag{36′}$$

where $E = M_1 v_1^2 / 2$ and k is Boltzmann's constant. It is evident that this correction is significant only at very low projectile energies.

One may note that the stopping power in the eV region is in general a rather uncertain quantity. However, most recent investigations[26–28] point at a power law

$$S_0(v) \simeq \text{const} \times v^{\alpha} \tag{35′}$$

with $1 \lesssim \alpha \lesssim 2$. In that case, Eq. (30) yields

$$S(v_1) \simeq S_0(v_1) \left[1 + \frac{\alpha+2}{3} \frac{\langle v_2^2 \rangle}{v_1^2} \left[\frac{\alpha-1}{2} - \frac{M_2}{M_1} \right] \right] . \tag{37}$$

Obviously, for $\alpha > 1$ and $M_1 \gg M_2$, the stopping-power correction becomes *positive,* unlike in (36), and velocity rather than energy dependent. Note, however, that (37) only holds in the limit of $v_1^2 \gg \langle v_2^2 \rangle$.

Unlike (37), Eq. (36′) is rigorous, provided (35) is valid. Therefore, the stopping power becomes negative for $E < 3kT/2$, i.e., the projectile is *accelerated* up to its equilibrium energy.

The straggling function corresponding to (35′) is easily shown[2] to have the form

$$W_0(v) \simeq \text{Const} \times v^{\alpha+2} \; , \tag{38}$$

with a constant differing from that in Eq. (35) [cf. Eq. (40) below)]. Again, for $\alpha = 1$, a rigorous result can be derived from Eq. (29), i.e.,

$$W(v_1) = W_0(v_1) \left[1 - \frac{10}{3} \frac{M_2 \langle v_2^2 \rangle}{M_1 v_1^2} + \frac{M_2^2 \langle v_2^4 \rangle}{(M_1 v_1^2)^2} \right] + \tfrac{2}{3} M_2 \langle v_2^2 \rangle S_0(v_1) \; . \tag{39}$$

If W_0 and S_0 are related according to Ref. 2,

$$\frac{W_0}{S_0} = \frac{3}{7} \frac{4 M_1 M_2}{(M_1 + M_2)^2} E \quad \text{for } \alpha = 1 \; . \tag{40}$$

it is readily seen that for $M_1 \gg M_2$ and $M_1 \ll M_2$, the term containing S_0 is the leading correction to W_0 in (39). Thus, the straggling correction tends to be *positive.*

For arbitrary values of α, Eq. (32) yields

$$W(v_1) \simeq W_0(v_1) \left[1 + \frac{\langle v_2^2 \rangle}{v_1^2} \frac{\alpha+4}{3} \left[\frac{\alpha-1}{2} - 2 \frac{M_2}{M_1} \right] \right] + \tfrac{2}{3} M_2 \langle v_2^2 \rangle S_0(v_1) \; . \tag{41}$$

Some results of this section have been utilized in the analysis of stopping measurements of very slow recoil atoms in gases.[28]

IV. STOPPING IN A FREE-ELECTRON GAS

A. General remarks

The stopping of a point charge in an electron gas can be described at different levels of sophistication, as far as the many-body nature of the electron gas is concerned. In Lindhard's self-consistent description,[13] the interaction is essentially that of a dynamically screened point charge and individual electrons on the one hand, as well as plasma modes on the other hand.

Although the present theory cannot be expected to describe the stopping in an electron gas with a similar amount of rigor as the dielectric theory, one may find it useful to compare the predictions of the kinetic description with those of the dielectric description in order to determine the limitations of the former.

In order to ensure a meaningful comparison, we must include the Pauli principle in our considerations. Note that no limitations were imposed on the range of final electron velocities in Eqs. (17) and (23).

For simplicity, as well as for the sake of comparison with the results of Refs. 13 – 15, we shall consider mainly the degenerate Fermi gas in this section. Then, the Pauli principle requires that

$$v_2 < v_F \tag{42a}$$

and

$$v_2' > v_F \tag{42b}$$

for allowed scattering events, where v_F is the Fermi velocity. While the requirement (42a) is well accounted for by the factor $f(\vec{v}_2)$ in Eq. (10), which means

$$f(\vec{v}_2)=\begin{cases}\dfrac{3}{4\pi v_F^3} & \text{for } 0\le v_2\le v_F\\ 0 & \text{otherwise}\end{cases} \tag{43}$$

for a degenerate Fermi gas, Eq. (42b) needs to be considered separately. This can be achieved most readily by addition of a set of correction terms ΔS and ΔW to the stopping cross section S and the straggling parameter W, which read

$$\Delta S=-\int_{V_2'<v_F} T\,d\sigma,\quad \Delta W=-\int_{v_2'<v_F} T^2 d\sigma\,, \tag{44}$$

respectively. These expressions will be evaluated subsequently.

B. Stopping cross section at high velocity

Let us first evaluate the stopping cross section from Eq. (30′) disregarding the Pauli principle. The stopping cross section for an electron gas at rest is given by[13]

$$S_0=\frac{4\pi e_1^2e^2}{mv_1^2}\operatorname{arccosh}\frac{mv_1^2}{\hbar\omega_0}\quad\text{for } mv_1^2>\hbar\omega_0\,, \tag{45}$$

where ω_0 is the plasma frequency and $m=m_2$ the electron mass.

For later purposes, it will be convenient to evaluate Eq. (30′) for the more general form

$$S_0(v_1)=\frac{4\pi e_1^2e^2}{mv_1^2}f(v_1)\,. \tag{46}$$

One then obtains

$$S(v_1)\simeq\frac{4\pi e_1^2e^2}{mv_1^2}\left[f+\frac{\langle v_2^2\rangle}{v_1^2}\left(-\tfrac{1}{3}v_1f'+\tfrac{1}{6}v_1^2f''\right)+\frac{\langle v_2^4\rangle}{v_1^4}\left(-\tfrac{1}{15}v_1f'+\tfrac{1}{15}v_1^2f''-\tfrac{1}{30}v_1^3f_1'''+\tfrac{1}{120}v_1^4f''''\right)+\cdots\right], \tag{47}$$

where $f'=df(v_1)/dv_1$, etc. Now, inserting (45), or

$$f(v_1)\simeq\ln\frac{2mv_1^2}{\hbar\omega_0}-\left[\frac{\hbar\omega_0}{2mv_1^2}\right]^2-\cdots\,, \tag{48}$$

one readily finds

$$S(v_1)\simeq\frac{4\pi e_1^2e^2}{mv_1^2}\left[\ln\frac{2mv^2}{\hbar\omega_0}-\frac{\langle v_2^2\rangle}{v_1^2}-\frac{1}{2}\frac{\langle v_2^4\rangle}{v_1^4}-\left[\frac{\hbar\omega_0}{2mv_1^2}\right]^2\right] \tag{49}$$

up to terms of order v_1^{-4}. Equation (49) is a well-known result. It has been derived rigorously for the Fermi gas at absolute zero.[14] Indeed, in that case

$$\langle v_2^2\rangle=\tfrac{3}{5}v_F^2,\quad \langle v_2^4\rangle=\tfrac{3}{7}v_f^4\,, \tag{50}$$

with v_F being the Fermi velocity. After insertion of these averages into (49), one obtains exactly the result given in Ref. 14. It is thus found that the present formalism, which is based on the assumption of scattering of *individual* electrons on the self-consistent Hartree potential set up by the penetrating ion, correctly describes the stopping power including all known orders of "shell corrections."

In addition, one may conclude that Eq. (49) can also be applied to a Fermi gas at *nonzero temperature.* This result has been derived rigorously[29] up to the term proportional to v_1^{-2}.

C. Correction for Pauli principle: general procedure

In order to evaluate the corrections for the Pauli exclusion principle, Eqs. (44), we need to explicitly write down the scattering cross section $d\sigma$ in velocity variables $\vec{v}_2'$. This can be accomplished by starting in the center-of-mass system, C_s, where we can write

$$d\sigma_0(|\vec{v}_1-\vec{v}_2|,\theta)=d\sigma_0(u_2,\theta)d^3u_2'\frac{\delta(u_2'-u_2)}{u_2^2}\times\frac{\delta((\vec{u}_2'\cdot\vec{u}_2)/u_2^2-\cos\theta)}{2\pi} \tag{51}$$

for elastic collisions and azimuthal symmetry. Since we deal with the case $m_2\ll m_1$ only, we have

$$\vec{V}=\vec{v}_1,\quad \vec{w}_2=\vec{u}_2=\vec{v}_2-\vec{v}_1\,. \tag{52}$$

These relations will be used throughout the rest of this section.

Through the use of Eq. (2b), Eq. (51) can be transformed to $\vec{v}_2'$ variables.

$$d\sigma_0 = d\sigma_0(u_2,\theta)\frac{u_2 d^3 v_2'}{\pi} \times \delta(v_2'^2 - 2\vec{v}_2'\cdot\vec{v}_1 + v_1^2 - u_2^2) \times \delta(\vec{u}_2\cdot\vec{v}_2' - \vec{u}_2\cdot\vec{v}_1 - u_2^2\cos\theta) \ . \quad (53)$$

Noting that T, according to Eq. (5), can be written as

$$T = \frac{m}{2}(v_2'^2 - v_2^2) \ , \quad (54)$$

and that the bounds in Eq. (44) do not contain the angular variable, we can integrate over the latter and obtain

$$d\sigma_0 = d\sigma_0(u_2,\theta)\frac{dv_2'^2}{\pi}\frac{1}{[b^4-(v_2'^2-a^2)^2]^{1/2}} \quad (55)$$

with

$$a^2 = v_1^2 + u_2^2 + 2\vec{v}_1\cdot\vec{u}_2\cos\theta \ , \quad (56)$$

$$b^2 = 2[v_1^2 u_2^2 - (\vec{v}_1\cdot\vec{u}_2)^2]^{1/2}\sin\theta \quad (57)$$

in the range where the square root in (55) is real, and zero otherwise.

Combining (54) and (55) and carrying out the integrations over v_2', one finds

$$\int_{(v_2')} T\,d\sigma_0 = \begin{cases} m\,d\sigma_0(u_2,\theta)\frac{1}{2}(a^2-v_2^2) & \text{for } a^2+b^2 \le v_F^2 \\ m\,d\sigma_0(u_2,\theta)\frac{1}{2\pi}\left[(a^2-v_2^2)\arccos\frac{a^2-v_F^2}{b^2} - [b^4-(a^2-v_F^2)^2]^{1/2}\right] & \text{for } a^2-b^2 \le v_F^2 \le a^2+b^2 \end{cases} \quad (58)$$

and

$$\int_{(v_2')} T^2 d\sigma_0 = \begin{cases} m^2 d\sigma_0(u_2,\theta)\frac{1}{4}[b^4/2+(a^2-v_2^2)^2] & \text{for } a^2+b^2 \le v_F^2 \\ m^2 d\sigma_0(u_2,\theta)\frac{1}{4\pi}([b^4/2+(a^2-v_2^2)^2]\arccos\frac{a^2-v_f^2}{b^2} \\ \quad +(2v_2^2-\frac{1}{2}v_F^2-\frac{3}{2}a^2)[b^4-(a^2-v_F^2)^2]^{1/2}) & \text{for } a^2-b^2 \le v_F^2 \le a^2+b^2 \ . \end{cases} \quad (59)$$

From here one could, in principle, proceed along the scheme applied in Sec. II D. For present purposes, it is sufficient to go over to the low- and high-velocity limits in order to estimate the significance of these corrections.

D. High-velocity limit: Role of plasma resonances

Note that the upper choice of the stopping cross section in Eq. (58) applies to *unrestricted* scattering events [$v_F = \infty$ in Eq. (44)]. Thus, one may conclude from Eq. (58) that the Pauli principle cuts away all stopping contributions from the range

$$a^2+b^2 < v_F^2 \ , \quad (60a)$$

it provides a correction within the range

$$a^2-b^2 \le v_F^2 \le a^2+b^2 \ , \quad (60b)$$

and it does not affect the stopping cross section (nor the straggling parameter) for

$$v_F^2 < a^2-b^2 \ . \quad (60c)$$

Now, at high velocities, $v_1 \ll v_F$, the condition (60a) is obeyed for small values of θ only; expansion up to second order in θ shows (60a) to be equivalent to

$$\theta < \theta_c = \frac{1}{v_1^2}\{[v_1^2 v_F^2 - (\vec{v}_1\cdot\vec{v}_2)^2]^{1/2} - [v_1^2 v_2^2 - (\vec{v}_1\cdot\vec{v}_2)^2]^{1/2}\} \ , \quad (61)$$

i.e., all energy transfers

$$T \lesssim T_c \simeq \frac{1}{2}mv_1^2\theta_c^2 \quad (62)$$

are suppressed. Obviously, T_c is of the order of magnitude of the Fermi energy $\frac{1}{2}mv_F^2$. The limiting energy transfer between the regimes of Eqs. (60b) and (60c) is slightly higher than T_c but of the same order of magnitude, i.e., independent of v_1.

It follows that the Pauli principle does not affect those contributions to the stopping power that stem from energy transfers within the range $T_c' \lesssim T \leq 2mv_1^2$, where T_c' is of the order of the Fermi energy.

Note that T_c is intermediate between the minimum energy transfer[13]

$$\epsilon_1 \simeq \frac{(\hbar\omega_0)^2}{2mv_1^2} \tag{63}$$

and the maximum energy transfer $\epsilon_2 = 2mv_1^2$. Energy transfers between ϵ_1 and $\simeq \hbar\omega_0$ are known to be due to plasma resonance excitation.[13,14] Such excitations have been disregarded from the very beginning.

One may thus conclude that in the high-velocity limit, only those portions of the stopping and straggling integrals are affected by the Pauli principle, which stem from low momentum transfers, i.e., from plasma resonances. These contributions are not described properly in the present description from the very beginning.

The reader may ask why the present theory, although applicable only to high momentum transfer (individual particle) scatterings, was able to deliver correct shell corrections to the *total* stopping power, cf. Sec. IV B. The reason is the equipartition rule for the stopping power of the electron gas,[14] from which follows that shell corrections proportional to $\langle v_2^{2n} \rangle / v_1^{2n}$ *to all orders* $n \geq 1$ receive equal contributions from energy transfers to plasma resonances and single-electron excitations, respectively. Since single-electron processes are described with a reasonable degree of rigor in the present treatment, the validity of the calculated shell corrections is just a manifestation of the equipartition rule. Some aspects of the equipartition rule are discussed explicitly in the Appendix.

E. Straggling at high velocities

Straggling obeys quite different partition rules. They have been derived and are listed in the Appendix. One finds that large momentum transfers dominate. Let us, therefore, consider the regimes of large and small energy transfers separately.

Take first large momentum transfers, and disregard the Pauli principle. According to Eqs. (A5) and (A13b), we have

$$W_0 = 4\pi e_1^2 e^2 \left[1 - \text{const} \times \frac{\hbar\omega_0}{2mv_1^2} \right] \tag{64}$$

with

$$\text{const} = [1 + (\epsilon^* / \hbar\omega_0)^2]^{1/2} + \ln\{[1 + (\hbar\omega_0/\epsilon^*)^2]^{1/2} - \hbar\omega_0/\epsilon^*\} , \tag{64a}$$

where $\epsilon^* = \hbar^2 k^{*2}/2m$ defines the lower limit for high momentum transfers, $\hbar k \geq \hbar k^*$. Moreover, we have

$$S_0 = \frac{4\pi e_1^2 e^2}{mv_1^2} L_0 \tag{65}$$

with

$$L_0 = \tfrac{1}{2} \ln \frac{2mv_1^2}{\epsilon^*} , \tag{65'}$$

if we disregard terms of order v_1^{-4}. Insertion of (64) and (65) into Eq. (32') yields

$$(W)_{>\epsilon^*} = 4\pi e_1^2 e^2 \left[1 + \frac{1}{3} \frac{\langle v_2^2 \rangle}{v_1^2} \ln \frac{2mv_1^2}{\epsilon^*} - \frac{\langle v_2^2 \rangle}{v_1^2} - \text{const} \times \frac{\hbar\omega_0}{2mv_1^2} \right] \tag{66}$$

up to terms of order v_1^{-2}. Here, the shell correction terms

$$4\pi e_1^2 e^2 \frac{\langle v_2^2 \rangle}{v_1^2} \left[\frac{1}{3} \ln \frac{2mv_1^2}{\epsilon^*} - 1 \right] \tag{66a}$$

must be compared with those following from the dielectric treatment, Eq. (A14b),

$$4\pi e_1^2 e^2 \frac{\langle v_2^2 \rangle}{v_1^2} \left[\frac{1}{3} \ln \frac{4mv_1^2}{\hbar\omega_0} - \frac{7}{8} - \text{Const} \right] \tag{66b}$$

with

$$\text{Const} = \frac{1}{3} \left[\frac{\epsilon^*}{\hbar\omega_0} \right]^4 - \left[\frac{1}{3} \left[\frac{\epsilon^*}{\hbar\omega_0} \right]^2 - \frac{1}{2} \right] \times \frac{\epsilon^*}{\hbar\omega_0} [1 + (\epsilon^* / \hbar\omega_0)^2]^{1/2} . \tag{67}$$

The difference between the parentheses in (66a) and (66b) amounts to 0.2130 for $\epsilon^* = \hbar\omega_0$. Note in particular that the logarithmic terms in v_1 are in agreement with each other.

Let us, next, consider low momentum transfers. From physical considerations, one would expect this straggling contribution to be insensitive to electronic motion, i.e., the shell correction ought to be zero. W is then given by W_0 only, i.e., according to Eq. (A 13a),

$$(W)_{<\epsilon^*}=4\pi e_1^2 e^2 \frac{\hbar\omega_0}{2mv_1^2}\left[\ln\frac{4mv^2}{\hbar\omega_0}-1+\text{const}\right]. \tag{68}$$

Comparison with Eq. (A 14a) shows that a shell correction

$$\text{Const}\times\langle v_2^2\rangle/v_1^2$$

has been disregarded in this manner. Combine, then Eqs. (66) and (68) to obtain the total straggling parameter

$$W=4\pi e_1^2 e^2\left[1+\left[\frac{1}{3}\frac{\langle v_2^2\rangle}{v_1^2}+\frac{\hbar\omega_0}{2mv_1^2}\right]\ln\frac{4mv^2}{\hbar\omega_0} -\frac{\langle v_2^2\rangle}{v_1^2}\left[1-\frac{1}{3}\ln\frac{\hbar\omega_0}{2\epsilon^*}\right]-\frac{\hbar\omega_0}{2mv_1^2}\right], \tag{69}$$

which differs from the result derived recently,[29]

$$W=4\pi e_1^2 e^2\left[1+\left[\frac{1}{3}\frac{\langle v_2^2\rangle}{v_1^2}+\frac{\hbar\omega_0}{2mv_1^2}\right]\ln\frac{4mv^2}{\hbar\omega_0} -\left[\frac{7}{8}\frac{\langle v_2^2\rangle}{v_1^2}+\frac{\hbar\omega_0}{2mv_1^2}\right]\right], \tag{69'}$$

by

$$\delta W=-4\pi e_1^2 e^2\frac{\langle v_2^2\rangle}{v_1^2}\left[\frac{1}{8}-\frac{1}{3}\ln\frac{\hbar\omega_0}{2\epsilon^*}\right]. \tag{70}$$

The value of the parentheses is 0.3560 for $\epsilon^*=\hbar\omega_0$. It could be brought to disappear with the choice $\epsilon^*=0.3436\hbar\omega_0$. Since the logarithmic terms dominate in Eqs. (69) and (69′), this difference is considered insignificant. Its origin is assumed to be caused mainly by scattering events in the region specified by Eqs. (59) and (60b).

F. Stopping and straggling at low velocity

Let us next evaluate the stopping cross section $S(v_1)$ in the low-velocity limit. According to (33), we need $S_0(v)$ in the velocity range $0\le v\le v_F$. Since Eq. (45) is a high-velocity result, we can expect to obtain valid results by inserting (45) into (33) only if v_F is large, i.e., in the limit of high electron density.

By differentiation of (45) one finds

$$\frac{2}{3v_2}S_0+\tfrac{1}{3}S_0'=\frac{1}{3}\frac{4\pi e_1^2 e^2}{mv_2^2}\frac{2mv_2}{\hbar\omega_0}\times\left[\left[\frac{mv_2^2}{\hbar\omega_0}\right]^2-1\right]^{-1/2},$$

and hence

$$S(v_1)\simeq\frac{4\pi e_1^2 e^2 v_1}{mv_F^3}\,\text{arccosh}\frac{mv_F^3}{\hbar\omega_0} \tag{71}$$

at low velocity, $v_1 \ll v_F$.

Before analyzing this result, we need to consider a possible correction due to the Pauli exclusion principle. It is convenient to work in $\vec{u}_2'$ rather than $\vec{v}_2'$ variables. With spherical coordinates,

$$\vec{u}_2'=u_2(\cos\theta,\sin\theta\cos\psi,\sin\theta\sin\psi), \tag{72}$$

(51) reads

$$d\sigma_0=d\sigma_0(u_2,\theta)\frac{d\psi}{2\pi}, \tag{73}$$

while

$$T\simeq mv_1v_2[-\cos\chi(1-\cos\theta)+\sin\chi\sin\theta\cos\psi] \tag{74}$$

to the lowest power in v_1 ($\ll v_F$), where χ is the angle between $\vec{v}_2$ and $\vec{v}_1$. The condition $v_2'>v_F$ reads

$$v_2^2-2v_2v_1\cos\chi(1-\cos\theta)+2v_2v_1\sin\chi\sin\theta\cos\psi>v_F^2, \tag{75}$$

where terms of second order in v_1 have been neglected. We note that v_2 must be close to v_F, i.e.,

$$v_2=v_F-\delta v, \tag{76}$$

hence Eq. (75) reads

$$\delta v<v_1[-\cos\chi(1-\cos\theta)+\sin\chi\sin\theta\cos\psi]. \tag{77}$$

Thus, the leading term in the stopping cross section takes on the form

$$S=\int d^3v_2 f(v_2)\frac{u_2}{v_1}\int T\,d\sigma_0 \simeq\tfrac{3}{2}mv_Fv_1\int d\sigma_0(v_F,\theta)\int d\cos\chi\int\frac{d\psi}{2\pi}[-\cos\chi(1-\cos\theta)+\sin\chi\sin\theta\cos\psi]^2, \tag{78}$$

with a boundary condition arising from (76) and (77) as well as $v_2 < v_F$,

$$-\cos\chi(1-\cos\theta)+\sin\chi\sin\theta\cos\psi>0\ . \qquad (79)$$

After (79) is rewritten in the form

$$2\sin\frac{\theta}{2}\left|-\cos\chi\sin\frac{\theta}{2}+\sin\chi\cos\frac{\theta}{2}\cos\psi\right|>0\ , \qquad (80)$$

one may evaluate the integral (78) easily to obtain

$$S(v_1)=mv_Fv_1\sigma^{(1)}(v_F)\ . \qquad (81)$$

After insertion of (18), (81) reduces to (71). Thus, the Pauli exclusion principle does not generate a correction in the leading term of the stopping cross section. This result is well known.[24,30]

The straggling parameter is found in the same manner after another factor T, Eq. (74), has been added to the integral (78). One finds

$$W(v_1)=3(mv_Fv_1)^2\int d\sigma_0(v_F,\theta)\sin^3\frac{\theta}{2} \qquad (82)$$

to the leading order in v_1. This result is in striking contrast with Eq. (34), which was found by ignoring

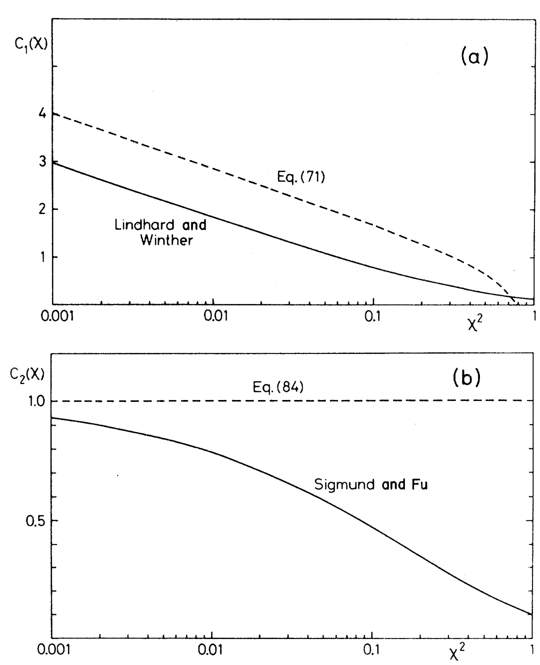

FIG. 2. (a) Low-velocity stopping power for free-electron gas. Solid curve: $C_1(\chi)$ according to Ref. 14, relation to stopping cross section specified by Eq. (85). Dotted curve: Present result, Eq. (71). χ^2 is the density parameter specified by Eq. (87). (b) Same as (a) for straggling. Solid curve: $C_2(\chi)$ according to Ref. 29 [cf. Eq. (86)]. Dotted curve: Present result, Eq. (84).

the Pauli principle. Note in particular that Eq. (82) predicts a v_1^2 dependence while (34) shows a linear behavior in v_1.

The integral in Eq. (82) is not readily expressible in terms of $\sigma^{(1)}(v_F)$ and $\sigma^{(2)}(v_F)$, i.e., of $S_0(v_F)$ and $W_0(v_F)$. In order to find a *qualitative* estimate, insert the *unscreened* Coulomb cross section,

$$d\sigma_0(v_F,\theta)=\frac{2\pi e_1^2e^2}{(mv_1^2)^2}\frac{d(\sin\theta/2)}{\sin^3\theta/2}\ , \qquad (83)$$

which yields

$$W(v_1)=4\pi e_1^2e^2\frac{3}{2}\frac{v_1^2}{v_F^2}\ . \qquad (84)$$

Figures 2(a) and 2(b) show the results obtained in the present approach compared with those of the dielectric theory.

Instead of Eq. (71), Lindhard and Winther[14] obtained

$$S(v_1)=\frac{4\pi e_1^2e^2v_1}{mv_F^3}C_1(\chi)\ , \qquad (85)$$

while the following result[29] must be compared with Eq. (84):

$$W(v_1)=4\pi e_1^2e^2\frac{3}{2}\frac{v_1^2}{v_F^2}C_2(\chi)\ , \qquad (86)$$

C_1 and C_2 being functions of the density parameter

$$\chi^2=\frac{e^2}{\pi\hbar v_F} \qquad (87)$$

or

$$\frac{2mv_F^2}{\hbar\omega_0}=\frac{\sqrt{3}}{\chi}\ . \qquad (87')$$

Figure 2(a) shows that Eq. (71) overestimates the stopping cross section at all but the lowest electron densities, but that the relative difference decreases with increasing electron density, in accordance with the expectation expressed in the beginning of this paragraph. The main physical reason for the difference is thought to be the insistence on *dynamic* screening implied by Eq. (45), rather than the *static* screening entering into Eq. (85).

Figure 2(b) shows a similar discrepancy for the straggling parameter, although the relative difference is less pronounced at high density but more pronounced at low density. Note, however, that (84) has been evaluated under the *additional* simplifying assumption of *unscreened* Coulomb scattering.

G. Discussion

It was the purpose of this rather extensive discussion of stopping in an electron gas to test the capability of the present approach against accurate predictions on the basis of a well-defined model. With regard to the stopping cross section, it was found that Eq. (30′), i.e., the high-velocity expansion, predicts shell corrections of both first and second order correctly, even when applied to excitation of plasma modes where the binary-encounter picture cannot be expected to be valid. This behavior was ascribed to the equipartition rule. At low velocities, Eq. (33) overestimates the stopping cross section of an electron gas by $\sim 25-100\%$ in the density range in question [cf. Fig. 2(a)], the difference being most pronounced at low electron densities. Therefore, the accuracy of predictions of the stopping cross section based upon Eq. (28′) must be expected to deteriorate as the velocity decreases, unless the estimate (45) for S_0 is improved.

With regard to straggling, quite accurate results have been found at high velocities on the basis of Eq. (32′), although it was crucial to consider the partition of the straggling parameter into high and low momentum transfers. Unlike in the case of the stopping cross section, the straggling parameter at low velocities is strongly affected by the Pauli exclusion principle, even to the extent that Eq. (34) predicts a linear velocity dependence while the Pauli principle generates a quadratic velocity dependence. For the intermediate velocity regime, a similar statement applies as the one made above on the stopping cross section.

V. ELECTRONIC STOPPING IN GASES

A. Stopping cross section at high velocities

Before applying the present scheme to the stopping of particles by atoms or molecules, we must give some consideration to the question of what values of S_0 and W_0 have to be adopted. Since (18) followed from (17) in the limit of

$$v_2 \ll v_1 \, , \tag{88}$$

S_0 and W_0 ought to be understood as the leading terms in the respective expansions in powers of v_2/v_1. Note that this convention does not preclude the presence of higher-order terms in v_1^{-1} in either S_0 or W_0. Indeed, in case of the Fermi gas, a term proportional to $(\hbar\omega_0/2mv_1^2)^2$ occurs in S_0 besides the Bethe logarithm, according to Eq. (49); similarly, a term proportional to $\hbar\omega_0/2mv_1^2$ was found to contribute to W_0 [cf. Eq. (64)]. Both terms refer to the *static* properties of an electron gas. In case of an atom or molecule, the mean excitation energy I takes over to some extent the role of the plasma frequency.[13] This quantity, defined in the conventional way[3,4]

$$\log I = \sum_n f_{n0} \ln(E_n - E_0), \quad \sum_n f_{n0} = 1 \tag{89}$$

with the atomic or molecular levels E_n ($n = 0,1,2,\ldots$), and the associated dipole oscillator strengths f_{n0} is, of course, not a purely static quantity. On the other hand, it enters only logarithmically into the Bethe expression of the stopping cross section.

Writing the stopping cross section of an atom in the form

$$S(v) = \frac{4\pi e_1^2 e^2}{mv^2} Z L(v) \, , \tag{90}$$

where Z is the atomic number, one may expand L in powers of e_1, i.e.,

$$L(v) = L^{(0)}(v) + L^{(1)}(v) + L^{(2)}(v) + \cdots \, . \tag{91}$$

with

$$L^{(i)}(v) = L_0^{(i)} + \frac{\langle v_2^2 \rangle}{v^2}\left(-\tfrac{1}{3} v L_0^{(i)\prime} + \tfrac{1}{6} v^2 L_0^{(i)\prime\prime}\right) + \frac{\langle v_2^4 \rangle}{v^4}\left(-\tfrac{1}{15} v L_0^{(i)\prime} + \tfrac{1}{15} v^2 L_0^{(i)\prime\prime} - \tfrac{1}{30} v^3 L_0^{(i)\prime\prime\prime} + \tfrac{1}{120} v^4 L_0^{(i)\prime\prime\prime\prime}\right) + \cdots \, , \tag{92}$$

according to Eq. (47), where the index 1 has been dropped from v_1. Inserting the Bethe expression

$$L_0^{(0)} = \ln \frac{2mv^2}{I} \tag{93}$$

into (92) we find immediately that

$$L^{(0)} = \ln \frac{2mv^2}{I} - \frac{\langle v_2^2 \rangle}{v^2} - \frac{1}{2} \frac{\langle v_2^4 \rangle}{v^4} - \cdots \, , \tag{94}$$

in agreement with the kinetic part—i.e., the main contribution—of the conventional expression for shell corrections.[4] In contrast, Bohr's classical formula[31]

$$L_0^{(0)}=\ln\frac{v^3}{\text{const}}$$

would yield

$$L^{(0)}=\ln\frac{v^3}{\text{const}}-\frac{3}{2}\frac{\langle v_2^2\rangle}{v^2}-\frac{3}{4}\frac{\langle v_2^4\rangle}{v^4}-\cdots\,, \tag{95}$$

i.e., a 50% increase in shell corrections.

The Barkas correction[32–34] $L_0^{(1)}$ can be written in the form[34]

$$L_0^{(1)}=\frac{3\pi e_1 e I}{2\hbar m v^3}\ln\frac{2mv^2}{I}\,. \tag{96}$$

Then, Eq. (92) yields an *order-of-magnitude estimate* of the shell correction $L_1^{(1)}$ to the Barkas correction, so that

$$L^{(1)}\simeq L_0^{(1)}+L_1^{(1)}$$
$$\simeq\frac{3\pi e_1 e I}{2\hbar m v^3}\left[\ln\frac{2mv^2}{I}+3\frac{\langle v_2^2\rangle}{v^2}\left[\ln\frac{2mv^2}{I}-1\right]+\cdots\right] \tag{97}$$

While the accuracy of this result is limited due to deviations from equipartition, the main conclusion to be drawn from Eq. (97) is that shell corrections in the Barkas effect are *positive* and significantly more important on a relative scale than in the Bethe term, i.e., the leading power of e_1.

The Bloch correction[35] can be written in the form[34]

$$L_0^{(2)}=-1.202\frac{e_1^2e^2}{\hbar^2v^2} \tag{98}$$

at not too low velocities. Equation (93) yields a shell correction $L_1^{(2)}$ so that

$$L^{(2)}\simeq L_0^{(2)}+L_1^{(2)}$$
$$=-1.202\frac{e_1^2e^2}{\hbar^2v^2}\left[1+\frac{5}{3}\frac{\langle v_2^2\rangle}{v^2}+\cdots\right], \tag{99}$$

i.e., again an *enhancement* in comparison with the bare Bloch correction (98).

It appears likely that terms like $L_1^{(1)}$ and $L_1^{(2)}$ in Eqs. (97) and (99) need to be taken into account in a detailed discussion of higher-order e_1 corrections to the Bethe stopping formula.[36] This point was made some time ago.[37]

With regard to the range of validity of expansions like (94), (97), and (99), one may notice that the averages $\langle v_2^2\rangle$ and $\langle v_2^4\rangle$ receive contributions from widely different velocity ranges, in accordance with the atomic shell structure. Splitting the mean excitation energy (89) into contributions from the individual shells,[38]

$$\log I=\sum w_k \log I_k \tag{100}$$

with

$$\sum_k w_k=1\,,$$

we may write (93) in the form

$$L_0^{(0)}=\sum_k w_k\ln\frac{2mv^2}{I_k}\,, \tag{93$'$}$$

so that (94) reads

$$L^{(0)}=\sum_k w_k\left[\ln\frac{2mv^2}{I_k}-\frac{\langle v_2^2\rangle^k}{v^2}-\frac{1}{2}\frac{\langle v_2^4\rangle^k}{v^4}-\cdots\right], \tag{94$'$}$$

where $\langle v_2^2\rangle^k$ is the average square velocity of an electron in the kth shell. Obviously, (94′) ceases to be valid as soon as the conditions $v^2\gg\langle v_2^2\rangle^k$, $v^4\gg\langle v_2^4\rangle^k$ are no longer valid for the *innermost* shell.

An evaluation of the complete expression (28′) for the stopping cross section based on Eq. (93′) has been performed recently, with promising results.[39] A discussion of relativistic effects on the stopping cross section of inner-shell electrons has been presented separately.[40,41]

B. Stopping cross section at low velocities

When evaluating the stopping cross section at low velocities from Eq. (33) on the basis of the Bethe formula for S_0, we should note again the high-velocity nature of S_0. This implies that such an estimate may be valid for fast atomic electrons, i.e., inner-shell electrons. It appears appropriate, therefore, to start from Eq. (93′) rather than (93).

Equations (33), (90), and (93′) yield

$$S(v)\simeq\frac{4\pi e_1^2e^2}{m}Z_{\frac{2}{3}}v\sum_k w_k\langle v_2^{-3}\rangle_k\,, \tag{101}$$

where

$$\langle v_2^{-3} \rangle_k = \int_{\sqrt{I_k/2m}}^{\infty} 4\pi v_2^2 dv_2 \, f_k(v_2) v_2^{-3} \tag{101a}$$

and $f_k(v_2)$ is the (ground-state) velocity distribution of electrons in the kth shell, normalized according to

$$\int_0^\infty f_k(v_2) 4\pi v_2^2 dv_2 = 1 \; . \tag{101b}$$

Since low velocities contribute substantially to the average in Eq. (101a), it appears appropriate to include deviations from the first Born approximation, i.e., to extend (93′) by a term analogous to (96),

$$L_0^{(1)} = \sum w_k \frac{3\pi e_1 e I_k}{2\hbar m v^3} \ln \frac{2mv^2}{I_k} \; . \tag{96′}$$

Evaluation of Eq. (33) by insertion of Eqs. (90) and (96′) yields a leading correction ΔS to the stopping cross-section equation (101), which is of the order of magnitude

$$\Delta S \simeq \frac{4\pi e_1^2 e^2}{m} Z \times \tfrac{2}{3} v \sum_k w_k \frac{3\pi e_1 e I_k}{2\hbar m} \left\langle v_2^{-6} \left[1 - \tfrac{3}{2} \ln \frac{2mv_2^2}{I_k} \right] \right\rangle_k , \tag{102}$$

the average $\langle \; \rangle_k$ being defined in analogy with (101a). Introducing the variable $\zeta = v_2 (2m/I_k)^{1/2}$, one may rewrite (101) and (102) in the form

$$S(v) = \frac{4\pi e_1^2 e^2}{m} Z \tfrac{2}{3} v \sum_k w_k \int_1^\infty 4\pi \frac{d\zeta}{\zeta} f_k(\zeta \sqrt{I_k/2m}\,) \tag{101′}$$

and

$$\Delta S(v) = \frac{4\pi e_1^2 e^2}{m} Z \tfrac{2}{3} v \sum_k w_k \frac{3\pi e_1 e}{\hbar \sqrt{I_k/2m}} \int_1^\infty 4\pi \frac{d\zeta}{\zeta^4} f_k(\zeta \sqrt{I_k/2m}\,)(1 - 3 \ln\zeta) \; . \tag{102′}$$

It is evident that the integrals over ζ exclude a large fraction of the electrons in the respective shells from contributing to the stopping power; it appears also that even the K shell contributes to low-velocity stopping, and that the Barkas correction is most pronounced for stopping due to outer-shell electrons, as it is well known for velocities beyond the stopping power maximum.[32–34]

A numerical evaluation of Eq. (101′) will be attempted separately. It is noteworthy, however, that the first correction term to (101′) is positive, i.e., that S bends *upward* when leaving the linear regime. Indeed, in the case that $S_0(v')$ drops to zero at some velocity v_0, Eq. (28′) yields the following expansion, valid for $v < \frac{1}{2}(I_k/2m)^{1/2}$,

$$S(v) = \frac{4\pi}{3} v \int_0^\infty f(v_2) v_2 dv_2 [2S_0(v_2) + v_2 S_0'(v_2)] + \frac{2\pi}{15} v^3 \int_0^\infty f(v_2) v_2 dv_2 [4S_0''(v_2) + v_2 S_0'''(v_2)]$$
$$+ \frac{\pi}{210} v^5 \int_0^\infty f(v_2) v_2 dv_2 [6S_0''''(v_2) + v_2 S_0'''''(v_2)] \; . \tag{103}$$

After insertion of (93′), the term proportional to v^3 in Eq. (103) reads

$$\frac{4\pi e_1^2 e^2}{m} Z \tfrac{2}{5} v^3 \sum_k w_k \int_{\sqrt{I_k/2m}}^\infty 4\pi \frac{dv'}{v'^3} f_k(v') ,$$

which is positive definite, and becomes comparable with (101) as $2mv^2/I_k$ increases toward 1 for the outermost shell.

C. Straggling at high velocities

The leading term in an expansion of the straggling parameter W in powers of v_2/v is Bohr's straggling expression,[42]

$$W_0 = 4\pi e_1^2 e^2 Z \; . \tag{104}$$

A superscript has not been included since higher-order e_1 corrections have not yet been evaluated, although *one* source of such a contribution, geometric correlation between target electrons, has been shown to be significant.[43,25,26,44,45]

If (104) and (90), in conjunction with (93), are inserted into Eq. (32′), one obtains

$$W(v) \simeq 4\pi e_1^2 e^2 Z \left[1 + \frac{2}{3} \frac{\langle v_2^2 \rangle}{v^2} \ln \frac{2mv^2}{I} - \frac{\langle v_2^2 \rangle}{v^2} \right] . \tag{105}$$

If, on the other hand, the stopping cross section is split into contributions from the individual shells [cf. Eq. (93′)] one finds

$$W(v)\simeq 4\pi e_1^2 e^2 Z\left[1+\sum_k w_k \frac{\langle v_2^2\rangle^k}{v^2}\times\left[\frac{2}{3}\ln\frac{2mv^2}{I_k}-1\right]\right], \tag{106}$$

$\langle v_2^2\rangle^k$ being defined as in Eq. (94′).

Equation (105) can be compared with the expression given by Fano (Sec. 5 of Ref. 4)

$$W(v)\simeq 4\pi e_1^2 e^2 Z\left[1+\frac{2}{3}\frac{\left\langle\left[\sum_i^Z \vec{v}_i\right]^2\right\rangle_0}{Zv^2}\ln\frac{2mv^2}{I_1}\right], \tag{105′}$$

where

$$\ln I_1=\frac{\sum_n (E_n-E_0)f_{n0}\ln(E_n-E_0)}{\sum_n (E_n-E_0)f_{n0}} \tag{107}$$

and $\langle\ \rangle_0$ indicates the ground-state expectation value.

Equation (106) may be brought into the form

$$W(v)\simeq 4\pi e_1^2 e^2 Z\left[1+\frac{2}{3}\frac{\langle v_2^2\rangle}{v^2}\left[\ln\frac{2mv^2}{I_1'}-1\right]\right] \tag{106′}$$

with

$$\ln I_1'=\frac{\sum_k w_k\langle v_2^2\rangle^k \ln I_k}{\sum_k w_k\langle v_2^2\rangle^k}, \tag{107′}$$

which has a similar structure as $\ln I_1$ [cf. Eqs. (107) and (111) below]. Equation (106′) differs from (105′) by the absence of correlation terms of the type

$$\left\langle\sum_{i\neq j}^{Z}\vec{v}_i\cdot\vec{v}_j\right\rangle_0, \tag{108}$$

an obvious consequence of the assumption of binary scattering events. The term $-2\langle v_2^2\rangle/3v^2$ is absent in Eq. (105′), since corrections of this order have been deliberately omitted in Ref. 4.

Let us now compare the present results with those found for the free-electron gas, and concentrate on the terms containing $\ln v^2$. The coefficient of that term reads

$$\frac{1}{3}\frac{\langle v_2^2\rangle}{v^2}+\frac{\hbar\omega_0}{2mv^2} \tag{109}$$

for the electron gas [cf. Eq. (69′)], and

$$\frac{2}{3}\frac{\langle v_2^2\rangle}{v^2} \tag{110}$$

for the atomic case [cf. Eq. (105)], the common factor $4\pi e_1^2 e^2 Z$ being omitted in the comparison. Obviously, (109) and (110) are, in general, not identical.

Now, the first term in Eq. (109) arises from high momentum transfers [cf. Eq. (A14b) in the Appendix] while the second is due to plasma resonances even for the *static* electron gas [cf. Eq. (A13a) in the Appendix]. On the other hand, inspection of Fano's procedure for deriving Eq. (109)—which *also* shows a factor $\frac{2}{3}$ in front of the logarithm, like Eq. (110)—indicates that low and high momentum transfers *each* contribute a term proportional to $\langle v_2^2\rangle/3v^2$ to Eq. (110). Thus, the remaining difference is in the contribution of low momentum transfers to the straggling correction, where the electron gas yields a term

$$\frac{\hbar\omega_0}{2mv^2}=\frac{I}{2mv^2} \tag{109′}$$

while for an atom, one finds

$$\frac{1}{3}\frac{\langle v_2^2\rangle}{v^2}, \tag{110′}$$

apart from correlation terms.

On the other hand, the following sum rule is satisfied for atomic systems[46] (correlation terms still being ignored):

$$\sum (E_n-E_0)f_{n0}=\tfrac{2}{3}m\langle v_2^2\rangle, \tag{111}$$

i.e., Eq. (110′) can be approximated by

$$\frac{\sum (E_n-E_0)f_{n0}}{2mv^2}, \tag{112}$$

which is strikingly similar to, although not identical with (109′) since I is found by a different averaging procedure than the numerator in Eq. (112) [cf. Eq. (89)]. However, the two quantities must have similar scaling properties and may be close in magnitude for a reasonably narrow excitation spectrum.

It appears justified, therefore, to conclude that the seeming disparity between (109) and (110), while inherent in the different physics of resonance excitations in the two systems, and interesting in principle, need not be substantial in a numerical sense. From a more conceptual point of view, one may draw the conclusion that only the first term in the straggling correction (109) is a shell correction—namely the contribution from high momentum transfers—while the second term arises from the *static* properties of the electron gas. A similar distinction with regard to static properties is not feasible in the atomic case.

The presence of a logarithmic term like that in Eq. (106′) was first pointed out by Williams[47] and was discussed subsequently by Livingston and Bethe,[38] who also gave the correct factor $\frac{2}{3}$. The seeming discrepancy in the terms containing $\langle v_2^2\rangle$ in Eqs. (69) and (105) was observed in Ref. 44, and ascribed to the application of approximate sum rules in Ref. 4. This latter assertion has not been confirmed by the present work.

Interestingly enough, if Bloch's expression for the stopping cross section of an atom,[35]

$$S_0=\frac{4\pi e_1^2 e^2}{mv^2} Z\left\{\ln\frac{2mv^2}{I} +\mathrm{Re}\left[\psi(1)-\psi\left(1-\frac{iee_1}{\hbar v}\right)\right]\right\}, \tag{113}$$

is inserted into Eq. (32′), together with Bohr's expression for W_0, Eq. (104), one finds

$$W=4\pi e_1^2 e^2 Z\left[1+\frac{2}{3}\frac{\langle v_2^2\rangle}{v^2}\left\{\ln\frac{2mv^2}{I}+\mathrm{Re}\left[\psi(1)-\psi\left(1-\frac{iee_1}{\hbar v}\right)\right]\right\}-\frac{\langle v_2^2\rangle}{v^2}\right], \tag{114}$$

where $\psi(\xi)=d\ln\Gamma(\xi)/d\xi$. The middle term in the square brackets of Eq. (114) is identical with that found by Titeica[48] after a thorough application of Bloch's treatment to the straggling problem.

Although the present scheme appears to consistently reproduce the leading corrections to the straggling parameter at high velocities, some caution is indicated with regard to terms like $-\langle v_2^2\rangle/v^2$ in Eqs. (106) and (114). Indeed, a binding correction of relative order $\sim I/2mv^2$ ought to be applied to Bohr's straggling expression W_0, in analogy with the occurrence of I in the Bethe expression S_0. According to Eq. (32′), such a term yields corrections of higher order in the terms proportional to $\langle v_2^2\rangle$, but due to its occurrence in the leading term W_0, it competes with other corrections proportional to v^{-2}. It is not obvious at this stage how the precise magnitude of this correction can be determined within the present scheme in a consistent manner.

D. Straggling at low velocities

At low velocities, Eqs. (34), (90), and (93′) yield

$$W(v)\simeq 4\pi e_1^2 e^2 Z \times\frac{2}{3}v\sum_k w_k\left\langle\frac{1}{v_2}\ln\frac{2mv_2^2}{I_k}\right\rangle_k , \tag{115}$$

the notation being the same as in Sec. IV B. The magnitude of this quantity will be evaluated along with the corresponding stopping-power values. At this point, the most noticeable result is the linearity of W in velocity, in distinct contrast to the parabola behavior[49] predicted for the free-electron gas [cf. Eq. (86) and Ref. 29]. Moreover, it is readily shown, by the same procedure as applied to S in

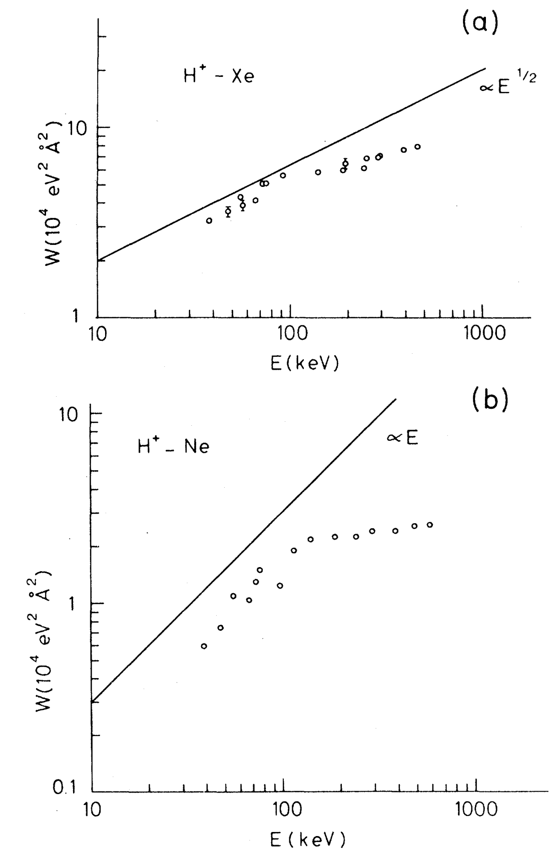

FIG. 3. Straggling parameters measured for protons penetrating gas targets. Replotted from Ref. 45. (a) xenon; (b) neon.

Sec. V B, that the next term in an expansion of $W(v)$ in powers of v, is of *third order.* Thus, the velocity dependence of the straggling parameter of a point charge in an atomic gas appears to be a useful test on the validity of a free-electron gas description to the stopping parameters of an *atom,* i.e., the basis of the dielectric theory of stopping.[6]

Figure 3 shows measured straggling parameters for protons on Xe and Ne, taken from Ref. 45, in a double-logarithmic plot. There appears to be evidence in favor of a linear dependence at low velocities of W on velocity in case of xenon, and a quadratic dependence in case of neon. The evidence is not compelling in either case. Extension of the measurements down to even lower energies, and elimination of charge-exchange straggling by measuring on very thin gas layers, might shed some more light on this point. For heavier ions, a clear bendover toward linearity in velocity was already documented in Ref. 45.

VI. SUMMARY

This section summarizes the main results.

(1) On the basis of a binary-encounter description of elastic scattering events between moving particles, expressions have been derived that relate stopping power and straggling for a projectile penetrating a medium in internal motion to the stopping parameters of an equivalent medium at rest.

(2) These relationships are valid at nonrelativistic velocities for all target-to-projectile mass ratios. They involve the velocity distribution of target particles as well as kinematic factors, but unlike in conventional binary-encounter stopping theory, the interaction is not specified.

(3) The relationships are applied to media with an iostropic velocity distribution of the constituent particles. They could also be applied in the presence of a drift velocity, i.e., to a stopping medium in macroscopic motion.

(4) A high-speed expansion yields corrections to stopping power and straggling of order $\langle v_2^2 \rangle / v_1^2$, where $\langle v_2^2 \rangle$ is the mean square target velocity and v_1 the projectile speed. Higher-order corrections have also been evaluated.

(5) A low-speed expansion yields expressions for stopping power and straggling that are both linear in projectile velocity. The next nonvanishing terms are of third order in velocity.

(6) When applied to problems involving nuclear stopping, the description yields corrections to the stopping power, which may be positive or negative, depending on velocity and mass ratio. Both the energy ratio and the velocity ratio may be pertinent in determining these corrections. At low enough projectile velocity, the stopping power may change sign.

(7) When applied to stopping of low-speed ions in a free-electron gas, the description needs to be modified by inclusion of the Pauli principle. While this is known not to affect calculated stopping powers, straggling is strongly affected and turns from a linear dependence on projectile velocity to the well-known square dependence. Except at high electron densities, the calculated values for both stopping power and straggling exceed those evaluated on the basis of the dielectric description of stopping in the Fermi gas.

(8) When applied to stopping of high-speed ions in a free-electron gas, the description yields the two leading shell corrections to the stopping power in agreement with dielectric theory and, in accordance with the partition of energy loss into plasma modes and single-particle excitations—which is discussed in detail for the case of straggling—correct shell corrections to leading order to the straggling parameter.

(9) When applied to stopping of high-speed ions in gases, the description yields shell corrections that agree with literature values both in case of stopping power and straggling, but if an expansion in powers of $\langle v_2^2 \rangle / v_1^2$ is avoided, the description allows to estimate stopping powers and straggling down to velocities where even outer-shell corrections become sizable. The accuracy is expected to be best for the inner shells.

(10) The description allows order-of-magnitude estimates of shell corrections to Barkas and Bloch corrections.

(11) A seeming disparity between the leading correction terms to the Bohr straggling parameter evaluated for atomic targets and a free-electron gas, respectively, is reconciled by means of the observation that the two systems differ in zero order. The difference is shown to lie in the low-momentum-transfer events.

(12) Expressions have been derived for the stopping power and straggling of gases at low velocity, both linear in projectile velocity, which involve parameters entering the Bethe theory of stopping as well as atomic velocity distributions for the individual shells. Numerical evaluations have not yet been reported.

(13) It is shown that with increasing velocity, the stopping power bends *upward* from the linear dependence.

(14) It is pointed out that an unambiguous determination of the velocity dependence of the straggling parameter of a gas at low velocity might give valuable information on the range of validity of the dielectric theory of stopping when applied to atomic targets.

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APPENDIX: PARTITION OF MEAN ENERGY LOSS AND STRAGGLING IN FERMI GAS

An approximate equipartition of the *stopping power* of a high-speed particle between dipole resonance excitation and free-electron scattering was first observed by Bethe[3]; these observations have been generalized to include shell corrections by Walske[5] and Fano.[4] Equipartition at a given *energy transfer* exceeding a well-defined minimum value has been established by Lindhard and Winther[14] for the special case of a free-electron gas. With regard to straggling, it is well known that the leading contribution stems from scattering events with high momentum transfer,[1,42] and more recent work[52] indicated that this may prevail even to the leading correction to Bohr straggling. This appendix serves the purpose of deriving expressions for the partition of the straggling parameter of a free-electron gas on the basis of a recently developed formalism.[29] As a check on the validity of the scheme, known results on equipartition of stopping power[14] are rederived.

In the notation of Ref. 29, the stopping power of a free-electron gas reads

$$\frac{dE}{dx}=\frac{-4\pi e_1^2 e^2}{mv^2}\rho L \tag{A1}$$

with[53]

$$L=L^{(0)}+L^{(1)}+\cdots \tag{A2}$$

and

$$L^{(0)}=\int_0^\infty \frac{dk}{k}\Theta(\hbar kv-\alpha_k)\ , \tag{A3a}$$

$$L^{(1)}=-\frac{2}{3}\frac{\langle mv_2^2\rangle}{(\hbar\omega_0)^2}\int_0^\infty \frac{dk}{k}\epsilon_k\left[-\frac{4\epsilon_k^2}{(\hbar\omega_0)^2}\Theta(\hbar kv-\epsilon_k)+\frac{4\epsilon_k^2}{(\hbar\omega_0)^2}\Theta(\hbar kv-\alpha_k)+\frac{4\alpha_k^2-(\hbar\omega_0)^2}{2\alpha_k}\delta(\alpha_k-\hbar kv)\right]\ , \tag{A3b}$$

where ρ is the electron density, $\epsilon_k=\hbar^2k^2/2m$, and

$$\alpha_k^2=\epsilon_k^2+(\hbar\omega_0)^2\ . \tag{A4}$$

The subscript 1 has been dropped from v_1. Θ represents a step function, $\Theta(\xi)=\int_{-\infty}^{\xi}\delta(t)dt$.

Similarly, it was found[29] that

$$\Omega^2=4\pi e_1^2e^2\rho x(w^{(0)}+w^{(1)}+\cdots)\ , \tag{A5}$$

where

$$w^{(0)}=\frac{1}{mv^2}\int_0^\infty \frac{dk}{k}\alpha_k\Theta(\hbar kv-\alpha_k) \tag{A6a}$$

and

$$w^{(1)}=-\frac{4}{3}\frac{\langle v_2^2\rangle}{v^2}\int_0^\infty \frac{dk}{k}\frac{\epsilon_k}{\hbar\omega_0}\left[-\frac{2\epsilon_k^3}{(\hbar\omega_0)^3}\Theta(\hbar kv-\epsilon_k)+\frac{8\alpha_k^4-12\alpha_k^2(\hbar\omega_0)^2+(\hbar\omega_0)^4}{4\alpha_k(\hbar\omega_0)^3}\Theta(\hbar kv-\alpha_k)+\frac{4\alpha_k^2-(\hbar\omega_0)^2}{4\hbar\omega_0}\delta(\hbar kv-\alpha_k)\right]\ . \tag{A6b}$$

Noting that the step function $\Theta(\hbar kv-\alpha_k)$ limits the integration in the second term of the integrand in (A3b) and (A6b) to the interval

$$mv^2-[(mv^2)^2-(\hbar\omega_0)^2]^{1/2}=\epsilon_1\le\epsilon_k\le\epsilon_2=mv^2+[(mv^2)^2-(\hbar\omega_0)^2]^{1/2}\,, \tag{A7}$$

and that, for swift projectiles,

$$\epsilon_1\simeq\frac{(\hbar\omega_0)^2}{2mv^2},\quad \epsilon_2\simeq 2mv^2\,, \tag{A8}$$

we split the integrals in (A3) and (A6) into low-k and high-k regimes, $\epsilon_k \lessgtr \epsilon^*$, respectively, with

$$\frac{(\hbar\omega_0)^2}{2mv^2}\ll\epsilon^*\ll 2mv^2\,, \tag{A9}$$

ϵ^* being kept flexible otherwise.

Evaluating (A3) and (A6) in the low-k regime, keeping only terms of order up to v^{-2}, one finds

$$(L^{(0)})_{\epsilon_k<\epsilon^*}\simeq\tfrac{1}{2}\ln\frac{\epsilon^*(2mv^2)}{(\hbar\omega_0)^2}\,, \tag{A10a}$$

$$(L^{(1)})_{\epsilon_k<\epsilon^*}\simeq-\frac{\langle v_2^2\rangle}{2v^2}\,, \tag{A10b}$$

$$(w^{(0)})_{\epsilon_k<\epsilon^*}\simeq\frac{\hbar\omega_0}{2mv^2}\left[\ln\frac{4mv^2}{\hbar\omega_0}+[1+(\epsilon^*/\hbar\omega_0)^2]^{1/2}-1+\ln\{[1+(\hbar\omega_0/\epsilon^*)^2]^{1/2}-\hbar\omega_0/\epsilon^*\}\right]\,, \tag{A11a}$$

$$(w^{(1)})_{\epsilon_k<\epsilon^*}\simeq\frac{\langle v_2^2\rangle}{v^2}\left\{\frac{1}{3}\left[\frac{\epsilon^*}{\hbar\omega_0}\right]^4-\left[\frac{1}{3}\left[\frac{\epsilon^*}{\hbar\omega_0}\right]^2-\frac{1}{2}\right]\frac{\epsilon^*}{\hbar\omega_0}[1+(\epsilon^*/\hbar\omega_0)^2]^{1/2}\right\}\,. \tag{A11b}$$

The complementary contributions for $\epsilon_k>\epsilon^*$ can be found easily by comparison with the respective complete expressions.[29] Equation (A10a) demonstrates the well-known equipartition of the Bethe stopping formula[3,4,13,14]; there is *strict* equipartition for the choice

$$\epsilon^*=\hbar\omega_0\,. \tag{A12}$$

Equation (A10b) demonstrates strict equipartition of the first shell correction, in agreement with a general result proved in Ref. 14. Note that this equipartition is independent of the choice of ϵ^* so long as (A9) holds.

The straggling terms depend obviously on the accurate choice of ϵ^*. From (A11a) and Ref. 29, one finds that

$$(w^{(0)})_{\epsilon_k<\epsilon^*}=\frac{\hbar\omega_0}{2mv^2}\left[\ln\frac{4mv^2}{\hbar\omega_0}-1+\text{const}\right]\,, \tag{A13a}$$

$$(w^{(0)})_{\epsilon_k>\epsilon^*}=1-\text{const}\times\frac{\hbar\omega_0}{2mv^2}\,, \tag{A13b}$$

where the constant has the value 0.5328 for $\epsilon^*=\hbar\omega_0$. This demonstrates the fact[1] that the leading straggling contribution stems exclusively from high momentum transfers, $\epsilon_k>\epsilon^*$, but that the logarithmic correction term for the *static* electron gas originates in plasma resonance excitation.

Finally, from (A11b) and Ref. 29, one finds

$$w^{(1)}_{\epsilon_k<\epsilon^*}=\text{Const}\times\frac{\langle v_2^2\rangle}{v^2}\,, \tag{A14a}$$

$$(w^{(1)})_{\epsilon_k>\epsilon^*}=\frac{\langle v_2^2\rangle}{v^2}\left[\tfrac{1}{3}\ln\frac{4mv^2}{\hbar\omega_0}-\frac{7}{8}-\text{Const}\right]\,, \tag{A14b}$$

where the constant has the value 0.5690 for $\epsilon^*=\hbar\omega_0$.

This demonstrates that the logarithmic shell correction to the straggling parameter originates in high momentum transfers, while both small and large momentum transfers contribute to the term proportional to $\langle v_2^2\rangle/v^2$.

*Permanent address.

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