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Energy losses by slow ions and atoms to electronic excitation in solids*

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We consider the theory of energy losses by slow ions and atoms to electronic excitations in an electron gas. Predictions of the theory are compared with experimental data on ion penetration in several different solids. We also compare the stopping power obtained from linear-response theory with that found from numerically computed phase shifts for electron scattering on the screened potential of an ion. The stopping power of an electron gas for slow, singly ionized He atoms is calculated from linear-response theory, using a wave function for the bound electron determined self-consistently in the electron gas.

I. INTRODUCTION

The stopping power of a medium for an energetic ion or atom is of recurring interest in physics. The instance in which v_0, the speed of the projectile traveling in a solid, is much less than some characteristic average velocity of electrons in the solid is of special interest in cases such as the slowing and reflection of hydrogen atoms impinging on the inner wall of a controlled thermonuclear reactor.[1] This problem has furnished motivation for the recent Monte Carlo studies by Oen and Robinson,[2] which have been carried out in order to estimate the number and energy of ions reflected from a metal surface. These workers have employed the atomic-collision theories of Lindhard, Scharff, and Schiøtt,[3] and Firsov[4] to estimate energy losses by ions in the metals.

We here reexamine the theory of energy loss by slow protons and He^+ ions in an electron gas as a function of electron-gas density. We suggest procedures for using these results to determine energy loss in the inhomogeneous electron gases existing in real metals.

We present, in Sec. II, a survey of theories relevant to the slow-proton problem, giving stopping power in an electron gas as a function of gas density. This density is characterized by the standard electron-spacing parameter r_s, usually called the one-electron radius, and defined by

$$\tfrac{4}{3}\pi r_s^3 = n_0^{-1} ,$$

where n_0 is the number density of electrons in the electron gas and r_s is measured in units of $a_0 = \hbar^2/me^2$, the first Bohr radius.

The present paper is of broader scope and emphasizes somewhat different aspects than the work of Trubnikov and Yavlinskii.[5] They were interested in seeing if the energy loss is proportional to projectile velocity at low energies. Agreement with data was perceived by them as being qualitatively satisfactory.

All of the results here are expressed in hartree atomic units ($e = \hbar = m_e = 1$). This means that the units of energy are hartree Ry ($\simeq 27.2$ eV). The results are clarified whenever other units are more expedient.

In hartree atomic units, the Fermi momentum p_F, wave vector k_F, and velocity v_F are identical, and in a degenerate electron gas, one has for instance

$$k_F = (\alpha r_s)^{-1} ,$$

where $\alpha = (4/9\pi)^{1/3}$. Also, the plasma energy in these units is

$$\omega_P = (3/r_s^3)^{1/2} \text{ hartree Ry} .$$

The one-electron radius $r_s = (3/4\pi n)^{1/3}$, where n is the electron density. If it is desired to express the Fermi energy E_F in Bohr Ry ($\simeq 13.6$ eV), one simply has to square k_F:

$$E_F = k_F^2 = (\alpha r_s)^{-2} \text{ Bohr Ry} .$$

In Sec. III, we examine the possibility of energy losses by the mechanism of plasmon excitation, going beyond linear theory to examine higher-order processes.

We return to linear theory in the ensuing sections, and in Sec. IV obtain the stopping power as a function of r_s for a He^+ ion moving with velocity $v_0 \ll v_F$ in an electron gas. Although the bound electron is subject to a screened potential, rather than the bare Coulomb potential, binding is shown to exist over a large range of r_s values.

Section V describes a phase-shift calculation of the stopping power in which electrons at the Fermi surface are viewed as scattering from the screened potential of a proton. The phase shifts are nu-

merically obtained and forced to satisfy the Friedel sum rule. This procedure gives a criterion for determining the screening length for the potential.

All of the results are compared and displayed graphically along with the limited amount of data presently available in this low-energy realm.

II. COMPARISON OF ELEMENTARY THEORIES

The classic treatment of electronic stopping power is that of Fermi and Teller.[6] They were interested to see if the intrinsic lifetime of a muon with velocity $v_0 \ll v_F$ is comparable to the time required for it to slow to rest in the medium. Arguing that the degeneracy of an electron gas restricts participation of the struck electrons to those within an approximate range v_0 of v_F, they found the energy loss per unit distance traversed in the medium to be

$$\frac{dW}{dR} = \frac{2v_0}{3\pi} \ln\frac{1}{\alpha r_s} . \tag{1}$$

If this is multiplied on the right-hand side by 52, it gives dW/dR in eV/Å. For $r_s \ll 1$ and $v_0 \ll v_F$ the Fermi-Teller formula gives an especially simple standard of comparison. In the present instance, it is viewed as a limiting case for a proton intruder which results when a hydrogen atom impinges on a metal. The atom almost certainly loses its electron into the anonymity of the electron gas upon entering, and is thereafter bombarded from all sides by a nearly isotropic flux of the conduction electrons. Those which collide with the slowly moving ion take away a bit more energy than they bring to such encounters, and these dissipations eventually bring the ion to rest. The probability of ionization will be examined in Secs. IV and V.

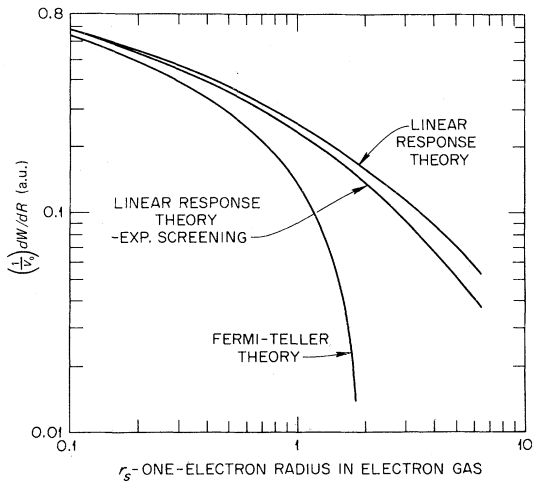

FIG. 1. Comparison of calculations of quantity $v_0^{-1} dW/dR$ (a.u.) for a slow proton in an electron gas. The results are expressed as a function of the one-electron radius r_s.

In 1954, Lindhard,[7] in a pioneering paper, showed how to do a many-body self-consistent treatment of the response of an electron gas to a perturbation. He thereby found an explicit expression for the linear-response function of the electron gas. His procedure was to consider the assembly of electrons in a manner similar to that used in passing from the microscopic form of Maxwell's equations in vacuum to their corresponding form inside matter. The momentum-frequency Fourier component $\phi_{\vec{k},\omega}$ of the electric potential was found to satisfy

$$\epsilon_{\vec{k},\omega} k^2 \phi_{\vec{k},\omega} = 4\pi \rho_{\vec{k},\omega} , \tag{2}$$

where $\rho_{\vec{k},\omega}$ is the Fourier component of the source density of electric charge. If one considers a swift proton as a classical point charge moving at constant velocity v_0 in the gas, elementary electrodynamics leads to

$$\frac{dW}{dR} = \frac{2}{\pi v_0^2} \int_0^\infty \omega\, d\omega \int_{\omega/v_0}^\infty \frac{dk}{k} \operatorname{Im}\left(-\frac{1}{\epsilon_{\vec{k},\omega}}\right) \text{ a.u.} \tag{3}$$

Lindhard's expression for $\epsilon_{\vec{k},\omega}$ may then be used to find dW/dR. This result gives an improvement over the Fermi-Teller formula in the limit $v_0 \ll v_F$, viz.,

$$\frac{dW}{dR} = \frac{2v_0}{3\pi}\left[\ln\left(1+\frac{\pi}{\alpha r_s}\right) - \frac{1}{1+\alpha r_s/\pi}\right] \text{ a.u.} , \tag{4}$$

as shown by Ritchie.[8] For an intruder of charge Z_1, this formula, and the Fermi-Teller formula, each have a factor of Z_1^2 multiplying the right-hand side. For $r_s \ll 1$, Eq. (4) reduces to Eq. (1).

Equation (4) is derived using an approximate form for $\epsilon_{\vec{k},\omega}$ which is equivalent to assuming that the potential about an ion is exponentially screened by density fluctuations in the electron gas. Actually, the potential about the ion has a long oscillatory tail decreasing as $Z_1 r^{-3} \cos(k_F r + \phi)$, corresponding to the existence of Friedel oscillations.[9] If v_0 increases much beyond v_F an oscillatory wake appears in the trail of the ion.[10] These oscillations constitute then an important mode of energy loss for swift protons, and may bind an electron in the wake. While we present results without the assumption of exponential screening, in addition to the results shown in Eq. (4), we do not consider the high speeds of wake-riding situations here. The results for $v_0^{-1} dW/dR$ in linear-response theory, and in linear-response theory with exponential screening are each shown in Fig. 1 as a function of r_s. Also shown is the Fermi-Teller result.

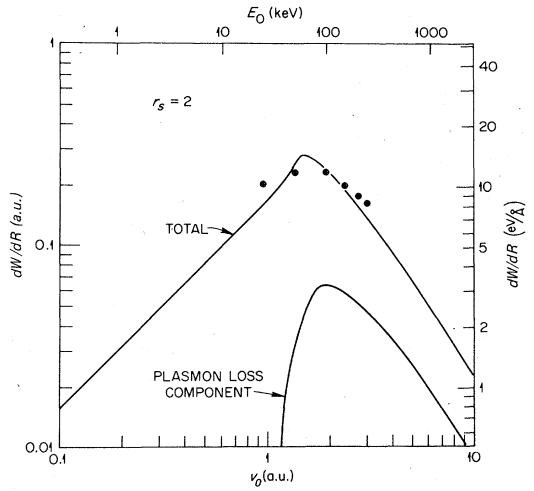

FIG. 2. Variation of energy-loss function dW/dR with proton velocity (v_0). The solid curve was computed for $r_s = 2.07$ (A1) from Eq. (3). The contribution of plasmon excitation is displayed separately. The dots show experimental data of Young (Ref. 11).

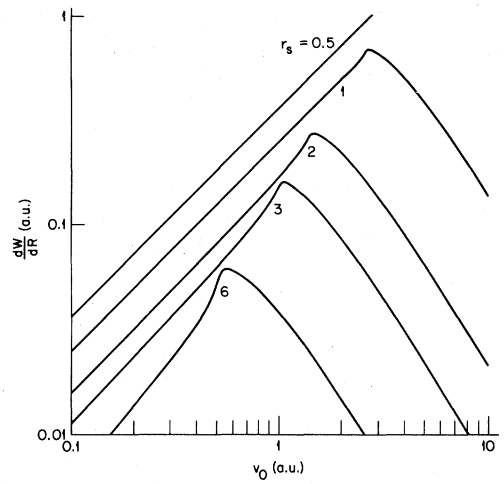

FIG. 3. The total energy-loss function (dW/dR) as a function of proton velocity (v_0) for several values of the one-electron radius r_s of an electron gas.

III. POSSIBILITY OF PLASMON EXCITATION

At higher velocities than v_F, the plasmon-loss mechanism must be considered. In Fig. 2, we show the variation of the total dW/dR (a.u.) with v_0 for a proton at an electron-gas density approximately equal to that of aluminum. The total is computed from Eq. (3) using the Lindhard dielectric function. The contribution from plasmon excitation is shown separately in the figure. Experimental data are shown in this figure as dots and are taken from the work of Young.[11]

Figure 3 shows the total dW/dR computed as was done for Fig. 2, but results are displayed for several different values of r_s. The energy-loss function dW/dR remains linear at high proton velocities for the smaller values of r_s (higher densities of the electron gas). It is interesting that plasmons are not excited until fairly high proton energies (over 8 keV) even for $r_s = 6$. This is the case because there is a mismatch in energy and momentum transfer between a plasmon and a low-energy proton. At a given energy loss, the slow proton must transfer an amount of momentum which may be too large for the plasmon to accept. Although a proton with an energy of several keV might be expected to create many 15-eV quanta of the plasmon in aluminum, this just does not occur in a linear theory.

It is conceivable that higher-order processes might break the "selection rule" just described. Two possible compound processes are shown in Figs. 4(a) and 4(b). The contribution of the first of these (scatter of the proton from a metal core ion with accompanying plasmon emission) has been calculated and found to be negligible for slow protons. The reason for this lack of significance is sensible in view of the fact that, as in bremsstrahlung, the contribution is proportional to the square of the acceleration of the deflected particle. For a proton this acceleration in deflecting from a metal core ion is small.

The diagram of Fig. 4(b) offers another possible higher-order process, but it has not yet been analyzed in detail.

A projectile may excite surface plasmons while impinging on a metal surface. We have made a rough estimate of the energy lost by a slow proton approaching a surface at near-grazing incidence, and find losses which are probably small compared with losses to volume excitations. It is most likely that the contribution is even less for atomic projectiles; a hydrogen atom has a much weaker electric interaction with the surface than

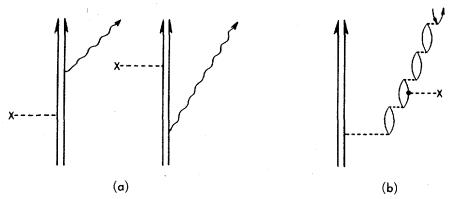

FIG. 4. (a) Feynman diagrams in which a proton scatters from an ion core and emits a plasmon. Both time orderings are shown. (b) Feynman diagram in which a proton gives rise to a string of polarization bubbles (electron-hole pairs) with an elastic scattering of one of the electrons or holes. The elastic scattering vertex must be inserted alternatively in all bubbles.

a proton has. We show only the result of this calculation, the energy loss at the surface being given in atomic units by

$$\Delta\omega = \frac{2\omega_s}{3v_F}\left(\frac{v_0}{v_F}\right)^2 \frac{1}{\cos\theta} , \tag{5}$$

where θ is the angle between $\vec{v}_0$ and the surface normal, and ω_s is the surface-plasma energy. Using $v_0 = 0.1$, $v_F = 1$, $\omega_s = 1$, and $\cos\theta = 0.02$, the loss is only 5 eV.

IV. LINEAR-RESPONSE THEORY FOR A PARTIALLY IONIZED INTRUDER

In the Fermi-Thomas model of a degenerate electron gas, an ion that travels with speed $v_0 \ll v_F$ induces a surrounding, spherically symmetric polarization of the medium that screens the electric potential of the ion. If Z_1 is the ion's charge, the potential at a distance r from the ion is found in this form of the random-phase approximation to be

$$V(r) = Z_1 e^{-\kappa r}/r , \tag{6}$$

where the inverse screening length κ is given by

$$\kappa = 3\alpha/(r_s)^{1/2} . \tag{7}$$

Since r_s for real metals has an approximate range given by $1.5 \lesssim r_s \lesssim 6$, κ ranges over values given by $0.6 \lesssim \kappa \lesssim 1.3$.

For a proton intruder, the calculation of Rogers, Graboske, and Harwood[12] shows that the potential $V(r)$ in Eq. (6) can only marginally bind an electron. They found by numerical integration that the number of bound states under the influence of $V(r)$ is for the lowest energy states

$$n^* = 0.5829 + 0.4993 Z_1 \kappa^{-1} \quad (\text{for } n^* < 10) . \tag{8}$$

A simple calculation with the Bohr model for a circular orbit also shows the marginal nature of such binding for $Z_1 = 1$. In an electron gas, the binding energy calculated relative to vacuum must be altered by adding the magnitude of the work function, so the binding is weaker than Eq. (8) indicates. This was considered by Callaway[13] in his discussion of the autoionization of positronium in an electron gas. Also, the binding is weaker due to the exchange interaction, as shown by Isenberg.[14]

Since $V(r)$ is not self-consistent (due to the polarization of the electronic medium by the presence of an electron in orbit), it is possible that the binding is actually a bit stronger than that given by Eq. (8). We consider this and calculate the binding energy for an electron in orbit about an intruder of charge Z_1 using a self-consistent potential. The calculation involves first finding this potential, and then variationally computing the binding energy assuming a wave function equal to

$$u(r) = (Z_2^3/\pi)^{1/2} e^{-Z_2 r} , \tag{9}$$

where Z_2 is the parameter to be varied in minimizing the total energy of the electron.

The self-consistent potential for the electron is given by

$$V_{sc}(r) = -Z_1 e^{-\kappa r}/r + V(\kappa, Z_2, r) - V(0, Z_2, r) , \tag{10}$$

where

$$V(\kappa, Z_2, r) = \int d^3r'\, u^*(r') u(r') \frac{e^{-\kappa|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} . \tag{11}$$

Then,

$$\Delta V = V(\kappa, Z_2, r) - V(0, Z_2, r) \tag{12}$$

is the potential at the position of the electron due to polarization engendered in the electron gas by the electron itself.

We find that

$$V(\kappa, Z_2, r) = \frac{16 Z_2^4}{(4Z_2^2 - \kappa^2)^2} \times \left[\frac{e^{-\kappa r}}{r} - \frac{e^{-2Z_2 r}}{r}\left(1 + \frac{r(4Z_2^2 - \kappa^2)}{4Z_2}\right)\right] . \tag{13}$$

The Hamiltonian H_{sc} satisfies the Schrödinger equation given in atomic units as

$$H_{sc} u(r) = \frac{-1}{2r}\frac{\partial^2}{\partial r^2}[ru(r)] + V_{sc}(r) u(r) = E_{sc} u(r) . \tag{14}$$

The expected value of H_{sc} using Eq. (9) is found to be

$$\langle H_{sc}\rangle = \frac{Z_2^2}{2} - \frac{4 Z_1 Z_2^3}{(2Z_2 + \kappa)^2} - \frac{5Z_2}{8} + \frac{Z_2^3}{2(2Z_2 + \kappa)^4}(\kappa^2 + 8Z_2\kappa + 20Z_2^2) . \tag{15}$$

A sixth-order polynomial results from setting the derivative of $\langle H_{sc}\rangle$ with respect to Z_2 equal to zero. The solutions found numerically for the case of $Z_1 = 2$ (e.g., an α particle, which might be expected to bind an electron), and for κ given by Eq. (7), were substituted into Eq. (15) to obtain the binding energy. Relative to vacuum, $\langle H_{sc}\rangle$ ranges from the limiting value of -5.3 eV as $r_s \to 0$ down to the value -54.4 eV as $r_s \to \infty$. The latter is the value obtained for the ground-state energy of an electron in orbit about an α particle with no electron-gas present, as one would expect.

The value as $r_s \to 0$ of $\langle H_{sc}\rangle$ is not changed by taking $Z_1 = 0$, and so represents a self-binding of the electron due to polarization of the surrounding electrons. This contribution to the binding is in-

dependent of Z_1, and thus is present also for an electron in orbit about a proton. The subtraction of the work function weakens the binding calculated in this manner, but does not always make the binding energy positive even for r_s as large as the values it assumes for real metals. For example, for $r_s=2$, the $Z_1=0$ case gives a binding energy relative to vacuum of −4.1 eV, which is a bit larger in magnitude than the work function for aluminum. The presence then of a proton would increase the magnitude of the binding energy to a point that would in this model cause an electron to be bound. In fact, this model neglects additional physical effects that weigh against such binding. For instance, we have neglected to account for the influence of the Lindhard linear-response function beyond the form it gives for $V(r)$ in Eq. (6) in using the random-phase approximation, and have used only the Fermi-Thomas expression for the inverse screening length. Also, we have neglected the influence of the metal core ions, which tend to strip the intruder of the bound electron. We should actually account for exchange as well, and it is thought then on balance that an improved model would deny any binding of an electron to a proton in a real metal in agreement with experiment.

We expect that an electron will be bound to an α particle over a large range of r_s. For example, the minimum value of $\langle H_{sc}\rangle$ at $r_s=1$ is found in our model to be about −24 eV relative to vacuum, becoming even more negative at larger r_s. The stopping power in this case must then be calculated for a charge density of the intruder that accounts for the bound electron. The results should converge to those of a bare α particle at low r_s, and should approach those of a proton at high r_s, where the binding is very strong, since the low-energy stopping power is independent of the intruder's mass.

We assume that the electron is bound in its lowest energy state around the α particle. Therefore, the charge density generated by the moving He^+ ion may be written

$$\rho = Z_1\delta(\vec{r}-\vec{v}_0t) - Z_3|u(\vec{r}-\vec{v}_0t)|^2 , \tag{16}$$

where $\vec{v}_0t$ describes the position of the ion at time t, and $u(\vec{r})$ is the wave function for the bound electron. The value of Z_3 actually is unity for the He^+ ion, but is indicative of the number of electrons in the charge cloud in other instances.

The Fourier transform of ρ may be written

$$\rho_{\vec{k},\omega} = [F(k^2)]^{1/2}\delta(\omega-\vec{k}\cdot\vec{v}_0) , \tag{17}$$

where $F(k^2)$ is given below.

Proceeding in an analogous way to the classical derivation of Eq. (3), one finds the ion's energy loss per unit distance traversed in the medium to be

$$\frac{dW}{dR} = \frac{1}{4\pi^4 v_0}\int \frac{d^3\vec{k}}{k^2}F(k^2) \times \int_0^\infty \omega\, d\omega\, \mathrm{Im}\left(\frac{-1}{\epsilon_{\vec{k},\omega}}\right)\delta(\omega-\vec{k}\cdot\vec{v}_0) . \tag{18}$$

Following Lindhard, we introduce, in atomic units, the variables

$$x = 2\omega/k_F^2 \quad \text{and} \quad z = k/2k_F , \tag{19}$$

and for $v_0 \ll v_F$, the general linear-response function,

$$\epsilon_{\vec{k},\omega} = 1 + (1/\pi z^2 k_F)[f_1(x,z) + if_2(x,z)]$$

reduces to the result, valid for small x,

$$\epsilon_{\vec{k},\omega} \simeq 1 + (1/\pi z^2 k_F)(1 + i\pi x/8z) . \tag{20}$$

Introducing $\zeta = (Z_2/k_F)^2$, one finds for $F(k^2) = \tilde{F}(z^2)$ that

$$\tilde{F}(z^2) = 4\pi^2[Z_1 - Z_3\zeta^2/(z^2+\zeta)^2]^2 . \tag{21}$$

When this result is used with Eq. (20) in Eq. (18) one finds the "reduced" stopping power for a slow ion in an electron gas. For purposes of graphical comparison we compute $v_0^{-1}\,dW/dR$, which is found in this instance to be

$$\frac{1}{v_0}\frac{dW}{dR} = Q^2 A\left(\frac{\pi}{\alpha r_s}\right) + \frac{Z_3\zeta^2}{\lambda^2}\left[\left(\frac{3Z_3\zeta^2}{\lambda^2} - 2Z_1\right)A\left(\frac{1}{\zeta}\right) + QU + Z_3Y\right], \tag{22}$$

where

$$\lambda = \alpha r_s/\pi - \zeta = (\alpha r_s/\pi)(1 - Z_2^2\pi\alpha r_s) ;$$

$$Q = Z_1 - Z_3\zeta^2/\lambda^2 ;$$

$$U = \frac{8}{3\pi\lambda}\left[\frac{\alpha r_s}{\pi}\ln\left(1+\frac{\pi}{\alpha r_s}\right) - \zeta\ln\left(1+\frac{1}{\zeta}\right)\right];$$

$$Y = \frac{\zeta^2}{9\pi}\left(\frac{1}{\zeta^2} - \frac{6}{\zeta\lambda} - \frac{\zeta+3}{(\zeta+1)^3} + \frac{6(\zeta+2)}{\lambda(\zeta+1)^2}\right);$$

and

$$A(x) = (2/3\pi)[\ln(1+x) - 1/(1+x)] .$$

For a very-high-density electron gas, the screening length κ^{-1} from Eq. (7) is so much less than the orbital radius of the bound electron that the full nuclear charge is effective in causing excitations. The quantity ζ^2/λ^2 in this high-density limit is negligible, so $Q \simeq Z_1$ and one has the subsequent reduction of Eq. (22) to

$$\frac{1}{v_0}\frac{dW}{dR} \simeq \frac{2Z_1^2}{3\pi}\left[\ln\left(\frac{\pi}{\alpha r_s}\right) - 1\right] \text{ a.u.} , \tag{23}$$

which is the high-density limit of Lindhard's result for a bare intruder particle of charge Z_1.

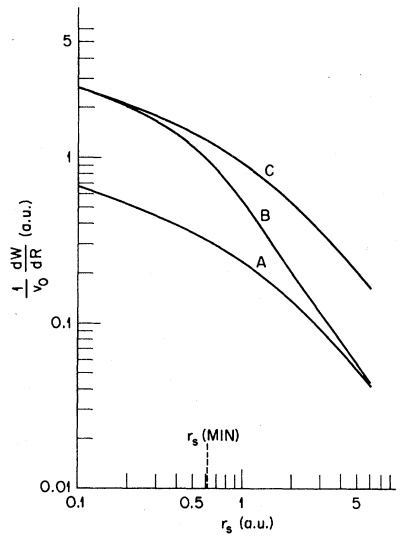

FIG. 5. Variation of $v_0^{-1}\,dW/dR$ with r_s as found for a slow He^+ ion from Eq. (22) (curve B), as found in linear response theory for a bare proton (curve A), and for an α particle (curve C) with $v_0 \ll v_F$ in each case.

In the case of a very-low-density electron gas, the orbit radius of the bound electron is much less than the screening length of the medium. The potential seen by this electron is then very nearly the bare Coulomb potential of the nucleus of the ion. In this limit, $\xi^2/\lambda^2 \to 1$, and $Q \to Z_1 - Z_3$, while Z_2 approaches the value of the nuclear charge. The results of Eq. (22) then approach those of a particle intruder of effective charge equal to the square root of $(5Z_3^2 - 4Z_1Z_3 + Z_1^2)$. In the case of an He^+ ion intruder, $Z_1 = 2$, and $Z_3 = 1$. Therefore, the low-density limit of the stopping power for this ion will be nearly equal to that found for a bare proton, the binding of the electron to the α particle being strong enough to evince this behavior in the rarefied medium in this low-energy realm.

The graph of $v_0^{-1}\,dW/dR$ as a function of r_s as obtained from Eq. (22) for the case of an He^+ ion is shown as curve B in Fig. 5. Also shown is $v_0^{-1}\,dW/dR$ for a bare proton (curve A), and a bare α particle (curve C), calculated from Eq. (4) multiplied by $Z_1^2 = 1$ in the former case and $Z_1^2 = 4$ in the latter case. The limiting cases discussed above may be discerned in Fig. 5 quite clearly.

Shastry, Jha, and Rajagopal[15] have given an improved formula for κ over the Fermi-Thomas result shown in Eq. (7). Using a self-consistent many-body approximation to the static dielectric constant of an electron gas, they found that, in lieu of the value of κ from Eq. (7), one has $\kappa = 2\sqrt{x}$, where

$$x = \frac{\alpha r_s/\pi}{1 - (\alpha r_s/\pi)[1 - x\ln(1 + 1/x)]} \,. \tag{24}$$

This equation may be solved in only a few iterations if recast in the form

$$x = \frac{c + [c^2 + 4\ln(1 + 1/x)]^{1/2}}{2\ln(1 + 1/x)} \,, \tag{25}$$

where $c = 1 - \pi/\alpha r_s$, but it makes only about a 2% change in the results of Fig. 5. The effects of Eq. (25) are also assessed in the next section.

V. PHASE-SHIFT CALCULATION OF STOPPING POWER FOR A SLOW PROTON

It is well appreciated that linear-response theory is suspect at real metallic densities, since even though self-consistent, it is essentially based on the first Born approximation. An improved calculation can be performed beginning with consideration of the diagrammatic perturbation series shown in Fig. 6. If one sums all the terms in this infinite series, including the effect of the Pauli principle in restricting electron states to those outside the occupied Fermi sphere, *but only in the very last transition*, one finds a quite simple result. One is able to express the energy-loss function dW/dR for a proton in the electron gas as[16]

$$\frac{dW}{dR} = v_0 v_F n_0 \sigma_{tr} \,, \tag{26}$$

where σ_{tr} is the usual transport cross section. It is given in terms of the scattering cross section by

$$\sigma_{tr} = \int d\sigma (1 - \cos\theta) = \frac{4\pi}{k_F^2} \sum_{l=0}^{\infty} (l+1)\sin^2(\delta_l - \delta_{l+1}) \,, \tag{27}$$

where θ is a scattering angle in the proton's frame, and δ_l is the phase shift of the lth partial wave for scattering of electrons at the Fermi surface from the screened potential of the proton.

Although we first performed a Wentzel-Kramers-

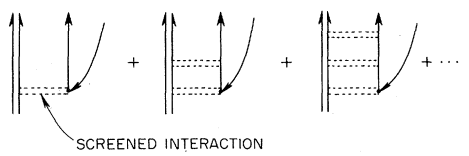

FIG. 6. Sum of Feynman diagrams representing the scattering of electrons in the medium on the proton. The basic interaction is assumed to be a screened Coulombic one, as in Eq. (6). Multiple scattering occurs with specific account of the operation of the exclusion principle only following the last interaction.

Brillouin (WKB) calculation of the δ_l, the error in this approximation motivated us to perform a numerical integration for the phase shifts. We have done this by direct numerical integration of the Schrödinger equation's radial part:

$$\left(\frac{d^2}{dr^2}+k^2-\frac{l(l+1)}{r^2}-\frac{2e^{-\kappa r}}{r}\right)u_l(r)=0\ , \qquad (28)$$

where $k=k_F=(\alpha r_s)^{-1}$ in the frame of the proton.

A technique that lends itself to easier computation of phase shifts has been given by Calogero.[17] He has been able to reduce the information in the Schrödinger equation to the form of a nonlinear first-order differential equation for a function $\delta_l(r)$, called the phase function. The asymptotic value of $\delta_l(r)$ as $r\to\infty$ is the phase-shift δ_l. The only boundary condition needed in this instance is $\delta_l(0)=0$, and the phase shifts calculated in this manner do not suffer from the typical modπ ambiguity if the differential equation is written

$$\frac{d\delta_l(r)}{dr}=-\frac{V(r)}{k}\left[\hat{j}_l(kr)\cos\delta_l(r)-\hat{n}_l(kr)\sin\delta_l(r)\right]\ , \qquad (29)$$

where $\hat{j}_l$ and $\hat{n}_l$ are Ricatti-Bessel functions. They may be written in closed form in terms of coskr and sinkr and their arguments, since they are related to the ordinary fractional-order Bessel functions $J_{\pm(l+1/2)}$:

$$\hat{j}_l(x)=(\tfrac{1}{2}\pi x)^{1/2}J_{(l+1/2)}(x)\ ;$$
$$\hat{n}_l(x)=(-1)^{l+1}(\tfrac{1}{2}\pi x)^{1/2}J_{-(l+1/2)}(x)\ . \qquad (30)$$

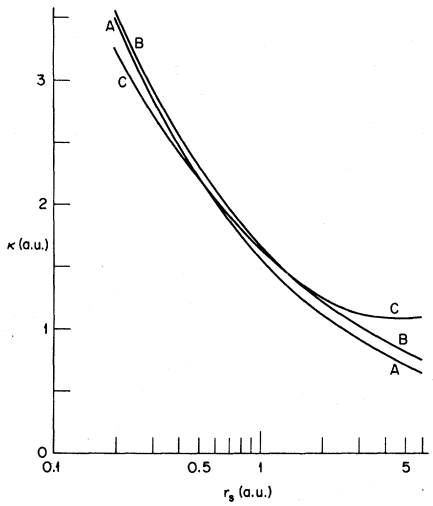

FIG. 7. Variation of the inverse screening length (κ) with the one-electron radius (r_s). Curve A gives the Fermi-Thomas results, Eq. (6); curve B gives the results of setting $\kappa=2\sqrt{x}$ with x obtained from Eq. (25); and curve C gives the values of κ dictated by Eq. (32).

For example, in the $l=0$ case one has that the s-wave phase function $\delta_0(r)$ satisfies the simple equation

$$\frac{d\delta_0(r)}{dr}=-\frac{V(r)}{k}\sin^2[kr+\delta_0(r)]\ , \qquad (31)$$

which may be numerically integrated with a programmable calculator for the Fermi-Thomas screened potential.

Calogero's method also yields the number of bound states, which he discerns from Levinson's theorem. In the terms of a graph of $\delta_l(r)$ versus r, a bound state is discerned whenever the phase function displays a plateau near multiples of π. The method is thus a bit confusing when bound states occur, since it is easy to confuse such plateaus with the actual asymptote, which is reached only for values of the radial coordinate beyond which the potential is negligible compared to k^2.

In determining the inverse screening length κ in $V(r)$, we used first the improved formula given by Eq. (25). As anticipated, this gave satisfactory results only for $r_s\lesssim 2.5$, the Friedel sum rule being satisfied to within 1.7% at $r_s=2$. This rule is

$$1=\frac{2}{\pi}\sum_l(2l+1)\delta_l\ . \qquad (32)$$

The deviation in the results from Eq. (32) was about 90% for $r_s=6$. Therefore, κ was chosen to make the phase shifts satisfy Eq. (32). Figure 7 shows a graph of κ found in this manner as a function of r_s (curve C), and also shows κ obtained from Eq. (7) (curve A) and κ obtained from Eq. (25) (curve B). It was only necessary to carry the sum in Eq. (32) to $l=9$ in obtaining the results shown as curve C in Fig. 7.

The results of our calculation of the stopping power from numerical computation of the phase shifts and subsequent use of Eqs. (27) and (26) are shown in Fig. 8, where we plot $v_0^{-1}dW/dR$ vs r_s. Also shown are predictions of other relevant theories, and some of the experimental data of Arkhipov and Gott.[18] Their data on stopping power is proportional to v_0 as expected in the low-energy range, but their values of $v_0^{-1}dW/dR$ are about 0.3 a.u. for Cu and Al, which is substantially larger than theory predicts. Such measurements are extremely difficult to carry out, and it is expected that the data points probably should have large error bars on them.

It might be mentioned that a WKB computation was found to yield values (10–20)% higher than those shown in curve D of Fig. 8, the error being less at higher r_s. These results are not shown in Fig. 8.

The value of r_s appropriate to Al was determined simply from the associated valence-band density, while the value of r_s for C was found from a Hartree-Fock calculation of the density in a spherically averaged Wigner-Seitz cell.[19] Figure 9 shows calculated r_s vs r values for C and Al. We used the maximum r_s in both curves, arguing that a slow proton tends to stay as far from the lattice ions as possible. A more detailed calculation would involve averaging the results similar to those of Fig. 8 over the distribution of density and r_s encountered by the proton in its trajectory through the lattice. In effect, one would consider the space-varying density of electrons in a solid as an ensemble of electron gases of varying densities. This procedure has been used with good effect by Lindhard and co-workers[20,21] to compute the stopping power of atomic systems for high velocity ($v_0 > v_F$) charges.

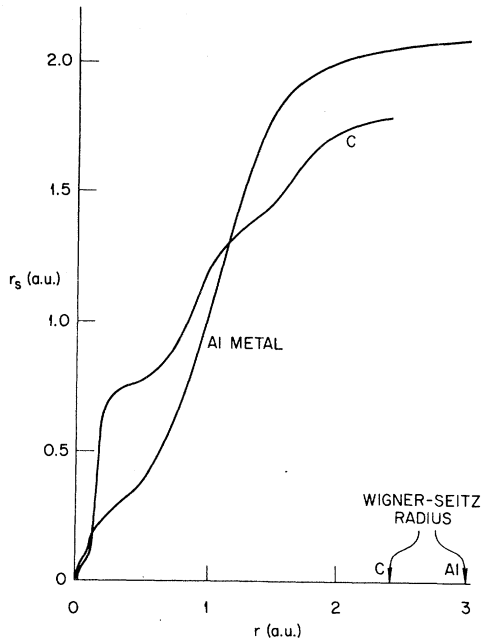

FIG. 9. The equivalent one-electron radius $r_s(r)$ plotted vs position in the Wigner-Seitz cell for aluminum metal and for carbon.

VI. CONCLUSIONS

Motivated by questions of radiation damage to the inner wall of a thermonuclear reactor, we have studied dW/dR, the energy loss per unit path length of slowly moving protons and α particles in an electron gas. Linear-response theory has been employed to evaluate this quantity in electron gases of various densities. In addition we have evaluated dW/dR by numerical evaluation of the phase shift of an electron at the Fermi surface scattering on the screened potential of the projectile. We find quite good agreement (±10%) over the range of densities existing in real metals. We have investigated, in a self-consistent manner, the effect of polarization in the medium on the binding of an electron to an He^+ projectile and have evaluated the energy loss for this case. Comparison of our results with available limited experimental data is made.

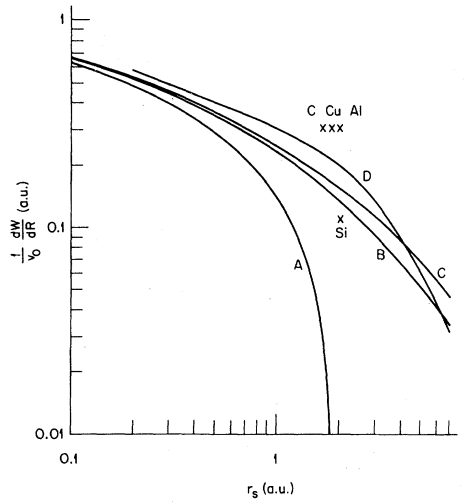

FIG. 8. Comparison of theoretical predictions and experimental data on $v_0^{-1}dW/dR$ as a function of the one-electron radius (r_s) in the case of a slow-proton intruder in a solid. Curve *A* gives the Fermi-Teller results [Eq. (1)]; curve *B* gives the results of linear-response theory with exponential screening [Eq. (4)]; curve *C* gives the predictions of general linear-response theory; and curve *D* gives the results of a numerical integration of the equations for the phase shifts and use of Eqs. (26) and (27).

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