

Nonlinear stopping power and energy-loss straggling of an interacting electron gas for slow ions

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Theoretical calculations of the basic quantities that characterize the stopping of an interacting electron gas for slow ions are presented. An appropriate low-frequency expansion for the imaginary part of the density response function has been used to modify well-known results for the noninteracting electron gas. The inner dissipative nature of the elementary electron-hole excitation is characterized by a complex local-field correction function. The basic quantities are expressed in terms of the phase shifts determined from a nonlinear density-functional formalism.

I. INTRODUCTION

The problem of energy loss of charged particles in a degenerate electron plasma has been studied by many authors using a variety of approaches. The theoretical descriptions are based on an assumption that the system is of linear-dissipative nature. It should be emphasized, however, that this linearity does not imply any physical restrictions on the permissible value of the mean density fluctuations of the system.¹

After the pioneering work of Fermi and Teller² some calculations were done within the framework of dielectric theory. In this formalism the absorption of energy and momentum by the system appears as a finite imaginary operator in the equations for the retarded field. For the noninteracting electron gas Lindhard³ determined the relevant propagator to first order in the coupling constant e^2 . The first explicit calculation which goes beyond the Fermi-Teller result was performed by Ritchie.⁴ In his stopping-power calculation, Ashley⁵ used a phenomenological damping constant in the Mermin⁶ form of the dielectric function. Static⁷ and dynamic⁸ local-field corrections have been introduced to improve the previous noninteracting results. Recently, Hu and Zaremba⁹ have determined an expression for the quadratic density response function to obtain the Z^3 correction to the stopping power of a slow ion moving in a homogeneous electron gas. An extension of the free-electron propagator formalism to the stopping power and screening problems of the very-high-density electron gas was done by Nagy,¹⁰ using a relativistic covariant many-body theory¹¹ for point particles and neglecting vacuum polarization effects.

As an alternative theoretical background, besides the dielectric formalism, the classical binary-encounter approximation (BEA) can be used to describe the pure elastic scattering between the intruder ion and the particles of the target. After the work of Trubnikov and Yavlin-skii,¹² Sigmund,¹³ and, later, Ferrariis and Arista¹⁴ demonstrated the usefulness of this kinetic approach. From a more rigorous point of view, several works have

been done to treat the response of an electron system to a localized time-dependent perturbation (LTDP) induced by the incoming ion and to calculate the stopping power. Blandin *et al.*¹⁵ have performed their calculation in the framework of the Keldysh formalism. Very recently, Schonhammer¹⁶ has given a didactic description within the general scattering theory for an electron gas of independent constituents.

In order to clarify the connection between the above-mentioned methods, the following considerations may be done. In the dielectric formalism the scattering potential is immediately given. This method is exact for a high-density electron gas. For this density, in the examined static limit, the Friedel sum rule¹⁷ is automatically satisfied via the first Born approximation for the forward scattering amplitude. In the appropriate (static) limit the expressions of both the BEA and the LTDP methods require the knowledge of this potential. Furthermore, a higher-order Born series for the scattering amplitude may be adequate, provided that the potential does not support bound states.¹⁸

Model potentials have been used¹⁹ to calculate phase shifts and the stopping power. The more powerful density-functional theory (DFT) allows one to calculate the induced screened potential²⁰ and density fluctuation in a self-consistent way. The Friedel sum rule is a self-consistency condition²¹ on the scattering potential that model-potential calculations are forced to satisfy. At metallic densities of the electron gas the results of the DFT calculations for the quantities that characterize the stopping phenomenon differ markedly from those obtained from the dielectric description. Generally, the former results give a better agreement with the relevant experimental data. Explicit calculations for the stopping power within this formalism were first performed by Echenique *et al.*²² for H and He ions, and later were extended for higher ionic charges.²³ The energy-loss straggling²⁴ and the width of the particle states²⁵ have also been calculated in DFT. It is to be noted that the general improvements are due mainly to the correct phase-shift determination. In other words, these calculations reflect the

importance of *screening nonlinearities*. The response of the system remains *linear* to the external probe and this behavior is reflected in the determination of the available states for the density fluctuation near the Fermi level. The density-functional formalism has proven to be a very useful tool in calculating other atomic and electronic processes similar to the stopping power, such as the impurity resistivity,²⁶ the damping rate or friction coefficient²⁶ of a vibrating atom in a metal surface,²⁷ and diffusion of a heavy particle in metals within a path-integral approach.²⁸ The stopping-power results for the homogeneous electron gas serve as a background for averaging procedures when dealing with inhomogeneous (atomic) electron gases.²⁹

From a rigorous standpoint the *dynamic impurity* problem presents several complications. A many-body formalism is needed to treat the interaction with the surrounding medium and one also needs to use the Born-Oppenheimer conceptual scheme. On the other hand, the neglect of recoil, quantum effects in the motion of a massive particle, and the possibility of creating excitations in the internal state of the slow projectile (atomic-type processes) leave the problem more tractable.

In this paper, as an intermediate approach, we propose a method to take into account the interacting nature of the electrons in the medium *and* connect the formally different main approaches. These are the main purposes of this work. We determine in an appropriate way the imaginary part of the density response function and use the elastic scattering picture with correct phase-shift analysis in our transport problem. The organization of this paper is as follows. Section II deals with the method. In Sec. III our results are summarized, and comparison with earlier theoretical calculations as well as experimental data are made. Section IV is devoted to the conclusions.

II. THE METHOD

Using the density-response-function theory, it is easy to obtain the basic quantities that characterize the *composite* ion-electron gas system. These are³ the width of the particle states (related to the imaginary part of the particle self-energy) Γ , the stopping power dE/dR , and the straggling parameter Ω^2 . For the sake of unified description we introduce a physical auxiliary quantity. The differential-inverse mean free path for an ion with charge Z_1 moving with speed v in an electron gas is given by³⁰ (atomic units, with $e^2 = \hbar = m_e = 1$, are used throughout this paper, except where explicitly stated)

$$\frac{d^2\mu}{dq d\omega} = 2 \frac{q}{v^2} \frac{1}{(2\pi)^2} \left[\frac{4\pi Z_1}{q^2} \right]^2 \text{Im}\chi(q, \omega), \quad (1)$$

where $\chi(q, \omega)$ is the density-density response function related to the dielectric function via³¹

$$\epsilon^{-1}(q, \omega) = 1 - \frac{4\pi}{q^2} \chi(q, \omega). \quad (2)$$

From Eq. (1), one obtains

$$\Gamma = v \int dq \int d\omega \frac{d^2\mu}{dq d\omega}, \quad (3)$$

$$\frac{dE}{dR} = \int dq \int d\omega \omega \frac{d^2\mu}{dq d\omega}, \quad (4)$$

$$\Omega^2 = \int dq \int d\omega \omega^2 \frac{d^2\mu}{dq d\omega}. \quad (5)$$

In these equations the integration limits are determined by the impulse and energy conservation laws after connecting the system variables (q, ω) with the parameter (v) of the heavy moving ion. Here we adopt a formally exact representation³¹ for $\chi(q, \omega)$, which has the form of the Dyson equation

$$\chi^{-1}(q, \omega) = \chi_0^{-1}(q, \omega) + \frac{4\pi}{q^2} + \phi(q, \omega), \quad (6)$$

well known in the theory of Green functions.

In this equation, $\chi_0(q, \omega)$ is the complex Lindhard function,³ which may be introduced either in connection with linear response to an external probe or in terms of the interaction between the electrons themselves. The long-range correlations characteristic of the electron system have been taken into account explicitly by separating off the Coulomb interaction $4\pi/q^2$. Thus $\phi(q, \omega)$ represents the collisional part of the total effective interaction between density fluctuations. Note that in writing Eqs. (2), (6), and (8) we have used the notation and interpretation of Ref. 31.

The imaginary part of $\chi(q, \omega)$, the spectral function, is an odd function of ω with the causality property³²

$$\omega \text{Im}\chi(q, \omega) \geq 0. \quad (7)$$

This property is closely connected with the fact that the energy transfer per unit time from an external probe to a stable system in thermodynamical equilibrium is a non-negative quantity and is based on the existence of irreversible processes in thermodynamics. The equality holds only for reversible processes which are quasistatic, i.e., for $\omega = 0$ processes. When ϕ is replaced by zero, Eq. (6) gives the expression for the response function in the random-phase approximation (RPA). In the case where $\phi(q, \omega)$ is approximated by a pure real function $\phi(q)$, Eq. (6) reduces to the expression for the response function in the static mean-field approximation (SMFA). There is a well-known connection³¹ between $\phi(q, \omega)$ and the so-called dynamic local-field correction $G(q, \omega)$:

$$\phi(q, \omega) = - \frac{4\pi}{q^2} G(q, \omega). \quad (8)$$

Here $G(q, \omega)$ represents the short-range correlations between electrons in the homogeneous electron-gas system, and characterizes the *dynamic* electron-electron interaction. In SMFA, similarly to the quasiparticle-lifetime model, this self-energy correction to single-particle propagation is a pure real function (for a careful and detailed discussion see Ref. 33).

For small ω value we can write⁸

$$\text{Im}\chi(q, \omega) = \frac{\text{Im}\chi_0(q, \omega) + (4\pi/q^2)\chi_0^2(q)\text{Im}G(q, \omega)}{\{1 - (4\pi/q^2)\chi_0(q)[G(q) - 1]\}^2}, \quad (9)$$

where the denominator of this expression is the square of the static-electron-dielectric function^{34,31} $\epsilon_e(q)$. In Eq. (9) the abbreviations are

$$\text{Im}\chi_0(q, \omega) = \left[\frac{k_F}{\pi^2} \right] \frac{\pi \omega}{2 q k_F} \quad \text{for } q \leq 2k_F, \quad (10)$$

$$\begin{aligned} \chi_0(z) &= \left[\frac{k_F}{\pi^2} \right] f_1(z) \\ &= \left[\frac{k_F}{\pi^2} \right] \frac{1}{2} \left[1 + \frac{1-z^2}{2z} \ln \left| \frac{z+1}{z-1} \right| \right]. \end{aligned} \quad (11)$$

Here we have introduced the standard³ notation $z = q/(2k_F)$, where $k_F = 1.92/r_s$ and r_s is defined from the density

$$n = \frac{3}{4\pi r_s^3}.$$

The determination of $\text{Im}G(q, \omega)$ is a tough problem that requires a powerful many-body technique.³⁵ This quantity is related to the dissipative nature of the electron-hole excitation process.³³ We determine $\text{Im}G(q, \omega)$ according to the model of Gross and Kohn.³⁶ In this model the imaginary part of the dynamic local-field correction is given by (see the Appendix)

$$\text{Im}G(q, \omega) = a(n) \frac{q^2}{4\pi} \omega, \quad (12)$$

for small ω values, provided that the q dependence is valid in the range $0 \leq q \leq 2k_F$. The parameter $a(n)$ depends

only on the density of the system.

Equation (1), after the substitution of Eq. (9), gives an exact description for the energy loss of an infinitesimal external bare test charge (Z_1). It is easy to show (in the examined static limit) by this substitution that in Eq. (1) appears the square of the Fourier transform of the screened scattering potential

$$V(q) = \frac{4\pi Z_1}{q^2 \epsilon_e(q)}. \quad (13)$$

In this case, the elastic scattering between an electron and the screened test charge is described in the first Born approximation. The *remaining* part is the numerator of Eq. (9). It is determined by the time-dependent properties of fluctuations of the electron gas and may be treated *independently* of the presence of the incoming ion. This latter statement is equivalent to the assumption of the linear dissipative nature of the system. Because of this separability it seems natural to modify the *scattering part* only, for cases in which the ion charge is not infinitesimal, and the Born approximation is not justified. We shall demonstrate below that this modification gives all the well-known results.

We interpret $|V(q)|^2$ in terms of the nonrelativistic scattering theory by means of the substitution²⁵

$$|V(q)|^2 \rightarrow 4\pi^2 |F(\theta)|^2, \quad (14)$$

where $F(\theta)$ is the single elastic-scattering amplitude and $q = 2v_F \sin(\theta/2)$ is the momentum transfer ($v_F = k_F$ in a.u.). Thus with the aid of Eqs. (9)–(12) we obtain

$$L(p) = \frac{1}{2} \left[\frac{v_F}{\pi} \right]^2 \int_0^1 dy \int_0^\pi d\sigma(\theta, v_F) \left[2vv_F \sin \left[\frac{\theta}{2} \right] y \right]^p \left[1 + C \frac{12n}{\pi} a(n) f \left[\sin \frac{\theta}{2} \right] \right] \quad (15)$$

for the determination of the basic quantities that can be written

$$\Gamma = L(p=1), \quad (16)$$

$$\frac{dE}{dR} = \frac{1}{v} L(p=2), \quad (17)$$

$$W = \frac{1}{nv} \Omega^2 = \frac{1}{nv} L(p=3). \quad (18)$$

To obtain Eq. (15) we have used a simple variable change in the ω integration [see Eqs. (3)–(5)] via $\omega = (qv)y$.

In Eq. (15), $d\sigma$ is the usual differential cross section

$$d\sigma = 2\pi |F(\theta)|^2 \sin\theta d\theta, \quad (19)$$

and $f(z)$ is given by [$z = \sin(\theta/2)$]

$$f(z) = z[f_1(z)]^2, \quad (20)$$

which (from a numerical point of view) is expandable in a well-behaved convergent series for $0 \leq z \leq 1$, using [see Eq. (11)]

$$\ln \left| \frac{z+1}{z-1} \right| = 2 \sum_{k=1}^{\infty} \frac{z^{2k-1}}{2k-1}. \quad (21)$$

In Eq. (15), C is a parameter that we have introduced for the sake of uniformity in the numerical calculations. When $C=0$ Eq. (15) yields the well-known expressions of BEA,^{13–16,25,26} which are based on the noninteracting representation of the fluctuations. Consequently, $C=1$ refers to an interacting electron gas. The choice of C denotes two essentially different pictures of the electron system.

The above deduction is not rigorous in a mathematical sense. We think, on physical grounds, that it is true at least if the linear dissipative picture is true, provided that the multiple scattering can be ignored.³⁷ That is, if the particles of the incoming beam (the moving ions) represent a very diluted impurity concentration, the above substitution [Eq. (14)] does not violate the validity of the calculation.

The structure of Eqs. (9) and (15) shows the fact that the net scattering rate, in addition to the matrix elements

describing the single elastic scattering, must be proportional to the permissible value of the density fluctuations. This latter is *governed* by the numerator of Eq. (9) and has a deep connection with the one-body momentum distribution function³⁸ in a homogeneous electron gas.

For heavy ions at low velocities the screening can be regarded as static. A full discussion of the screening of a light dynamic impurity is considerably more complicated³⁹ than that of a heavy one, since the correlated motion of the interacting particles (electron-impurity) must be taken into account.⁴⁰ The problem of a light impurity in an electron gas cannot be ultimately reduced to a two-body problem, whatever effective interaction is used. This simple-scattering problem for light particles appears if we go beyond the first Born approximation and has the analogy of the recoil problem of a heavy particle.⁴¹

For finite mass impurity (M), the many-electron-impurity system is no longer separable into effective mass and relative coordinates, and one always has a many-body scattering problem with an associated noncancellation of the Fermi factors.⁴¹ These corrections for the infinite mass scattering amplitude appear first in the second Born approximation and can be expressed for small mass ratios as a power series in (m_e/M) . In this paper we *neglect* this recoil effect. For small (m_e/M) ratios it is probably not too difficult to consider the above effect in our scheme via a “modification” of the energy and impulse conservation, by a formal change $\omega \rightarrow \omega - q^2/2M$, and retaining the two-body effective scattering picture.⁴² Furthermore, the multiple-scattering problem between a light particle, let us say, a positron, and the electrons may be characterized by the approximate solution of a Bethe-Goldstone equation. In this description a virtual positronium state appears. In our case (heavy ion) the bound states appear in a natural way, at appropriate values of the phase shifts for the scattering in an effective one-body potential, according to the Levinson theorem.

III. RESULTS

In our scheme, as we have argued above (Sec. II), the remaining part is the determination of the elastic scattering amplitude. Thus the phase shifts are the central quantities. To describe the scattering potential and characterize *screening nonlinearities*, we apply the standard DFT (Ref. 23) method and perform our calculation within its local version.⁴³ In our calculation the “solid-state influence” of the environmental is reflected in the Friedel sum rule¹⁷ for scattering phase shifts at the (unperturbed) Fermi level. The total screening condition is satisfied by *scattering waves*.

In order to determine the basic quantities that characterize the stopping phenomenon (Γ , dE/dR , and W), we have used the phase shifts at the Fermi energy of an electron scattered off a spherically symmetric self-consistent atom potential. The calculated phase shifts satisfy the Friedel sum rule with high accuracy.

In Eq. (15) appear integrals of the type

$$I(m) = \int d\sigma(\theta, v_F) \sin^m \left[\frac{\theta}{2} \right], \quad (22)$$

as can be seen from the structure of Eqs. (15), (20), and (21). This type of integral can be written in the form

$$I(m) = \frac{\pi}{2v_F^2} \frac{1}{2^{m/2}} \sum_{\lambda} \sum_{\mu} (2\lambda+1)(2\mu+1) \times \{1 - \cos(2\delta_{\lambda}) - \cos(2\delta_{\mu}) + \cos[2(\delta_{\lambda} - \delta_{\mu})]\} J_{\lambda\mu}^{(m)}. \quad (23)$$

In Eq. (23) the quantity $J_{\lambda\mu}^{(m)}$ is defined by

$$J_{\lambda\mu}^{(m)} = \int_{-1}^1 dx (1-x)^{m/2} P_{\lambda}(x) P_{\mu}(x), \quad (24)$$

where the P_{λ} 's are the Legendre polynomials.

First, we focus our attention on the r_s dependence of the above-mentioned basic quantities for a proton and helium projectiles. In Figs. 1, 2, and 3 we have plotted Γ/v , $(dE/dR)/v$, and W/v^2 , respectively, as a function of the density parameter r_s . The curves labeled (a) and (c) in these figures have been calculated from Eq. (15) with the parameter $C=0$, and the ones labeled (b) and (d) with $C=1$. The curves labeled (a) and (b) correspond to the proton case; meanwhile the curves labeled (c) and (d) correspond to the helium case. Our results show that, if we take into account the dissipative nature of the electron-hole excitations ($C=1$), we obtain an increasing relative deviation with respect to the results based on the rigid electron-hole concept ($C=0$) as the density decreases. These deviations change almost continuously from about 10% ($r_s=1.5$) to about 20%

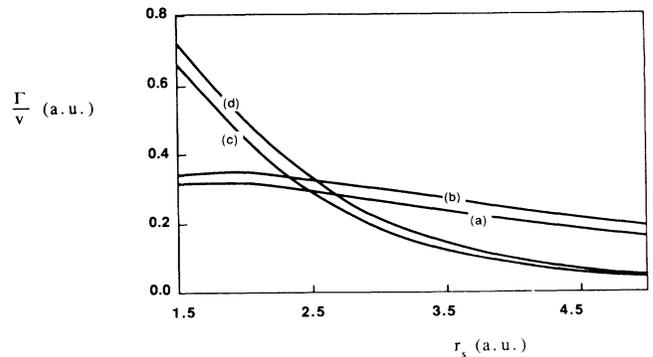


FIG. 1. Width of the particle states for a slow ion interacting with an electron gas as a function of r_s . Curves (a) and (c) are calculated from Eq. (15) with $C=0$ for a proton and helium intruders, respectively. Curves (b) and (d) are calculated from Eq. (15) with $C=1$ for a proton and helium intruders, respectively. See the text for the details.

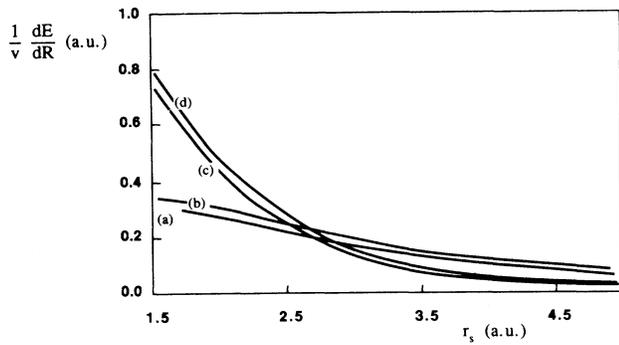


FIG. 2. Same as in Fig. 1 for the stopping power.

($r_s=5$). Of course, if r_s tends to zero, this deviation tends to zero as it should [see Eq. (A5) in the Appendix].

It is to be noted that we can obtain "fast" results using Eq. (15) if we suppose that only one phase shift ($l=0$) contributes to the scattering amplitude. In this case

$$I(m) = \frac{4\pi}{v_F^2} [1 - \cos(2\delta_0)] \frac{1}{m+2}. \quad (25)$$

For a proton intruder, $\delta_0 = \pi/2$ (the so-called unitary limit) gives a rather good approximation in the density range $3 \leq r_s \leq 5$, for the examined quantities.

We continue the analysis by comparing our theoretical results with some experimental data. In a recent experiment, Blume *et al.*,⁴⁴ adopting the

$$\frac{dE}{dR} = K\sqrt{E} \quad (26)$$

theoretically predicted form for the stopping power of a slow proton with kinetic energy E , have determined the value of K in units of $\sqrt{\text{eV}/\text{\AA}}$ (E must be put in eV) for a gold target. The experimental values in a $6 \text{ KeV} \leq E \leq 14 \text{ KeV}$ range are $K=0.09$ for the $\langle 110 \rangle$ channeling direction and $K=0.12$ for a polycrystalline target. We have obtained a very good agreement with these experimental data by taking $r_s=1.5$ ($K=0.11$) for

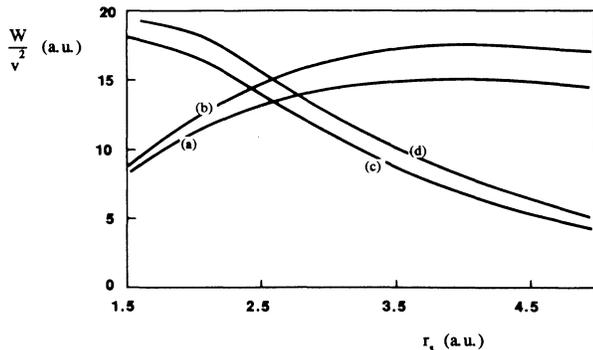


FIG. 3. Same as in Fig. 1 for the energy straggling parameter.

polycrystalline gold and $r_s=2$ ($K=0.094$) for the $\langle 110 \rangle$ channeling direction in our theoretical model for the stopping power [$C=1$ in Eq. (15)].

We have also studied the Z_1 dependence of the stopping power, comparing the experimental data of Böttiger and Bason⁴⁵ for the $\langle 110 \rangle$ channeling direction in a gold target with our theoretical model calculations in Fig. 4. The results show rather good agreement with the experimental data when we take $r_s=2$. This statement is valid both for positions and amplitudes of the oscillations. The only remaining deviation is in a small range around $Z_1=10$. This figure also gives some insight into the sensitivity of the calculated values with respect to the value of r_s (see the curve for $r_s=1.5$). According to the above results, it seems that $r_s=2$ is a reasonable physical choice to characterize the $\langle 110 \rangle$ channeling direction in gold.

In Fig. 5 we have plotted $(dE/dR)/v$ as a function of Z_1 (for $r_s=1.5$) to show the effect caused by taking into account the dissipative nature of the electron-hole excitations ($C=1$), in comparison with the rigid electron-hole concept ($C=0$). Depending on the concrete value of Z_1 (more physically, on the phase-shifts values), the difference is in the range 8–14%. Of course, the Z_1 oscillations reflecting the filling up of the bound states of the ion remain, as they must.²³

We compare our phase shifts with results of electron-neutral-atom scattering calculations. These calculations (Refs. 46 and 47) were performed for scattering electron energies below the first ionization threshold. In Ref. 46 the phase shifts were calculated by direct numerical integration of the scattering equations, for He and Ne, in

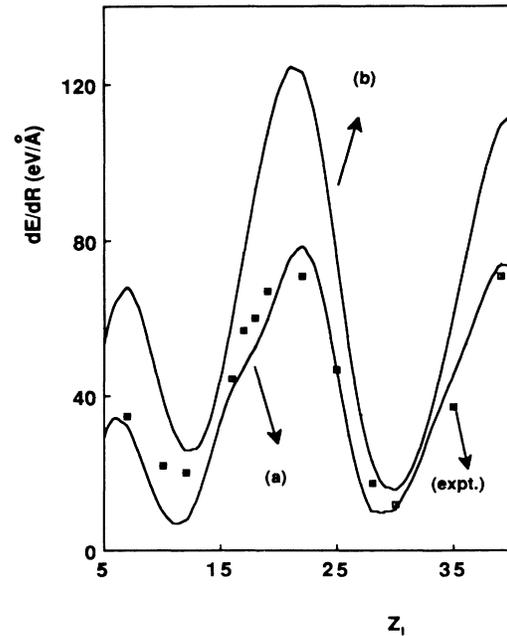


FIG. 4. Stopping power (in $\text{eV}/\text{\AA}$) as a function of the bombarding ion charge Z_1 for the $\langle 110 \rangle$ channeling direction in a gold target. The ion velocity is $v=0.68v_0$ (v_0 being the Bohr velocity). Curve (a) has been calculated with $r_s=2$, and curve (b) with $r_s=1.5$. The \square are experimental data from Ref. 45.

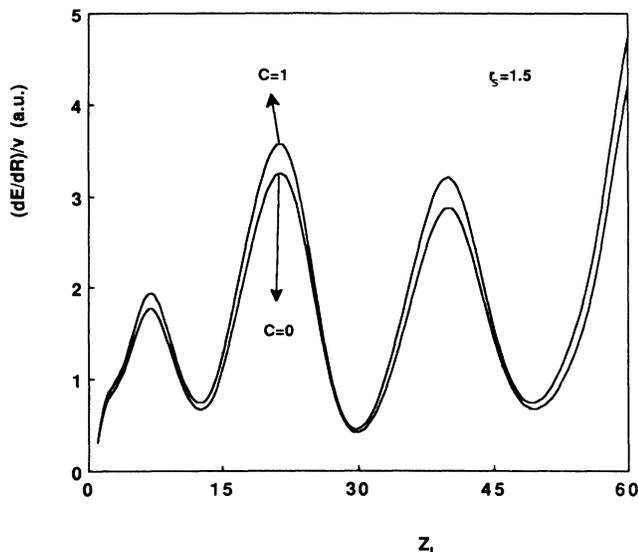


FIG. 5. Stopping power as a function of the ion charge Z_1 for a homogeneous electron gas with density parameter $r_s = 1.5$. See the text for the details.

the static approximation for the nonlocal exchange potential. Although this calculation was performed for an entirely different “environment condition,” we expect similarities with our calculation because of the very inert nature of the bound levels of inert-gas atoms. The results of Ref. 46 are shown in Figs. 6(a) and 6(b) as continuous lines, where we have plotted the phase shifts as a function of the scattering electron impulse (k). For He [Fig. 6(a)] only the $l=0$ phase shift has been plotted, and for Ne [Fig. 6(b)] both the $l=0$ and $l=1$ phase shifts. Our calculated values are denoted by \circ for the $l=0$ phase shift for He, and by \circ and \square for the $l=0$ and $l=1$ for Ne, respectively. Note that in this latter case (Ne) we subtract π from our δ_0 . These values are calculated in DFT at $k = k_F$ for $r_s = 2, 3, 4,$ and 5 . Figure 6(b) also contains data (denoted by \bullet for δ_0 and by \blacksquare for δ_1) obtained by the R -matrix method⁴⁷ for $k = 0.8, 0.9,$ and 1 . This calculation⁴⁷ includes the full static polarizability. We add a factor π to δ_0 and δ_1 of Ref. 47 to represent the calculated values in the figure.

By comparison we can establish an “overall agreement.” Some comments have to be added to our results. It is well known that the effective potential of an ion in a solid is similar to the optical potential of the free ion, but the polarization part (long-range correlation potential) in the effective potential is screened. Furthermore, in its local form the exchange and correlation potential always contains a self-interaction term. For higher r_s values (and therefore smaller k_F) the scattering length is not directly related to the phase shifts of an electron scattering off the self-consistent atom potential. It should be calculated from a self-consistent potential including the scattering electron itself, i.e., by a polarized orbital method within DFT.⁴⁸ In spite of these open questions in DFT, we think that for typical experimental materials

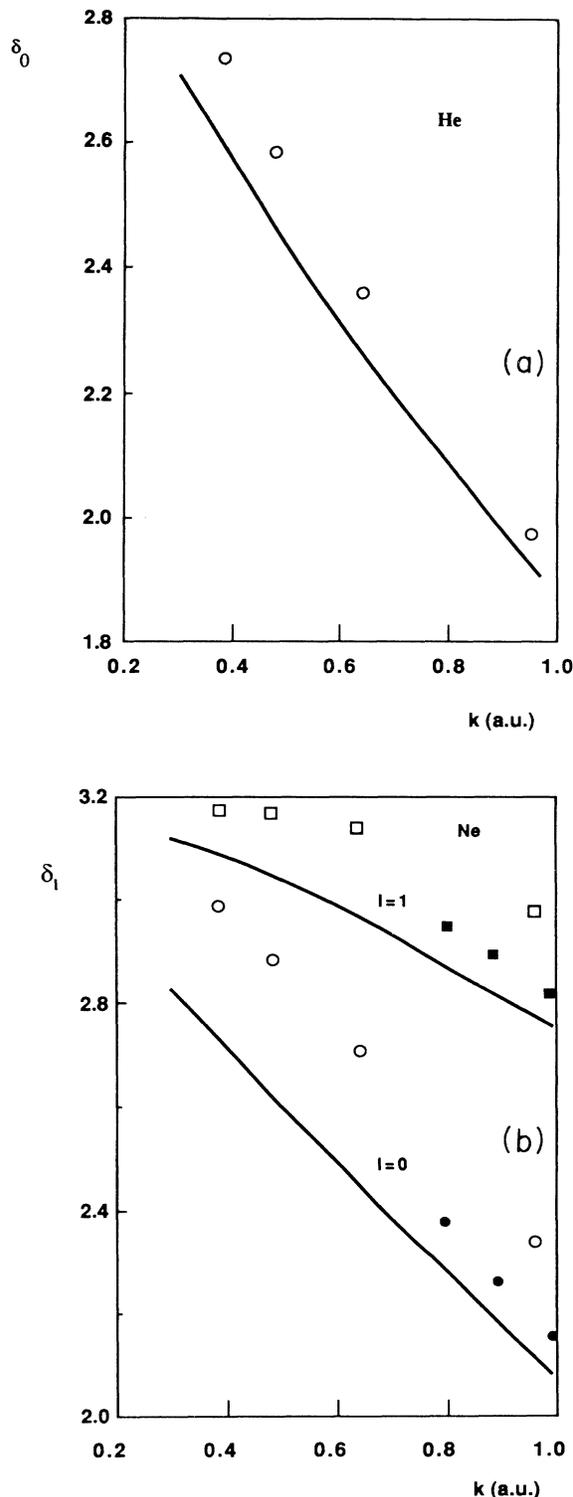


FIG. 6 (a) The $l=0$ phase shifts (δ_0) as a function of the scattering electron impulse for He. The results of Ref. 46 are denoted by a solid line. Our results are denoted by \circ . (b) The $l=0$ and $l=1$ phase shifts as a function of the scattering electron impulse for Ne. The results of Ref. 46 are denoted by a solid line. The results of Ref. 47 are denoted by \bullet for δ_0 and \blacksquare for δ_1 . Our results are denoted by \circ for δ_0 and by \square for δ_1 . See the text for the details.

($k_F \cong 1$) the accuracy of the phase shifts outlined in the embedding scheme is satisfactory enough as to be used in our problem if the Friedel sum rule is satisfied, as it is.

IV. CONCLUSIONS

In this paper we have developed a new method to calculate the basic quantities that characterize the stopping phenomenon of ions moving slowly through a uniform interacting electron gas. The main approximation to obtain the characteristic quantities in our method may be in the adopted *value* of $\text{Im}G(q, \omega)/\omega$, which is the quantity of central interest beyond the RPA to represent the inner dissipative nature of the electron-hole excitation process.

We have established that (i) all the well-known results of BEA for slow ions are based on the noninteracting representation of the density fluctuations in the homogeneous system; (ii) the essential difference between the main approaches, dielectric and BEA, is in the determination of the screened scattering potential. All the theories are based on the assumption that the system is of linear dissipative nature.

In agreement with the general expectation, our *numerical* results do not differ markedly from those which can be obtained by the standard binary-encounter theory, provided that the phase shifts are determined at the same level. Physically, this means that the imaginary part of the free-electron propagator characterizes the permissible density fluctuations (electron-hole excitations) together with the density of possible scattering states in an acceptable way for metallic densities of the degenerate electron plasma.

On the other hand, our calculated values are *systematically* in better agreement with the measured ones. The interacting nature of the electron gas can give measurable deviations with respect to a free-electron system, for the examined quantities.

More generally, our results based on ideas of charge neutrality at solid-state conditions and electron-hole excitation show that the electronic structure of a given slow heavy ion and its stopping are primary determined by the immediate environment in which it is immersed.

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APPENDIX: DETERMINATION OF THE $a(n)$ QUANTITY

According to the prescription of Gross and Kohn,³⁶ the approximate expression for $\text{Im}G(k, \omega)$ is as follows:

$$\text{Im}G(q, \omega) = a(n) \frac{q^2}{4\pi} \omega, \quad (\text{A1})$$

for small ω values, and

$$a(n) = c \left[\frac{d}{c} \right]^{5/3} (H_\infty - H_0)^{5/3}, \quad (\text{A2})$$

where $c = (23\pi/15)$ and $d = [\Gamma(\frac{1}{4})]^2 / (32\pi)^{1/2}$ are numerical constants. Using the notations

$$H_0 \equiv - \left[\frac{4\pi}{v_F^2} \right] \gamma_0, \quad (\text{A3})$$

$$H_\infty \equiv - \left[\frac{4\pi}{v_F^2} \right] \gamma_\infty, \quad (\text{A4})$$

after simple substitution within the last parentheses of Eq. (15), one obtains

$$\left[1 + \frac{12n}{\pi} a(n) f \left[\sin \frac{\theta}{2} \right] \right] = \left[1 + 3.88 r_s^{1/3} (\gamma_0 - \gamma_\infty)^{5/3} f \left[\sin \frac{\theta}{2} \right] \right]. \quad (\text{A5})$$

Here the density-dependent γ_0 and γ_∞ factors result from the compressibility and third-frequency-moment sum rule, respectively,⁴⁹ and generally $\gamma_0 > \gamma_\infty$. The final form of these factors is

$$\gamma_0 = \frac{1}{4} + \frac{\pi}{12} \alpha r_s^2 \frac{\partial \epsilon_c}{\partial r_s} - \frac{\pi}{24} \alpha r_s^3 \frac{\partial^2 \epsilon_c}{\partial r_s^2}, \quad (\text{A6})$$

$$\gamma_\infty = \frac{3}{20} + \frac{11}{20} \pi \alpha r_s \epsilon_c + \frac{13}{20} \pi \alpha r_s^2 \frac{\partial \epsilon_c}{\partial r_s}, \quad (\text{A7})$$

where $\alpha = (4/9\pi)^{1/3}$, and the correlation energy ϵ_c (Ref. 50) is measured in rydbergs. At metallic densities of the electron gas these factors vary slowly, and typical values are

$$\gamma_0 \cong 0.263, \quad \gamma_\infty \cong 0.075, \quad (r_s = 2).$$

For completeness, γ_0 is a monotonically growing function as a function of r_s , while γ_∞ has a weak minimum value at about $r_s = 5$ [$\gamma_\infty(r_s = 5) \cong 0.064$].

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¹L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, Oxford, 1980), Pt. 1, p. 387.

²E. Fermi and E. Teller, *Phys. Rev.* **72**, 399 (1947).

³J. Lindhard, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. **28** (1954).

⁴R. H. Ritchie, *Phys. Rev.* **114**, 644 (1959).

⁵J. C. Ashley, *Nucl. Instrum. Methods* **170**, 197 (1980).

⁶N. D. Mermin, *Phys. Rev. B* **1**, 2362 (1970).

⁷Yu. S. Sayasov, *Z. Phys. A* **313**, 9 (1983).

- ⁸I. Nagy, J. László, and J. Giber, *Z. Phys. A* **321**, 221 (1985); S. Tanaka and S. Ichimaru, *J. Phys. Soc. Jpn.* **54**, 2537 (1985); B. Dabrowski, *Phys. Rev. B* **34**, 4989 (1986).
- ⁹C. D. Hu and E. Zaremba, *Phys. Rev. B* **37**, 9268 (1988).
- ¹⁰I. Nagy, *J. Phys. B* **19**, L421 (1986).
- ¹¹S. A. Chin, *Ann. Phys. (N.Y.)* **108**, 301 (1977).
- ¹²B. A. Trubnikov and Yu. N. Yavlinskii, *Zk. Eksp. Teor. Fiz.* **48**, 253 (1965) [*Sov. Phys.—JETP* **21**, 167 (1965)].
- ¹³P. Sigmund, *Phys. Rev. A* **26**, 2497 (1982).
- ¹⁴L. de Ferrariis and N. R. Arista, *Phys. Rev. A* **29**, 2145 (1984).
- ¹⁵A. Blandin, A. Nourtier, and D. W. Hone, *J. Phys. (Paris)* **37**, 369 (1976).
- ¹⁶K. Schonhammer, *Phys. Rev. B* **37**, 7735 (1988).
- ¹⁷J. Friedel, *Philos. Mag.* **43**, 153 (1952); J. S. Langer and V. Ambegaokar, *Phys. Rev.* **121**, 1090 (1961); D. C. Langreth, *ibid.* **150**, 516 (1966).
- ¹⁸R. G. Newton, *Scattering Theory of Waves and Particles* (Springer, New York, 1982), pp. 273–295.
- ¹⁹T. L. Ferrell and R. H. Ritchie, *Phys. Rev. B* **16**, 115 (1977); A. Cherubini and A. Ventura, *Lett. Nuovo Cim.* **44**, 503 (1985); B. Apagyi and I. Nagy, *J. Phys. C* **20**, 1465 (1987); **21**, 3845 (1988).
- ²⁰C. O. Almbladh, U. von Barth, Z. D. Popovic, and M. J. Stott, *Phys. Rev. B* **14**, 2250 (1976); P. Jena and K. S. Singwi, *ibid.* **17**, 3518 (1978).
- ²¹C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1987), p. 343.
- ²²P. M. Echenique, R. M. Nieminen, and R. H. Ritchie, *Solid State Commun.* **37**, 779 (1981).
- ²³M. J. Puska and R. M. Nieminen, *Phys. Rev. B* **27**, 6121 (1983); P. M. Echenique, R. M. Nieminen, J. C. Ashley, and R. H. Ritchie, *Phys. Rev. A* **33**, 897 (1986); P. M. Echenique, *Nucl. Instrum. Methods B* **27**, 256 (1987); A. Arnau, P. M. Echenique, and R. H. Ritchie, *ibid.* **33**, 138 (1988).
- ²⁴J. C. Ashley, A. Gras-Martí, and P. M. Echenique, *Phys. Rev. A* **34**, 2495 (1986).
- ²⁵I. Nagy, A. Arnau, and P. M. Echenique, *Phys. Rev. B* **38**, 9191 (1988).
- ²⁶E. G. d'Agliano, P. Kumar, W. Schaich, and H. Suhl, *Phys. Rev. B* **11**, 2122 (1975).
- ²⁷M. Persson and B. Hellsing, *Phys. Rev. Lett.* **49**, 662 (1982).
- ²⁸F. Sols and F. Guinea, *Phys. Rev. B* **36**, 7775 (1987).
- ²⁹J. Lindhard and M. Scharff, *Phys. Rev.* **124**, 128 (1961); I. Nagy and J. László, *Phys. Lett. A* **112**, 95 (1985); H. Ascolani and N. R. Arista, *Phys. Rev. A* **33**, 2352 (1986); A. Ventura, *Nuovo Cimento* **10D**, 43 (1988).
- ³⁰C. J. Tung, R. H. Ritchie, J. C. Ashley, and V. E. Anderson, Oak Ridge National Laboratory Report No. ORNL-TM-5188, 1976, p. 5.
- ³¹A. A. Kugler, *J. Stat. Phys.* **12**, 35 (1975).
- ³²L. P. Kadanoff and P. C. Martin, *Ann. Phys. (N.Y.)* **24**, 419 (1963).
- ³³F. Green, D. Neilson, and J. Szymanski, *Phys. Rev. B* **35**, 124 (1987); F. Green, D. Neilson, D. Pines, and J. Szymanski, *ibid.* **35**, 133 (1987).
- ³⁴R. W. Shaw, Jr., *J. Phys. C* **3**, 1140 (1970).
- ³⁵S. Ichimaru, *Rev. Mod. Phys.* **54**, 1017 (1982); R. G. Dandrea, N. W. Ashcroft, and A. E. Carlsson, *Phys. Rev. B* **34**, 2097 (1986).
- ³⁶E. K. U. Gross and W. Kohn, *Phys. Rev. Lett.* **55**, 2850 (1985); **57**, 923(E) (1986); N. Iwamoto and E. K. U. Gross, *Phys. Rev. B* **35**, 3003 (1987).
- ³⁷W. Jones and N. H. March, *Theoretical Solid State Physics* (Dover, New York, 1985), Vol. 2, pp. 741–746.
- ³⁸J. Callaway and N. H. March, in *Solid State Physics*, edited by H. Ehrenreich and D. Turnbull (Academic, New York, 1984), Vol. 38, p. 158.
- ³⁹C. Zhang, N. Tzoar, and P. M. Platzman, *Phys. Rev. B* **37**, 7326 (1988).
- ⁴⁰A. Rubaszek and H. Stachowiak, *Phys. Rev. B* **38**, 3846 (1988).
- ⁴¹A. J. Heeger, in *Solid State Physics*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1969), Vol. 23, pp. 347–348.
- ⁴²I. Nagy, A. Arnau, and P. M. Echenique (unpublished).
- ⁴³O. Gunnarsson and B. I. Lundqvist, *Phys. Rev. B* **13**, 4274 (1976).
- ⁴⁴R. Blume, W. Eckstein, H. Verbeek, and K. Reichelt, *Nucl. Instrum. Methods* **194**, 67 (1982).
- ⁴⁵J. Bøttiger and F. Bason, *Radiat. Effects* **2**, 105 (1969).
- ⁴⁶L. D. Thomas, *J. Comput. Phys.* **13**, 348 (1973).
- ⁴⁷W. C. Fon, K. A. Berrington, and A. Hibbert, *J. Phys. B* **14**, 323 (1981).
- ⁴⁸M. J. Stott and E. Zaremba, *Phys. Rev. A* **21**, 12 (1980); D. Mahan, *ibid.* **22**, 1780 (1980).
- ⁴⁹N. Iwamoto, *Phys. Rev. A* **30**, 3289 (1984).
- ⁵⁰S. H. Vosko, L. Wilk, and M. Nusair, *Can. J. Phys.* **58**, 1200 (1980); N. Iwamoto, *Phys. Rev. B* **38**, 4277 (1988).