Stopping power of a two-dimensional electron gas for heavy particles

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The velocity dependence of the stopping power of a two-dimensional noninteracting electron gas for heavy in-plane ions is calculated. The transport cross section required in the kinetic treatment is determined for a bare Coulomb potential. Detailed analytical and illustrative numerical results are derived. The problem of screening is also discussed.

I. INTRODUCTION

Electronic excitations play an important role for the energy losses of particles moving through an electron gas. Note that if the stopping medium is in thermal equilibrium, a particle slows down until its kinetic energy approaches the equilibrium value. If the incoming particle has a large mass, the description of the motion of the heavy particle in terms of a classical trajectory presents a reasonable approximation. Here we assume a straightline trajectory for the heavy ion, which means that its kinetic energy must be larger than the equilibrium value of the stopping medium. The electrons are treated as noninteracting. We study the steady-state limit, i.e., we do not investigate the transient behavior after switching on the potential of the incoming ion.

In the frame of reference of the heavy projectile the independent electrons are scattered by a fixed potential. In this kinetic treatment the average momentum transfer suffered by the scattering electrons is the source of the retarding force (stopping power) experienced by the projectile in the slowing-down process. This force is a basic quantity in various solid-state physical problems, too. $1-4$ A nice example is the phenomenon of quantum dissipation.

A dielectric treatment of the retarding force, for a two-dimensional system, was presented by Bret and Deutsch using the random-phase approximation (RPA) for the linear response function.⁶ In this perturbative mean-field method the system constituents respond to the sum of the external and induced fields as free particles. The retarding force is calculated from the induced electric field at the site of the perturbing particle.

We have to emphasize that the connection between the kinetic and the dielectric treatments is not trivial.⁸ One might give explicit statements only a posteriori, i.e., performing calculations in both approximations.⁷ The kinetic approximation is a nonperturbative method for electron-hole excitations while the dielectric approach, although it takes into account plasmon excitations, corresponds to a first-order Born approximation. The plasmon channel gives negligible contributions in two-dimensional systems according to the RPA.⁶

There is a steady interest in the two-dimensional electron gas since it has been demonstrated how to realize experimentally this system confined to a plain with a continuously varying density.⁶ A kinetic treatment for stopping allows a diagnostic tool for two-dimensional electron systems in many fields of applications. Metal-oxide semiconductor devices are good, real examples. The descriptions of scattering,¹³ projectile screening,¹⁹ and thus expressions for the stopping power depend significantly on the dimensionality of the target. An investigation for two-dimensional system is, therefore, of nterest from obvious theoretical^{$4-6$} and experimenta points of view.

The paper is organized as follows. In Sec. II, we give a short but self-contained formulation of our kinetic framework appropriate for two- and three-dimensional (3D) electron gases. The heavy ion is characterized solely by its velocity v . The basic expression of the transport cross section in 2D for a bare Coulomb potential is given in Sec. III. Analytical and numerical calculations of the stopping power for 2D, together with possible applications, are presented in Sec. IV. Finally, we summarize our results in Sec. V. We use Hartree atomic units throughout this work.

II. THE STOPPING POWER

For an external potential with inversion symmetry moving through a noninteracting electron gas of dimension (D) two or three, one obtains the following expression for the stopping power: $8-10$

$$
S(D) = \frac{2}{(2\pi)^D} \int d^D p f(\epsilon_p) v_r \frac{\mathbf{v}_r \mathbf{v}}{v} \sigma_{\text{tr}}(D, v_r) \ . \tag{2.1}
$$

Here f denotes the Fermi function, $\varepsilon_p = p^2/2$ are freeelectron energies, and $v_r = v - p$ is the relative velocity

$$
v_r = (v^2 + p^2 - 2vp \cos\varphi)^{1/2} \tag{2.2}
$$

The integration over the isotropic electron velocity spectrum is carried out using the standard method $¹¹$ </sup>

$$
\frac{2}{(2\pi)^D} \int d^D p f = \frac{1}{\pi} K_{D-1} \int d p p^{D-1} f \int_0^{\pi} d \varphi (\sin \varphi)^{D-2} ,
$$
\n(2.3)

in which K_D has the following form:

$$
K_D = 2^{1-D} \pi^{-D/2} |\Gamma(D/2)|^{-1} . \tag{2.4}
$$

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It is easy to show that

$$
\frac{\mathbf{v}_r \mathbf{v}}{v} = v - p \cos \varphi \tag{2.5}
$$

The momentum-transfer (or transport) cross sections (σ_{tr}) in Eq. (2.1) are given in partial-wave representation

$$
\sigma_{\rm tr}(3D, v_r) = \frac{4\pi}{v_r^2} \sum_{l=0}^{\infty} (l+1) \sin^2[\delta_l(v_r) - \delta_{l+1}(v_r)] , \quad (2.6)
$$

for $3D$, and¹³

$$
\sigma_{\rm tr}(2D, v_r) = \frac{4}{v_r} \sum_{m=0}^{\infty} \sin^2[\delta_m(v_r) - \delta_{m+1}(v_r)] , \quad (2.7)
$$

for 2D, where δ 's are the scattering phase shifts.

To implement the above-formulated approach, knowledge of the scattering potential is essential. The 3D case is well documented, $^{14, 15}$ therefore it appears of interest to investigate the retarding force S for an in-plane projectile, i.e., for 2D. Using Eqs. (2.1) – (2.5) we can write

$$
S(2D) = \frac{1}{\pi^2} \int dppf (p^2/2)
$$

$$
\times \int_0^{\pi} d\varphi (v - p \cos \varphi) v_r \sigma_{tr}(2D, v_r) . \quad (2.8)
$$

The aim of the present investigation is to focus on the velocity dependence of the stopping power in 2D. In order to obtain results for comparison with subsequent calculations this paper is devoted mainly to a bare Coulomb potential $V(r) = -Z_1/r$. Here Z_1 denotes the charge of the heavy projectile.

III. $\sigma_{tr}(2D, v_r)$ FOR COULOMB POTENTIAL

Applying the well-known¹⁶ result for scattering Coulomb wave functions in 2D, we can write

$$
\delta_m(v_r) - \delta_{m+1}(v_r) = \tan^{-1} \frac{Z_1}{v_r(m+1/2)} \tag{3.1}
$$

We continue with standard expressions of trigonometry

$$
\sin^2(\tan^{-1}x) = \frac{x^2}{1+x^2}
$$
 (3.2)

and

$$
\sum_{m=0}^{\infty} \frac{1}{(2m+1)^2 + y^2} = \frac{\pi}{4y} \tanh \frac{\pi y}{2} \tag{3.3}
$$

By using Eqs. (3.1) – (3.3) in Eq. (2.7) we arrive at

$$
\sigma_{\rm tr}(2D, v_r) = Z_1 \frac{2\pi}{v_r^2} \tanh \frac{\pi Z_1}{v_r} \tag{3.4}
$$

The exact cross section is independent of the sign of Z_1 . In contrast to the 3D case the transport cross section in 2D is a finite quantity even for bare Coulomb potential. In the first-order Born approximation $(Z_1/v_r \rightarrow 0)$ one obtains

$$
\sigma_{tr}^{B}(2D, v_r) = Z_1^2 \frac{2\pi^2}{v_r^3} , \qquad (3.5)
$$

while in the opposite, i.e., classical limit $(Z_1/v_r \rightarrow \infty)$

$$
\sigma_{tr}^{cl}(2D, v_r) = |Z_1| \frac{2\pi}{v_r^2} , \qquad (3.6)
$$

is the appropriate expression. By simple comparison, we can conclude

$$
\sigma_{\text{tr}}(2\mathbf{D}) \leq \sigma_{\text{tr}}^B(2\mathbf{D})
$$

and

$$
2.7) \t\t \sigma_{tr}(2D) \leq \sigma_{tr}^{cl}(2D) , \t\t (3.7)
$$

for arbitrary scattering velocity v_r .

IV. RESULTS

A useful expression can be obtained for the stopping power if we use $\sigma_{tr}^{B}(2D, v_r)$. The result will be quantitatively appropriate for a high-density electron gas and arbitrary velocity of the projectile. With $\sigma_{tr}^{B}(2D,v_r)$ in Eq. (2.8) the angular integration is straightforward and reads

$$
\int_0^{\pi} d\varphi \frac{v - p \cos \varphi}{v^2 + p^2 - 2pv \cos \varphi} = \begin{cases} \pi/v & \text{for } (p/v) < 1 ,\\ 0 & \text{for } (p/v) > 1 .\end{cases}
$$
 (4.1)

The electron density (n_0) determines the chemical potential (μ) in a standard way for 2D:

$$
n_0 = \frac{kT}{\pi} \ln(1 + e^{\mu/k} \, , \tag{4.2}
$$

as follows from the norm integral. Here T is the temperature and k is the Boltzmann constant. The Fermi velocity is defined as $p_F = (2\pi n_0)^{1/2}$.

Introducing the new variable u in the Fermi function via

$$
u = \frac{1}{kT} \left[\mu - \frac{p^2}{2} \right],
$$
\n(4.3)

and taking into account the constraint of Eq. (4.1), together with μ from Eq. (4.2), the integration over the electron velocity spectrum in Eq. (2.8) becomes simple. We arrive at the desired analytical expression

$$
S(2D) = Z_1^2 \frac{2\pi}{v} kT[(\alpha_1 + \alpha_2) - \ln(e^{\alpha_1} + e^{\alpha_2} - 1)], \qquad (4.4)
$$

where $\alpha_1 = v^2/2kT$ and $\alpha_2 = p_F^2/2kT$. It is easy to show that $S(2\text{ D}) \geq 0$ for arbitrary velocity which is due to the infinite mass $(M \rightarrow \infty)$ assumption for the projectile. Practically, Eq. (4.4) is valid if $Mv^2/2 \gg \max(kT, p_F^2/2)$.

In applications to solid-state physical problems, like friction, orthogonality (or overlap) exponent for deplacing a potential by a short distance (a) , and quantum dissipation, $1-5$ $T=0$ is the usually considered limit. From Eq. (4.4) we obtain

$$
S(2D) = \begin{cases} Z_1^2 \pi v & \text{for } v < p_F, \\ Z_1^2 2\pi^2 n_0 / v & \text{for } v > p_F. \end{cases}
$$
 (4.5)

This equation confirms the expected asymptotic behaviors of $S(2D)$ at zero temperature

$$
S(2D) = \begin{cases} n_0 v p_F \sigma_{\text{tr}}(2D, p_F) & \text{for } v \ll p_F, \\ n_0 v^2 \sigma_{\text{tr}}(2D, v) & \text{for } v \gg p_F, \end{cases}
$$
(4.6)

which are simply obtained from Eq. (2.8) for wellbehaved $\sigma_{tr}(2D, v_r)$.

For a high-temperature 2D plasma if $kT \gg (v^2/2,$ $p_F^2/2$) a series expansion of Eq. (4.4) gives

$$
S(2D) = Z_1^2 \frac{\pi^2}{kT} n_0 v \tag{4.7}
$$

Of course, the high-velocity form in Eq. (4.5) holds at arbitrary temperature if the velocity is high enough $v \gg \max(\sqrt{kT}, p_F)$.

The asymptotic forms given by Eq. (4.6) are useful with $\sigma_{\rm tr}(2D, v_r)$ of Eq. (3.4) and $\sigma_{\rm tr}^{cl}(2D, v_r)$ of Eq. (3.6), too. Particularly, the classical expression $\sigma_{tr}^{cl}(2D)$ gives a constant value for $S(2D)$ at high velocity of the incoming ion. With Eqs. (3.4) or (3.6) one has to perform numerical integrations to obtain the detailed velocity dependence of $S(2D)$. In the following we present results obtained at $T=0$, for a fixed density of the system $p_F = 2$. Figure ¹ shows our numerical results as a function of the projectile velocity v, for $|Z_1| = 1$. The curve, based on application of the first-order Born approximation has a marked peak at $v = p_F$; see Eq. (4.5). The curve which is based on the classical approach tends to a fixed asymptotic value. Finally, the curve which is based on the exact Coulomb expression of the transport cross section has a plateaulike maximum, and, in agreement with the constraint of Eq. (3.7), is below the other ones. Even for a high density of the system $(p_F=2)$ the exact result is smaller than the first-order Born result, and the two curves merge only asymptotically for $v \gg p_F$.

As we have stated in Sec. II, the knowledge of the

FIG. 1. Stopping power S of a 2D zero-temperature electron gas for heavy unit charges as a function of the projectile velocity v: First-order Born approximation (dash-dotted curve), classical approximation (dashed curve), and exact treatment (solid curve) for a bare Coulomb potential. The density of the system is fixed by $p_F = 2$.

scattering potential is essential in our theoretical framework. Because of the electron time delay in scattering there is induced electron density or hole around the projectile depending on the sign of its charge. In other words, in further accomplishments of the theory one must take into account the question of self-consistency. In the 3D case the answer to this question is well docu-In the 3D case the answer to this question is well documented.^{14,15} In the remaining part of this section, as a first step, we incorporate the screening using linearized Thomas-Fermi theory in 2D. Then, to remain consistent, we apply a first-order Born approximation for the scattering amplitude to describe scattering by the screened potential. Therefore, this treatment is appropriate for a high-density 2D gas and for low-velocity repulsive intruders. The problems of nonlinearity¹⁷ (therefore the charge sign, i.e., Barkas effect¹⁵) and bound states¹⁸ are left for further investigations.

The screened potential in a static, linearized Thomas-Fermi theory is the following:¹⁹

$$
V(r) = -\frac{Z_1}{r} \left[1 - \frac{\pi c r}{2} [\mathbf{H}_0(c r) - Y_0(c r)] \right], \quad (4.8)
$$

where H_0 and Y_0 are Struve and Neumann functions, respectively. The screening constant c has a simple form: $c = 2(1-e^{-\alpha_2})$. The transport cross section, at a v_r scattering velocity, is given by

$$
\sigma_{\rm tr}^B(2{\rm D},c,v_r) = \frac{4\pi Z_1^2}{v_r^3} \int_0^1 dz \frac{z^2}{(z+\beta)^2 \sqrt{1-z^2}} ,\qquad (4.9)
$$

in which $\beta = c/2v_r$. The integration in Eq. (4.9) is straightforward and we obtain

 $\sigma_{\rm tr}^B(2{\rm D},c,v_r)$

$$
=Z_1^2 \frac{2\pi^2}{v_r^3} \left[1 - \frac{2}{\pi} \frac{\beta}{1-\beta^2} \left[1 - \frac{\beta^2}{\sqrt{|1-\beta^2|}} F(\beta)\right]\right],
$$
\n(4.10)

where the function F is the following:

$$
F(\beta) = \begin{cases} \ln[(1+\sqrt{1-\beta^2})/\beta] & \text{for } \beta < 1 ,\\ (\pi/2) - \sin^{-1}(1/\beta) & \text{for } \beta > 1 . \end{cases}
$$
(4.11)

For high densities ($p_F \gg 1$, thus $\beta \rightarrow 0$) we recover our previous result given by Eq. (3.5). The above result may be applicable in the first expression of Eq. (4.6) to obtain, i.e., the overlap⁵ parameter $K = [S(D)/v]a^2/(2\pi)$. At high velocities $(v, =v)$ the screening (and plasmons⁶) does not play a significant role in 2D for stopping calculations.

V. SUMMARY

We have presented a treatment of stopping power in a two-dimensional electron gas. We started with the kinetic theory of slowing-down processes. Then we described the transport cross section for a bare Coulomb potential.

We derived detailed analytical and illustrative numerical results for the stopping power. Finally, we discussed the problem of screening. To achieve a full self-consistency of screening and stopping of heavy ions in a 2D electron gas further developments are needed.

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