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Nonlinear calculation of the stopping power of a two-dimensional electron gas for heavy particles

Andrey Krakovsky
Department of Physics, New York University, New York, New York 10003

Jerome K. Percus
Department of Physics and Courant Institute of Mathematical Sciences, New York University, New York, New York 10003

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We present a nonlinear calculation of the stopping power of a two-dimensional electron gas in its ground state at metallic and overmetallic densities ($1<r_s<10$) for slow heavy repulsive intruders (antiprotons). We employ a scattering (kinetic) approach with the effective scattering potential coming from the profile equation of the Sjölander-Stott theory. A similar calculation in three dimensions shows excellent agreement with the density-functional theory results. In two dimensions, we obtain a stopping power which falls in between the bare Coulomb and linear screening potential treatments.

I. INTRODUCTION

Over the past 20 years there has been a steady interest in the two-dimensional (2D) quantum electron gas. One of the basic characteristics of such a gas is its stopping power with respect to charged intruders. The stopping power is the energy lost by the ion due to the retarding force in the medium per unit length of its trajectory. Recent experimental availability of beams of heavy negative ions[1] has triggered further interest in this field. These experiments contain important information about the effective scattering potential (see below) and, consequently, electron correlations. In actual calculations of the stopping power one usually employs the jellium model, in which the electrons are distributed over a neutralizing positive background. The situation in three dimensions is rather well known.[2] Recently, a scattering (kinetic) treatment of the stopping power of a 2D electron gas has appeared.[3] Briefly, kinetic treatment refers to the following. If the incoming ion has a large mass, its trajectory remains classical to a reasonable approximation. The electrons are treated as noninteracting and the effect of the ion on the electron gas is described in terms of an effective potential. In the reference frame of this ion the electrons are scattered by an effective potential, and the retarding force arises because of momentum transfer. Knowledge of the effective potential is crucial for the kinetic approach.

Another approach to the problem of retardation in the electron gas is to calculate the net field at the location of the ion through the medium response. This (dielectric) treatment for 2D electron gas was presented in Ref. 4. The authors used the random phase approximation linear response function. However, as was pointed out in Refs. 3 and 5, there is no direct connection between kinetic and dielectric treatments. The quality of results can be judged only by comparing results of both approaches. The kinetic approach is nonperturbative, while the dielectric approach, essentially, corresponds to the first Born approximation, which is far less reliable in two dimensions than in three dimensions. Nevertheless, so far, the shortcoming of both techniques has been the absence of nonlinear screening effects. The ability to treat nonlinear screening effects is essential for experimental implications, because it is well known that the response of an electron gas even to a charge of ± 1 is highly nonlinear.

In this work we present a kinetic treatment of the stopping power using a nonlinearly screened scattering potential based on the Sjölander-Stott (SS) theory. We calculate the stopping power of a slow heavy repulsive intruder in the ground state of an electron gas ($T=0$) at metallic and over-metallic densities. We compare our results for three dimensions with the 3D density-functional theory calculation of Nagy *et al.*[8] to demonstrate that our procedure produces reliable results. Then, we present our 2D calculation and compare them with results in Ref. 3. As is expected, in the metallic region our stopping power falls in between the results obtained by employing bare Coulomb and linearized Thomas-Fermi (linear screening) effective potentials. We use atomic units throughout this work.

II. FORMALISM

One of the simplest nonlinear approaches to the problem of an impurity in the electron gas is the SS theory.[6] In the metallic range in three dimensions it was known for a long time to produce reliable results for a repulsive impurity. Recently it was shown that the same holds in two dimensions:[7] one can reliably describe the effect of a repulsive impurity on the two-dimensional electron gas at metallic and overmetallic densities with the SS theory. We will use the profile equation resulting from the SS theory[6,7] to calculate the induced electron density around the intruder, and deduce the effective potential acting on the noninteracting electrons. This (nonlinear) effective potential will serve as input to the kinetic treatment of stopping power.[9]

The relation between the stopping power and the scattering potential can be obtained in a straightforward fashion. In general, the stopping power in the kinetic approach is given by[3]

$$S(D)=\frac{2}{(2\pi)^D}\int d^D p F(\varepsilon_p)\, v_r \frac{\mathbf{v}_r\cdot\mathbf{v}}{v}\,\sigma_{\mathrm{tr}}(D,v_r). \qquad (1)$$

Here, $D=2,3$ is the dimension of the system, F is the Fermi distribution, σ_{tr} is the transport cross section, $\varepsilon_p=p^2/2$ the

free-electron energy, and the relative velocity $\mathbf{v}_r=\mathbf{v}-\mathbf{p}$ has magnitude (φ is the relative angle)

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

We will be concerned here with a slow intruder. In this case, for a well-behaved $\sigma_{\rm tr}$, stopping power (1) reduces to

$$S(D)=nvp_F\sigma_{\rm tr}(D,p_F). \tag{3}$$

Here, n is the electron density, $p_F=\sqrt{2}/r_s$ for two dimensions and $p_F=(9\pi/4)^{1/3}/r_s$ for three dimensions, r_s being the Seitz radius. The transport cross sections are given by[10]

$$\sigma_{\rm tr}(2D,\ v_r)=\frac{4}{v_r}\sum_{m=0}^{\infty}\sin^2[\,\eta_m(v_r)-\eta_{m+1}(v_r)] \tag{4}$$

for 2D, and[11]

$$\sigma_{\rm tr}(3D,\ v_r)=\frac{4\pi}{v_r^2}\sum_{l=0}^{\infty}(l+1)\sin^2[\,\delta_l(v_r)-\delta_{l+1}(v_r)] \tag{5}$$

for 3D. The η_m and δ_l are the scattering phase shifts in two dimensions and three dimensions, respectively. As the intruder is considered to be heavy and slow, it is a good approximation to consider a static effective potential.[8]

Below, we will compare our results for three dimensions with the three-dimensional density-functional theory calculation[8] in order to show that our procedure is capable of reliably treating nonlinear effects. This fact will allow us to apply this procedure in two dimensions.

A. 3D calculation

We perform a calculation for a negative ion of charge -1 (antiproton). As was mentioned above, we will be concerned with slow repulsive intruders, and calculating induced density in the static limit becomes a good approximation. We start from the (static) profile equation resulting from the SS theory,[6] written in terms of the dimensionless momentum $q\to q/k_F$:

$$n_q^{\rm ind,3D}=f^{\rm 3D}(q)\left[\,1+\int_0^{\infty}k^2\,dk\left(\,1+\frac{q^2-k^2}{2qk}\times\ln\left|\frac{k+q}{k-q}\right|\right)n_k^{\rm ind,3D}\right]. \tag{6}$$

Here, $n_q^{\rm ind,\,3D}$ is the Fourier transform of the induced electron density, and $f^{\rm 3D}(q)$ is the induced density in the linear response approximation:

$$f^{\rm 3D}(q)=\chi_q u_q, \tag{7}$$

χ_q being the linear response, $u_q=-4\pi Ze^2/q^2$ the impurity potential, and Z the impurity charge. We employ the linear response function from the work of Farid *et al.*[12] After obtaining the induced density, we deduce the effective potential and calculate scattering phase shifts. We would like to remark on the Friedel sum rule (FSR), as it is an essential ingredient of the majority of the effective potential calculations. Usually, one uses the FSR in order to organize a self-consistent procedure. The free parameters of the effective potential are adjusted in such a way as to enforce the FSR. In our case there is no need for that. Instead, it provides an extra test for our effective potential. Indeed, we find that FSR is satisfied within the 0.5% accuracy. Our results for the stopping power together with results of Ref. 8 are shown in Fig. 1. Both results agree within the 3% accuracy. This agreement allows us to carry out the same procedure in two dimensions. In the next paragraph we apply our technique to the 2D electron gas.

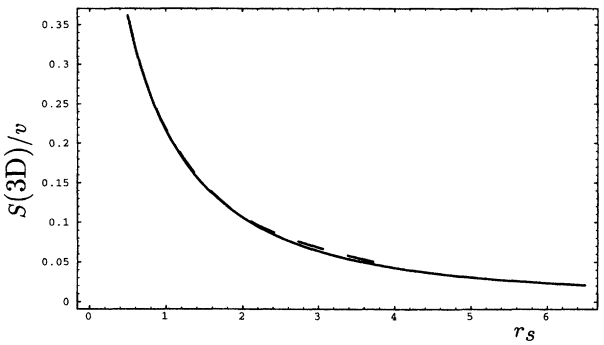

FIG. 1. The stopping power of 3D electron gas for a slow antiproton ($Z=-1$) as a function of the Seitz radius r_s; v is the projectile velocity. Solid line, present theory; dashed line, density-functional theory results of Nagy *et al.* (Ref. 8).

B. 2D calculation

In two dimensions the SS profile equation takes on the form[7] (momentum is dimensionless)

$$n_q^{\rm ind,\,2D}=f^{\rm 2D}(q)\left(\,1+\int_0^{\infty}k\,dk\,\frac{\Phi(\,q,k\,)}{\sqrt{k^2+q^2}}\,n_k^{\rm ind,\,2D}\right) \tag{8}$$

with the same notation: $f^{\rm 2D}(q)$ is the induced electron density in the linear response approximation. It is given by (7) now with χ_q the 2D linear response, and $u_q=-2\pi Ze^2/q$. For the 2D linear response we use extrapolated numerical results of Neilson *et al.*[13] The extrapolated $f^{\rm 2D}(q)$ (for $1<r_s<20$) is

$$f^{\rm 2D}(q)=\frac{Z\,2\sqrt{2}\,r_s}{2\sqrt{2}\,r_s+q^3-r_sF_q(r_s)}, \tag{9}$$

with

$$F_q(x)=\begin{cases}a_1(x)\,q+a_2(x)\,q^2 & \text{if } q\leqslant 2,\\ a_1(x)\,q+a_2(x)\,q^2 & \\ \quad+[b_1(x)\,(q-2)^2+b_2(x)\,(q-2)^3]/q & \text{if } q>2,\end{cases} \tag{10}$$

$$a_1(x)=0.06x,$$

$$a_2(x)=0.69-0.028x-0.0004x^2,$$

$$b_1(x)=-14.8+1.38x-0.02x^2\ ,$$

$$b_2(x)=3.5933-0.674x+0.01347x^2\ .$$

Our $f^{\rm 2D}(q)$ incorporates the correct high- and low-q dependence with the fit function $F_q(x)$ interpolating in between.

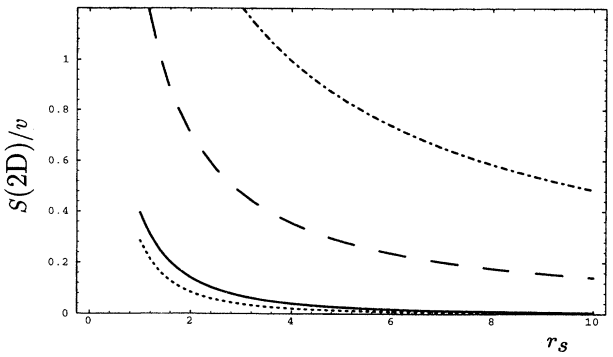

FIG. 2. Same as in Fig. 1 for 2D electron gas. Solid line, present theory; dashed line, bare Coulomb (BC); dotted line, linearized Thomas-Fermi (LTF), numerical; dash-dotted line, LTF in the first Born approximation effective potentials.

The function $\Phi(q,k)$ in (8) results from angular integration. In terms of special functions it is given as

$$\Phi(q,k)=\frac{q}{\pi}\left(\frac{K[-2a_{q,k}/(1-a_{q,k})]}{\sqrt{1-a_{q,k}}}+\frac{K[2a_{q,k}/(1+a_{q,k})]}{\sqrt{1+a_{q,k}}}\right)-\frac{a_{q,k}k}{4}\,{}_2F_1\left(\frac{3}{4},\frac{5}{4},2,a_{q,k}^2\right), \tag{11}$$

where

$$a_{q,k}=\frac{2qk}{k^2+q^2}\,.$$

We repeat the same procedure as in three dimensions: calculate the scattering phase shifts from the effective potential η_m and then the 2D stopping power is given by (3, 4).

Our results for the stopping power are shown in Fig. 2. We compare them with the stopping power for the bare Coulomb (BC) potential with exact phase shifts, and linearized Thomas-Fermi (LTF) potential, both of them linear treatments. LTF potential is given by[14]

$$V(r)=-\frac{Z}{r}(1-\pi r[H_0(2r)-Y_0(2r)])\,, \tag{12}$$

where H_0 and Y_0 are Struve and Neumann functions, respectively. For LTF we present exact first-order Born approximation for scattering and our nonperturbative numerical results. The exact calculation of transport cross sections for BC and LTF in the first Born approximation was done in Ref. 3:

$$\sigma_{\rm tr}^{\rm BC}(2{\rm D},v_r)=Z\,\frac{2\pi}{v_r^2}\tanh\frac{\pi Z}{v_r}\,, \tag{13}$$

$$\sigma_{\rm tr}^{{\rm LTF},(1)}(2{\rm D},v_r)=Z^2\frac{2\pi^2}{v_r^3}\left[1-\frac{2}{\pi}\frac{v_r}{v_r^2-1}\left(1-\frac{g(v_r)}{v_r\sqrt{|1-v_r^2|}}\right)\right] \tag{14}$$

with

$$g(v_r)=\begin{cases}\frac{\pi}{2}-\arcsin v_r & \text{for } v_r<1\\ \ln(v_r+\sqrt{v_r^2-1}) & \text{for } v_r>1\,.\end{cases}$$

As one expects, our results for the stopping power are significantly lower than those for the BC potential, and higher than for the LTF potential. The results produced by the LTF in the first Born approximation would be reliable for high densities ($r_s\ll 1$), and as we see, in the metallic range it does even worse than BC.

III. CONCLUSION

We have presented a nonlinear calculation of the stopping power of the 2D gas in its ground state at densities $1<r_s<10$ for slow repulsive intruders (antiprotons). Calculations were performed using a scattering (kinetic) approach with a nonlinear effective potential resulting from the SS profile equation. Our results constitute a significant and important improvement over the recent (linear) results in this field[3,4] from both experimental and theoretical points of view. Using our technique it is possible to obtain the 2D stopping power for intermediate and large velocities of repulsive intruders. This requires a dynamical effective potential, which in our context means a reliable knowledge of dynamical response. This problem will be the subject of our next publication. We would like to note that our approach cannot be applied to attractive intruders (protons) at metallic densities because the SS theory fails to describe an incipient bound state. A nonlinear treatment of the stopping power of 2D electron gas for attractive intruders remains a focus of future research.

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[9] It is well known that in three dimensions SS produces overscreening by a hole: the impurity-electron pair-correlation function goes negative in a small region around the impurity. However, this does not have any significant effect on our calculation. In two dimensions we also have a signature of the overscreening by

a hole, this effect being less pronounced and persisting over the smaller density domain and range of repulsive impurity charges. As in three dimensions, it does not affect our results.

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