# Electronic stopping power of electron gases for slow antiparticles

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The stopping power of slow antiparticles penetrating electron gases are evaluated within a scattering theory approach to the energy-loss problem. The required effective scattering potential is obtained from a self-consistent density-functional calculation. A relationship of the stopping power $S \propto |Z|^b$ ($b$ is in the range of 0.7–0.9) at low velocities is found, in contrast to the $Z^2$ dependence predicted by the linear-response theory. The diffuse distribution of partial wave contributions of screening electrons in the case of antiparticles is quite different from that for normal particles and is thought to be the main reason for the monotonic increment of the stopping power as a function of $|Z|$. [S0163-1829(97)00210-5]

## I. INTRODUCTION

Recently, the advent of experiments about antiprotons[1,2] passing through condensed matter gives additional regions for theoretical studies. On one hand, the dependence of the interaction between particles and solids on the sign of the projectile charge, such as Barkas effect,[3] can be studied directly. On the other hand, the stopping characteristics of antiparticles themselves need to be investigated. Antiparticles are difficult to find in the common environment, and up to now, people have known little on the structures of antiparticles. It seems not quite meaningful to evaluate the stopping power for an antiparticle, except for an antiproton which can be considered as a point charge. This may be one reason that we have not, so far, found an article dealing with the stopping problem for antiparticles heavier than the antiproton passing through condensed matter at low velocities. However, if we consider a negative nuclear charge embedded in an electron gas, the stopping problem can still be treated as a process of electron-hole pair excitation and the collective response of electrons to the embedded charge.

In the field of energy loss of normal particles (with positive nuclear charges) at low velocities, the fact that stopping powers oscillate with the atomic number of the incident ion is well known.[8] However, as to the antiparticles, only the stopping quantities of antiproton have been studied carefully,[3–7] the problem of the stopping power as a function of negative nuclear charge in the low velocities' region still remains open. The interaction of antiparticles with electron gases may give us a new view of physical phenomena and deserves study. In the present paper, this problem will be taken into account and a comparison with the case of normal particles will be given.

## II. THEORY AND METHOD

There are many methods to calculate the stopping power for slow ions penetrating condensed matter. One approach commonly used is based on linear-response theory as applied to the model of a uniform electron gas,[9] in which the stopping power of a medium for a charged particle, with charge $Z$, is given by

$$\frac{dW}{dR}=\frac{2Z^2}{\pi v^2}\int_0^\infty \omega d\omega \int_{\omega/v}^\infty \frac{dk}{k}\,\mathrm{Im}\left[-\frac{1}{\epsilon(k,\omega)}\right], \qquad (1)$$

where $\epsilon(k,\omega)$ is the longitudinal dielectric function for the stopping medium. Hartree atomic units, in which $e=\hbar=m=1$, were used throughout this paper. At low velocities ($v \ll v_F$, where $v_F$ is the Fermi velocity of the medium), an expression was obtained by Ritchie,[10] using the random-phase approximation for the dielectric function valid for small $\omega$ and $k \leqslant k_F$ (where $k_F$ is the Fermi momentum), which is equivalent to assuming that the potential around an ion is exponentially screened by density fluctuations in the electron gas. The result is

$$\frac{dW}{dR}=Z^2\left(\frac{2v}{3\pi}\right)\left[\ln\left(1+\frac{\pi}{\alpha r_s}\right)-\frac{1}{1+\alpha r_s/\pi}\right], \qquad (2)$$

where $\alpha=(4/9\pi)^{1/3}$, $r_s=(3/4\pi n)^{1/3}$ is the "one-electron radius" (the radius of a sphere containing, on average, one electron), and $n$ is the electron density. A parametrized Thomas-Fermi-von Weizsäcker dielectric function, in which the parameter λ is set by the nuclear-cusp condition, was recently used to calculated the stopping quantities of an antiproton passing in an electron gas at slow velocities.[7] The advantage of this approach is that analytic expressions for the effective potential and induced hole density can be obtained.

Another method for the energy loss of ions impacting solids at low velocities is based on the scattering theory. For a massive projectile at low velocities the energy loss per unit path length can be written as[11]

$$\frac{dW}{dR}=nvv_F\sigma_{\mathrm{tr}}(v_F), \qquad (3)$$

where $\sigma_{\mathrm{tr}}$ is the usual transport cross section. In terms of the scattering cross section $\sigma$, $\sigma_{\mathrm{tr}}$ is given by

$$\sigma_{\mathrm{tr}}=\int d\sigma(1-\cos\theta) \qquad (4)$$

$$=\frac{4\pi}{k_F}\sum_{l=0}^{\infty}(l+1)\sin^2[\delta_l(E_F)-\delta_{l+1}(E_F)], \qquad (5)$$

 

TABLE I. Phase shifts of antiparticles, related Friedel sum, and cusp condition ($r_s=2.0$).

| Charge | $\delta_0$ | $\delta_1$ | $\delta_2$ | $\delta_3$ | $\delta_4$ | FSR | NCC |
|---|---|---|---|---|---|---|---|
| −0.5 | −0.3989 | −0.0912 | −0.0152 | −0.0041 | −0.0010 | −0.5006 | 1.0013 |
| −1.0 | −0.7073 | −0.1941 | −0.0422 | −0.0081 | −0.0018 | −1.0015 | 1.9946 |
| −2.0 | −1.1814 | −0.4070 | −0.1097 | −0.0230 | −0.0048 | −2.0086 | 3.9977 |
| −3.0 | −1.5190 | −0.6084 | −0.1922 | −0.0455 | −0.0088 | −2.9940 | 6.0005 |
| −4.0 | −1.8295 | −0.7935 | −0.2825 | −0.0749 | −0.0148 | −3.9980 | 8.0064 |
| −5.0 | −2.0984 | −0.9638 | −0.3762 | −0.1102 | −0.0233 | −4.9987 | 9.9645 |

where $\theta$ is the scattering angle in the projectile's frame, and $\delta_l(E_F)$ is the phase shift of the $l$th partial wave for scattering of electrons at the Fermi surface from the screened potential of the projectile. The stopping power is rewritten as[12]

$$\frac{dW}{dR}=\frac{3v}{k_F r_s^3}\sum_{l=0}^{\infty}(l+1)\sin^2[\delta_l(E_F)-\delta_{l+1}(E_F)]. \qquad (6)$$

The problem of the low-velocity stopping is then reduced to the determination of the effective scattering potential. In the present paper we have used the density-functional formulation of Hohenberg and Kohn,[13] and Kohn and Sham[14] to calculate the self-consistent potential due to a static charge submerged in an electron gas. In the density-functional theory (DFT) the one-electron Schrödinger equation can be written as

$$\left[-\frac{\nabla^2}{2}+V(r)+v^{xc}(r)\right]\Psi_i(r)=E_i\Psi_i, \qquad (7)$$

and the electron density is

$$n(r)=\sum_i |\Psi_i(r)|^2. \qquad (8)$$

The potential $V$ is that seen by an electron as a result of the screening of the ion by the electron gas. It is found that a fast negatively charged trailing ion can bind electrons in its wake-riding states.[15] Wake effects are not significant at low velocities and the potential caused by an antiparticle with negative charges is repulsive to electrons, no bound states exist and the screening charge is only composed of the scattering states of the electron gas. The exchange and correlation potential $v^{xc}$ is a local potential depending on the total density $\rho(r)$. We have only dealt with spin-compensated systems in our calculations, although the results could be easily extended in a straightforward manner to magnetic systems. The local-density approximation for exchange and correlation has been used with the parametric formulation given by Gunnarsson and Lundqvist.[16] Equations (7) and (8) are solved self-consistently to get the phase shifts for the conduction band as a function of the energy, and then obtain the charge density. This kind of method has also been applied by Nagy,[4] who obtained the effective screened potential not by a self-consistent calculation, but by taking a one-parametric trial form of strictly finite range, and found that the effective potential around an antiproton is more extended than that of a proton at metallic densities. Nagy *et al.*[5] have also calculated the antiproton stopping power with DFT and found that the screening charge density of antiprotons is more diffuse than that of protons. In the present paper we extend the calculation from the case of antiproton to higher charge antiparticles aiming at finding some overall laws governing the dynamical screening of electron gases to antiparticles.

## III. RESULTS AND DISCUSSION

The validity of our calculation is tested by two conditions. The first one is the Friedel sum rule (FSR), which relates the scattering phase shifts to the total impurity charge $Z$ by the formula

$$Z=\frac{2}{\pi}\sum_{l=0}^{\infty}(2l+1)\delta_l(E_F). \qquad (9)$$

The second is the nuclear-cusp condition (NCC) nonperturbative constraint, which for the total electron density $n(r)$ at the position of an impurity with charge $Z$ reads[17]

$$\left.\frac{n'(r)}{n(r)}\right|_{r=0}=-2Z\mu, \qquad (10)$$

where $\mu$ denotes the reduced mass of the electron-impacting nucleus (two-body) system and $n'(r)$ is the derivative of $n(r)$ with respect to $r$. Considering the mass of a nucleus is much heavier than an electron, $\mu$ approximately equals 1.

In Table I the calculated phase shifts for scattering of electrons at the Fermi surface for antiparticles from $Z=-0.5$ to $-5.0$ ($r_s=2.0$), the Friedel sum and the nuclear-cusp condition are listed. From this table it is evident that our results conform to these two conditions very well. Besides, the phase shifts of $Z=-1.0$ are in good agreement with those of Nagy *et al.*[6] It ensures that the induced electron density, the effective potential, and the stopping power of antiparticles can be confidently given.

Figure 1 shows a comparison of our result of the reduced stopping power $Q=(dW/dR)(vZ^2)^{-1}$ with that of Nagy *et al.*,[7] a parametric calculation. The solid line corresponds to our results, and the dashed and dotted lines are from Ref. 7 with parameter $\lambda=4.304$ and $\lambda=1.0$, respectively. The density parameter is $r_s=2.0$. From this figure one finds that, at least in the range of $|Z|\leqslant 1.0$, the present self-consistent result has a same trend of the $|Z|$ dependence of the stopping power as that obtained by the parametric calculation.

In Fig. 2 the stopping powers of different electron gases with density parameter $r_s$ from 1.5 to 4.0 for antiparticles with $Z=-1$ to $-10$ are given. It can be clearly seen that the stopping power of different electron gases as a function of the charge of antiparticles is nearly linear. The relationship

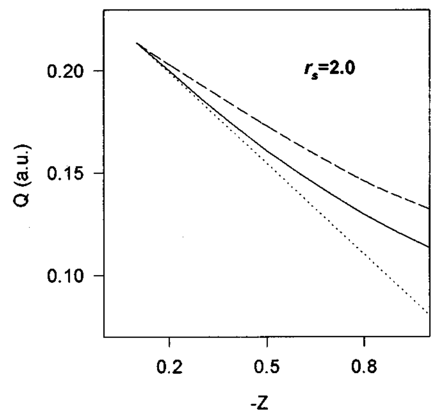


FIG. 1. Reduced stopping power $Q=(dW/dR)(vZ^2)^{-1}$ of an electron gas ($r_s=2.0$) as a function of the charge $|Z|$. The solid line are the results from DFT, and the dashed and dotted lines are those from Ref. 7, with parameters $\lambda=4.304$ and $\lambda=1.0$, respectively.

between $-(dW/dR)/v$ and $-Z$ can be approximated as $-(dW/dR)/v\propto(-Z)^b$. After fitting our results we obtain that the parameter $b$ is about 0.7–0.9 when $r_s$ is in the range of 1.5–4.0, which is greatly different from the $Z^2$ dependence predicted by Eq. (2), the result of the linear-response theory. The linear-response theory assumes that the induced electric field is linear to the external charge. This linearity is reasonable only in the limit in which the external source gives rise to a small perturbation of the initial charge distribution in the material. In order to find to what extent the linear-response theory could give a reasonably quantitative description of slow antiparticles, we have done calculations for $|Z|\leqslant10^{-2}$ and $r_s=2.0$. The results are shown in Fig. 3. The solid line is the results based on the density-functional theory and the dotted line is from Eq. (2). From this figure we can see that the results from these two different theories are in reasonably good agreement with each other. Only in this range, $|Z|\leqslant10^{-2}$, we may say that the projectile can be represented as a small perturbation, and the linear-response theory will be valid when projectiles of low velocities are considered.

From the results given above it is evident that even an antiproton, when passing solid material at low velocities,

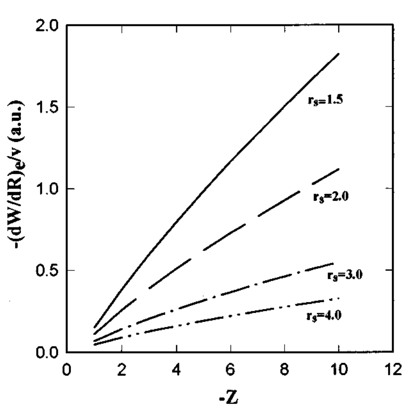


FIG. 2. The electronic stopping power of electron gases with density parameter $r_s=1.5$ to 4.0 for antiparticles with $-Z=1$ to 10 at low velocities.

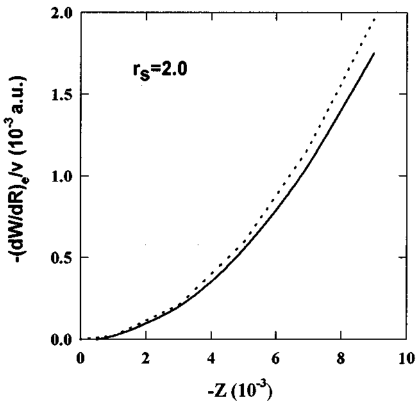


FIG. 3. The electronic stopping power of an electron gas ($r_s=2.0$) for antiparticles $|Z|\leqslant0.01$. The solid and dotted lines are the results from DFT and linear-response theory, respectively.

cannot be considered as a small perturbation to the electron-density distribution in the medium. The existence of an antiparticle greatly changes the electron-density distribution of the medium. Due to the repulsive potential generated by the antiparticle a screening hole is created, which is opposite to the case of a normal particle, where a pile up of electrons is formed. It is helpful to make a comparison of the stopping power of an electron gas for antiparticles with that for normal particles. In Fig. 4 the stopping powers of an electron gas with $r_s=2.0$ for antiparticles and normal particles as a function of $|Z|$ are plotted. The solid line refers to the antiparticles and the dotted line is for normal particles whose data are from Ref. 8 (also based on a self-consistent DFT calculation). It can be seen that the stopping power of electron gases for antiparticles and normal particles have remarkably different $|Z|$ dependence behaviors. This difference stems from the different distribution of phase shifts. In order to investigate the distribution of phase shifts, we decompose the screening charge (hole) to a different $l$ component according to the definition

$$Z_l=\frac{2}{\pi}(2l+1)\delta_l(E_F), \tag{11}$$

and define the percentage of contribution of the $l$th partial wave as

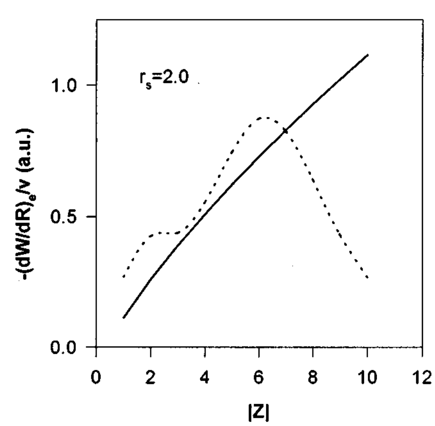


FIG. 4. The electronic stopping power of an electron gas ($r_s=2.0$) for antiparticles and normal particles from $|Z|=1$ to 10. The solid and dotted lines are the results for antiparticles (present work) and normal particles (Ref. 8), respectively.

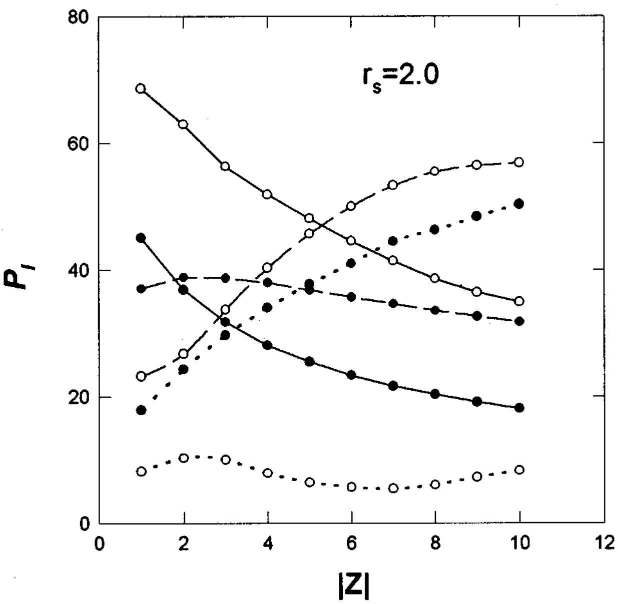


FIG. 5. The percentage of screening contribution of partial waves $P_l$ as a function of $|Z|$ from $|Z|=1$ to 10. Solid lines: $P_0$, dashed lines: $P_1$, dotted lines: $P_{l>1}$. Full circles: antiparticles, empty circles: normal particles.

$$P_l=\left|\frac{Z_l}{Z}\right|=\frac{2}{\pi}(2l+1)\left|\frac{\delta_l(E_F)}{Z}\right|\times 100\%. \qquad (12)$$

In Fig. 5 $P_0$, $P_1$, $P_{l>1}$ for antiparticles and normal particles with $|Z|$ from 1 to 10 are plotted with $r_s=2.0$. The solid lines refer to $P_0$, the dashed lines to $P_1$, and the dotted lines to $P_{l>1}$. The symbols of full circles represent the antiparticles and empty circles represent the normal particles. Although the $P_l$ is obtained from the phase shift at the Fermi surface, it actually reflects the total profiles of the phase shifts within the whole energy range at a certain partial wave $l$, e.g., $P_l$ reflects the properties of the total screening electrons of partial wave $l$. It can be seen from Fig. 5 that in the case of $|Z|=1$, the screen contribution from the partial wave $l=0$ is dominant and the $P_0$ of antiparticles from $|Z|=1$ to 10 is lower nearly one half than that of normal particles. This explains the reason why the stopping power of electron gases for an antiproton is lower than that for a proton. It is also evident that in the case of normal particles, the $P_1$ is quite larger than other partial waves' contributions from $|Z|=6$–10, and in the case of antiparticles, there is no a significantly dominant partial wave's contribution in the total range from $Z=-1$ to $-10$. From $Z=-2$ on, the contribution from partial wave $l=0$ is smaller than that from $l=1$, and from $Z=-5$ on, the contribution from partial waves $l=1$ is smaller than that from $l>1$. The concentration of screening electrons on partial wave $l=1$ is the main reason of the stopping power oscillation for normal particles, and the more diffuse distribution of the screening contribution on partial waves causes the monotonic increment of the stopping power for antiparticles. This conclusion is based on the following. Since the contribution of partial wave $l=1$ to screening is dominant for the normal particles when $Z$ is greater than 6, $\delta_1$ will increase with $Z$ and become larger than $\pi/2$. According to Eq. (6), it is easy to understand that the concentrated contribution from $l=1$ partial wave can cause an oscillation of $dW/dR$ as $Z$ is changed. However, the contribution from all the partial waves are more diffusely distributed among different partial waves for antiparticles. The phase shift $\delta_l$ is usually less than $\pi/2$, when the largest part of screening electrons are contributed by this partial wave $l$. As a result, the stopping power for antiparticles will change monotonously with $|Z|$. Additionally, this diffusive distribution of partial wave contributions of screening electrons gives rise to the more diffuse screening potentials and electron densities for the case of antiparticles embedded in electron gases than those for normal particles, which explains the findings of Refs. 4 and 5.

In summary, we have analyzed the stopping power of electron gases for antiparticles at low velocities within the density-functional theory and found the nearly linear relationship between the stopping power and the charges $|Z|$. The linear-response theory is valid when $|Z|\ll 1$ in the range of low velocities. The diffuse distribution of partial wave contributions of screening electrons in the case of antiparticles is quite different from that of normal particles and is thought to be the main reason for the monotonic increment of the stopping power as a function of $|Z|$.

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