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Scattering-theory formulation of stopping powers of a solid target for protons and antiprotons with velocity-dependent screening

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The scattering theory formulation of the stopping power of a homogeneous electron gas is implemented by consistent velocity-dependent potentials, which are needed to calculate transport cross sections for bare intruders. The method of volume averaging, over the Wigner-Seitz atomic cell of a solid Al target, is employed to characterize inhomogeneities of the electronic system and define average stopping powers for cases of protons and antiprotons. The theoretical results for average energy losses of both projectiles are in remarkable agreement with recent experimental data over a broad range of projectile velocities. [S1050-2947(98)50909-2]

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I. INTRODUCTION

The stopping power of matter for energetic charged particles is of recurring interest in physics. The understanding of the slowing down of these particles is of great fundamental and applied relevance. Generally, it is important to know accurately the stopping power for a broad range of projectile velocities in order to interpret experiments and justify our physical ideas for slowing down processes.

Theoretically, stopping power has been considered since the early days of atomic physics; for textbooks, see Refs. [1,2]. As in most areas of physics a general approach to stopping power involves models, where the stopping matter is approximated by simpler systems, such as a degenerate electron gas [3] or sets of harmonic oscillators [4].

We reexamine here the theory of energy loss by protons (p) and antiprotons $(\bar{p})$ in an electron gas as a function of the projectile velocity v. For the electron-gas model there are two general approaches.

One of these is based on perturbative treatments of response function theory. The linear response treatment [5] provides a qualitative description of the stopping power. Its result is independent of the charge sign of the charged projectile. The quadratic response treatment [6] improves our physical understanding for the asymptotic limits, i.e., for a high-density electron gas and/or a high-velocity projectile. Around the measured [7] stopping maximum in real targets, these treatments are not able to account quantitatively for the strong influence of unit-charge $(Z=\pm 1)$ projectiles.

The second approach to the stopping power of an electron gas is the scattering theory formulation [8–11]. At present, this theory treats the electron gas as a quantum-statistical ideal system of independent constituents. The influence of the heavy projectile on this system is modeled by a spherically symmetric screened potential. The assumption [8–11] of a central potential allows the application of the standard partial-wave method in order to obtain one-electron scattering phase shifts that are needed to characterize the energy-loss process.

In this Rapid Communication we present a survey of the scattering theory supplemented by a physically motivated treatment for consistent velocity-dependent screening, giving stopping powers of a solid Al target for protons $(Z=1)$ and antiprotons $(Z=-1)$. We use Hartree atomic units $(e^2=\hbar=m_e=1)$ throughout this work.

II. THEORY AND RESULTS

For a common one-body potential with spherical symmetry moving with constant velocity $\mathbf{v}$ through a homogeneous (h) electron gas of given density n_0, one obtains the following expression for the stopping power [8–11]:

$$\left(\frac{dE}{dx}\right)_h = \frac{2}{(2\pi)^3}\int d^3\mathbf{p} f^0(p^2/2) v_r \frac{\mathbf{v}_r\cdot\mathbf{v}}{v}\sigma_{tr}(v_r). \quad (1)$$

Here $f^0(p^2/2)$ denotes the distribution function (step function at $T=0$ temperature) of the ideal system of independent constituents, and $\mathbf{v}_r=\mathbf{v}-\mathbf{p}$ is the relative velocity $v_r^2=v^2+p^2-2vp\cos\varphi$. In the formally *exact* solution [10], given by Eq. (1), the distribution function enters linearly, and thus, for heavy projectile and potential with inversion symmetry, the Pauli principle does not impose a restriction [12].

The momentum-transfer (or transport) cross section $\sigma_{tr}(v_r)$ in Eq. (1) is given in partial-wave representation by

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

where δ_l's are one-electron scattering phase shifts. Of course, to implement the above-formulated approach, knowledge of the scattering potential is essential. This potential represents the effect of the heavy charged intruder on the model system. Here we take the additional step of determining the scattering potential in a consistent way and thus implement the formal result.

Our starting equation to construct a consistent, velocity-dependent screening is the linearized Thomas-Fermi-Weizsäcker equation [13]

$$(-\tfrac{1}{2}\nabla^2+b)\omega(r)+\sqrt{n_0}V(r)=0, \quad (3)$$

where $V(r)$ is the self-consistent screened potential of the projectile. This screened potential contains, via the Poisson equation, the properly normalized induced charge density $[\delta n(r)]$ of this approach $\delta n(r)=2\sqrt{n_0}\omega(r)$ and depends on the parameter b. The ''wave-function'' $\omega(r)$ of Eq. (3) is determined, at short distances $(r\to 0)$, by the Coulomb part $(-Z/r)$ of the potential and the Laplace term. In the static $(v=0)$ situation b is a so-called (Pauli) pseudopotential [14], representing the kinetic energy of electrons. Precisely, this kinetic-energy-like nature of the extra term b in Eq. (3) gives the physical motivation to consider b as a consistency parameter in a velocity-dependent construction.

The self-consistent solution of Eq. (3) for the screened potential has the following form [13]:

$$V(r)=-\frac{Z}{r}e^{-\alpha r}\left[\frac{e^{\gamma r}+e^{-\gamma r}}{2}+\frac{b}{4\alpha\gamma}(e^{\gamma r}-e^{-\gamma r})\right], \quad (4)$$

in which α and γ are characterized by

$$\alpha^2=\frac{b}{2}+\sqrt{4\pi n_0}, \quad (5a)$$

$$\gamma^2=\frac{b}{2}-\sqrt{4\pi n_0}. \quad (5b)$$

Note that $V(r)$ may have an oscillatory behavior as a function of the model parameters b and n_0.

The normalization constraint for the total induced density (a constraint that is inherently included in the above parametric treatment) may be expressed by a condition for scattering one-electron phase shifts caused by the self-consistent potential. This condition for static $(v=0)$ charged projectiles is the well-known Friedel sum rule [15]. In two independent recent publications [16,17] an extension of this rule to velocity-dependent screening was established.

Their result is as follows in Born approximation for the scattering amplitude [16,17]:

$$Z=\tilde{V}(q=0)\frac{p_F}{\pi^2}\left[\frac{1}{2}+\frac{p_F^2-v^2}{4p_Fv}\ln\left|\frac{v+p_F}{v-p_F}\right|\right], \quad (6)$$

where $\tilde{V}(q)$ is the Fourier transform of the screened potential. The Fermi velocity is defined as $p_F=(3\pi^2 n_0)^{1/3}$ and can be expressed by $p_F=1.92/r_s$, where r_s is the Wigner-Seitz radius. Now, in the present parametric case $\tilde{V}(q=0)=Zb/(2n_0)$, and one obtains from Eq. (6) the desired consistent form of the parameter b as

$$b(v,p_F)=\frac{2}{3}p_F^2\left[\frac{1}{2}+\frac{p_F^2-v^2}{4p_Fv}\ln\left|\frac{v+p_F}{v-p_F}\right|\right]^{-1}. \quad (7)$$

Clearly, according to our motivation, this pseudopotential term has a special kinetic-energy-like form for both limits of v, viz., $b\sim p_F^2$ or $b\sim v^2$, respectively at a fixed r_s value.

Our theoretical framework becomes, with this equation, a closed one. We shall use the above $b(r_s,v)$ in Eqs. (5a), (5b), and (4), and calculate $\delta_l(v_r)$ values to Eqs. (2) and (1) by numerical solution of the scattering Schrödinger equation at $v_r^2/2$ scattering energies for cases of $Z=\pm 1$. Next, we perform the double integration $(d^3\mathbf{p}=2\pi p^2\sin\varphi dpd\varphi)$ in Eq. (1) numerically to obtain stopping powers for a given r_s Wigner-Seitz radius and fixed v values, $v\in[0,4]$.

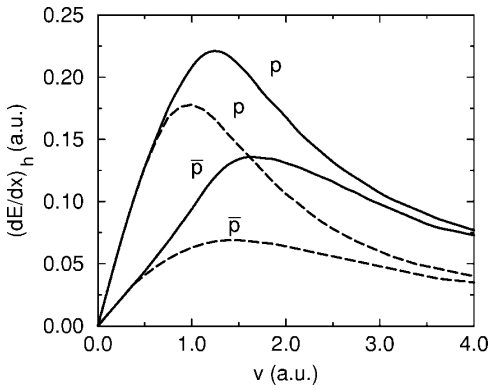

FIG. 1. The stopping power of a homogeneous electron gas with $r_s=2.07$, as a function of the projectile velocity v, for protons (p) and antiprotons $(\bar{p})$. The solid curves are based on consistent velocity-dependent potentials, while the dashed ones are based on the corresponding static potentials.

In the following we present our numerical results, first for a homogeneous electron gas of given r_s. The numerical value of r_s is fixed by the valence density of an Al target: $r_s=2.07$ [18]. In order to show the influence of a consistent velocity-dependent screening, we compare, in Fig. 1, its results (solid curves) with those obtained by the statically-screened-potential approximation (dashed curves). Our results for protons (p) and antiprotons $(\bar{p})$ show, in both cases, remarkable charge-sign dependences. Apart from the low-velocity range $(v<1)$ the dynamical screening acts to enhance the stopping powers for both projectiles. In the high-velocity, Bethe-like $(v\gg 1)$ limit the corresponding curves merge, showing that the problem becomes a perturbative one, asymptotically. Furthermore, in this high-velocity range the velocity-dependent screening gives a stopping power about two times higher than the static-potential approximation.

The dynamical result has the expected [1–6] asymptotic form in the Bethe limit

$$\left(\frac{dE}{dx}\right)_h=Z^2\frac{4\pi n_0}{v^2}\ln\frac{2v^2}{\omega_p}, \quad (8)$$

where $\omega_p=\sqrt{4\pi n_0}$ is the classical plasma frequency. In addition, we note that at low velocities $(v\ll p_F)$ the present results (for $Z=\pm 1$) are in very reasonable agreement with those based on the so-called ''impurity-form'' of the stopping power [the low-velocity form of Eq. (1)]:

$$\left(\frac{dE}{dx}\right)_h=n_0 v p_F\sigma_{tr}(p_F), \quad (9)$$

and self-consistent static potentials of density-functional theory (DFT) within its Kohn-Sham orbital version [19,20] or Thomas-Fermi-Weizsäcker iterative version [13].

The above results are important for the case of a homogeneous electron gas characterized, solely, by its r_s value. This condition, namely, the constancy of r_s, is best satisfied for a real solid target at exceptional, i.e., channeling condi-

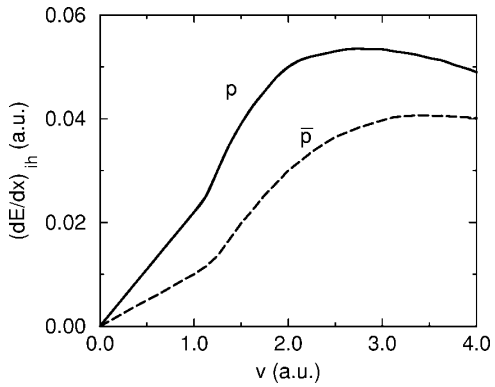

FIG. 2. The inhomogeneity correction [see Eqs. (10) and (11)] obtained by volume averaging over a Wigner-Seitz solid-state atom of the Al target. The results are plotted for protons (p) and antiprotons ($\bar{p}$) as a function of the projectile velocity v.

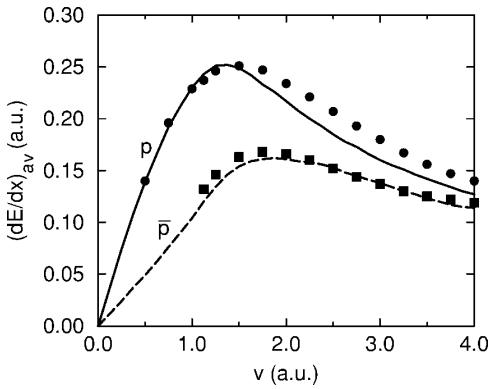

FIG. 3. The average stopping power [see Eq. (10)] of an Al target for protons (p) and antiprotons ($\bar{p}$) as a function of the projectile velocity v. The experimental data are denoted by ● for protons [25] and by ■ for antiprotons [7].

tions. Therefore, the next natural step in the implementation of a consistent theory for random incidence situations [7] is to take into account the inhomogeneity of the electron system. Within the framework of an electron-gas model this is achieved via the so-called local plasma density approximation (LPDA) [1,2,21]. In this empirically successful method, the inhomogeneous electron gas of a solid-state target atom is described by a distance-dependent, equivalent, one-electron radius $r_s(r)$ [18], where r is measured from the fixed nucleus. Earlier [21] and more recent [22–24] results, obtained within the LPDA, even for slow ions, provide an *a posteriori* justification for the success of this old rule of empirical nature.

In the following we present our velocity-dependent results, obtained by combining Eq. (1) with local $r_s(r)$ density parameters and the LPDA for a realistic electron density [18] in a spherically averaged Wigner-Seitz cell. This density was calculated by the Hartree-Fock method. The equivalent one-electron radius $r_s(r)$ is almost constant ($r_s=2.07$; valence part) for $2<r<R_W$ (see Fig. 9 of Ref. [18]) and tends to zero quite smoothly as $r\rightarrow 0$. The cell radius is $R_W=3$, as prescribed by the target atomic density. Note that all of our previous velocity-dependent equations, needed for Eq. (1), include the $r_s(r)$ values, besides the velocity parameter v.

The volume-averaged (av) stopping power is calculated, according to the LPDA method, as

$$\left(\frac{dE}{dx}\right)_{av}=\frac{3}{R_W^3}\int_0^{R_W}dr\,r^2\left\{\left(\frac{dE}{dx}\right)_h[r_s(r)]\right\}, \qquad (10)$$

at given v values. Furthermore, it is useful to define and introduce the following quantity:

$$\left(\frac{dE}{dx}\right)_{ih}=\left(\frac{dE}{dx}\right)_{av}-\left(\frac{dE}{dx}\right)_h \qquad (11)$$

to characterize the inhomogeneity (ih) correction. The last term of the right-hand side of Eq. (11) refers to the uniform gas (see Fig. 1) with $r_s=2.07$.

The results, obtained by a careful numerical procedure for the quantity of Eq. (11), are plotted in Fig. 2 as a function of the velocity of protons (p) and antiprotons ($\bar{p}$). By comparing with Fig. 1, one can see that this correction is very small at low velocities. At intermediate and higher velocities this contribution becomes an important one. In the interesting range of the stopping-power maximum and beyond it (see Fig. 1), the correction term is almost constant, especially for protons. Furthermore, the correction term is essentially bigger for the positive particle than for a repulsive one.

Our final results for solid-state conditions are exhibited in Fig. 3, together with recent experimental points for the average (av) stopping power [see Eq. (10)]. One can observe a remarkable agreement with measured antiproton data [7] and only moderate deviations from the measured proton data [25] for an Al target. This latter deviation may be the consequence of the so-called charge-exchange contribution. This contribution is not considered in the present work. According to prediction [26] this term may be about 10% in the investigated velocity range beyond the stopping maximum, and thus would result in an even better agreement for the attractive, proton intruder.

III. CONCLUSIONS

In this Rapid Communication we have investigated the important problem of energy losses of proton and antiproton projectiles in a solid Al target. We applied the scattering theory formulation of the stopping power and implemented it with a consistent determination of the velocity dependence in a common one-body scattering potential required for the transport cross-section calculations. We have modeled the real solid target by an inhomogeneous electron gas and used the LPDA in order to define average quantities for stopping powers.

We investigated the special role of the inhomogeneity correction and finally compared our theoretical results with relevant experimental predictions. A remarkable agreement was established. This agreement shows that the present (easily controllable) model and the physical ideas behind it are successful in interpreting an important and fundamental phenomenon in the field of charged-particle interaction with matter.

Our optimization of the central potential was based on the linear version of the Friedel sum rule. Therefore, the nonlinear effects (charge-sign dependencies in stopping) are due to

the exact quantum solution of the scattering problem. The fully consistent determination of a central potential based on the general form of the velocity-dependent Friedel sum rule [16,17] needs further examination.

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