Non-linear calculation of antiproton stopping powers at finite velocities using the extended Friedel sum rule

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Abstract

We calculate the energy loss of antiprotons in an electron gas for non-relativistic velocities by numerical integrations of the radial Schrödinger equation and using an extension of the Friedel sum rule to finite velocities. The calculations cover a wide range of velocities and electron-gas densities, including the range of interest for solid targets. The non-linear calculations are compared with the results of linear theory obtained from the dielectric formulation. A convergence between both calculations is obtained for high velocities and high electron-gas densities. The results show the importance of non-linear effects in the interaction of antiprotons with solids, in particular for energies below and around the stopping power maximum. Tabulated results are presented for a wide range of antiproton energies (5 keV to 3 MeV) and electron-gas densities ($n_e$ values from 0.2 to 4). These results are applied to calculate antiproton stopping powers of various solids, obtaining good agreement with experiments. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

The interaction of charged particles with matter has been a subject of great interest both for the advance of the knowledge of the basic interaction processes, as well as for a multitude of practical applications. The perturbation theory developed by Bethe [1] predicted a $Z^2$-dependence of the stopping power with projectile charge $Z$. Later on, experiments with positive and negative pions in matter [2], as well as experiments with ion beams [3], provided evidence of higher-order terms ($Z^3$-effects) in the perturbative expansion.

These effects were theoretical studied by various authors using different perturbation models [4–9], or using non-linear approaches such as density functional theory (DFT) [10], or alternative approaches based on trial potentials to represent non-linear screening conditions [11].

The study of non-linear effects in the energy loss is a powerful approach to test and improve the precision of various theoretical models aiming to describe the interaction process, and the advantage of using antiprotons as test particles (instead of protons or positive ions) was also pointed out [12]; the basic difference lies in the absence of electron capture and loss events when using negative particles. In this sense, antiprotons may be considered the ideal test particles that permit to isolate and study the basic coupling mechanism.
On the other hand, the recent advances in experimental techniques have made possible to obtain low-energy antiprotons with energies down to a few tens of keV’s [13], and to carry out measurements of antiproton stopping powers for energies around and below the stopping maximum [14,15]. These studies are also relevant to the growing field of muon applications in materials science, using both positive and negative muons [16], where adequate models to calculate muon stopping powers and ranges are required [17].

This paper is an extension of a previous work [18] where we used the “extended Friedel sum rule” (EFSR) [19] to calculate the energy loss of protons and antiprotons in Al and Si. Here we extend our previous study and present a full set of non-linear calculations of antiproton energy losses, covering the range of non-relativistic velocities and the whole range of electron densities that may be required for applications to solid targets. The results are tabulated in order to make them available for further calculations or applications to specific materials. Finally, we apply this method to calculate the stopping powers of various solids and compare them with experiments.

2. Formulation

The generalization of the Friedel sum rule to finite velocities was developed in Ref. [19]; we give here only a brief description of the formulation. The extended sum rule for a particle with velocity $v$ and charge $Z_i e$ (with $Z_i = -1$ for antiprotons) may be written in the form

$$2 \pi \sum_{l=0}^\infty (2l + 1) G_l(v, v_F) = Z_i,$$  \hspace{1cm} (1)

where $v_F$ is the Fermi velocity of the solid. The function $G_l(v, v_F)$ represents the contribution of each $l$-wave component to the screening charge, and may be expressed as an integral over a displaced Fermi sphere (DFS) of the corresponding phase-shift contribution, as follows:

$$G_l(v, v_F) = \frac{1}{4\pi} \int_{\text{DFS}} \left[ \frac{d\delta_l(k)}{dk} \right] d\Omega dk$$

$$= \int_{k_{\min}}^{k_{\max}} \left[ \frac{d\delta_l(k)}{dk} \right] g(k, v) dk,$$  \hspace{1cm} (2)

where $k_{\min} = \max\{0, v - v_F\}$ and $k_{\max} = v + v_F$. The function $g(k, v)$ takes into account the angular part of the integration over the DFS, and the expressions for the cases $v < v_F$ and $v > v_F$ were given in [19]. $\delta_l(k)$ is the phase shift of the electron wave function, and $k$ is the wave vector corresponding to the relative electron–ion motion $(k = mv_i/h$, where $\vec{v}_i = \vec{v}_e - \vec{v})$. The derivative $[d\delta_l(k)/dk]$ gives the contribution of each $l$-wave component to the accumulation of screening charge around the intruder charge. From these expressions one may retrieve the usual Friedel sum rule in the low-velocity limit ($v \ll v_F$), and a perturbative form of the sum rule for high velocities ($v \gg v_F$) [19].

The scattering potential was modeled by a simple screened potential, whose screening parameter $x$ is adjusted in a self-consistent way for each velocity $v$, using the extended sum rule. In this way, the changes in the screening conditions due to dynamical effects are taken into account in an average way by changing the screening parameter $x$. We have shown previously [19] that this procedure yields good agreement with more elaborate calculations using DFT [20].

Once the self-consistent condition is achieved, we calculate the transport cross section (TCS) $\sigma_{tr}$, from the usual expression

$$\sigma_{tr}(k, v) = \frac{4\pi}{k^2} \sum_{l=0}^\infty (l + 1) \sin^2 \left[ \delta_l(k, v) - \delta_{l-1}(k, v) \right].$$  \hspace{1cm} (3)

We note in Eq. (3) that $\delta_l$ and $\sigma_{tr}$ also depend on the ion velocity $v$ because of the optimization of the scattering potential (by the adjustment of the screening parameter $x = x(v)$).

Finally, we calculate the stopping power $S = -\langle dE/dx \rangle$ by integrating $\sigma_{tr}$ over the distribution of electron velocities in a Fermi sphere ($0 \leq v_e \leq v_F$) and over the range of relative electron–ion velocities $k = |\vec{v}_i|$ (with $|v - v_e| \leq k \leq |v + v_e|$) [19].
\[ S(v, r_s) = \frac{1}{4\pi^2v^2} \int_0^{v_F} v_e dv_e \int_{|v-v_e|}^{v} dk k^4 \sigma_{\pi} \times (k, v) \left[ 1 + \frac{v^2 - v_e^2}{k^2} \right], \]  

(4)

dthis yields the stopping power for any (non-relativistic) ion velocity and for each chosen value of the electron gas parameter \( r_s = 1.919/v_F = 0.621n^{-1/3} \), where \( n \) is the electron gas density (atomic units are used here).

The results of these calculations will be analyzed next.

3. Results and discussion

The calculations presented here have been made for a potential of the form

\[ V(r) = \left(-\frac{Z_1}{r}\right)\exp\left(-\alpha r\right), \]

where \( Z_1 = -1 \). The screening parameter \( \alpha \) was adjusted for each antiproton velocity as described before. The required number of phase shifts was of the order of \( 10^{-4} \) at low velocities but increases strongly with ion velocity, because the value of \( \alpha \) decreases like \( \sim \omega_{\pi}/v \) for \( v \gg v_F \) (weak screening), and so the maximum \( l \)-number \( (l_{\max} \sim \alpha v / \omega_{\pi}) \) increases like \( \sim v^2 \), and hence the convergence of the partial-wave series becomes slower. For the largest velocities considered here \((\sim 10 \text{ a.u.)}\) we included up to 600 phase shifts to maintain a good precision in the results. However, the high-\( l \) terms may be approximated very closely by semiclassical integrals [19], which speeds up the process. Calculations with this method have been always straightforward, and no difficulties with the convergence to the self consistent solutions were ever found.

We show in Fig. 1 the results for: (a) the screening parameter \( \alpha \), and (b) the stopping power \( S \), as a function of the antiproton energy, for a set of values of \( r_s \). The solid lines are the results of the present calculations, whereas the dashed lines show the asymptotic values predicted by the dielectric (RPA) model, namely: \( \alpha_{\text{RPA}}(v) \equiv \omega_{\pi}/v \), and

\[ S_{\text{RPA}}(v) \cong \left(\frac{\omega_{\pi}}{v}\right)^2 \left[ \frac{2v^4}{\omega_{\pi}} - \frac{3v_F^2}{5} \right]. \]  

(5)

The vertical bars in part (a) indicate the antiproton energies \( E_0 = 0.5m_p v_F^2 \). For velocities \( v \ll v_F \) the values of \( \alpha \) are nearly constant (static screening), but for \( v \gg v_F \) they approach the linear prediction of the dielectric model, \( \alpha \sim \omega_{\pi}/v \), in a very close way. In a similar way, the stopping power values converge to Eq. (5) at high velocities.

The results in the low-velocity limit are analyzed in Fig. 2, which shows together the \( \alpha \)-values and the low-velocity stopping coefficient, \( S/v \), in atomic units. The dashed lines are the values from the RPA model [21], for \( v \ll v_F \), given respectively by \( \alpha_{\text{RPA}}(0) = \sqrt{3}\omega_{\pi}/v_F = 1.563/\sqrt{r_s} \), and
Finally, in order to facilitate applications of the present calculations to different target materials, we provide in Tables 1 and 2 a set of values of the screening parameter $\alpha$ and corresponding stopping powers, for $r_s$ values between 0.2 and 4, and antiproton energies between 5 keV and 3 MeV. Some applications of these results will be discussed next.

4. Applications

In previous calculations [18], the EFSR model was used to represent the contribution to the stopping power due to valence electrons, which is usually the main contribution for low and intermediate energies. In that approach, the additional contribution from inner shells was incorporated using the harmonic oscillator model, including up to second-order terms in the perturbative expansion [22,23]. The approach in this case hinges in two different models: the non-linear EFSR method and the second-order oscillator model.

In order to obtain a self-contained and fully non-linear description, we apply here a different approach based on the so-called “local density approximation”, which considers the inhomogeneous electron density within the solid (as calculated by solid-state theory methods), and where the parameter $r_s$ varies according to the local

![Image of Figure 2: Low-velocity limit. Values of $\alpha$ and stopping coefficient $S/V$, in atomic units, as a function of $r_s$. (-- --) Results of the present calculations; (---) RPA values.](image)

Table 1

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electron density. In this method, the energy loss is averaged by integrating through a Wigner–Seitz cell representing the state of the target atoms in the solid. This approach was first introduced by
Lindhard and Scharff [24], and was later used by many other authors, yielding in many cases good results, although one may note that a clear justification of the approach was not given so far. In the present calculations, realistic representations of the electron density distributions obtained by previous authors were used [25], and the \( r_s \) dependence of the energy loss was obtained by spline interpolation of the values in Table 2.

The results of the calculations are shown in Fig. 3(a)–(d), for Si, Cu, Ag and Au, respectively, and compared with the experimental measurements of antiproton stopping powers from [15]. In the case of Si, the results of previous calculations [18] using a combination of non-linear and perturbative models are also shown. The spread of the experimental values is larger for the heavier targets, but in all cases a satisfactory comparison with the calculated values is observed.

To conclude this study, we present in Fig. 4 a prediction of the antiproton stopping power of carbon, showing both the cases of amorphous and graphite carbon (with different Wigner–Seitz radii of 1.31 and 1.25, respectively).

5. Summary

Non-linear calculations of the energy loss of antiprotons in a free electron gas have been performed for a wide range of velocities and target densities through a self-consistent approach, using the extension of the Friedel sum rule to finite velocities, together with the TCS method.

The calculations have been compared with the results of the perturbative RPA model and the convergence of the EFSR to the RPA results has been shown in the appropriate limits of large velocities and high electron gas densities. Important non-linear effects arise for low and intermediate energies.

The EFSR–TCS method provides a closed approach to the study of non-linear effects in a wide range of velocities. In particular, the present calculations include the relevant range of energies around the stopping power maximum, which is usually the most complex range for stopping power calculations.

Tabulated results have been produced, covering the relevant range of antiproton energies and electron densities, which may be used in further applications.

We have applied here these values to calculate the energy loss of antiprotons in various solids showing a good comparison with available experimental data.

The results can be further applied to calculate the energy loss of negative muons and pions in various target materials, as well as the corresponding penetration ranges.

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