

Stopping characteristics for a slow antiproton

I. Nagy,* A. Arnau, P. M. Echenique, and E. Zaremba†

Departamento de Física de Materiales, Facultad de Química, Universidad del País Vasco, Apartado 1072, San Sebastián 20080, Spain

(Received 8 March 1991; revised manuscript received 27 June 1991)

The energy loss, straggling, and dynamic width of slow antiprotons passing through an electron gas have been evaluated within a scattering-theory approach to the stopping-power problem. The required effective scattering potential is obtained from both a self-consistent density-functional calculation and a pseudo-linear-response treatment of the screening nonlinearities. The two methods give similar results. Comparison of the examined quantities with the case of protons reveals a marked difference in the metallic-density range.

The availability of antiparticle beams has made it possible to study the dependence of the interaction between particles and solids on the sign of the projectile charge (Z_1). Recent experiments by Andersen *et al.*,¹ using incident-beam energies in the range $0.5 < E < 3$ MeV, have shown the different energy losses experienced by protons and antiprotons traversing silicon foils. They observe that the difference becomes more significant as the energy of the incident beam is decreased. With the planned extension^{1,2} of the experiments to even lower energies (100 keV), it will be feasible to measure the antiproton stopping power down to the stopping-power maximum. Motivated by these rapid experimental developments in the measurements and the obvious theoretical interest in the influence of the sign of the projectile charge, we have investigated the slowing-down process at still lower energies, i.e., below the stopping-power maximum.

The physical quantities characterizing the stopping phenomena are the dynamic width of the particle states (Γ), the stopping power (dE/dR), which is the energy loss per unit path length, and the energy-loss straggling (W). Within the electron-gas model these quantities can be calculated at low projectile velocities in terms of a differential scattering cross section $d\sigma(v_F, \theta)$ for a statically screened spherically symmetric potential. One finds^{3,4}

$$\Gamma = \frac{3}{2}nv \int d\sigma(v_F, \theta) \sin \frac{\theta}{2}, \quad (1)$$

$$\frac{1}{v} \frac{dE}{dt} = \frac{dE}{dR} = 2nvv_F \int d\sigma(v_F, \theta) \sin^2 \left[\frac{\theta}{2} \right], \quad (2)$$

$$W = 3(vv_F)^2 \int d\sigma(v_F, \theta) \sin^3 \left[\frac{\theta}{2} \right], \quad (3)$$

where v is the ion velocity and v_F is the Fermi velocity of the electrons. Atomic units are used in this paper. The electron density is given in terms v_F by $n = v_F^3 / (3\pi^2)$. θ is the scattering angle, and the differential cross section is required for electrons moving at the Fermi velocity. We note that in a very recent article Møller pointed out the

feasibility of measuring W for slow antiprotons,² which is an additional motivation for the calculation of this quantity.

At the low ion velocities of interest, the stopping phenomena are governed by electron-hole-pair excitations and Γ can be interpreted as the total integrated excitation rate. It is the key quantity in the interpretation of experimental energy spectra using a convolution method.⁵ Furthermore, one can introduce a quantity defined as

$$\langle \epsilon \rangle = \frac{dE/dt}{\Gamma}, \quad (4)$$

which represents the average pair excitation energy.⁶ It may find application in studies of electron transport as in the process of secondary-electron emission.⁷

All of the above quantities can be calculated using linear-response theory.⁸ This description is valid only in the high-electron-density limit and is equivalent to the use of the first-order Born approximation for the scattering cross section. Within this theory a good approximation to the screened scattering potential is the simple Yukawa potential (Thomas-Fermi) $V(r) = -(Z_1/r)e^{-\alpha r}$ with screening parameter $\alpha = 2(v_F/\pi)^{1/2}$. The stopping-power quantities can then be obtained analytically, and one finds (for a unit charge)

$$\Gamma = \frac{1}{2}v\chi^2 \left[\frac{1}{\chi} \arctan \frac{1}{\chi} - \frac{1}{1+\chi^2} \right], \quad (5)$$

$$\frac{dE}{dR} = v \frac{2}{3\pi} \left[\ln \left[1 + \frac{1}{\chi^2} \right] - \frac{1}{1+\chi^2} \right], \quad (6)$$

$$W = 3v^2\pi^3\chi^4 \left[3 \left[1 - \chi \arctan \frac{1}{\chi} \right] - \frac{1}{1+\chi^2} \right], \quad (7)$$

where $\chi^2 = 1/\pi v_F$. The extension of these results to the second-order Born approximation is feasible and has been carried out for the stopping power by Nagy and Echenique⁹ and Sørensen.¹⁰ However, some modification of the linearly screened scattering potential is necessary, both from the point of view of formal consistency¹¹ and quantitative accuracy.¹²

TABLE I. Lowest six angular momentum quantum numbers antiproton phase shifts δ_1 calculated at the Fermi energy in KS DFT.

r_s	$-\delta_0$	$-\delta_1$	$-\delta_2$	$-\delta_3$	$-\delta_4$	$-\delta_5$
0.2	0.184 787	0.090 447	0.051 671	0.031 518	0.020 016	0.013 163
0.5	0.340 635	0.135 220	0.061 123	0.029 263	0.014 465	0.007 344
1.0	0.509 178	0.168 202	0.058 118	0.020 757	0.005 442	0.002 822
1.5	0.623 477	0.184 313	0.050 297	0.013 481	0.003 642	0.000 997
2.0	0.707 902	0.194 043	0.041 887	0.007 952	0.000 858	0.000 272
3.0	0.825 753	0.204 814	0.025 900	0.000 612	0.000 164	0.000 074
4.0	0.908 961	0.210 592	0.010 983	0.003 754	0.000 428	0.000 010

At typical metallic densities ($v_F \sim 1$), the asymptotic expansion breaks down as a result of the strong non-linearity of the interaction of the probe charge with the electrons, and so a nonperturbative calculation of the scattering is needed. The most accurate potentials available are from self-consistent nonlinear screening calculations^{13,14} done in the Kohn-Sham (KS) scheme^{15,16} of density-functional theory (DFT). On the other hand, an approximate nonlinear solution can be obtained using a parametrized Thomas-Fermi-von Weizsäcker (TFW- λ) dielectric function in which the parameter λ is used to satisfy a nonperturbative constraint (nuclear-cusp condition). The advantage of this approach is that analytic forms for the potential and induced density¹⁷ (see also Ref. 18) can be obtained. The stopping power for a slow antiproton has been calculated^{12,17} using both approaches, which give nearly the same results for various

densities. More importantly, the results show a marked difference in comparison to those of a proton.^{11,19–22} The same conclusion was arrived by Sørensen¹⁰ by means of self-consistent DFT calculations at two electron-gas densities ($r_s = 0.543$ and 2.17). His results for proton and antiproton stopping powers are in quantitative agreement with ours, except for the case of the proton at the lower density, which in his calculations is problematic. At this density the screened potential supports a bound state, which is included in our calculations and leads to a significantly weaker scattering potential than obtained when screening by the bound state is excluded.

To complete our understanding about the influence of the sign of the charge on the stopping phenomena, we here present the results for Γ , W , and $\langle \epsilon \rangle$. We have used the Fermi-level phase shifts of the self-consistent screened potentials to determine the differential scattering cross

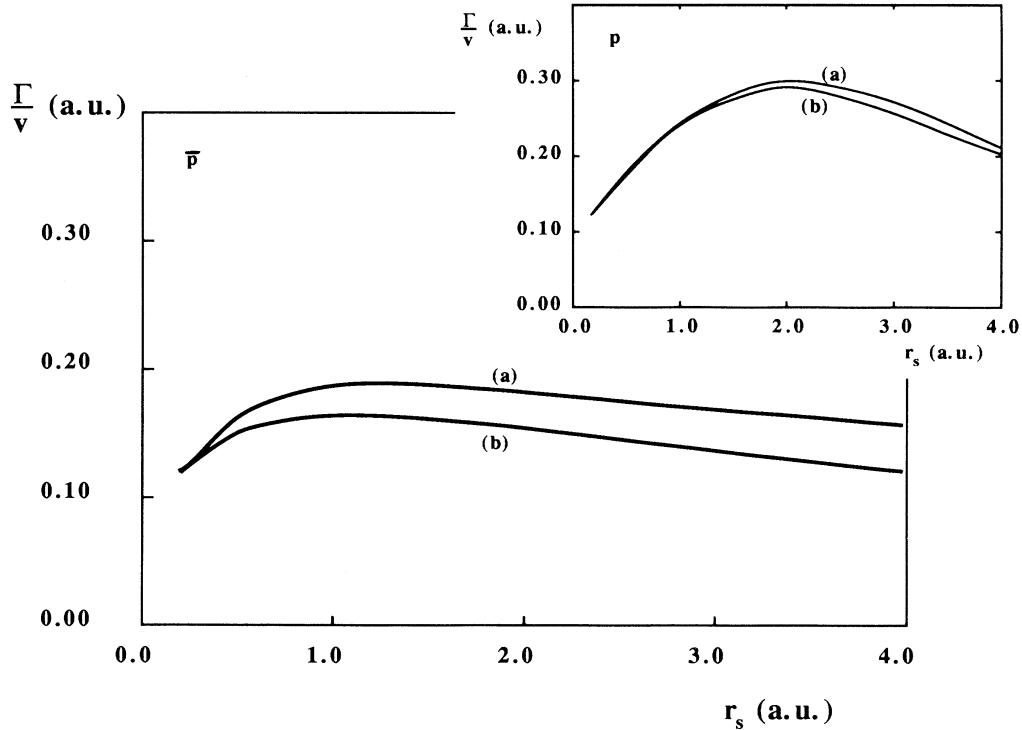


FIG. 1. Width of the particle states (Γ) calculated for protons (p) and antiprotons (\bar{p}) within the scattering-theory approach using KS DFT [curve (b)] and TFW- λ [curve (a)] descriptions of the scattering potential.

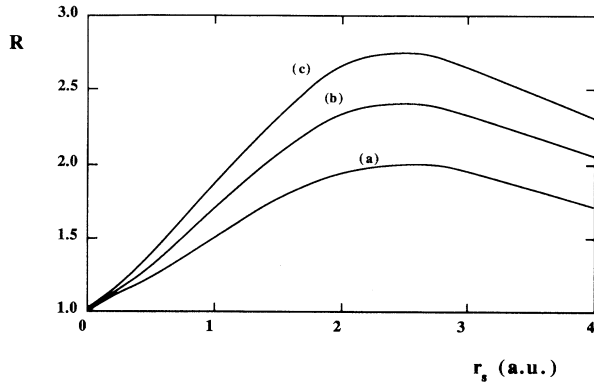


FIG. 2. Ratios of proton to antiproton values as a function of r_s , using the KS DFT approach: (a) width of the projectile state, (b) stopping power, and (c) straggling.

section $d\sigma(v_F, \theta)$ [see Eqs. (1)–(3)]. Table I contains the first six phase shifts for an antiproton as a function of the density parameter $r_s = [3/(4\pi n)]^{1/3}$ in the range $0.2 \leq r_s \leq 4$, obtained in the KS DFT. At metallic densities the leading phase shift (δ_0) is relatively insensitive to changes in the density of the system. A similar conclusion holds in the case of protons. As is well known,^{13,14} δ_0 for protons is about $\pi/2$, while for antiprotons it is roughly one-half of this value. This large difference in the leading phase shift results in significantly different stopping characteristics for protons and antiprotons, as shown in detail below.

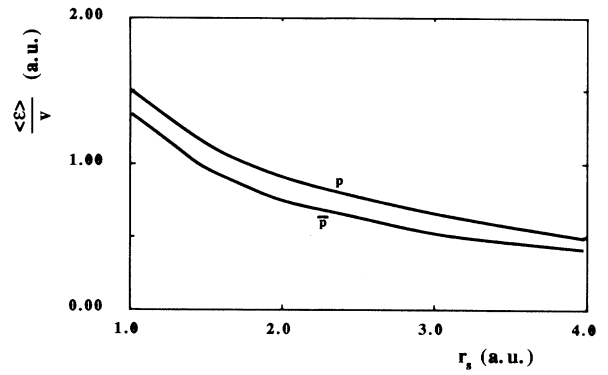


FIG. 3. Average energy $\langle \epsilon \rangle$ of an electron-hole excitation as a function of r_s for protons (p) and antiprotons (\bar{p}) using the KS DFT approach.

In Figs. 1 and 2 we show the width of the particle states (Γ/v) and energy-loss straggling (W/v^2) as a function of r_s for antiprotons (\bar{p}) using the TFW- λ [curves (a)] and KS DFT [curves (b)] approaches to calculate the scattering potential. The curves in the inset refer to the same quantities for a proton (p). Figures 1 and 2 show the sensitivity of these two quantities to the sign of the projectile charges. At typical metallic densities the results obtained in both approaches agree within 10%.

In Fig. 3 we plot $\langle \epsilon \rangle$, as defined in Eq. (4), as a function of r_s for protons (curve p) and antiprotons (curve \bar{p}) obtained in KS DFT. It is not very sensitive to the sign

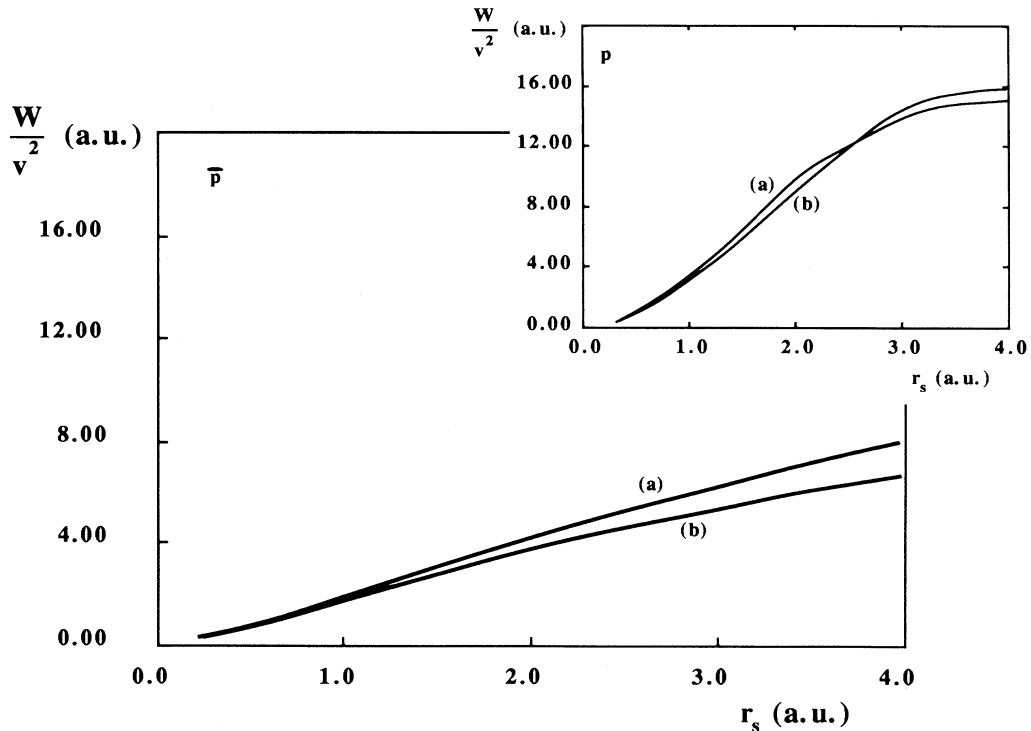


FIG. 4. Energy-loss straggling (W) for protons (p) and antiprotons (\bar{p}). The notation is the same as in Fig. 1.

of the charge of the bombarding particle and is close to the value $\langle \epsilon \rangle \sim vv_F$ to be expected on the basis of classical arguments. The ratios (R) of the proton and antiproton Γ and W are plotted in Fig. 4 as a function of r_s , together with the same ratio for the stopping power taken from Ref. 12. It can be seen that these ratios are of the order of two in the metallic density range ($2 < r_s < 4$) and increase in the order Γ , dE/dR , and W as a result of the different weighting factors of the scattering cross section [see Eqs. (1)–(3)].

It should be noted that the linear-response values one obtains from Eqs. (5)–(7) for the antiproton are in acceptable agreement (within 20%) with those obtained in the self-consistent KS DFT calculation for the antiproton, even though the Thomas-Fermi and KS DFT screened potentials differ markedly.^{12,23} An examination of the leading phase shift (δ_0) provides a simple explanation. In the first-order Born approximation, the phase shift δ_0 for our Yukawa potential is given by⁴

$$\delta_0 = -\frac{\pi}{2} \chi^2 \ln \left[1 + \frac{1}{\chi^2} \right]. \quad (8)$$

The numerical values from Eq. (8) are fortuitously close to those given in Table I. Qualitatively, the mistake one makes in choosing a linearly screened potential is “compensated” by the use of the first-order Born approximation; neither of these approximations is quantitatively accurate.

In summary, we have investigated the behavior of the stopping characteristics for slow antiprotons. A notable dependence on the sign of the projectile charge is found; nonlinear effects are therefore significant for the quantities examined.

We gratefully acknowledge financial support by Eusko Jaurlaritza, Euskal Herriko Unibertsitatea, Gipuzkoako Foru Aldundia, and the Comision Asesora de Investigación Científica y Técnica (DGICYT). One of us (E.Z.) was supported by a grant from the Natural Science and Engineering Research Council of Canada. P.M.E. acknowledges help and support by Iberduero S.A. One of us (I.N.) was supported in part by the Hungarian Research Found OTKA, Grant No. 517/1990.

*Permanent address: Quantum Theory Group, Institute of Physics, Technical University of Budapest, Budapest, H-1521, Hungary.

†Permanent address: Department of Physics, Queen’s University, Kingston, Ontario, Canada K7L 3N6.

¹L. H. Andersen *et al.*, Phys. Rev. Lett. **62**, 1731 (1989).

²S. P. Møller, Nucl. Instrum. Methods B **48**, 1 (1990).

³I. Nagy, A. Arnau, and P. M. Echenique, Phys. Rev. B **38**, 9191 (1988).

⁴P. M. Echenique, I. Nagy, and A. Arnau, Int. J. Quantum Chem. Quantum Chem. Symp. **23**, 521 (1989).

⁵A. Närmann, R. Monreal, P. M. Echenique, F. Flores, W. Heiland, and S. Schubert, Phys. Rev. Lett. **64**, 1601 (1990).

⁶E. J. Sternglass, Phys. Rev. **108**, 1 (1957).

⁷J. Calera-Rubio, A. Gras-Martí, N. R. Arista, M. M. Jakas, Z. Sroubek, and G. Falcone, Surf. Sci. **251/252**, 136 (1991).

⁸J. Lindhard, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. **28**, 8 (1954).

⁹I. Nagy and P. M. Echenique, in Proceedings of the 12th Werner Brandt International Conference on the Penetration of Charged Particles in Matter, edited by R. H. Ritchie and P. M. Echenique, National Technical Information Service, U.S. Department of Commerce (1989), p. 111.

¹⁰A. H. Sørensen, Nucl. Instrum. Methods B **48**, 10 (1990).

¹¹C. D. Hu and E. Zaremba, Phys. Rev. B **37**, 9268 (1988).

¹²I. Nagy, A. Arnau, P. M. Echenique, and E. Zaremba, Phys.

Rev. B **40**, 11 983 (1989).

¹³E. Zaremba, L. M. Sander, H. B. Shore, and J. H. Rose, J. Phys. F **7**, 1763 (1977).

¹⁴C. O. Almbladh, U. von Barth, Z. D. Popovic, and M. J. Stott, Phys. Rev. B **14**, 2250 (1976).

¹⁵P. Hohenberg and W. Kohn, Phys. Rev. **136**, B964 (1964).

¹⁶W. Kohn and L. J. Sham, Phys. Rev. **140**, A1333 (1965).

¹⁷I. Nagy, B. Apagyi, and K. Ladányi, Phys. Rev. A **42**, 1806 (1990).

¹⁸F. Perrot and N. H. March, Phys. Rev. A **42**, 4884 (1990).

¹⁹P. M. Echenique, R. M. Nieminen, and R. H. Ritchie, Solid State Commun. **37**, 779 (1981).

²⁰P. M. Echenique, R. M. Nieminen, J. C. Ashley, and R. H. Ritchie, Phys. Rev. A **33**, 897 (1986).

²¹P. M. Echenique, F. Flores, and R. H. Ritchie, in *Dynamic Screening of Ions in Condensed Matter*, Vol. 43 of *Solid State Physics*, edited by H. Ehrenreich and D. Turnbull (Academic, New York, 1990), p. 229.

²²I. Nagy, B. Apagyi, and K. Ladányi, in *Interaction of Charged Particles with Solids and Surfaces*, Vol. 271 of *NATO Advanced Study Institute, Series B: Physics*, edited by F. Flores, H. M. Urbassek, N. R. Arista, and A. Gras-Martí (Plenum, New York, 1991).

²³I. Nagy, A. Arnau, P. M. Echenique, and K. Ladányi, Phys. Rev. A **43**, 6038 (1991).