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Z_1^3 corrections to the energy widths of the states of protons and antiprotons in an electron gas

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Abstract

The energy widths of the states of protons and antiprotons moving at arbitrary velocities in a homogeneous electron gas are evaluated within a quadratic response theory and the random-phase approximation (RPA). It is found that at low and intermediate velocities the Z_1^3 correction causes a considerable reduction in the energy width of the states of antiprotons, though it is found to be less important than in the evaluation of both the stopping power and the energy-loss straggling. © 1998 Elsevier Science B.V.

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1. Introduction

The problem of energy losses suffered by moving ions interacting with matter has been of long-standing interest in physics [1–5]. The basic quantities that characterize the distribution of electronic energy losses are the energy width of particle states Γ, which is related to the imaginary part of the self-energy, the stopping power $-\mathrm{d}E/\mathrm{d}x$, and the energy-loss straggling $\mathrm{d}\Omega^2/\mathrm{d}x$. The energy width of the particle states Γ is essentially the integrated value of the differential probability of transferring energy $\hbar\omega$ to the electron gas in a single inelastic excitation process. By weighting $\hbar\omega$ and $(\hbar\omega)^2$ with this differential probability, the stopping power and the energy-loss straggling are obtained, respectively. Although Γ is not a directly observable quantity, a systematic development of the theoretical description requires its knowledge.

It is well known that linear response theories represent a good approximation when the projectile velocity is much greater than the average velocity of target electrons. The importance of nonlinearities in the evaluation of the stopping power was demonstrated, in the low-velocity limit, by Echenique et al. [6] using density-functional

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theory (DFT). Nonlinear density-functional calculations of the energy-loss straggling and the energy width of the states of slow ions have also been reported [7,8], and nonlinear results have been found to be significantly different from those obtained within linear response theory. On the other hand, since the early measurements by Barkas et al. [9] of the energy loss of positive and negative pions it is nowadays well known that deviations from the Z_1^2 (Z_1 represents the projectile charge) stopping power predicted within linear response theories are still significant at velocities over the Fermi velocity of the target, and the necessity of taking Z_1^3 corrections into account has been shown [10–14]. A quadratic response theory for the interaction of charged particles with an electron gas has been developed [13,14], and calculations, within this theory, of the stopping power of an electron gas for ions moving with arbitrary nonrelativistic velocities have provided good agreement with measurements of the energy loss of protons and antiprotons in silicon [13]. A calculation of the Z_1^3 correction to the energy-loss straggling and the energy width of the states of ions moving in an electron gas has been reported only very recently [15], in the low velocity limit.

In this paper we investigate, within the full random-phase approximation (RPA), the Z_1^3 correction to the energy width of the states of ions moving with arbitrary nonrelativistic velocity in an electron gas. The results throughout this paper will be expressed in Hartree atomic units, i.e., $\hbar = m = e = 1$.

2. Theory and results

Considering an ion of charge Z_1 moving with velocity $\boldsymbol{v}$ through a homogeneous electron gas, the energy width of the states of the ion Γ can be expressed in terms of the probability of transferring momentum $\boldsymbol{q}$ and energy ω to the electron gas, $P(\boldsymbol{q},\omega)$, as [16]

$$\Gamma = \int \mathrm{d}\boldsymbol{q} \int_0^\infty P(\boldsymbol{q},\omega)\ \mathrm{d}\omega. \tag{1}$$

An explicit expression for this probability is given, up to third order in the projectile charge, in Ref. [14], by following a perturbation-theoretical analysis of the many-body interactions between the moving charge and the electron gas. Using this probability and the RPA, one finds from Eq. (1):

$$\begin{aligned}\Gamma &= \Gamma_{\mathrm{L}} + \Gamma_{\mathrm{Q}} \\ &= 2Z_1^2 \int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^3} v_{\boldsymbol{q}}\ \mathrm{Im}(-\epsilon^{-1}_{\boldsymbol{q},\omega})\theta(\omega) \\ &\quad - 4Z_1^3 \int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^3} v_{\boldsymbol{q}} \int \frac{\mathrm{d}^3\boldsymbol{q}_1}{(2\pi)^3} v_{\boldsymbol{q}_1} v_{\boldsymbol{q}-\boldsymbol{q}_1} \\ &\quad [f_1(\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1) + f_2(\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1) \\ &\quad + f_3(\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1)]\theta(\omega),\end{aligned} \tag{2}$$

where the subscripts L and Q denote linear and quadratic contributions, respectively, $\epsilon_{\boldsymbol{q},\omega}$ is the longitudinal dielectric function, $v_{\boldsymbol{q}}$ is the Fourier transform of the electron–electron bare Coulomb interaction, $v_{\boldsymbol{q}} = 4\pi/\boldsymbol{q}^2$, $\theta(x)$ is the Heaviside function,

$$\begin{aligned}&f_1(\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1) \\ &= \mathrm{Im}\ \epsilon^{-1}_{\boldsymbol{q},\omega}\ \mathrm{Re}\ \epsilon^{-1}_{\boldsymbol{q}_1,\omega_1}\ \mathrm{Re}\ \epsilon^{-1}_{\boldsymbol{q}-\boldsymbol{q}_1,\omega-\omega_1}\ \mathrm{Re}\, M^{\mathrm{s}}_{\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1},\end{aligned} \tag{3}$$

$$\begin{aligned}&f_2(\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1) \\ &= \mathrm{Re}\ \epsilon^{-1}_{\boldsymbol{q},\omega}\ \mathrm{Re}\ \epsilon^{-1}_{\boldsymbol{q}_1,\omega_1}\ \mathrm{Re}\ \epsilon^{-1}_{\boldsymbol{q}-\boldsymbol{q}_1,\omega-\omega_1} H^{\mathrm{s}}_{\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1},\end{aligned} \tag{4}$$

$$\begin{aligned}&f_3(\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1) = \\ &- 2\mathrm{Im}\ \epsilon^{-1}_{\boldsymbol{q},\omega}\ \mathrm{Im}\ \epsilon^{-1}_{\boldsymbol{q}_1,\omega_1}\ \mathrm{Re}\ \epsilon^{-1}_{\boldsymbol{q}-\boldsymbol{q}_1,\omega-\omega_1} H^{\mathrm{s}}_{\boldsymbol{q}_1,\omega_1,\boldsymbol{q},\omega},\end{aligned} \tag{5}$$

with

$$\omega = \boldsymbol{q}\cdot\boldsymbol{v}, \tag{6}$$

$$\omega_1 = \boldsymbol{q}_1\cdot\boldsymbol{v}_1. \tag{7}$$

$M^{\mathrm{s}}_{\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1}$ represents the symmetrized quadratic density–density response function, and $H^{\mathrm{s}}_{\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1}$ is related to the imaginary part of $M^{\mathrm{s}}_{\boldsymbol{q},\omega,\boldsymbol{q}_1,\omega_1}$ [14].

Calculations of both linear and quadratic energy widths of protons moving in an electron gas with $r_{\mathrm{s}} = 2, 4$, and 6, as obtained from Eqs. (2)–(7), are presented in Fig. 1. The corresponding inverse mean free paths, Γ_{L}/v and Γ_{Q}/v, are exhibited in Fig. 2. The sum of linear and quadratic energy widths of protons and antiprotons with $r_{\mathrm{s}} = 2$ are shown, as a triple dot–dashed curve and a dash–dotted curve, respectively, in Fig. 3. For comparison, the linear (short-dashed curve)

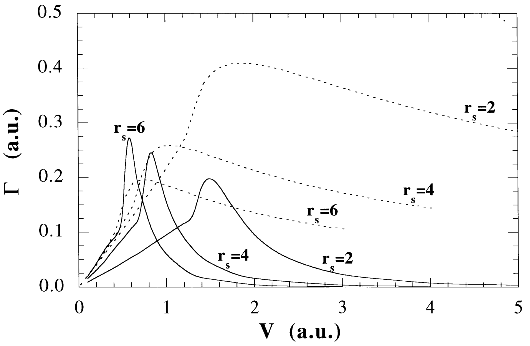

Fig. 1. The linear (short–dashed curves) and quadratic (solid curves) energy widths of states of protons, in an electron gas with $r_s = 2$, 4, and 6, as a function of the projectile-velocity.

and quadratic (solid curve) energy widths of protons for $r_s = 2$ are also displayed in Fig. 3. An inspection of Figs. 1 and 3 indicates that the quadratic contribution to both the energy width and the inverse mean free path is, at velocities above the maximum, much smaller than the linear contribution, showing a good convergence, at high velocities, of the Z_1 expansion. In Fig. 4 the sum of linear and quadratic inverse mean free paths of protons and antiprotons are shown as a triple dot–dashed curve and a dash–dotted curve, respectively.

The low-velocity limit of the Z_1^3 correction to the energy width of the states of charged particles moving in an electron gas has been investigated recently [15], by using the low-frequency limit of the

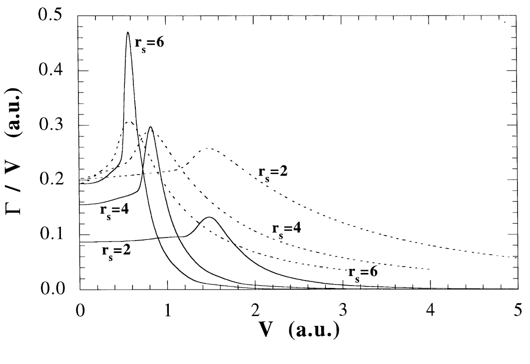

Fig. 2. The linear (short–dashed curves) and quadratic (solid curves) contributions to the inverse mean free path of protons, in an electron gas with $r_s = 2$, 4, and 6, as a function of the projectile-velocity.

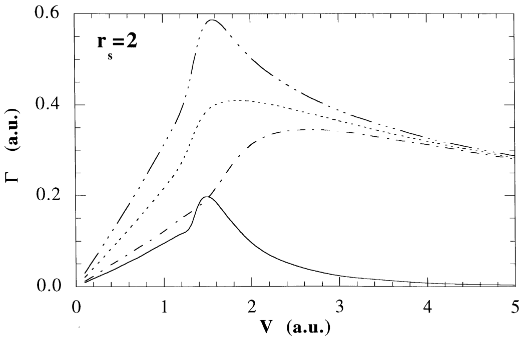

Fig. 3. The sum of the linear and quadratic energy widths of states, $\Gamma = \Gamma_L + \Gamma_Q$, of protons (triple dot–dashed curve) and antiprotons (dash–dotted curve) in an electron gas with $r_s = 2$. The short-dashed curve and solid curve represent the linear and quadratic contributions to the energy width of states of protons, respectively.

full RPA linear and quadratic response functions. Within the low-velocity limit, a full nonlinear calculation of the energy width of the states of both protons and antiprotons was also presented in Ref. [15], as obtained by following a scattering theory approach in which the statically screened potential was determined by solving self-consistently a Hartree one-body equation, showing that the quadratic response theory of Ref. [14] is accurate, in the case of antiprotons, to describe nonlinearities for all electron densities with $r_s \leqslant 2$.

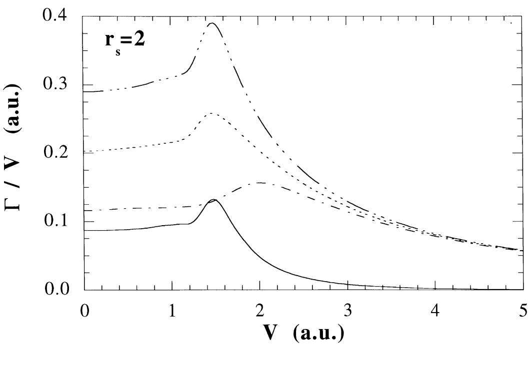

Fig. 4. The sum of the linear and quadratic inverse mean free paths, $\Gamma/v = \Gamma_L/v + \Gamma_Q/v$, of protons (triple dot–dashed curve) and antiprotons (dash–dotted curve) in an electron gas with $r_s = 2$. The short-dashed curve and solid curve represent the linear and quadratic contributions to the inverse mean free path of protons, respectively.

Accordingly, the results presented in Figs. 3 and 4 for the total contribution, up to third order in the projectile charge, to the energy width and the inverse mean free path of antiprotons are expected to be accurate for arbitrary nonrelativistic velocities.

For completeness, our total RPA energy width is presented in Fig. 5, as obtained in the low-velocity limit up to third order in the projectile charge and as a function of the electron density parameter r_s, in the case of both protons and antiprotons. Since exchange and correlation are absent in our RPA treatment, we have also represented, in the same figure, full nonlinear self-consistent Hartree calculations, i.e., DFT calculations with exchange and correlation contributions to the effective screened potential excluded, like the ones presented in Ref. [15]. While in the case of antiprotons for $r_s \leqslant 2$ our quadratic response calculations show a good agreement with the corresponding full nonlinear results, in the case of protons the quadratic response calculations appear to be accurate only at very high electron densities ($r_s < 1$). Our quadratic calculations overestimate, at metallic densities, the energy width of the states of slow protons. This is a consequence of slow positive ions being able to carry with them a number of electrons [6].

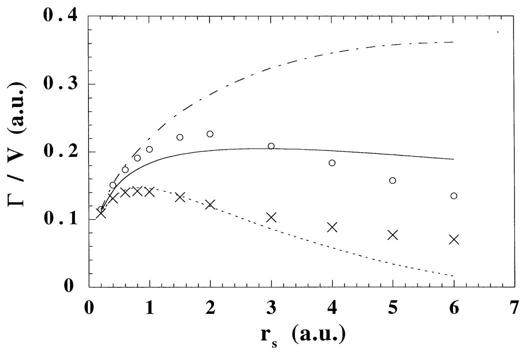

Fig. 5. A comparison of the inverse mean free paths of the perturbation theory down to Z_1^3 order within the RPA, $\Gamma/v = \Gamma_L/v + \Gamma_Q/v$, for slow protons (dash–dotted curve) and antiprotons (short-dashed curve), with those of fully nonlinear Hartree calculation to all orders in Z_1 for protons (circles) and antiprotons (crosses). The solid curve represent the linear contribution to the inverse mean free path, Γ_L/v, for $|Z_1| = 1$.

3. Summary and conclusions

We have calculated Z_1^3 corrections to the energy widths of the states of protons and antiprotons moving with arbitrary nonrelativistic velocities in a uniform electron gas, within a quadratic response theory and the RPA. At high velocities (after the plasmon threshold), the quadratic response theory provides an accurate estimate of the full nonlinear correction to the energy widths of the states of protons and antiprotons moving in an electron gas. Within a full nonrelativistic projectile-velocity range the present quadratic response theory provides an accurate description of nonlinearities in the energy width of the states of antiprotons in many solids used in experiments ($r_s \leqslant 2.5$). A comparison with results obtained within linear response theory indicates that at low and intermediate velocities the Z_1^3 correction reduces significantly the energy width of states of antiprotons.

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