Nonlinear calculations for the width of particle states

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The energy width of the states of slow ions interacting with an electron gas has been calculated using the density-functional formalism to calculate an effective one-electron potential. Our results show the same behavior as the stopping power and straggling parameter when comparisons with dielectric theory are made. The agreement between the dielectric and nonlinear density-functional results is improved when a local-field correction is taken into account in the dielectric formalism.

The problem of slow ions moving with constant velocity v ($v \ll v_F$, v_F being the Fermi velocity of electrons in the conduction band) is of special interest in cases such as the slowing and reflection of hydrogen atoms impinging on the inner wall of a controlled thermonuclear reactor[1] as well as in astrophysical studies and in surface analytical techniques. A many-body formalism[2,3] is needed to treat the complicated nature of the interaction. Because of this complexity, approximations must be made to solve the problem in a tractable way.[4-6] An essential step is to introduce an appropriate local potential to describe the interaction of the electrons with the incoming ion.[7-14]

Using linear response theory it is easy to obtain the basic quantities that characterize the composite system.[15] These are the width of the particle states Γ, the stopping power dE/dR, and the straggling parameter W. The width of the particle states is essentially the integrated value of the differential probability for energy transfer ω in a single inelastic excitation process. For slow, heavy ions this elementary process is the particle-hole generation. Furthermore, by weighting ω and ω^2 with the above differential probability, dE/dR and W, respectively, can be obtained. Thus, although Γ (related to the imaginary part of the self-energy) is not a directly observable quantity, a systematic development of the theoretical description requires its knowledge.

The low-velocity expression for Γ in dielectric theory is given by (atomic units are used throughout this paper)

$$\Gamma = \frac{v}{(2\pi)^3} \int_0^{2v_F} dq\, q^2 \left[\frac{V(q)}{\epsilon(q)} \right]^2 , \tag{1}$$

where $V(q)$ is the Fourier transform of the bare Coulomb potential, $\epsilon(q)$ is the electron dielectric function,[8] and v is the ion velocity. In this case the elastic scattering between the electron and the screened ion is described in the first Born approximation. If we interpret this result in terms of nonrelativistic scattering theory and make the substitution

$$\frac{V(q)}{\epsilon(q)} \leftrightarrow -2\pi f(\theta) ,$$

where $f(\theta)$ is the scattering amplitude and $q = 2v_F \times \sin(\theta/2)$ is the momentum transfer, we obtain for the width of the states

$$\Gamma = \tfrac{3}{2} nv \int_0^{\pi} d\sigma(\theta, v_F) \sin\left[\frac{\theta}{2} \right] . \tag{2}$$

Here n is the electron gas density, and $d\sigma$ is the differential cross section at the Fermi energy.

Similarly (see the Appendix), the well-known results for the stopping power[11,16] and straggling parameter[17] can be obtained:

$$\frac{dE}{dR} = 2nvv_F \int_0^{\pi} d\sigma(\theta, v_F) \sin^2\left[\frac{\theta}{2} \right] , \tag{3}$$

$$W = 3(vv_F)^2 \int_0^{\pi} d\sigma(\theta, v_F) \sin^3\left[\frac{\theta}{2} \right] . \tag{4}$$

Equation (2) allows us to calculate Γ in terms of the phase shifts for the elastic scattering of an electron by the self-consistent potential of the ion in the electron gas. One finds

$$\Gamma = \frac{3\pi nv}{4\sqrt{2} v_F^2} \sum_l \sum_m (2l+1)(2m+1)\{1 - \cos(2\delta_l) - \cos(2\delta_m) + \cos[2(\delta_l - \delta_m)]\} J_{lm} , \tag{5}$$

where δ_l are the phase shifts at the Fermi energy and the quantity J_{lm} is defined by

$$J_{lm} = \int_{-1}^{1} dx (1-x)^{1/2} P_l(x) P_m(x) , \tag{6}$$

and the P_l's are the Legendre polynomials. We have used the phase shifts calculated by Puska and Nieminen[18,19] using density-functional theory (DFT) with the parametrization given by Gunnarsson and Lundqvist[20] for the local exchange and correlation potential. The results obtained for the width of the states for $r_s = 1.5$ and $r_s = 3.0$ [$r_s = (3/4\pi n)^{1/3}$)] are shown in Fig. 1, where we have plotted Γ/v as a function of the ion charge Z_1. The curves show the characteristic Z_1 oscillations that can be explained in terms of the ion effective charge.[21-23] These oscillations have also been found for the stopping

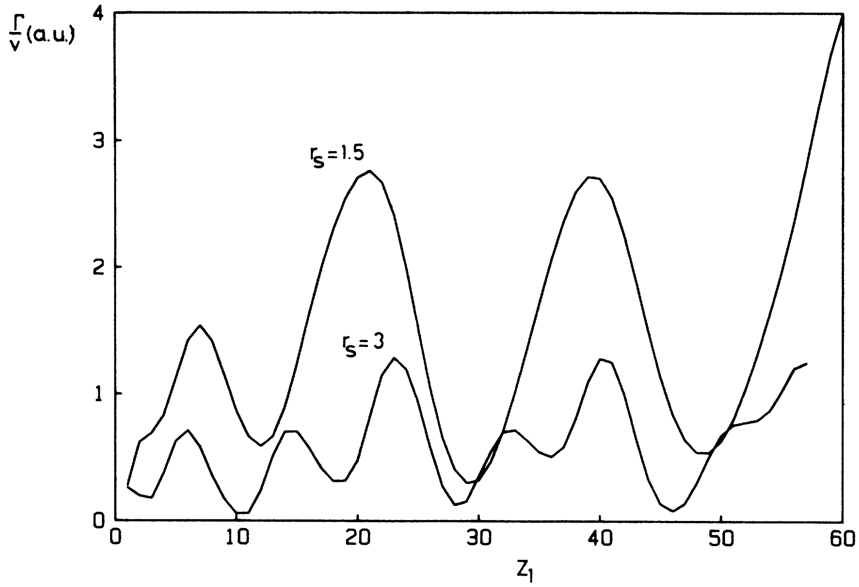

FIG. 1. Width of the particle states for a slow ion interacting with an electron gas of density parameter $r_s = 1.5$ and $r_s = 3.0$. We have plotted Γ/v as a function of the ion charge Z_1. The curves show the characteristic Z_1 oscillations.

power[24,25] and straggling parameter.[26] If an effective charge Z_1^* is defined in an operational manner

$$Z_1^* = \left(\frac{dE/dR\,|_{Z_1}}{dE/dR\,|_{Z_1=1}} \right)^{1/2}, \tag{7}$$

we find that $\Gamma/v(Z_1^*)^2$ is about 0.31 within 30% for $r_s = 1.5$ and for $r_s = 3.0$ it is about 0.28 within 15%. Similar behavior has been found for the straggling parameter.[22,26] That is, most of the oscillatory behavior in Γ/v shown in Fig. 1 is due to the variation in ion effective charge as defined by Eq. (7).

In Fig. 2 we have plotted Γ/v as a function of r_s for $Z_1 = 1$ and $Z_1 = 2$ and compare with dielectric-theory (DT) results without local-field correction [random-phase approximation (RPA)] and with a local-field correction.[8,27] The DFT results are given by the curves labeled $Z_1 = 1$ for a proton and $Z_1 = 2$ for a helium nucleus. The width of the states is smaller for a helium nucleus than that for a proton with the same velocity for $r_s \gtrsim 2.5$. The curves labeled DT1 (without local-field correction) and DT2 (with local-field correction) in Fig. 2 are the dielectric theory results for a proton calculated from Eq. (1). These are about 0.2 and 0.3 respectively for $1.5 \lesssim r_s$

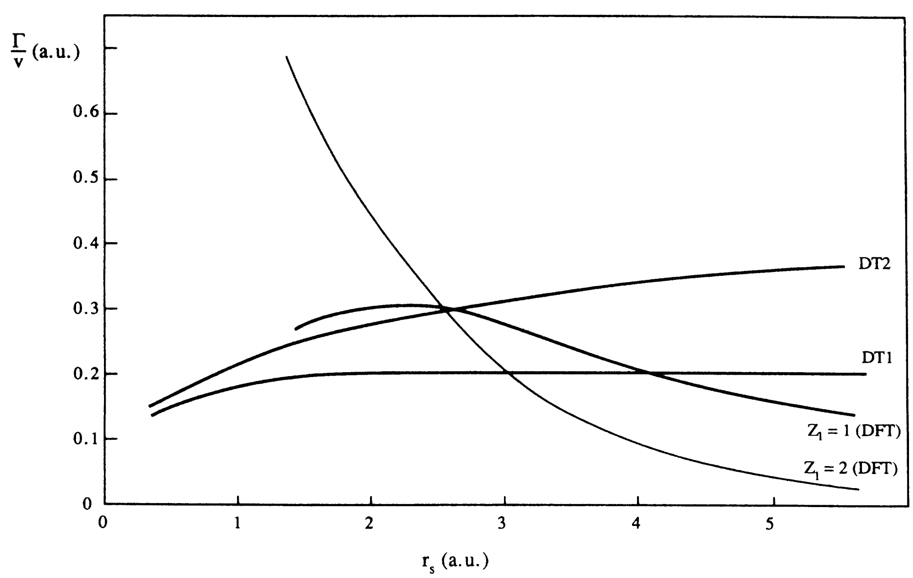

FIG. 2. Width of the particle states for a slow ion interacting with an electron gas as a function of r_s. Curve labeled DT1 is the dielectric-theory result, without local-field correction, for a proton and DT2 with local-field correction. The curve labeled $Z_1 = 1$ is the nonlinear DFT result for a proton. (The one labeled $Z_1 = 2$ is the nonlinear DFT result for a helium nucleus.)

≤ 4.0. If we compare the DFT result with DT1 we see that it is about 50% greater when $1.5 \leq r_s \leq 3.0$. In this density range the agreement with DT2 is better. Nevertheless, it is clear that significant correction to the RPA results are to be expected when refined descriptions of exchange and correlation (local field factor[27]) are included in the response function. For high r_s values the nonlinear DFT result is smaller than the dielectric theory one. Lowest-order perturbation theory must obviously break down when the projectile can bind an electron.[28] For the straggling parameter and the stopping power the same behavior have been found[29,30] in this region of r_s values. For very small r_s ($r_s < Z_1^{-2}$) values the two theories (DT and DFT) tend toward agreement independently of the charge of the projectile.

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APPENDIX

Equation (2) has been derived in a heuristic didactic way. From the general theoretical results of Ref. 4, with the substitution

$$\omega = \mathbf{q}\cdot\mathbf{v} = qv\cos\phi ,$$

and taking into account that for low ion velocities $q = 2v_F \sin(\theta/2)$ it is easy to obtain an expression, $L(n)$, for the determination of the basic quantities

$$L(n) = \frac{1}{2}\left[\frac{v_F}{\pi}\right]^2 \int_0^{\pi/2} d\phi \sin\phi \times \int_0^{\pi} d\sigma(\theta, v_F)\left[2vv_F \sin\left[\frac{\theta}{2}\right]\cos\phi\right]^n . \tag{A1}$$

From Eq. (A1)

$$\Gamma = L(n=1) ,$$

$$\frac{dE}{dR} = \frac{1}{v}\frac{dE}{dt} = \frac{1}{v}L(n=2) ,$$

$$W = \frac{1}{nv}\frac{d}{dt}[\langle(\Delta E - \langle\Delta E\rangle)^2\rangle] = \frac{1}{nv}L(n=3) .$$

Neglect of recoil is the major approximation that has been made in deriving Eq. (A1). Such an approximation is justified when the impulse of the slow heavy ion is much bigger than the Fermi impulse. In this case the center-of-mass velocity corresponds to the velocity of the intruder.

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