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DENSITY FUNCTIONAL CALCULATION OF STOPPING POWER OF AN ELECTRON GAS FOR SLOW IONS*

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We describe the first calculation of the stopping power of an electron gas for slow ions using the density-functional formalism. We evaluate the nonlinear self-consistent potential around the ion and from scattering theory determine the energy loss directly. Comparison with the results of linear theory is made.

The theory of stopping power of solids for energetic ions is of continuing interest in physics. The case of slow ions, i.e., ions moving with much less than the average velocity of the electrons in the solid, is important in cases such as the slowing and reflection of hydrogen atoms impinging on the inner wall of a controlled thermonuclear reactor.[1] Recently Oen and Robinson[2] have carried out Monte Carlo studies to estimate the number and energy of ions reflected from a metal surface.

We here summarize briefly theoretical work on the stopping power of an electron gas for a slow ion. Some numerical results that we have obtained from density functional theory are described.

Fermi and Teller[3] were the first to calculate the energy loss per unit path length of a charged particle moving with velocity $\underline{v}$ much less than the Fermi velocity $\underline{v}_F$. Their result for an intruder of charge Z_1 can be written as

$$\frac{dW}{dR} = Z_1^2 \frac{2v}{3\pi} \ln\left(\frac{1}{\alpha r_s}\right) \tag{1}$$

where v is the particle speed, r_s is the one-electron radius, $r_s = (3/4\pi n)^{1/3}$ where n is the electron density, and $\alpha = (4/9\pi)^{1/3}$. We use atomic units throughout ($e = \hbar = m = 1$).

Within linear response theory the stopping power for a classical point charge moving at constant velocity $\underline{v}$ can be written as

$$\frac{dW}{dR} = \frac{2Z_1^2}{\pi v^2} \int_0^\infty \omega d\omega \int_{\omega/v}^\infty \frac{dk}{k} \operatorname{Im}\left(\frac{-1}{\epsilon(k,\omega)}\right) \tag{2}$$

where $\epsilon(k,\omega)$ is the longitudinal dielectric function for the stopping medium. An improvement over the Fermi-Teller formula can be obtained[4] from this, using an approximation to the full RPA[5] dielectric constant for an electron gas, valid when $\omega = 0$ and $k/k_F \lesssim 1$. Here $\underline{k}_F$ is the Fermi momentum. This is equivalent to assuming that the potential about an ion is exponentially screened by density fluctuations in the electron gas. One obtains

$$\frac{dW}{dR} = Z_1^2 \frac{2v}{3\pi}\left[\ln\left(1+\frac{\pi}{\alpha r_s}\right) - \frac{1}{1+\alpha r_s/\pi}\right] \tag{3}$$

as shown by Ritchie.[4] For $r_s \ll 1$, Eq. (3) reduces to Eq. (1).

Recently Ferrell and Ritchie[6] have calculated from linear response theory the stopping power for slow, singly ionized He atoms. They also considered an alternative approach to determining the energy loss of slow ions in terms of scattering theory.[6] Electrons at the Fermi surface are viewed as being scattered by the screened potential of the ion. The stopping power for a slow ion can be written as[6-8]

$$\frac{dW}{dR} = \frac{3v}{k_F r_s^3} \sum_{\ell=0}^{\infty} (\ell+1)\sin^2\left[\delta_\ell(E_F) - \delta_{\ell+1}(E_F)\right] \tag{4}$$

where $\delta_\ell(E_F)$ are the phase shifts at the Fermi energy for scattering of an electron on a spher-

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ically symmetric self-consistent potential. Since the ion is moving slowly compared with the electrons at the Fermi surface, we can use the results of a static calculation for such potential. Recent work by Almbladh, et al., and others[9] shows that nonlinear calculations of the density fluctuations and induced potential differ markedly from the ones obtained with linear response theory.

We have used the density functional formalism of Hohenberg and Kohn and Kohn and Sham[10] to calculate the self-consistent potential due to a static proton and a He nucleus submerged in an electron gas at metallic densities. The local density approximation for exchange and correlation has been used with the parametrization given by Gunnarsson and Lundqvist.[11] Except at the highest densities, a doubly occupied bound state exists below the bottom of the conduction band.

The scattering phase shifts at the Fermi level satisfy the Fridel sum rule to a good accuracy. Those phase shifts were used in Eq. (4) to tabulate the stopping power. The results of our calculations are shown in Fig. 1 together with the linear theory predictions. Curve A was calculated in linear response theory, Eq. (3), for $Z_1 = 1$ while Curve B was computed from the same equation for $Z_1 = 2$. We show in Curve C the results of a calculation by Ferrell and Ritchie[6] of the stopping power for a slow, singly ionized He atom calculated from linear response theory, using a wave function for the bound electron determined self-consistently in the electron gas. Curves D and E were computed from the density functional approach for a proton and a He nucleus, respectively.

As r_s decreases toward values << 1, our results tend toward agreement with linear theory. That is, Curve D, computed by the density functional method for a proton, approaches Curve A,

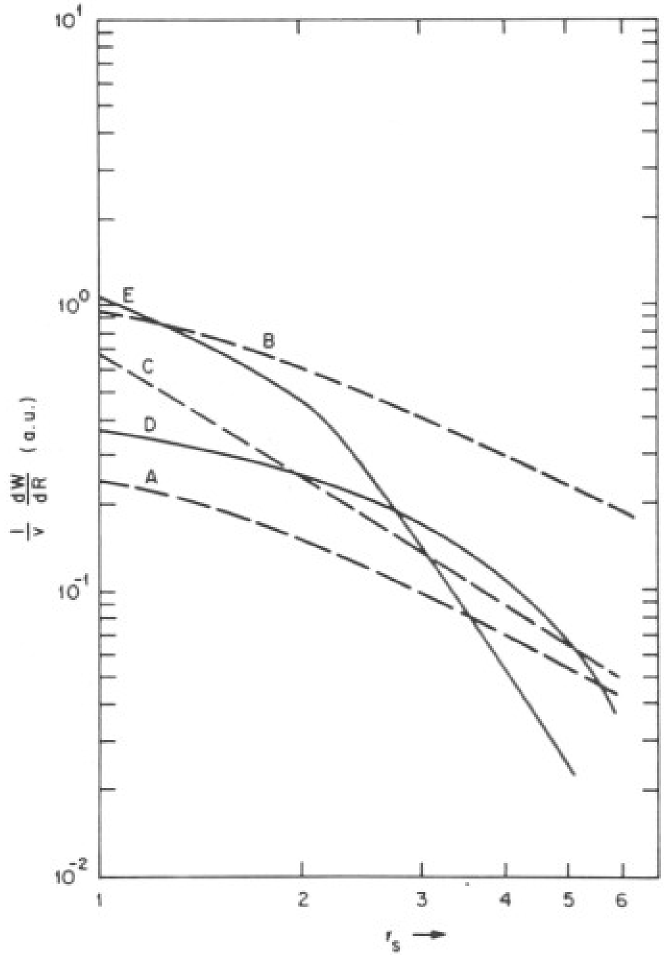

Fig. 1. Variation of v^{-1} dW/dR with r_s as found in a linear response theory for a proton (Curve A) and for a He nucleus (Curve B). Curve C shows the results of Ferrell and Ritchie's calculation (Ref. 6) for a slow, singly ionized He atom. Curves D and E show the results of the present work for protons and He nuclei, respectively. In all of these calculations, we take $v << v_F$.

calculated from Eq. (3) using $Z_1 = 1$. It is interesting that for $r_s \lesssim 1.2$, Curve E, computed for a He nucleus, actually lies above Curve B, computed from Eq. (3) taking $Z_1 = 2$. However, they approach the same value as $r_s \to 0$. As r_s increases, the energy loss for both H and He decreases more rapidly than predicted by linear theory due to the fact that bound states of atomic character develop, thereby tending to screen out interactions with the electron gas. The energy loss of a He nucleus at large r_s is smaller than that of a proton at the same r_s value. This can be understood in terms of atomic scattering cross sections for zero-energy electrons on the respective atoms. For those electrons the scattering lengths on He and H atoms are 1.44 and 2.39 atomic units, respectively.[12] The ratio of electron scattering cross section on hydrogen to that on helium at very low energies is then $(2.39/1.44)^2 = 2.75$, while at $r_s = 5$ the ratio of the stopping powers for protons and He nuclei is nearly the same, viz., 2.61, in our calculation. This confirms the qualitative expectation that an ion moving in a very low-density electron gas experiences energy loss nearly equal to that computed as if the electrons of the medium scatter independently from the fully neutral atomic form of the ion.

In conclusion, we have evaluated the stopping power of an electron gas for slow protons and He nuclei using the density functional formalism to compute the nonlinear self-consistent potential around the ion. The results of our calculation differ from the ones obtained with linear response theory in that the atomic character of the projectile is fully accounted for in the present work at all values of r_s.

We are currently extending this work to ions with $Z_1 > 2$ in order to study "Z_1-fluctuations" in energy loss of slow ions in matter.[13]

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References

1. J. T. Hogan and J. F. Clarke, Journal of Nuclear Materials 53, 1 (1974).
2. O. S. Oen and M. T. Robinson, Nuclear Instruments and Methods 132, 647 (1976).
3. E. Fermi and E. Teller, Physical Review 72, 399 (1947).
4. R. H. Ritchie, Physical Review 114, 644 (1959).
5. J. Lindhard, Kongelige Danske Videnskabernes Selskab, Matematsik-Fysiske Meddelelser 28(8) (1954).
6. T. L. Ferrell and R. H. Ritchie, Physical Review B 16, 115 (1977).
7. N. F. Mott and H. Jones [The Theory and Properties of Metals and Alloys (Dover, 1958) p. 294] employ this model in Born approximation to estimate the contribution of impurity scattering to the resistivity of metal.
8. J. Finneman, dissertation (The Institute of Physics, Aarhus Univ., 1968), unpublished.
9. C. O. Almbladh, U. von Barth, Z. D. Popovic and M. J. Stott, Physical Review B 14, 2250 (1976); P. Jena and K. S. Singwi, Physical Review B 17, 3518 (1978).
10. P. Hohenberg and W. Kohn, Physical Review B 136, 964 (1964); W. Kohn and L. J. Sham, Physical Review A 140, 1133 (1965).
11. O. Gunnarsson and B. Lundqvist, Physical Review B 13, 4274 (1976).
12. K. Smith, R. P. McEachran and P. E. Fraser, Physical Review 125, 553 (1962); G. F. Drukarev, The Theory of Electron-Atom Collisions (Academic Press, 1965).
13. J. H. Ormrod, J. R. MacDonald and H. E. Duckworth, Canadian Journal of Physics 43, 275 (1965); B. Fastrup, P. Hvelplund and C. A. Sautter, Kongelige Danske Videnskabernes Selskab, Matematsik-Fysiske Meddelelser 35(10) (1966); L. Eriksson, J. A. Davies and P. Jespersgaard, Physical Review 161, 219 (1967); F. H. Eisen, Canadian Journal of Physics 46, 561 (1968). For references to experiment and theory in this area, see J. S. Briggs and A. P. Pathak in Atomic Collisions in Solids, Eds., S. Datz, B. R. Appleton and C. D. Moak (Plenum Press, 1975) p. 15.