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Collective Oscillations in Many Electron Atoms. II* Scattering and Slowing Down

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Abstract

The slowing down of fast charged particles by their interaction with many electron atoms is considered using the hydrodynamic version of the Thomas–Fermi model. The agreement obtained with experiment is excellent over a wide range of parameters but worsens as the velocity of the charged particle decreases.

1. Introduction

In a former paper (Monaghan 1973, hereinafter referred to as Part I) the small oscillations of the Thomas–Fermi model (Bloch 1933*a*) were examined and the radial and dipole modes of oscillation were calculated. In the present paper, the numerical and analytical results of Part I are applied to the problem of the slowing down of fast charged particles by their interaction with many electron atoms which may be ionized. The classical picture of the process, together with its generalization to the quantum mechanical case, has been given by Jackson (1962). The paper by Bloch (1933*a*) is fundamental for the present investigation.

2. Equations of Motion

As in Part I, the motion of the atomic electrons is assumed to be described by the Eulerian equation of motion with an equation of state appropriate to a degenerate electron gas. If ρ is the mass density of the electrons, $\rho \boldsymbol{f}$ the Coulomb force per unit volume due to the particles of the atom and U the Coulomb potential between an electron and a passing external charge then the equation of motion is

$$\rho\,\partial \boldsymbol{v}/\partial t + \rho(\boldsymbol{v}\,.\,\nabla)\boldsymbol{v} = -\nabla p + \rho(\boldsymbol{f} - \mu^{-1}\nabla U), \tag{1}$$

where μ is the mass of an electron. The unperturbed equation is

$$0 = -\nabla p_0 + \rho_0 \boldsymbol{f}, \tag{2}$$

which, as was shown in Part I, may be manipulated to give the Thomas–Fermi equation. For small motions, equation (1) can be linearized to become

$$\rho_0\,\partial \boldsymbol{v}/\partial t = -\nabla \delta p + \delta\rho \boldsymbol{f} - \rho_0\,\mu^{-1}\nabla U, \tag{3}$$

where, as with the approximations used in Part I, $\delta \boldsymbol{f}$ has been neglected. Using

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equation (2) and recalling that for a fully degenerate electron gas

$$p = \text{const.}\, \rho^{5/3}, \tag{4}$$

we find that

$$\partial \boldsymbol{v}/\partial t = -\nabla(W\delta\rho) - \mu^{-1}\nabla U, \tag{5}$$

where $W = 5p_0/3\rho_0^2$.

Since the forces are conservative and the fluid is barytropic, we can choose

$$\boldsymbol{v} = \nabla\Phi, \tag{6}$$

so that equation (5) becomes

$$\partial\Phi/\partial t + W\delta\rho + \mu^{-1}U = 0. \tag{7}$$

The equation of continuity for the perturbed motion then takes the form

$$\partial(\delta\rho)/\partial t + \nabla.(\rho_0\nabla\Phi) = 0. \tag{8}$$

If the potential U is due to a charge Qe moving in a straight line with velocity v and impact parameter b then

$$U = -Qe^2\{(b-x)^2 + (vt-y)^2 + z^2\}^{-\frac{1}{2}}. \tag{9}$$

Here a cartesian coordinate system has been used, with origin at the centre of the atom, the y axis parallel to $\boldsymbol{v}$, and the z axis perpendicular to the plane containing $\boldsymbol{v}$ and the centre of the atom. It should be noted that equation (9) is only valid provided the deviation of the passing particle is negligible. It would be straightforward, though complicated, to deal with the case where the trajectory is no longer a straight line but it is convenient, and practical, to assume that v is sufficiently large to justify the straight line approximation.

Provided the particle passes outside the atom, or at most penetrates the low density outer region, equation (9) may be replaced by

$$U = -Qe^2(b^2+v^2t^2)^{-\frac{1}{2}}\{1 + (bx+vty)/(b^2+v^2t^2)\}. \tag{10}$$

The first term of equation (10) does not enter the equations of motion because it contributes nothing to ∇U. On neglecting this term we have

$$U = -Qe^2(b^2+v^2t^2)^{-3/2}(bx+vty). \tag{11}$$

The presence of x and y in equation (11) shows that the dipole modes corresponding to the spherical harmonic Y_{lm}, with $l = 1$ and $m = \pm 1$, are driven by the disturbing potential U. The equations of motion can therefore be solved by expanding Φ and $\delta\rho$ in terms of the eigenfunctions for the $l = 1$ modes. This expansion can be written

$$\Phi = \sum_j \Phi_j(B_{ja}\sin\theta\cos\phi + B_{jb}\sin\theta\sin\phi), \tag{12}$$

$$\delta\rho = \sum_j \eta_j(A_{ja}\sin\theta\cos\phi + A_{jb}\sin\theta\sin\phi), \tag{13}$$

where Φ_j and η_j are the radial parts of the eigenfunctions as calculated in Part I and B_{ja}, B_{jb}, A_{ja} and A_{jb} are functions of time. Substituting equations (12) and (13) into (7) and (8) we find (recalling equation (30) and the orthogonality condition (33) of Part I) that

$$\dot{B}_{ja} + w_j A_{ja} = \frac{Qe^2 b}{\mu H_j w_j (b^2 + v^2 t^2)^{3/2}} \int \eta_j r^3 \, \mathrm{d}r \tag{14}$$

and

$$\dot{A}_{ja} = B_{ja} w_j , \tag{15}$$

with

$$H_j = \int \Phi^2 r^2 W^{-1} \, \mathrm{d}r ,$$

where w_j is an eigenvalue for the dipole oscillation. The equations for B_{jb} and A_{jb} are the same as equations (14) and (15) except that vt replaces b in the numerator of (14).

3. Energy Loss

We now obtain an expression for the energy of the atom after the particle has receded to infinity by multiplying equation (5) by $\rho_0 \boldsymbol{v}$ and integrating over the atomic volume. We no longer consider U since its contribution is negligible when $t \to \infty$. If ΔE is the energy of excitation then

$$\mathrm{d}\Delta E/\mathrm{d}t = \int \{\rho_0 \boldsymbol{v} . \partial \boldsymbol{v}/\partial t + \rho_0 \boldsymbol{v} . \nabla(W \delta\rho)\} \, \mathrm{d}\tau . \tag{16}$$

By elementary manipulations and the use of equation (8), equation (16) becomes

$$\frac{\mathrm{d}\Delta E}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \int \{\tfrac{1}{2}\rho_0 v^2 + \tfrac{1}{2} W(\delta\rho)^2\} \, \mathrm{d}\tau . \tag{17}$$

The energy of excitation is therefore given by

$$\Delta E = \int \{\tfrac{1}{2}\rho_0 v^2 + \tfrac{1}{2} W(\delta\rho)^2\} \, \mathrm{d}\tau . \tag{18}$$

Substituting equations (12) and (13) into (18), and using the orthogonality relations for η_j and Φ_j, gives

$$\Delta E = \tfrac{2}{3}\pi \sum_j H_j w_j^2 (B_{ja}^2 + A_{ja}^2 + B_{jb}^2 + A_{jb}^2) . \tag{19}$$

Equations (14) and (15), together with their counterparts for B_{jb} and A_{jb}, may be solved by standard methods. Letting $t \to \infty$, we find that

$$A_{ja}^2 + B_{ja}^2 = \left(\frac{Qe^2}{\mu H_j w_j}\right)^2 \left| b \int_{-\infty}^{\infty} \frac{\exp(\mathrm{i} w_j t) \, \mathrm{d}t}{(b^2 + v^2 t^2)^{3/2}} \right|^2 \left(\int \eta_j r^3 \, \mathrm{d}r \right)^2 , \tag{20}$$

$$A_{jb}^2 + B_{jb}^2 = \left(\frac{Qe^2}{\mu H_j w_j}\right)^2 \left| v \int_{-\infty}^{\infty} \frac{t \exp(\mathrm{i} w_j t) \, \mathrm{d}t}{(b^2 + v^2 t^2)^{3/2}} \right|^2 \left(\int \eta_j r^3 \, \mathrm{d}r \right)^2 . \tag{21}$$

The integrals over t occurring in equations (20) and (21) can be written in terms of the modified Bessel functions K_n. Substituting into equation (19) we find that

$$\Delta E = \left(\frac{Q^2 e^4}{\mu^2 v^4}\right)\tfrac{8}{3}\pi \sum_j w_j^2 H_j^{-1}\{K_1^2(\xi_j)+K_0^2(\xi_j)\}\left(\int \eta_j r^3\,\mathrm{d}r\right)^2,$$

where

$$\xi_j = w_j b v^{-1}. \tag{22}$$

If there are N atoms per unit volume, the energy loss of the particle per unit length of path due to distant collisions is

$$(\mathrm{d}E/\mathrm{d}R)_{\mathrm{far}} = 2\pi N \int_{b_1}^{\infty} \Delta E\, b\, \mathrm{d}b. \tag{23}$$

The choice of b_1 is discussed in Section 4. Substituting for ΔE in equation (23) gives

$$(\mathrm{d}E/\mathrm{d}R)_{\mathrm{far}} = \tfrac{8}{3}\pi\left(\frac{Q^2 e^4}{\mu^2}\right)2\pi N v^{-2}\sum_j H_j^{-1}\left(\int \eta_j r^3\,\mathrm{d}r\right)^2 \xi_j K_0(\xi_j) K_1(\xi_j), \tag{24}$$

where ξ_j is now given by $w_j b_1 v^{-1}$. By making use of the parameters used in Part I, equation (24) can be written as

$$(\mathrm{d}E/\mathrm{d}R)_{\mathrm{far}} = (Q^2 e^4/\mu v^2)\, 4\pi N Z \sum_j q_j \xi_j K_0(\xi_j) K_1(\xi_j), \tag{25}$$

where

$$q_j = v_j^2 x_0^{9/2}\left(\int_0^1 \Phi_j \phi^{1/2} u^{5/2}\,\mathrm{d}u\right)^2 \Big/ 5\int_0^1 \Phi_j^2 \phi^{1/2} u^{3/2}\,\mathrm{d}u. \tag{26}$$

An often used approximation is based on the observation that $K_n(x)$ decreases exponentially for $x \gg 1$ and that

$$K_0(x) \simeq \ln 2x^{-1} \qquad \text{and} \qquad K_1(x) \simeq x^{-1} \qquad \text{for} \qquad x \ll 1. \tag{27}$$

Substituting these approximations into equation (25) and introducing the classical oscillator strength

$$f_j = Z q_j,$$

we find that

$$(\mathrm{d}E/\mathrm{d}R)_{\mathrm{far}} \simeq 4\pi N Q^2 e^4 \mu^{-1} v^{-2} \sum_j f_j \ln(2v/b_1 w_j). \tag{28}$$

The total energy loss is found by adding the energy loss due to close collisions. For fast particles, Bloch (1933*b*) has estimated this contribution to be

$$(\mathrm{d}E/\mathrm{d}R)_{\mathrm{close}} \simeq 4\pi N Q^2 e^4 \mu^{-1} v^{-2} Z \ln(2\mu v b_1/1\cdot 1\hbar). \tag{29}$$

If we define an average frequency $\bar{w}$ by

$$\sum_j f_j \ln w_j = Z \ln \bar{w} \tag{30}$$

and use the sum rule in its approximate form

$$\sum_j f_j \simeq Z, \tag{31}$$

we can combine equations (28) and (29) to give

$$(\mathrm{d}E/\mathrm{d}R)_{\text{total}} \simeq 4\pi N Q^2 e^4 \mu^{-1} v^{-2} Z \ln(2\mu v^2/1\cdot 1\hbar\bar{w}). \tag{32}$$

This formula is in essential agreement with the quantum mechanical formula. Nevertheless the foregoing analysis is not satisfactory for it is not always true that the sum over all frequencies is consistent with the approximations (27). It is preferable, as done in Section 4, to estimate the energy loss due to distant collisions more accurately.

4. Numerical Results and Discussion

It is convenient to follow Lindhard and Scharff (1953) and introduce quantities L and X defined by

$$L = (\mathrm{d}E/\mathrm{d}R)_{\text{total}}\, \mu v^2 (4\pi N Z Q^2 e^4)^{-1} \tag{33}$$

and

$$X = (v\hbar e^{-2})^2 Z^{-1}. \tag{34}$$

From the previous results we obtain

$$L = \ln(2\mu v b_1/1\cdot 1\,\hbar) + \sum_j q_j \xi_j K_0(\xi_j) K_1(\xi_j). \tag{35}$$

The choice of b_1 is not too critical because it does not occur in the most important terms. A rough estimate of it can be made by noting that it divides the collisions at the point where the typical period of the incoming particle is comparable with that of the orbital electrons, i.e.

$$v/b_1 \approx u/a \approx e^2\hbar^{-1} Z^{2/3} \mu e^2 Z^{1/3} \hbar^{-2}, \tag{36}$$

or

$$b_1 = v\hbar^3/\mu e^4 Z,$$

where the estimates of u and a have been taken from Lindhard and Scharff (1953). The scaling used in Part I is chosen so that

$$w_j = v_j Z\mu e^4 \pi^2 2^7/h^3 3\sqrt{5}, \tag{37}$$

and the numerical calculations show that

$$v_j \approx gj, \tag{38}$$

where g only depends on Z. Defining J by

$$J = \pi 3\sqrt{5}/16g, \tag{39}$$

the expression for L becomes

$$L = \ln(1\cdot 81\, X) + \sum_{j=1}^{\infty} (j/J)\, q_j K_0(j/J) K_1(j/J). \tag{40}$$

The evaluation of L is made difficult because the series converges very slowly. To overcome this difficulty the following procedure was adopted. The sum rules of

Part I show that

$$\sum_{j=1}^{\infty} q_j = 1 - Z^{-1} \tag{41}$$

and

$$\sum_{j=1}^{\infty} C_j \equiv \sum_{j=1}^{\infty} \left(\int_0^1 \Phi_j^2 \phi^{1/2} u^{5/2}\,\mathrm{d}u\right)^2 \Big/ \int_0^1 \Phi_j^2 \phi^{1/2} u^{3/2}\,\mathrm{d}u = \int_0^1 \phi^{1/2} u^{7/2}\,\mathrm{d}u\,, \tag{42}$$

while the numerical calculations show that

$$C_j \approx B/j^{3+\varepsilon} \tag{43}$$

By substituting equation (43) into (42) and (41), and using the Euler summation formula, B and ε can be estimated for various values of Z:

Z	B	ε	g
10	0·0235	0·191	0·0260
20	0·0166	0·113	0·0106
40	0·0118	0·0656	0·00455

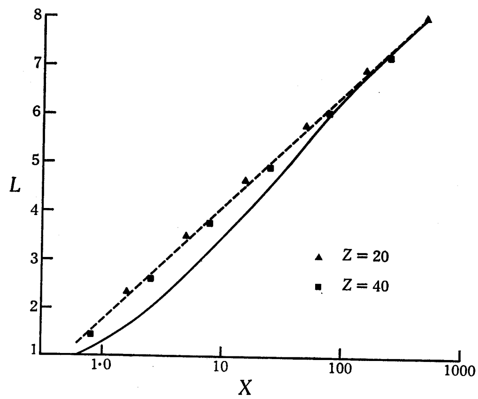

Fig. 1. Comparison of present theoretical results (dashed line) for L as a function of X (as defined by equations (33) and (34)) with a smooth curve (full line) through the experimental results of Lindhard and Scharff (1953).

Finally, with B and ε known, L can be estimated using the Euler summation formula to be

$$L \simeq \ln(1\cdot 81\,X) + J^{-\varepsilon} H \int_{J^{-1}}^{\infty} K_0(S)\,K_1(S)\,S^{-\varepsilon}\,\mathrm{d}S + \tfrac{1}{2} H J^{-1} K_0(J^{-1}) K_1(J^{-1})\,, \tag{44}$$

where $H = \frac{1}{5} g^2 x_0^{9/2} B$ and x_0 is the scaled radius defined in Part I. In the calculations reported here, the integral in the approximation (44) was performed analytically by taking the upper limit as $1\cdot 0$ and by using the approximation

$$-S K_0(S)\,K_1(S) \simeq \ln(\tfrac{1}{2}\alpha S) + S^2[\tfrac{1}{4}\{\ln(\tfrac{1}{2}\alpha S) - 1\} + \tfrac{1}{2}\{\ln(\tfrac{1}{2}\alpha S)\}^2]\,, \tag{45}$$

where $\ln \alpha = 0\cdot 577$.

The results are shown in Fig. 1, which includes for comparison experimental results taken from Lindhard and Scharff (1953). It is evident that for large X the Thomas–Fermi model gives an excellent description of the energy loss process but as X decreases the agreement with experiment becomes much less satisfactory. That the hydrodynamic model should be better for large v is brought out clearly by the phenomenological analysis of Lindhard and Scharff.

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