Aust. J. Phys., 1974, **27**, 667–72

Collective Oscillations in Many Electron Atoms. III* Photoabsorption

J. J. Monaghan

Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado 80302, U.S.A.; on leave from present address: Department of Mathematics, Monash University, Clayton, Vic. 3168.

Abstract

The generalization by Bloch of the Thomas–Fermi atom to time-dependent motion is applied to the calculation of the photoabsorption cross section. The results are in reasonable agreement with the experimental cross sections in the range of photon energies $0{\cdot}3Z$ eV $< \hbar\omega < 300Z$ eV, where Z is the atomic number of the atom.

Introduction

In the early part of this century, Bloch (1933) generalized the Thomas–Fermi atom (Thomas 1927; Fermi 1928) by applying classical hydrodynamics to the degenerate electron gas formed by the atomic electrons. Bloch confined his analysis to one particular problem: the transfer of energy from a passing charged particle to the Thomas–Fermi atom. Being unable to determine the modes of oscillation numerically, Bloch contented himself with estimating the parameter of his model from the experimental results for one element. The agreement with experiment for all other elements with large atomic numbers was found to be very satisfactory.

Recently the hydrodynamic model has been subjected to more careful numerical analysis. The photoabsorption cross section has been calculated by Ball *et al.* (1973) using the original Thomas–Fermi model with an infinite radius and, as a consequence, a continuous rather than a discrete spectrum of normal modes. In Part I of the present series (Monaghan 1973) the hydrodynamic model has been examined using Amaldi's correction which results in a finite radius for the neutral atom. The spectrum is discrete for this model and the analysis is a good deal simpler than that for the model used by Ball *et al.* The polarization has been computed in Part I and found to be in good agreement with experiment for ions and badly in error for neutral atoms. The parameters in the slowing down formula of Bloch (1933) have been estimated in Part II (Monaghan 1974) and the agreement with experiment is good for swiftly moving particles. In the present paper, the photoabsorption cross section will be determined using the results for the discrete-spectrum model.

Equations of Motion

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, ρf the coulomb force per unit volume and U

* Part II, *Aust. J. Phys.*, 1974, **27**, 169–75.

the external potential per unit charge, the equation of motion becomes

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

where μ is the mass and e the charge 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, so that

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

In the following we shall adopt Cowling's (1942) approximation and neglect $\delta \boldsymbol{f}$. Using equation (2), and recalling that for a fully degenerate electron gas

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

we find

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

where $W = 5P_0/3\rho_0^2$. Since the forces are conservative, and the fluid barotropic, we can choose

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

so that equation (5) may be written

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

The equation of continuity for the perturbed motion is

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

For the case of photoabsorption we take U to be given by

$$U = \mathscr{E} r\cos\theta\sin\omega t, \tag{9}$$

where $\mathscr{E}$ is the amplitude of the electric field due to a plane electromagnetic wave. We assume that the field is turned on at $t = 0$.

It is evident from equation (9) that the oscillating field drives the $l = 1$, $m = 0$ modes of oscillation. The equation of motion can therefore be solved by expanding Φ and $\delta\rho$ in terms of the eigenfunctions for these modes. These expansions can be written

$$\Phi = \sum_j \Phi_j B_j \cos\theta, \qquad \delta\rho = \sum_j \eta_j A_j \cos\theta, \tag{10}$$

where Φ_j and η_j are known (see Part I). These functions satisfy the orthogonality relations

$$\int \Phi_j \Phi_k W^{-1} r^2\,\mathrm{d}r = H_j \delta_{kj}, \tag{11a}$$

$$\int \eta_j \eta_k W r^2\,\mathrm{d}r = \omega_j^2 H_j \delta_{kj}, \tag{11b}$$

$$\int \Phi_j \eta_k r^2\,\mathrm{d}r = \omega_j H_j \delta_{kj}. \tag{11c}$$

Furthermore

$$\Phi_j \omega_j = W\eta_j \qquad \text{and} \qquad \eta_j \omega_j + \nabla.(\rho_0 \nabla \Phi_j) = 0, \tag{12}$$

where ω_j is the frequency of the jth mode.

Substituting the expansions (10) into equations (7) and (8), and using the relations (11) and (12), we find

$$\dot{B}_j + \omega_j A_j + \frac{e\mathscr{E} \sin \omega t}{\mu H_j \omega_j} \int \eta_j r^3 \, \mathrm{d}r = 0 \tag{13a}$$

and

$$\dot{A}_j = \omega_j B_j. \tag{13b}$$

The boundary conditions on equations (13) are that there is no motion at $t = 0$. The solutions are readily found to be

$$B_j = \frac{F(\omega_j)}{\omega_j^2 - \omega^2}\Big(\cos(\omega t) - \cos(\omega_j t)\Big) \tag{14a}$$

and

$$A_j = \frac{F(\omega_j)}{\omega_j^2 - \omega^2}\left(\frac{\omega_j}{\omega}\sin(\omega t) - \sin(\omega_j t)\right), \tag{14b}$$

where

$$F(\omega_j) = -\frac{\omega e\mathscr{E}}{\mu H_j \omega_j} \int \eta_j r^3 \, \mathrm{d}r. \tag{15}$$

Energy Transfer

The energy transferred to the atom at time t is given by

$$\Delta E = \int \{\tfrac{1}{2}\rho_0 (\nabla \Phi)^2 + \tfrac{1}{2} W \eta^2\} \, \mathrm{d}V. \tag{16}$$

This expression may be derived easily by multiplying equation (5) by $\rho_0 \boldsymbol{v}$ and integrating over the atomic volume. Using the equation of continuity we find

$$\frac{\mathrm{d}(\Delta E)}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\int \{\tfrac{1}{2}\rho_0 (\nabla \Phi)^2 + \tfrac{1}{2} W \eta^2\} \, \mathrm{d}V\right) = -e\mu^{-1} \int \rho_0 \boldsymbol{v}.\nabla U \, \mathrm{d}V. \tag{17}$$

Substitution of the expansions (10) into the expression for ΔE gives

$$\Delta E = \tfrac{2}{3}\pi \sum_j \omega_j^2 H_j (B_j^2 + A_j^2). \tag{18}$$

Thus

$$\Delta E = \frac{2\pi e^2 \omega^2 \mathscr{E}^2}{3\mu^2} \sum_j \frac{1}{H_j}\left(\int \eta_j r^3 \, \mathrm{d}r\right)^2 \frac{R_j^2 + S_j^2}{(\omega_j^2 - \omega^2)^2}, \tag{19}$$

where

$$R_j = \cos(\omega t) - \cos(\omega_j t)$$

and

$$S_j = (\omega_j/\omega)\sin(\omega t) - \sin(\omega_j t).$$

By using the scaled variables introduced in Part I, we can write equation (19) in the form

$$\Delta E = \frac{e^2\mathscr{E}^2\omega^2 Z}{2\mu}\sum_j q_j \frac{R_j^2+S_j^2}{(\omega_j^2-\omega^2)^2}, \tag{20}$$

where Zq_j is the classical oscillator strength and q_j is defined by

$$q_j = \tfrac{1}{5}v_j^2 x_0^{9/2}\left(\int_0^1 \Phi_j \phi^{1/2} u^{5/2}\,\mathrm{d}u\right)^2 \Big/ \int_0^1 \Phi_j^2 \phi^{1/2} u^{3/2}\,\mathrm{d}u \tag{21}$$

and

$$\omega_j = v_j Z(\mu e^4\pi^2 2^7/h^3 3\sqrt{5}) \equiv v_j K, \tag{22}$$

where x_0 is the radius of the atom when the unit of length is taken to be

$$\frac{3^{2/3}h^2}{\pi^{4/3}\mu e^2 Z^{1/3}2^{13/3}} = \frac{0{\cdot}468\times 10^{-10}}{Z^{1/3}}\ \text{m}. \tag{23}$$

The function ϕ is the Thomas–Fermi function whose argument here is the variable $u = x/x_0$.

Because the frequencies ω_j are very close together, the summation in equation (20) can be written as an integral which is dominated (when t is very large) by the resonance term. Furthermore, since q_j is slowly varying, it can be evaluated at the resonance frequency and taken outside the integral. The dominant term in the integral is easily found to be

$$4\int_1^\infty (\omega_j^2-\omega^2)^{-2}\sin^2\{\tfrac{1}{2}(\omega-\omega_j)t\}\,\mathrm{d}j. \tag{24}$$

The numerical calculations in Part I show that

$$\omega_j \sim Kgj, \tag{25}$$

where g is a constant and K is defined by equation (22). Accordingly, the term (24) is approximately

$$\frac{t}{2\omega^2 Kg}\int_{-\infty}^{\infty} x^{-2}\sin^2 x\,\mathrm{d}x = \frac{\pi t}{2\omega^2 Kg}. \tag{26}$$

Thus

$$\Delta E \simeq (\pi e^2\mathscr{E}^2 Z/4\mu Kg)q_{\text{res}}\,t. \tag{27}$$

The incoming time-averaged flux of radiation is $c\mathscr{E}^2/8\pi$, and the cross section for photoabsorption is therefore

$$\sigma(\omega) = (2\pi e^2/\mu c)(Z/Kg)q_{\text{res}}. \tag{28}$$

The calculations in Parts I and II show that

$$q_j \sim \tfrac{1}{5}g^2 x_0^{9/2} B j^{-(1+\varepsilon)},$$

where $\varepsilon \ll 1$ and both B and ε depend on Z. At resonance we have

$$j \sim \omega/Kg \tag{29}$$

and therefore

$$\sigma(\omega) \simeq (2\pi e^2/\mu c)(Z/Kg)(\tfrac{1}{5}g^2 x_0^{9/2})\, B\,(Kg/\omega)^{1+\varepsilon}. \tag{30}$$

Because the Thomas–Fermi model is only a rough approximation, it is entirely adequate to approximate the cross section (30) by the use of certain scaling relations made evident by the numerical calculations. These scaling relations, for an n-times ionized atom with nuclear charge $+Ze$, are:

$$g = \text{const.}\{(n+1)/Z\}^{5/4}, \tag{31a}$$

$$x_0 = \text{const.}\{Z/(n+1)\}^{1/2}, \tag{31b}$$

$$B = \text{const.}\{(n+1)/Z\}^{1/2}. \tag{31c}$$

Evaluating the constants for $Z = 40$, and neglecting ε, we find

$$\sigma(\Omega) \simeq \left(\frac{(n+1)40}{Z}\right)^{3/4} \frac{0{\cdot}232\times 10^{-18}}{\Omega} \text{ cm}^2, \tag{32}$$

where

$$\Omega = (\hbar\omega \text{ in eV})/(27{\cdot}2Z \text{ eV}). \tag{33}$$

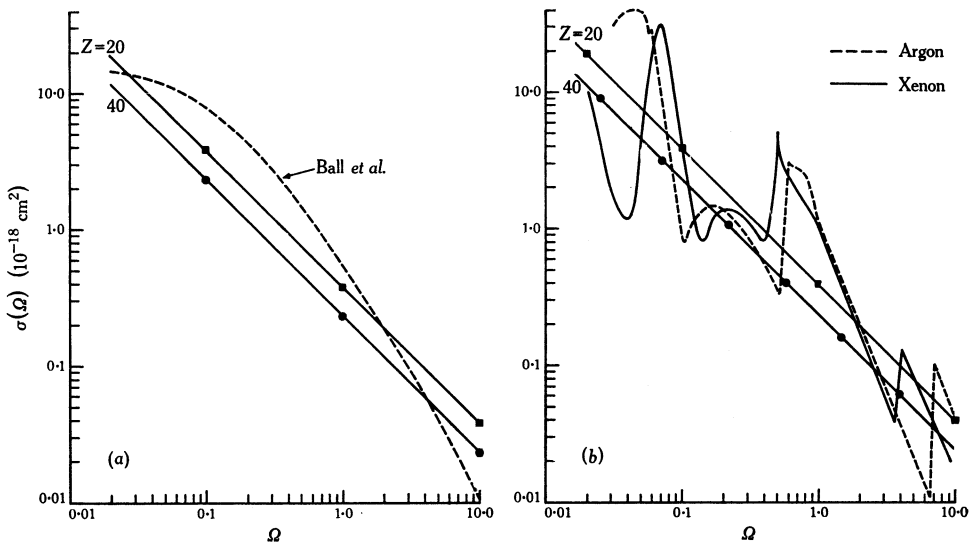

Fig. 1. Comparison of the present theoretical cross section (32) for $Z = 20$ and 40 (straight lines) with: (*a*) the result for $\sigma(\Omega)$ calculated by Ball *et al.* (1973), and (*b*) the experimental results for argon and xenon (Fano and Cooper 1968) shown as smooth curves which neglect fine structure. Note that the parameter Ω is as defined by equation (33).

Comparison with Experiment

The result (32) is compared with the cross section calculated by Ball *et al.* (1973) in Fig. 1*a*. The main difference is that the cross section calculated here is lower at low frequencies and falls off less rapidly. There is the further difference that the calculations of Ball *et al.* are based on the original Thomas–Fermi atom for which

σ is universal function of Ω, while the present calculations give a different curve for each Z.

In Fig. 1*b* we compare the cross section (32) with the experimental results for the elements argon and xenon (Fano and Cooper 1968) in the range of frequencies for which the approximations are expected to be reasonably valid. Evidently the expression (32) is only accurate to within 50% at a few selected points while elsewhere the agreement is just to within an order of magnitude. However, when the cross section is required for an integration over a wide range of frequencies, as is frequently the case in stellar calculations, the approximate expression (32) may be adequate since equation (28), from which it is obtained, satisfies the sum rule (see Part I)

$$\int \sigma(\omega)\,\mathrm{d}\omega \simeq Kg \sum_k \sigma(\omega_k) = \frac{2\pi e^2 Z}{\mu c}\left(1-\frac{n+1}{Z}\right). \tag{34}$$

If $n+1$ is replaced by n, equation (34) is the quantum mechanical result. It can be seen from Fig. 1*b* that the approximate cross sections do in fact average the peaks and valleys of the experimental cross sections rather well.

Conclusions

The Thomas–Fermi–Bloch model is expected to be a good approximation for those processes involving many atomic electrons. This restriction means that the absorption of photons with energies of a few electron volts, which may be attributed to the excitation of one or two outer electrons, is not adequately described. Similarly, one would not expect a good description of absorption involving energies of the order of Z^2 rydbergs, since these energies indicate absorption by K or L electrons. For intermediate energies the calculated $\sigma(\omega)$ should be reasonable although, since there is no shell structure in the model, the structure in the experimental cross section is outside the scope of the model.

Acknowledgment

This work was carried out while the author was a Visiting Fellow at the Joint Institute for Laboratory Astrophysics (JILA), University of Colorado, Boulder, Colorado, U.S.A.

References

Ball, J. A., Wheeler, J. A., and Fireman, E. L. (1973). *Rev. Mod. Phys.* **45**, 333.
Bloch, F. (1933). *Z. Phys.* **81**, 363.
Cowling, T. G. (1942). *Mon. Notic. Roy. Astron. Soc.* **101**, 367.
Fano, U., and Cooper, J. W. (1968). *Rev. Mod. Phys.* **40**, 441.
Fermi, E. (1928). *Z. Phys.* **48**, 73.
Monaghan, J. J. (1973). *Aust. J. Phys.* **26**, 597.
Monaghan, J. J. (1974). *Aust. J. Phys.* **27**, 169.
Thomas, L. H. (1927). *Proc. Cambridge Phil. Soc.* **23**, 524.

Manuscript received 6 June 1974