Calculation of free-free radiative absorption cross sections

Philip W. Coulter
Department of Physics and Astronomy, University of Alabama, University, Alabama 35486
(Received 18 May 1983)

One-photon free-free absorption cross sections are evaluated by means of an integral relationship involving electron-atom off-shell scattering amplitudes. Off-shell effects are explicitly calculated and compared to various on-shell approximations. This calculation shows that off-shell effects become small with increasing energy as expected. One of the on-shell approximations agrees with the exact result over the entire energy range under consideration to within a few percent. The only integrals which appear in the calculations are absolutely convergent in contrast to methods used in previous calculations.

I. INTRODUCTION

Free-free radiative absorption is important for determining opacities of stars,[1,2] the continuous spectra of atomic gases,[3] and the absorption of energy by plasmas in the laser-driven fusion process.[4] Polarized-orbital theory[5] has been used to compute accurate values for the H^- free-free absorption coefficient.[6,7] For more complex atoms, semiempirical methods[8,9] have been used. An *ab initio* calculation of the free-free one-photon absorption coefficient for Ar^- using many-body perturbation theory has been performed by Pindzola and Kelly.[10] First-order ground-state and final-state correlation diagrams were included, and second-order direct polarization diagrams were also considered.

One-photon free-free absorption cross sections can be evaluated approximately by using on-shell approxiations[11] which relate absorption amplitudes to elastic scattering amplitudes. On-shell approximations were used recently by Ritchie[12] to calculate one-photon free-free absorption cross sections for Ar^-. Elastic scattering phase shifts for electron on argon computed by Pindzola and Kelly[13] were used in this calculation. Ritchie obtained absorption cross sections in good agreement with the exact results of Pindzola and Kelly[10] at low electron energies. At higher energies, where the approximation should be better, Ritchie's results were not in good agreement with those of Pindzola and Kelly. He suggested that the source of this disagreement may be in neglecting an off-shell term in an integral relation for the absorption matrix element.

In this paper we have calculated one-photon free-free absorption cross sections for electrons scattering from Ar by using the integral relation mentioned above. This calculation involves computing off-shell elastic scattering amplitudes. The off-shell term was explicitly evaluated and found to be relatively less important at higher energies, in agreement with theoretical expectations. The method used to evaluate the absorption cross sections is fast, and we believe, more accurate than previous methods of evaluating absorption cross sections. Pindzola and Kelly[10] estimate that their results are reliable to within 10%. The method used here can be made accurate to within 1%.

The theory is presented in Sec. II. The numerical results and our conclusions are given in Sec. III.

II. THEORY

Using the dipole-velocity form of the radiative interaction and neglecting spin, the absorption cross section in the dipole approximation is given by

$$I_a=(1/2\pi)(I\alpha/E_p^2)a_0^4(m_e^2/\hbar^3)(k'/k)\,|\,M(\vec{k}',\vec{k})\,|^2\ , \tag{1}$$

where

$$M(\vec{k}',\vec{k})=\langle\psi_{\vec{k}'}^{(-)}(\vec{r})\,|\,\vec{\rho}\cdot(-i\vec{\nabla})\,|\,\psi_{\vec{k}}^{(+)}(\vec{r})\rangle\ . \tag{2}$$

I is the radiation intensity in W/cm^2, E_p is the photon energy in hartrees, $\vec{k}$ ($\vec{k}'$) is the initial (final) electron momentum in units of a_0^{-1}, $\vec{\rho}$ is a unit vector in the direction of polarization of the radiation, α is the fine-structure constant, and a_0 is the Bohr radius. The electron wave functions satisfy the Lippmann-Schwinger equation

$$\psi_{\vec{k}}^{(+)}(\vec{r})=e^{i\vec{k}\cdot\vec{r}}+[1/(2\pi)^3]\int d^3k'\,e^{i\vec{k}'\cdot\vec{r}}/(k^2-k'^2\pm i\epsilon)\langle e^{i\vec{k}'\cdot\vec{r}'}\,|\,V_{\vec{k}}(\vec{r}')\,|\,\psi_{\vec{k}}^{(+)}(\vec{r}')\rangle\ . \tag{3}$$

It is understood that the integral is evaluated in the limit $\epsilon\to 0$ ($\epsilon>0$) and we assume that the potential can be energy dependent.

If we define the off-shell scattering amplitude by

$$F(\vec{k}',\vec{k})=-(1/4\pi)\langle e^{i\vec{k}'\cdot\vec{r}}\,|\,V_{\vec{k}}(\vec{r})\,|\,\psi_{\vec{k}}^{(+)}(\vec{r})\rangle\ , \tag{4}$$

then it can be shown that[14] (since $k\neq k'$)

$$M(\vec{k}',\vec{k})=(2\pi a_0^2/E_p)\vec{\rho}\cdot[\vec{k}'F(\vec{k}',\vec{k})-\vec{k}F(\vec{k},\vec{k}')]$$
$$+(2/\pi)\int d^3k''\,\vec{\rho}\cdot\vec{k}''F(\vec{k}'',\vec{k})F(\vec{k}'',\vec{k}')/[(k'^2-k''^2+i\epsilon)(k^2-k''^2+i\epsilon)]\ . \quad (5)$$

It has been assumed that $V_{\vec{k}}(\vec{r})$ is invariant under time reversal and parity. The on-shell approximation derived by Low can be obtained by neglecting the last term and using an on-shell approximation for the off-shell amplitudes in the first term. It is this last term which Ritchie suggests may be larger than expected.

The rate at which electrons are scattered into solid angle $d\Omega'$ is given by ($I_a = d\Gamma_A/d\Omega'$/incident flux)

$$d\Gamma_A/d\Omega' = FN\alpha[a_0^2/(2\pi E_p)]k'\,|M(\vec{k}',\vec{k})|^2\ , \quad (6)$$

where F is the photon flux in $\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$, and N is the number of electrons per cm^3. We define a differential absorption "cross section" by

$$d\sigma_A/d\Omega' = F^{-1}N^{-1}d\Gamma_A/d\Omega'\ . \quad (7)$$

In order to obtain a total absorption cross appropriate for incident electrons with random velocities, we define

$$\sigma_A(\vec{k}',\vec{k}) = 1/4\pi\int d\Omega\,d\Omega'(1/2\pi)\alpha a_0^2/E_p k'\,|M(\vec{k}',\vec{k})|^2\ . \quad (8)$$

In computing $\sigma_A(\vec{k}',\vec{k})$ we assume a fixed photon polarization, average over the initial electron directions, and integrate over the final electron directions. σ_A has units of cm^5.

If we write $\psi^{(+)}$ as (assuming a central potential)

$$\psi^{(+)}_{\vec{k}}(r) = 4\pi\sum_{l,m} i^l\eta_l(k,r)Y^*_{lm}(\hat{k})Y_{lm}(\hat{r})\ , \quad (9)$$

then

$$F(\vec{k}',\vec{k}) = -4\pi\sum_{l,m} U_l(k',k)Y_{lm}(\hat{k}')Y^*_{lm}(\hat{k})\ , \quad (10)$$

where

$$U_l(k',k) = \int r^2 j_l(k'r)U_k(r)\eta_l(k,r)dr\ . \quad (11)$$

If we assume that the photon is linearly polarized along the z axis, then

$$M(\vec{k}',\vec{k}) = \sum_{l,l',m}(-1)^m X_{ll'}(k',k)\begin{bmatrix}1 & l & l'\\ 0 & 0 & 0\end{bmatrix}\begin{bmatrix}1 & l & l'\\ 0 & m & -m\end{bmatrix}Y_{l'm}(\hat{k}')Y^*_{lm}(\hat{k})\ , \quad (12)$$

where

$$X_{ll'}(k',k) = 8\pi^2\sqrt{(2l+1)(2l'+1)}\left[\frac{-2a_0^2}{E_p}[k'U_l(k',k)-kU_{l'}(k,k')]+\frac{4}{\pi}\Gamma_{ll'}(k',k)\right]\ , \quad (13)$$

and

$$\Gamma_{ll'}(k',k) = \int_0^\infty \frac{k''^3dk''}{(k^2-k'^2-i\epsilon)(k'^2-k''^2-i\epsilon)}U_l(k'',k)U_{l'}(k'',k')\ . \quad (14)$$

The total absorption cross section is

$$\sigma_A = \frac{\alpha a_0^2}{24\pi^2E_p}k'\sum_{l,l'}\begin{bmatrix}1 & l & l'\\ 0 & 0 & 0\end{bmatrix}^2|X_{ll'}(k',k)|^2\ . \quad (15)$$

III. RESULTS AND CONCLUSIONS

Hartree-Fock wave functions were used for the Ar atom and no attempt was made to account for polarization effects. A local approximation[15] was used for the exchange potential for the scattered electron. Because of this we do not expect our results to be in precise agreement with those of Pindzola and Kelly. The agreement is quite good, however, and improves as the energy increases.

Exact calculations of absorption cross sections are usually made by a direct evaluation of $M(\vec{k}',\vec{k})$ in Eq. (2). This integral is not absolutely convergent since both the initial and final wave functions represent free particles. The integrals can be evaluated in the usual way by introducing a factor of $e^{-\epsilon r}$ to make them convergent[6] and taking the limit as $\epsilon\to 0$. Pindzola and Kelly[10] calculated the integrals numerically up to $r=R$ and added an asymptotic part (from R to ∞) which may be calculated analytically by making the integral absolutely convergent. They varied R from $40a_0$ to $80a_0$ and estimate that this technique is accurate to better than 10%. These calculations were done using both the length and velocity formulations of the dipole approximation.

An advantage of using Eq. (5) to compute $M(\vec{k}',\vec{k})$ is that all of the integrals are convergent. In order to evaluate $M(\vec{k}',\vec{k})$ we must evaluate $U_l(k',k)$ and $\Gamma_{l'l}(k',k)$ in Eq. (13). The evaluation of $U_l(k',k)$ is straightforward, but the integral in Eq. (14) for $\Gamma_{ll'}(k',k)$ is slowly convergent. Fortunately it is possible to do the k'' integration exactly. Using the definition of the U_l [Eq. (11)], we see that

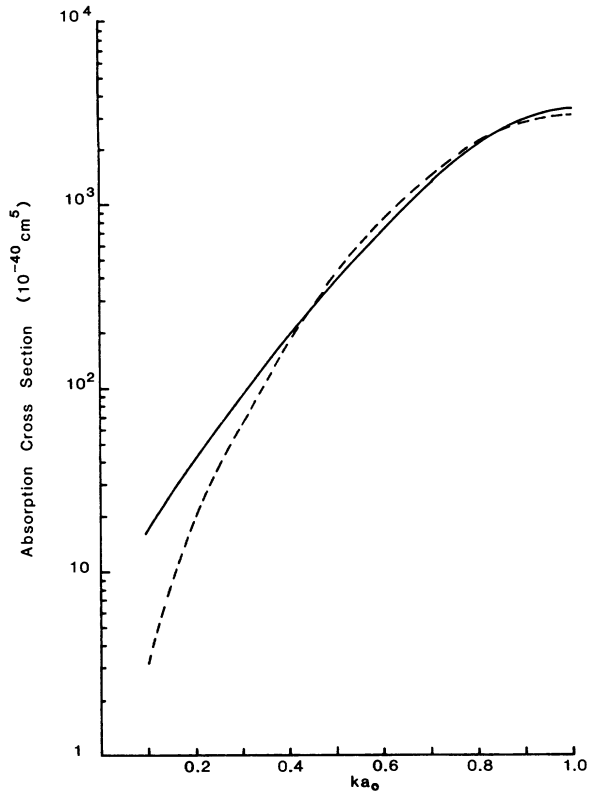

FIG. 1. Free-free one-photon absorption cross section for Ar^- at $\lambda=20000$ Å. The solid curve is the Hartree-Fock velocity form calculation of Pindzola and Kelly, Ref. 10. The dashed curve shows the results of the present calculation. Both calculations include $s\leftrightarrow p$ and $p\leftrightarrow d$ transitions.

$$\Gamma_{ll'}(k'k)=\int dr\,dr'\,r^2r'^2U_{k'}(r)U_k(r')\eta_l(k'r)\times\eta_{l'}(kr')F_{ll'}(k,k',r,r')\ , \tag{16}$$

where

$$F_{ll'}(k,k',r,r')=\int_0^\infty \frac{k''^3dk''}{(k^2-k''^2+i\epsilon)(k'^2-k''^2+i\epsilon)}\times j_l(k''r)j_{l'}(k''r')\ . \tag{17}$$

This integral can be done exactly in terms of spherical Bessel functions and spherical Hankel functions of the first kind by standard techniques. We note from Eq. (12) that l and l' differ by unity so that the integral is even in k''.

In Fig. 1 we compare our results for the free-free absorption cross section for e^- scattering from Ar in the presence of photons with a wavelength of 20000 Å to those obtained by Pindzola and Kelly[10] using a Hartree-Fock formalism without polarization or first-order correlation effects. The agreement between the two calculations is poor at low energies but improves at higher energies. Both calculations include partial waves up to $l=2$. At higher energies $l=3$ states are also important, but they were omitted by Pindzola and Kelly since the contribution of higher energies to the (thermal averaged) free-free absorption coefficient is negligible.

We checked the accuracy of the calculations by varying the grid distribution. We estimate that the results are accurate to within 1%. A calculation of the free-free absorption cross section at one energy for partial waves up to $l=2$ requires less than 1.5 min of computing time on a UNIVAC 1100/61 if the potential is known.

The on-shell approximation which can be obtained from Eq. (5) is

$$M(\vec{k}',\vec{k})=\frac{2\pi a_0^2}{E_p}\vec{\rho}\cdot[\vec{k}'F(\vec{k}',\vec{k})-\vec{k}F(\vec{k},\vec{k}')]\ . \tag{18}$$

The off-shell amplitudes, $F(\vec{k}',\vec{k})$ and $F(\vec{k},\vec{k}')$, may also be approximated by on-shell amplitudes. Ritchie examined the validity of the on-shell approximation by considering two different types of on-shell approximations. In one case he evaluated $M(\vec{k}',\vec{k})$ by replacing the off-shell scattering amplitudes by elastic amplitudes in which the electron energy (in Ry) is assumed to be $(ka_0)^2$, and in the other case the electron energy was assumed to be $(k'a_0)^2$ for both amplitudes. When he compared the absorption cross sections using these two different approaches, he found that they disagreed at low energies, but the disparity was very small at higher energies (approximately 1 Ry). However, Ritchie's on-shell results were significantly different from the exact results of Pindzola and Kelly near 1

TABLE I. Free-free radiative absorption cross sections for electrons scattering from Ar in the presence of photons with $\lambda=20000$ Å. In columns A, B, and C Eq. (18) is evaluated by using on-shell approximations. In column A we use elastic scattering amplitudes with $F(\vec{k}',\vec{k})$ and $F(\vec{k},\vec{k}')$ evaluated at electron energies (in Ry) of $(k'a_0)^2$ and $(ka_0)^2$, respectively. In column B $F(\vec{k}',\vec{k})$ and $F(\vec{k},\vec{k}')$ are both evaluated at $(k'a_0)^2$. In column C they are both evaluated at $(ka_0)^2$. The correct off-shell amplitudes are used to evaluate Eq. (18) in column D. The exact results, including all off-shell terms, are given in column E.

	Free-free radiative absorption cross sections (10^{-40} cm^5)				
ka_0	A	B	C	D	E
0.1	3.09	2.26	10.3	6.10	3.12
0.2	1.97×10^1	1.77×10^1	2.76×10^1	2.42×10^1	2.01×10^1
0.4	1.77×10^2	1.67×10^2	1.92×10^2	1.84×10^2	1.82×10^2
0.6	7.96×10^2	7.72×10^2	8.20×10^2	8.04×10^2	8.08×10^2
0.8	2.16×10^3	2.16×10^3	2.16×10^3	2.17×10^3	2.18×10^3
1.0	3.14×10^3	3.25×10^3	3.03×10^3	3.15×10^3	3.14×10^3

Ry. He suggested that the discrepancy might be due to neglecting the last term in Eq. (15).

We present our results in Table I for the free-free absorption cross section using several approximations as well as the exact calculation. At low energies we see that the various off-shell approximations as well as the exact on-shell calculations of Eq. (18) give results which differ widely with each other and with the exact calculation. At higher energies the various approximations agree reasonably well with each other and with the exact calculations. It is interesting to note that the off-shell approximation in column A of Table I gives results which are always in fairly good agreement with the exact calculations.[16] In this approximation $F(\vec{k}',\vec{k})$ and $F(\vec{k},\vec{k}')$ in Eq. (18) are replaced by elastic amplitudes evaluated at electron energies (in Ry) of $(k'a_0)^2$ and $(ka_0)^2$, respectively.

We have evaluated the free-free radiative absorption cross sections for electrons scattering from Ar by evaluating an integral relation for the absorption amplitude in terms of off-shell e,Ar scattering amplitudes. This method has the advantage that all of the integrals are absolutely convergent and can be done accurately. Off-shell effects were examined by making various on-shell approximations and comparing them to the exact calculation. It can be concluded that off-shell effects are important at low energies, but they become negligible at higher energies, as expected. One of the on-shell approximations was in good agreement with the exact result at all energies under consideration.

ACKNOWLEDGMENTS

The author thanks Dr. Burke Ritchie for several useful discussions. The calculations were done at the Charles Seebeck Computer Center at the University of Alabama.

[1]A. Pannekoek, Mon. Not. R. Astron. Soc. 91, 155 (1931).
[2]V. P. Myerscough and G. Peach, in *Case Studies in Atomic Collisions Physics II* (North-Holland, Amsterdam, 1972), p. 293.
[3]L. M. Biberman and G. C. Norman, Usp. Fiz. Nauk. 91, 193 (1967) [Soc. Phys.—Usp. 10, 52 (1967)].
[4]K. A. Brueckner and S. Jorna, Rev. Mod. Phys. 46, 325 (1974).
[5]A. Temkin, Phys. Rev. 107, 1004 (1957).
[6]J. L. Stilley and J. Callaway, Astrophys. J. 160, 245 (1970).
[7]K. L. Bell, A. E. Kingston, and W. A. McIlveen, J. Phys. B 8, 358 (1975).
[8]R. R. Johnson, J. Quant. Spectrosc. Radiat. Transfer 7, 815 (1967).
[9]S. Geltman, J. Quant. Spectrosc. Radiat. Transfer 13, 601 (1973).
[10]M. S. Pinzola and H. P. Kelly, Phys. Rev. A 14, 204 (1976).
[11]F. E. Low, Phys. Rev. 110, 974 (1958).
[12]B. Ritchie, Phys. Rev. 23, 2276 (1981).
[13]M. S. Pindzola and H. P. Kelly, Phys. Rev. A 9, 323 (1974).
[14]H. Kruger and M. Shultz, J. Phys. B 9, 1899 (1976); see, also Ref. (10).
[15]M. E. Riley and D. G. Truhlar, J. Chem. Phys. 63, 2182 (1975).
[16]This on-shell approximation breaks down in this energy region for higher proton energy ($\lambda = 2000$ Å, $E_p = 6.2$ eV). In order for it to remain valid we expect that the photon energy must be smaller than or at least comparable to the electron energy.