

Radiative Absorption Cross Section of an Electron in the Field of an Argon Atom

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The results of a numerical calculation of the radiative absorption cross section for an electron in the field of a neutral argon atom are reported. The atomic potential used is the same as used by Holtmark in his treatment of the Ramsauer effect. The light frequency is 4.318×10^{14} cps. This exact cross section is compared with three approximations which contain the phase shifts for elastic scattering. One of these approximations, the one due to Holstein, is found to differ very little from the exact cross section over a large range of initial electron energies.

INTRODUCTION

IN this paper, attention will be directed to the cross section for the absorption of a photon by an electron in the field of an argon atom. Only transitions between electron states in the continuum will be considered. The process is usually called "free-free absorptive transition" or "inverse bremsstrahlung."¹

The neutral argon atom is represented by a static central potential which is the same potential used by Holtmark² in his treatment of the Ramsauer effect in this atom. It is a Hartree atomic field modified by the inclusion of a polarization term $\sim r^{-4}$ for large distances r from the atomic nucleus. The frequency ν of the light used is 4.318×10^{14} cps which is the R_1 line of a ruby laser at 300°K.³

For this system, the results of a numerical calculation of the free-free absorption cross section will be reported. This cross section will be called the "exact" cross section.

Even with the availability of high-speed computers, the accuracy of a theoretical calculation of a cross section is limited by the inherent complexity of the many-electron system. The elastic cross sections have been measured for a large number of atoms and molecules over wide ranges of energy.⁴ This is not true for inelastic cross sections. It would therefore be useful if the inelastic-electron-scattering cross section could be expressed in terms of the elastic-scattering cross sections or quantities derived therefrom, viz., the scattering phase shifts. For the case where the neutral atom is represented by a static potential, in the limit of vanishing frequency of the radiation field one obtains the well-known result that the free-free absorptive cross section is proportional to the cross section for momentum transfer. For finite frequency no exact direct connection between elastic and inelastic cross sections

exists.⁵ Approximations leading to this type of connection were used by Ohmura and Ohmura^{6,7} for the absorption by H^- , and by Somerville⁸ for H_2^- . They include only the $0 \rightarrow 1$ and $1 \rightarrow 0$ partial wave transitions where 0 and 1 are the angular momentum of the electron and set the p wave scattering phase shift equal to zero. Somerville's expression was extended by Ashkin and Emtage⁹ to include higher partial wave transitions and phase shifts. Similar approximations have been used by Firsov and Chibisov.¹⁰ Recently Holstein¹¹ obtained another approximate expression for the cross section which can be calculated from the phase shifts. This result was obtained independently of an earlier field-theoretical work of Low¹² which claimed validity only when the light frequency is much less than the initial electron energy for the case of absorption.

These approximations of Somerville, Ashkin and Emtage, and Holstein have been evaluated numerically using phase shifts which we obtained for the present system and are compared with the "exact" cross section.

THE FORM OF THE CROSS SECTIONS

We follow the method given by Landau and Lifshitz¹³ to obtain the transition probability between wave functions of the continuous spectrum. The initial- and

⁵ An indirect connection between the elastic cross section and the inelastic radiative cross section does exist in the following sense. The effective scattering potential of a many-electron atom fully determines the inelastic electron scattering in the potential scattering approximation. V. Bargmann [Phys. Rev. **75**, 301 (1949)], and I. M. Gelfand and B. M. Levitan [Dokl. Akad. Nauk SSSR **77**, 557 (1951)] have developed methods for determining the potential of interaction between two colliding systems from the differential elastic scattering cross section when the latter is known as a function of energy and angle and in some cases polarization.

⁶ T. Ohmura and H. Ohmura, *Astrophys. J.* **131**, 8 (1960).

⁷ R. L. Taylor and B. Kivel, *J. Quant. Spectry. Radiative Transfer* **4**, 239 (1964).

⁸ W. B. Somerville, *Astrophys. J.* **139**, 192 (1964).

⁹ M. Ashkin and P. R. Emtage, 1964 (unpublished).

¹⁰ O. B. Firsov and M. I. Chibisov, *Zh. Eksperim. i Teor. Fiz.* **39**, 1770 (1960) [English transl.: *Soviet Phys.—JETP* **12**, 1235 (1961)].

¹¹ T. Holstein, Westinghouse Scientific Paper 65-1E2-GASES-P2, 1965 (unpublished).

¹² F. E. Low, *Phys. Rev.* **110**, 974 (1958).

¹³ L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon Press Ltd., London, 1958).

¹ H. A. Bethe and E. E. Salpeter, *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 35.

² J. Holtmark, *Z. Physik* **55**, 437 (1929).

³ Bela A. Lengyel, *Lasers* (John Wiley & Sons, Inc., New York, 1962), Table I, p. 115.

⁴ *Atomic and Molecular Processes*, edited by D. R. Bates (Academic Press Inc., New York, 1962).

final-state electron wave functions can be written

$$\psi_{\mathbf{k}}^{(\pm)}(\mathbf{r}) = (1/k) \sum_{l=0}^{\infty} (2l+1) i^l e^{\pm i\delta_l(k)} R_{kl}(r) P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}), \quad (1)$$

where $\psi^{(+)}$ is the initial state and has the asymptotic form

$$\psi_{\mathbf{k}}^{(+)} \sim e^{i\mathbf{k} \cdot \mathbf{r}} + \text{outgoing wave}, \quad (2)$$

where $\psi^{(-)}$ is the final state and has the asymptotic form

$$\psi_{\mathbf{k}}^{(-)} \sim e^{i\mathbf{k} \cdot \mathbf{r}} + \text{incoming wave}. \quad (3)$$

The wave vector \mathbf{k} is related to the energy E by $E = (\hbar k)^2/2m$, where m is the electron mass, $P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}})$ is the Legendre polynomial of the l th order, and the carets denote unit vectors. The radial function $v_{kl}(r) = R_{kl}(r)/r$ satisfies the radial Schrödinger equation

$$\frac{d^2 v_{kl}(r)}{dr^2} + \left[\frac{2mE}{\hbar^2} - \frac{2m}{\hbar^2} V(r) - \frac{l(l+1)}{r^2} \right] v_{kl} = 0, \quad (4)$$

where $V(r)$ is the total potential seen by the electron and v_{kl} satisfies the boundary conditions

$$v_{kl}(0) = 0 \quad (5)$$

$$v_{kl}(r) \sim \sin(kr - \frac{1}{2}\pi l + \delta_l(k)) \quad \text{for } r \rightarrow \infty. \quad (6)$$

Equation (6) defines $\delta_l(k)$ the l th scattering phase shift evaluated at the energy corresponding to the wave number k .

If we write the interaction of the radiation field as $eE_0 \mathbf{e} \cdot \mathbf{r} \cos \omega t$, then the transition rate from the direction $\hat{\mathbf{k}}_i$ into the solid angle $d\Omega(k_f)$ about the direction $\hat{\mathbf{k}}_f$ for light of frequency ω is

$$dW_{\Omega}(\hat{\mathbf{k}}_i, \hat{\mathbf{k}}_f) = (e^2 E_0^2 k_f / 16\pi^2 \hbar^3 m \omega^4) |(\psi_{\mathbf{k}_i}^{(+)}, \mathbf{e} \cdot \nabla V \psi_{\mathbf{k}_f}^{(-)})|^2 d\Omega(\hat{\mathbf{k}}_f), \quad (7)$$

where

$$(\hbar^2/2m)(k_f^2 - k_i^2) = \hbar\omega. \quad (8)$$

Equation (7) involves the gradient of the potential and is the most convenient form for our numerical calculation.¹⁴

The free-free absorption cross section $K(k_i)$ is obtained from $dW_{\Omega}(\hat{\mathbf{k}}_i, \hat{\mathbf{k}}_f)$ by averaging over initial directions $\hat{\mathbf{k}}_i$, integrating over final directions $\hat{\mathbf{k}}_f$, and dividing by the initial photon flux. The result per unit density of scattering centers is

$$K(k_i) = \frac{1}{3} (32\pi^2 \alpha a_0^5) \{ (E_L^3 k_f k_i^2)^{-1} \Sigma(k_i, k_f) \} \text{ cm}^5, \quad (9)$$

where $\alpha = e^2/\hbar c$ is the "fine structure constant," $a_0 = \hbar^2/me^2$ is the "radius of the first Bohr orbit," and the quantity in curly brackets is in atomic units (a.u.).¹⁵ In atomic units E_L , the energy of a ruby laser photon, is

$$E_L = \frac{1}{2} (k_f^2 - k_i^2) = 0.0657. \quad (10)$$

We have defined $\Sigma(k_i, k_f)$ by

$$\Sigma(k_i, k_f) = \sum_{l=0}^{\infty} [l |M(k_i, k_f, l-1)|^2 + (l+1) |M(k_i, k_f, l+1)|^2], \quad (11)$$

where

$$M(k_l, k_{l'}) = \int_0^{\infty} dr v_{kl}(r) \frac{\partial V}{\partial r} v_{k'l'}(r) \quad (12)$$

and $v_{kl}(r)$ satisfies Eq. (4) (in a.u.) and the conditions stated in Eqs. (5) and (6). The quantity $K(k_i)$ defined by Eq. (9) is what we call the "exact" cross section.

Somerville's approximation to the exact cross section is⁸

$$K_s(k_i) = a_0^5 \alpha \left(\frac{8\pi^2}{3} \right) \left\{ \frac{k_i^4 \sin^2 \delta_0(k_f) + k_f^4 \sin^2 \delta_0(k_i)}{k_i^2 k_f E_L^3} \right\} \text{ cm}^5. \quad (13)$$

A modified form of this expression which includes higher-order phase shifts is⁹

$$K_M(k_i) = (8\pi^2 \alpha a_0^5 / 3) \{ k_f / E_L^3 \} \bar{Q}_d(k_i) \text{ cm}^5, \quad (14)$$

where

$$\bar{Q}_d(k_i) = \sum_{l=0}^{\infty} (l+1) \times \{ (k_f/k_i)^{2l+2} \sin^2[\delta_l(k_i) - \delta_{l+1}(k_f)] + (k_i/k_f)^{2l+2} \sin^2[\delta_l(k_f) - \delta_{l+1}(k_i)] \}$$

and k_f/E_L^3 in Eq. (14) is in atomic units. When $E_L \ll k_i^2/2$, we have $k_i \approx k_f$ and

$$(2\pi/k_i^2) \bar{Q}_d(k_i) \approx (4\pi/k_i^2) \sum_l (l+1) \sin^2 \times [\delta_l(k_i) - \delta_{l+1}(k_i)] = Q_d(k_i), \quad (15)$$

where $Q_d(k_i)$ is the cross section for momentum-transfer collisions.¹⁶ When Eq. (15) is valid K_M may be written

$$K_M(k_i) = (4\pi \alpha a_0^5 / 3) \{ (k_i^3 / E_L^3) Q_d(k_i) \}. \quad (16)$$

Holstein¹¹ has developed an approximation to K which reduces to Eq. (16) when $E_L \ll k_i$. This expression may be written

$$K_H(k_i) = K_1(k_i) + K_2(k_i), \quad (17)$$

where

$$K_1(k_i) = \frac{8\pi \alpha a_0^5}{3} \left\{ \frac{k_f}{E_L^3} \left[\frac{E_f + E_i}{2} - (E_f E_i)^{1/2} \right] Q_0(k_m) \right\}, \quad (18)$$

$$K_2(k_i) = \frac{8\pi \alpha a_0^5}{3} \left\{ \frac{k_f (E_f E_i)^{1/2}}{E_L^3} Q_d(k_m) \right\}, \quad (19)$$

¹⁶ H. S. W. Massey and E. H. S. Burhop, *Electronic and Ionic Impact Phenomena* (Oxford University Press, London, 1952). The definition and notation given on p. 367 of this reference are the ones used in this paper.

¹⁴ Reference 1, p. 337.

¹⁵ Reference 1, p. 89.

and k_m is defined by

$$k_m^2 = k_i^2 + E_L \quad (\text{a.u.}) \quad (20)$$

In Eq. (18) Q_0 is the total elastic-scattering cross section

$$Q_0(k_m) = (4\pi/k_m^2) \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l(k_m) \quad (21)$$

and in Eq. (19) $Q_d(k_m)$ is the momentum transfer cross section. We have written K_H as a sum of two terms in order to display it in terms of the two elastic cross sections evaluated at a mean energy.

RESULTS AND DISCUSSION

The value of K , K_S , K_M , and K_H for a range of initial electron energies are given in Tables I and II. In Fig. 1 the exact and approximate cross sections are plotted against the initial electron energy in Rydberg units of energy (k_i^2 in atomic units). The Schrödinger equation was solved numerically for pairs of k_i and k_f related by Eq. (10) and for pairs of l and l' to obtain the matrix element M . The phase shifts for these k and l values were also obtained and used to evaluate Q_0 and Q_d .

An examination of the tables and the curves leads to the following conclusions. The Somerville approximation is seen to be a rather poor one for the present system over the whole range of initial electron energies studied. The modified Somerville approximation is in fair agreement with the "exact" cross section for energy $\gtrsim 0.2$ Ry but is likewise a poor approximation for smaller energies. These approximations are poor because they reflect too strongly the Ramsauer effect when compared to the exact cross section.

The Holstein approximation, on the other hand, is accurate over most of the energy range considered. The relative error $|K_H(E_i) - K(E_i)| / \frac{1}{2}(K_H + K)$ for $E_i \approx 0.02$ rydberg units of energy (≈ 0.27 eV) is $\approx 20\%$. For $E_i \approx 0.2$ Ry (≈ 2.7 eV) and $E_i \approx 1.5$ Ry (≈ 20 eV), the relative errors are $\approx 1.5\%$ and $\approx 6.5\%$, respectively.

When $E_m \gg E_i$, the estimated error given by Holstein is $|K_H - K| / \frac{1}{2}(K_H + K) \approx E_i^2 (\Delta E)^2$ where ΔE is the

TABLE I. The absorption cross sections K , K_S , and K_M .

Initial electron energy (Rydberg units)	Absorption cross section (10^{-38} cm 2)		
	K [Eq. (9)]	K_S [Eq. (13)]	K_M [Eq. (14)]
0.01	0.0238	0.0133	0.9900
0.0125	0.0236	0.0091	0.5372
0.015	0.0228	0.0065	0.3297
0.025	0.0247	0.0037	0.0943
0.04	0.0301	0.0083	0.0458
0.06	0.0395	0.0197	0.0469
0.1	0.0662	0.0485	0.0845
0.2	0.1877	0.1409	0.2417
0.4	0.6748	0.2933	0.7658
0.7	1.8891	0.4930	1.9468
1.0	2.4091	0.6009	2.5867
1.5	2.4805	0.6670	2.6749

TABLE II. The absorption cross section K_H .

Initial electron energy (Rydberg units)	Absorption cross section (10^{-38} cm 2)	
	K_H [Eq. (17)]	K_H [Eq. (17)]
0.0143	0.0169	0.0169
0.0343	0.0245	0.0245
0.0757	0.0527	0.0527
0.0870	0.0569	0.0569
0.0907	0.0657	0.0657
0.1057	0.0817	0.0817
0.1257	0.1018	0.1018
0.1343	0.1118	0.1118
0.1457	0.1334	0.1334
0.1657	0.1530	0.1530
0.2657	0.3285	0.3285
0.3343	0.4916	0.4916
0.4657	0.9155	0.9155
0.6343	1.6372	1.6372
0.7657	2.1446	2.1446
0.9343	2.4913	2.4913
1.0657	2.5733	2.5733
1.4343	2.5964	2.5964
1.5657	2.6421	2.6421

energy interval over which $Q_d(E)$ undergoes relative variations of order unity. From the calculated values of Q_d we find $\Delta E \approx 1$ Ry for $E \approx 1.5$ Ry, $\Delta E \approx 0.4$ for $E \approx 0.2$. This gives $E_i^2 / (1 \text{ Ry})^2 \approx 1.6\%$ and $E_i^2 / (0.4 \text{ Ry})^2$

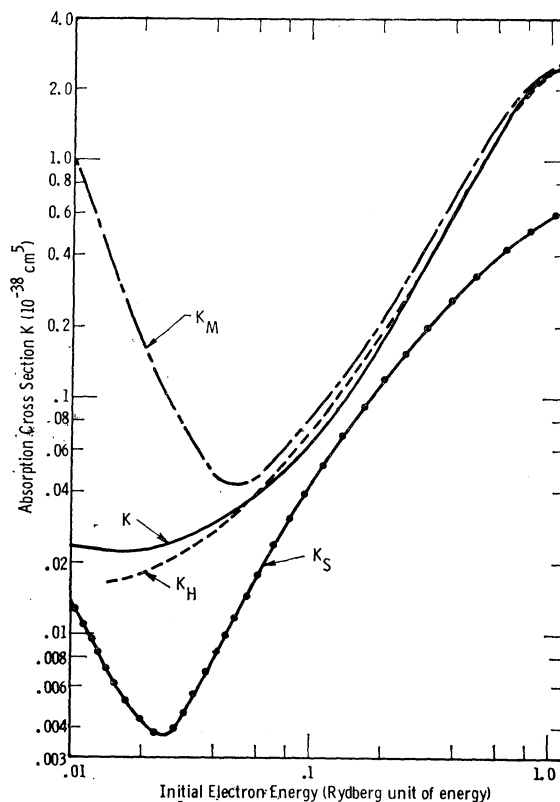


FIG. 1. Absorption cross section versus initial electron energy. K is the "exact" cross section and is defined by Eq. (9) of the text. K_S is Somerville's approximation and is defined by Eq. (13). K_M is a modification of Somerville's approximation and is defined by Eq. (14). K_H is Holstein's approximation and is defined by Eq. (17). The light frequency $\nu = \omega/2\pi = 4.318 \times 10^{14}$ cps.

$\approx 10\%$ which are in agreement with the errors given above. In view of the rapid variation of $Q_d(E_m)$ when $E_i \approx E_m \approx 0.02$ Ry the relatively small error in K_H is remarkable.

Phelps¹⁷ has used Holstein's approximation in a study of gas breakdown at optical frequencies due to a focused laser beam. Measured values of the elastic cross sections were used. The results of the present paper show that the use of Holstein's approximation for the cross section for free-free transitions in Phelps' study and similar applications is well justified except at very low energies.

¹⁷A. V. Phelps, Westinghouse Scientific Paper 65-1E2-GASES-P3, 1965 (unpublished).

This approximation is particularly useful when experimental values of Q_0 and Q_d are available. In fact we emphasize that the purpose of the present paper is to compare an exact numerical calculation with approximate calculations of the transition probability for a given model and not to provide accurate values of the cross section. It is generally known that this model does not reproduce exactly the experimental cross section.

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Electronic g Factors of the Low Levels of Ni I*

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Electronic g factors have been obtained for the seven lowest levels in Ni I by means of the atomic-beam magnetic-resonance technique. The results, in order of increasing excitation energy, are 3F_4 , 1.24968(3); 3F_3 , 1.08285(3); 3F_2 , 0.66954(3); 3D_3 , 1.33358(3); 3D_2 , 1.15106(3); 3D_1 , 0.49804(2); and 1D_2 , 1.01297(7). A re-analysis of the atomic spectrum involving configuration interaction with intermediate coupling has resulted in an improved set of parameters. The g values so computed are compared with the experimental results.

I. INTRODUCTION

IN recent years, hyperfine structure (hfs) studies have yielded more and more information on the details of atomic wave functions. Atomic species for which these studies can be made on several spectroscopic terms are especially attractive from this viewpoint. Ni I has three terms from two different configurations at sufficiently low excitation energy that the Boltzmann populations at atomic-beam temperatures should be sufficient for detailed hfs studies in the odd isotope Ni⁶¹. The present experiment was carried out to determine precise values for the electronic g factors of these low-lying states.

Of course, the measurement of atomic g factors with sufficient precision provides considerable information concerning the degree and nature of admixtures present in the atomic wave functions even without hfs studies. A computer program was employed to improve the fit to the observed energy levels of Ni I and from this description of the mixing to predict the g factors of the states for which comparison with experiment was possible.

II. EXPERIMENTAL DETAILS

The experiment was performed on the Argonne Mark II atomic-beam magnetic-resonance apparatus

which has been previously described.¹ Two-quantum flop-in transitions of the type ($J, m_J = 1 \leftrightarrow J, m_J = -1$) were detected in the even-even Ni isotopes with an electron-bombardment universal detector using mass analysis and a digital lock-in arrangement. The details of the detector are given in Ref. 1.

The source of (Ni) beam atoms was a graphite oven with a 0.010-in. slit, heated by electron bombardment. The Ni attacked the graphite if the oven became too hot, but because of the sensitivity of the detection scheme a sufficient beam intensity for the present purpose could be achieved at a modest temperature. A different oven scheme will presumably have to be used for hfs studies on Ni⁶¹ for which the intensity will be considerably lower ($\times 1/300$) as a result of both the smaller isotopic abundance and the nonzero nuclear spin.

The intensity of the homogeneous magnetic field in which the Ni transitions were induced was measured by observing resonances in the same field in a calibration beam of K³⁹ atoms from a separate oven. A surface-ionization detector was used to detect the K beam.

The number of levels for which measurements could be made is simply the number of levels for which the population in the beam is sufficiently great. The Boltzmann factor, which gives the expected relative

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¹W. J. Childs, L. S. Goodman, and D. von Ehrenstein, Phys. Rev. **132**, 2128 (1963).