

Coherent Scattering of Photons by Atomic Hydrogen*

M. H. MITTLEMAN† AND FRED A. WOLF

Lawrence Radiation Laboratory, University of California, Livermore, California

(Received May 10, 1962)

The cross section for the coherent scattering of light by atomic hydrogen is evaluated numerically below the first excitation threshold. The evaluation above threshold is discussed.

A FORMAL expression for the coherent cross section for the scattering of light by atoms was first obtained by Kramers and Heisenberg in 1925.¹ We have been unable to find any numerical evaluations of these results except in certain energy limits. We have therefore used a technique originally proposed by Schwartz and Tiemann² to obtain an expression suitable for numerical computation.

Our starting point is the Kramers-Heisenberg result for the differential elastic cross section,

$$d\sigma/d\Omega = r_0^2 |\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}' + \boldsymbol{\epsilon} \cdot \mathbf{Z}(k) \cdot \boldsymbol{\epsilon}' + \boldsymbol{\epsilon}' \cdot \mathbf{Z}(-k) \cdot \boldsymbol{\epsilon}|^2, \quad (1)$$

where the tensor $\mathbf{Z}(k)$ is given by the usual second-order perturbation expansion

$$\mathbf{Z}(k) = \frac{1}{m} \sum_n \frac{\langle 0 | \mathbf{p} | n \rangle \langle n | \mathbf{p} | 0 \rangle}{E_0 - E_n + \omega_k}. \quad (2)$$

Here $\boldsymbol{\epsilon}$ and $\boldsymbol{\epsilon}'$ are the initial and final polarization vectors, respectively, r_0 is the classical electron radius, k is the photon momentum, and ω_k is the photon energy. The dipole approximation for the photons has been used.

Simple invariance arguments suffice to show that \mathbf{Z} is proportional to the unit tensor. This yields the result,

$$d\sigma/d\Omega = r_0^2 (\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}')^2 |1 - P(k) - P(-k)|^2, \quad (3)$$

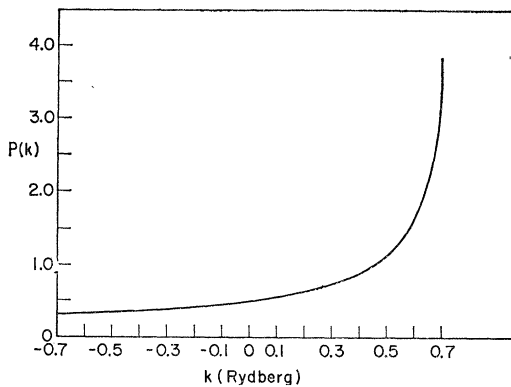


FIG. 1. $P(k)$ vs k .

* This work performed under the auspices of the U. S. Atomic Energy Commission.

† Physics Department, University of California, Berkeley, California.

¹ W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, New York, 1954), 3rd ed., p. 192.

² C. Schwartz and J. J. Tiemann, *Ann. Phys. (New York)* 2, 178 (1959).

where, in atomic units,

$$P(k) = -\frac{2}{3} \sum_n \frac{\langle 0 | \mathbf{p} | n \rangle \cdot \langle n | \mathbf{p} | 0 \rangle}{E_0 - E_n + k}. \quad (4)$$

It should be pointed out that Eq. (3) is just the Thomson cross section modified by the dynamic polarizability in the last bracket. Schwartz and Tiemann² have shown how to evaluate this sum. Briefly, the technique consists of defining the vector function

$$\boldsymbol{\Psi} = \sum_n \frac{|n\rangle \langle n | \mathbf{p} | 0 \rangle}{E_0 - E_n + k}, \quad (5)$$

which satisfies the differential equation

$$[E_0 + k - H] \boldsymbol{\Psi} = \mathbf{p} | 0 \rangle. \quad (6)$$

One then defines a new function $u(r)$ by

$$\boldsymbol{\Psi} = (\hat{r}/r^2) u(r) | 0 \rangle, \quad (7)$$

and its Laplace transform $S(p)$ which satisfies

$$\left[(p^2 - 2p + k) \frac{d}{dp} + 4p - 6 \right] S(p) = -\frac{6i}{p^4}, \quad (8)$$

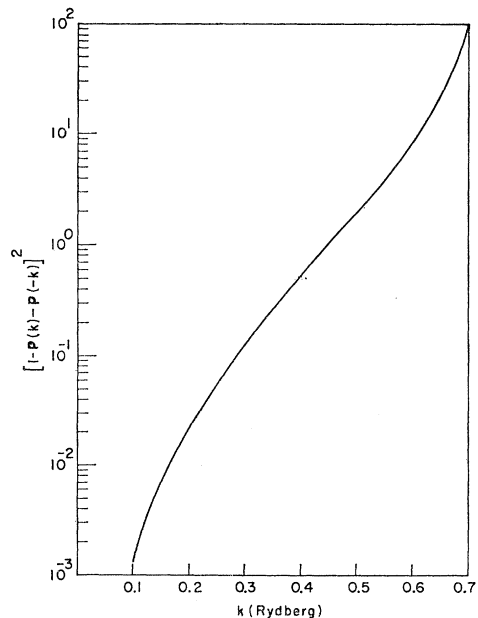


FIG. 2. $(d\sigma/d\Omega)/(d\sigma/d\Omega)_{\text{Thomson}}$ vs k .

and is related to the result by

$$P(k) = (8i/3)S(2). \quad (9)$$

The result is³

$$P(k) = \frac{16}{k^2} \left| \frac{1-\lambda}{1+\lambda} \right|^{1/\lambda} \int_1^{1/\lambda} \frac{dt}{(1+t)^4} (1-t^2\lambda^2) \left| \frac{1+\lambda t}{1-\lambda t} \right|^{1/\lambda} \quad (10)$$

where $\lambda = (1-k)^{1/2}$. This has been evaluated numerically with the aid of an IBM 650 in the range $-0.7 < k < 0.7$. Results are presented below. Figure 1 displays $P(k)$ in this range. Figure 2 gives the ratio of the cross section to the Thomson cross section vs k in units of rydbergs (13.6 eV). We note that $P(k) \rightarrow \frac{1}{2}$ as $k \rightarrow 0$ so that the cross section vanishes (as k^4) as the incident photon "sees" less and less atomic structure. In the high-energy limit, $P(k) + P(-k) \sim 1/k^2$ so that the binding becomes

³ This result has been obtained previously by Professor C. Schwartz (unpublished). We are indebted to him for making it available to us and for his instructive comments.

unimportant and the scattering takes place as though from a free electron.

$P(k)$ is singular for $k = \frac{3}{4}$, the first threshold. The singularity is, of course, nonphysical. We have omitted the finite linewidth from our description of the intermediate states in (4). Its inclusion would yield a slight shift of the eigenvalues E_n , making them complex. $P(k)$ would then exhibit a sharp finite peak at the threshold. If the linewidth were solely due to natural broadening, $P(k)$ would have the value

$$|P(\frac{3}{4})| \rightarrow \frac{2}{3}\alpha^{-2} = 1.25 \times 10^4, \quad (11)$$

yielding the extremely large and narrow resonance cross section. This value would be reduced and broadened if other broadening mechanisms were operative. We shall not pursue this further since the results will depend upon the experimental environment of the atom. An analytic continuation of (10) to the region above the first threshold can be obtained by an integration by parts, reducing the power of the singularity in the integrand.

Study of Electron Correlation in Helium-Like Systems Using an Exactly Soluble Model*

NEIL R. KESTNER† AND OKTAY SINANOĞLU

Sterling Chemistry Laboratory, Yale University, New Haven, Connecticut

(Received July 13, 1962)

The exact solution of a two-electron system in which the electron-electron interaction is Coulombic but the electron-nuclear attraction is a harmonic oscillator potential gives the following wave function: $\chi_1 \chi_2 f(r_{12})$, where the χ 's are one-particle spherical harmonic oscillator wave functions. The exact $f(r_{12})$ has only a small curvature in r_{12} , the distance between the two electrons. This exactly soluble model is used to gain some insight into electron correlation in actual two electron atoms and into the usual approximations. A variational trial function, $f(r_{12}) = 1 + \alpha r_{12}$, where α is a variable parameter, gives energies and even wave functions close to the exact solution. The correlation energy determined from an analytic Hartree-Fock solution and the average angle between the two electrons are somewhat less than in actual helium-like systems.

I. INTRODUCTION

FROM the early work of Hylleraas to the present, the main problem in the quantum mechanics of two-electron systems has been the choice of correct trial wave functions. The present state of this research is summarized by Löwdin.¹ The problem is to find the correct two-electron part of the wave function since the Hartree-Fock solution is the best one-electron result.

The studies of Fock,² Kinoshita,³ Kato,⁴ and others sought to obtain the form of a power series solution, hoping that a trial function of that form would rapidly converge to the exact wave function. Kinoshita's energy calculations on helium³ attest to this approach.

However, one cannot solve the two-electron atomic system exactly; nor can one obtain the coefficients of each term in a formal power series solution. To study the two-electron effects which represent the correlation in the motions of the two electrons, we consider here a model problem which can be solved exactly.

A single-particle Gaussian wave function of a spheri-

* This research was supported by a grant from the National Science Foundation.

† National Science Foundation Predoctoral Fellow.

¹ P. O. Löwdin, in *Advances in Chemical Physics*, edited by I. Prigogine (Interscience Publishers, Inc., New York, 1959), Vol. II, p. 207; P. O. Löwdin and L. Redei, *Phys. Rev.* **114**, 752 (1959).

² V. Fock, *Kgl. Norske Videnskab. Selskabs Forh.* **31**, 138, 145 (1958).

³ T. Kinoshita, *Phys. Rev.* **105**, 1490 (1957).

⁴ T. Kato, *Trans. Am. Math. Soc.* **70**, 195, 212 (1951).