PHYSICAL REVIEW A VOLUME 22, NUMBER 5 NOVEMBER 1980

Resonance scattering of Lyman-α radiation by hydrogen in the ground state

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(Received 10 March 1980)

We calculate the cross section for the resonance scattering of Lyman-α radiation by spinless nonrelativistic hydrogen atoms in the ground state using a two-level model. A generalization of Dirac's resonance scattering theory is used together with the exact matrix elements for the electromagnetic interaction. In contrast to the usual treatments in which only the dipole approximation for the matrix elements are taken, the shift in position of the resonance is finite and has a value of 75% of the Lamb shift of the $n = 1$ state. Whether this latter fact is significant in renormalization calculations is left open.

I. INTRODUCTION

The calculation of the resonance-scattering cross section for Lyman-α radiation is important for a variety of reasons. First of all, such scattering is extremely important in astrophysics, since hydrogen is the most abundant element in "empty" space. Hydrogen is also important in the higher portions of the earth's atmosphere, where it acts as a scatterer of solar radiation.

Another reason for calculating this cross section is that this is the simplest resonance cross section which one can calculate, since the wave functions are simple and since a two-level approximation, involving the ground state and the degenerate first excited state, is apt to be especially good. One may expect some insight into the methods of calculating resonance cross sections for more complicated atoms.

Still another reason is that the resonance line shape, which is identical to the line shape of Lyman-α radiation emitted by excited hydrogen, is related to the self-energy problem of quantum electrodynamics. As is well known, the position of resonance (or maximum intensity in the case of emission) is not precisely at the Lyman-α frequency, but is shifted. In the traditional calculations of this shift, the dipole approximation to the electromagnetic matrix elements is used, and the shift is infinite. Since the advent of renormalization theory one uses renormalization to obtain finite results.[1] Where resonance scattering is treated directly,[2] it is found that the shift is of the order of the Lamb shift of the energy levels.

In the present paper, we use Dirac's theory of resonance scattering.[3] In this theory only the matrix elements which have a resonant denominator in the usual perturbation-theory expansions are assumed to be nonzero. One is then led to a Hamiltonian whose eigenfunctions can be obtained exactly. The Dirac resonance theory is studied from a rigorous mathematical point of view by Friedrichs, and we are greatly influenced by his paper.[4]

However, we must modify the Dirac resonance theory somewhat to take into account the degeneracy of the first excited state of hydrogen. In our treatment we shall consider only the matrix elements of the electromagnetic interaction

$$H_I = i(e\hbar/Mc)\vec{A}\cdot\vec{\nabla}\ , \tag{1}$$

where M is the electron mass which connects the following states with each other by the emission of a photon from the vacuum: 1S, 2S, 2P. In contrast to the traditional treatments, we shall not use the dipole approximation, but instead we shall use *exact* matrix elements.[5,9] It will be seen that in contrast to earilier treatments, the shift in position of resonance will be *finite* without renormalization. Furthermore, this shift, when translated into shifts in energy level, is close to the Lamb shift for the ground state. We include *all* matrix elements of the two-level system, those which lead to "forbidden" (in the dipole approximation) as well as those which lead to "permitted" transitions. When we first carried out the calculations for the frequency shift using the techniques of the present paper,[6] we ignored the forbidden transitions. This calculation led to a frequency shift somewhat greater than one-half of the Lamb shift. [The line shape of emitted Lyman-α radiation was also calculated in Ref. 7, also taking into account only the permitted transition between the 1S state and the 2P states, using the exact matrix elements (calculated differently but agreeing with other matrix elements[5,6]), but with an unconventional treatment of the electromagnetic interaction. Exactly the same shift as found previously was obtained.[6]] The inclusion of matrix elements corresponding to forbidden transitions between the 2S and 2P states and between the 2P states themselves gives a substantial contribution to the shift. On the other hand, only the permitted transition from the 1S to the 2P state contributes to the natural line breadth. It would be interesting to see what contributions the $n=3$ states and two-photon intermediate states give. There should be no difficulty in calculating these contributions other than "book keeping." If the contributions are small, it would appear that the two-level single-photon theory is indeed a good approximation.

In short, the calculations of the present paper are of the kind that could have been done in the early 1930's had the exact matrix elements been used. The shift which we obtain corresponds to the raising of the ground state by an amount of 6297 MHz in frequency terms. The shift for the ground state calculated using renormalization theory is 8126 MHz.[8] Thus our calculation, which is completely free of infinities, gives 75% of the Lamb shift.

It ought to be mentioned that the inclusion of the effect of retardation is being treated in recent times by a number of writers (see, for example Ref. 10). However, the objectives and methods are very different from those of the present paper.

II. THE DIFFERENTIAL AND TOTAL CROSS-SECTIONS. THE RADIATION PATTERN OF THE SCATTERED RADIATION. COMPARISON WITH PHENOMENOLOGICAL THEORY

The quantity $k=2\pi/\lambda$ is the wave number of the incident and scattered radiation which is assumed to be near the wave number κ of Lyman-α radiation.

From the Bohr formula for the energy levels of hydrogen

$$\kappa a=\tfrac{3}{8}\alpha \;, \tag{2}$$

where a is the first Bohr radius of the hydrogen atom and α is the fine structure constant. The polarization of the radiation is most conveniently described by the helicity variable $\beta=\pm 1$. If $\beta=1$, the radiation is circularly polarized in the direction opposite to that of propagation, whereas if $\beta=-1$, the radiation is circularly polarized in the direction of propagation.

We shall assume that incident radiation of wave number k and helicity β propagates in the positive direction along the z axis from minus infinity and strikes the hydrogen atom in the ground state located at the origin. Let us denote by $\hat{\eta}$ the unit vector in the direction of propagation of the scattering radiation, and let us introduce the usual polar coordinates θ and ϕ by

$$\hat{\eta}=(\sin\theta\,\cos\phi,\ \sin\theta\,\sin\phi,\ \cos\theta). \tag{3}$$

We shall denote the cross section for the scattering of the photon with the same circular polarization in the direction $\vec{\eta}$ by $\sigma_1(\theta)$. This and the other cross sections are independent of ϕ. Then, $\sigma_1(\theta)\,d\Omega$ (where $d\Omega=\sin\theta\,d\theta\,d\phi$) gives the relative intensity of the radiation scattered in the solid angle $d\Omega$. Explicitly,

$$\sigma_1(\theta)=(9/4\kappa^2)F(k)\cos^4\tfrac{1}{2}\theta \;, \tag{4}$$

where $F(k)$ is the resonance function given by

$$F(k)=\frac{\gamma^2}{(k-\kappa-\delta)^2+\gamma^2} \;, \tag{5}$$

and in which the half-breadth γ and the resonance shift δ have the values (in cm^{-1})

$$\delta=-1.320, \quad \gamma=-1.046\times 10^{-2} \;. \tag{5a}$$

In terms of frequency (MHz) these quantities are

$$c\delta/2\pi=-6297, \quad c\gamma/2\pi=-49.9. \tag{5b}$$

The effect of δ is to change the position of resonance from κ to $\kappa+\delta$ and can be interpreted as an apparent increase of the ground-state energy with respect to the first excited state. The contributions of the permitted and forbidden transitions to δ are discussed in Sec. V.

The differential cross section for scattering of radiation whose circular polarization is *opposite* to that of the incident radiation is denoted by $\sigma_2(\theta)$ and given by

$$\sigma_2(\theta)=(9/4\kappa^2)F(k)\sin^4\tfrac{1}{2}\theta \;. \tag{6}$$

The differential cross section for scattering of photons of either polarization, but with the incident circular polarization still given by β, is denoted by $\sigma_T(\theta)$ and is just the sum of $\sigma_1(\theta)$ and $\sigma_2(\theta)$:

$$\sigma_T(\theta)=\sigma_1(\theta)+\sigma_2(\theta) \;.$$

One easily verifies that

$$\sigma_T(\theta)=(9/8\kappa^2)\,F(k)(1+\cos^2\theta) \;. \tag{7}$$

If the incident radiation is unpolarized, one averages over both values of β to obtain the cross section for the scattering of unpolarized incident polarization without distinquishing the polarization of the scattered radiation. Since $\sigma_T(\theta)$ is independent of $\beta, \sigma_T(\theta)$ also gives the differential scattering cross section for unpolarized incident radiation. It is of interest to note that the θ dependence of $\sigma_T(\theta)$ is identical to that predicted by the classical theory of resonance fluorescence.[11] In the quantum theory of scattering, we shall see that this dependence is due to the fact that in our approximation, only photons with angular-momentum-quantum number $j=1$ are scattered.

The total cross section Σ is given by

$$\Sigma=\int \sigma_T(\theta)\,d\Omega \;,$$

where the integration is taken over the entire sphere. We have

$$\sum = (6\pi/\kappa^2)F(k). \quad (8)$$

We can confront Eq. (8) with the phenomenological results of Mitchell and Zemansky.[12] By the use of detailed balance and relations between the Einstein A and B coefficients, one can construct a cross-section Σ' considered as a function of the frequency ν. It is shown that[12]

$$\int \Sigma' \, d\nu = \frac{\lambda_0^2}{8\pi} \frac{g_2}{g_1} \frac{1}{\tau} \quad , \quad (9)$$

where λ_0 is the wavelength of the resonant line, g_2 and g_1 are the degeneracies of the upper and lower states, and τ is the lifetime of the upper state. From Eq. (8)

$$\int \Sigma \, d\nu = \frac{c}{2\pi} \int \Sigma \, dk = \frac{3\pi c}{\kappa^2} \, |\gamma| \; . \quad (10)$$

But $\kappa = 2\pi/\lambda_0$. From the Heisenberg uncertainty principle

$$\tau(\Delta E) \sim \hbar \; , \quad (11)$$

where ΔE is the "width" of the excited state. The width of the excited state is $|2\gamma|$ in terms of wave numbers. However, $\Delta E = \hbar c \, |2\gamma|$. Then Eqs. (10) and (11) yield the following:

$$\int \Sigma \, d\nu \sim \frac{\lambda_0^2}{8\pi} \, 3 \, \frac{1}{\tau} \; . \quad (12)$$

Equation (12) agrees with the phenomenological result Eq. (9).

We can also give the radiation pattern for the scattered radiation. We shall give the case where the incident radiation is plane polarized. Let $\hat{i}_1, \hat{i}_2, \hat{i}_3$ be an orthonormal triad of unit vectors. We take the incident radiation to have the form

$$\vec{E}_{in}(\vec{x},t) = C\hat{i}_1 \sin k(\hat{i}_3 \cdot \vec{x} - ct) \; ,$$
$$\vec{H}_{in}(\vec{x},t) = C\hat{i}_2 \sin k(\hat{i}_3 \cdot \vec{x} - ct) \; . \quad (13)$$

The radiation scattered in the direction described by the unit vector $\hat{\eta}$ is

$$\vec{E}_{sc}(\vec{x},t) = (3/4\pi)[(\hat{i}_1 \times \hat{\eta}) \times \hat{\eta}]C[F(k)]^{1/2} \times \cos[k(\hat{\eta}\cdot\vec{x} - ct) + \Phi(k)] \; ,$$
$$\vec{H}_{sc}(\vec{x},t) = (3/4\pi)[\hat{i}_1 \times \hat{\eta}]C[F(k)]^{1/2} \times \cos[k(\hat{\eta}\cdot\vec{x} - ct) + \Phi(k)] \; , \quad (14)$$

where $\Phi(k)$ is defined by

$$\sin\Phi(k) = -[F(k)]^{1/2} = \gamma[(k-\kappa-\delta^2] + \gamma^2]^{-1/2} \; ,$$
$$\cos\Phi(k) = (k-\kappa-\delta)[(k-\kappa-\delta)^2 + \gamma^2]^{-1/2} \; . \quad (14a)$$

At resonance, $\Phi = \frac{1}{2} - \pi$. It is to be noted that $|(\hat{i}_1 \times \hat{\eta}) \times \hat{\eta}| = |\hat{i}_1 \times \hat{\eta}| = \sin\Theta$, where Θ is the angle between $\hat{i}_1$ and $\hat{\eta}$. Hence, the maximum radiation is in the $\hat{i}_2$, $\hat{i}_3$ plane, and there is no radiation in or opposite to the $\hat{i}_1$ direction.

III. EIGENFUNCTIONS OF THE UNPERTURBED HAMILTONIAN. EXACT MATRIX ELEMENTS

For the sake of brevity the remainder of the paper will be written as a direct extension of earlier work,[5] except that in the present paper the helicity will be denoted by β instead of λ as in[5] to prevent confusion with the wavelength λ. Equations from the previous paper[5] will have a prime attached to them.

The Hamiltonian of the atom interacting with the radiation field is the usual one:

$$H = H_A + H_P + H_I = H_0 + H_I \; , \quad (15)$$

where H_A is the usual Hamiltonian for the hydrogen atom, H_P is the Hamiltonian for the photon field given by the first of Eq. (37′), and H_I is the interaction of Eq. (1). As is customary, we ignore the $\vec{A}^2$ term. Of course, $H_0 = H_A + H_P$ is the unperturbed Hamiltonian.

The space of wave functions is spanned by the eigenfunctions of H_0. These eigenfunctions are direct products of atomic eigenfunctions and either vacuum states of the field or of n-photon states which we take to be in the energy- angular-momentum representation as discussed in Eqs. (41′)–(43′). Particular eigenfunctions will concern us:

(1) The state in which the atom is in the 1S state and the photon field is in the vacuum state will be designated by $|1\rangle$. The state in which the atom is in the 1S state and there is a photon in the state whose energy is $E_p = \hbar c k$, whose angular momentum is given by the quantum numbers j, m and whose helicity is given by β, will be denoted by $|1, E_p, j, m, \beta\rangle$.

(2) The analogous kets in which the atom is in the 2S state will be denoted by $|2\rangle$ and $|2, E_p, j, m, \beta\rangle$, respectively.

(3) In the case that the atom is in a 2P state with the magnetic quantum number $M(=0, \pm 1)$, and the photon field is in a vacuum state, the eigenket will be denoted by $|2, M\rangle$. When a photon is present the ket will be written $|2, M, E_p, j, m, \beta\rangle$.

Thus in our notation, the absence or presence of the quantum number M indicates whether the atomic state is an S state or P state. These three sets of kets are orthogonal to all other eigenkets of H_0. They are also orthogonal to each other. Within each set they satisfy the orthonormality relations

$$\langle 1|1\rangle = 1\,,$$
$$\langle 1,E_p,j,m,\beta|1,E_p',j',m',\beta'\rangle = E_p\delta(E_p-E_p')\delta_{jj'}\delta_{mm'}\delta_{\beta\beta'}\,,$$
$$\langle 1|1,E_p,j,m,\beta\rangle = 0\,,$$
$$\langle 2|2\rangle = 1\,,$$
$$\langle 2,E_p,j,m,\beta|2,E_p',j',m',\beta'\rangle = E_p\delta(E_p-E_p')\delta_{jj'}\delta_{mm'}\delta_{\beta\beta'}\,,$$
$$\langle 2|2,E_p,j,m,\beta\rangle = 0\,,$$
$$\langle 2,M|2,M'\rangle = \delta_{MM'}\,,$$
$$\langle 2,M,E_p,j,m,\beta|2,M',E_p',j',m',\beta'\rangle = \delta_{MM'}E_p\delta(E_p-E_p')\delta_{jj'}\delta_{mm'}\delta_{\beta\beta'}\,,$$
$$\langle 2,M|2,M',E_p,j,m,\beta\rangle = 0\,. \tag{16}$$

We shall take all matrix elements of H_I to be zero except those between the eigenfunctions introduced above. The only nonvanishing matrix elements are easily calculated from Eqs. (2a′) and (2b′) when one uses the appropriate radial wave functions for the hydrogen atom. The nonvanishing matrix elements are the following:

$$\langle n,E_p,j,m,\beta|H_I|2,M\rangle = \langle 2,M|H_I|n,E_p,j,m,\beta\rangle^* = -i\beta(e^2/a)(\alpha/\pi)^{1/2} \times \delta_{Mm}\delta_{j,1}G_n(ka)\,, \tag{17a}$$

where n is the principal quantum number 1 or 2, and the functions $G_n(x)$ are given by

$$G_1(x) = -(\tfrac{2}{3})^{1/2}x[x^2+(\tfrac{3}{2})^2]^{-2}\,,$$
$$G_2(x) = -(12)^{-1/2}x^3[x^2+1]^{-3}\,. \tag{17b}$$

Furthermore,

$$\langle n|H_1|2,M,E_p,j,m,\beta\rangle = \langle 2,M,E_p,j,m,\beta|H_1|n\rangle^* = -(-1)^m i\beta(e^2/a)(\alpha/\pi)^{1/2} \times \delta_{M,-m}\delta_{j,1}G_n(ka)\,. \tag{17c}$$

Finally,

$$\langle 2,M'|H_1|2,M,E_p,j,m,\beta\rangle = \langle 2,M,E_p,j,m,\beta|H_1|2,M'\rangle^* = -(-1)^{M'}\left(\frac{e^2}{a}\right)\left(\frac{\alpha}{\pi}\right)^{1/2}\begin{pmatrix}1 & 1 & 1\\ m & -M' & M\end{pmatrix} \times \delta_{j,1}A(ka)\,, \tag{17d}$$

where the function $A(x)$ is given by

$$A(x) = 2^{-1/2}x^2[x^2+1]^{-3}\,. \tag{17e}$$

As noted previously, $k = E_p/\hbar c$.

IV. EIGENFUNCTIONS OF THE PERTURBED HAMILTONIAN IN THE TWO-LEVEL APPROXIMATION

We shall denote the energy of the ground state of the hydrogen atom by E_1 and the energy of the first excited state by E_2. Clearly, $\kappa = (E_2 - E_1)/\hbar c$. We shall be interested in particular eigenfunctions of the Hamiltonian $H = H_0 + H_1$. They will be denoted by $|1,E_p,j,m,\beta)$ and will satisfy the set of integral equations symbolically given by

$$|1,E_p,j,m,\beta) = |1,E_p,j,m,\beta\rangle + \gamma_-(E_1+E_p-H_0)H_1|1,E_p,j,m,\beta)\,, \tag{18}$$

where $\gamma_-(x)$ [which is not to be confused with the half-width γ or the function $\gamma(x)$ which will be used later as a "half-width function")] is given by

$$\gamma_-(x) = \frac{P}{x} - i\pi\delta(x) = \lim_{\epsilon\to+0}\frac{1}{x+i\epsilon}\,, \tag{19}$$

where P means that the principal value of the integral is to be used when P/x is used as a factor in an integrand. The eigenfunction $|1,E_p,j,m,\beta)$ is an outgoing wave function in the sense of scattering theory.[13] In our discussion of scattering we shall, however, follow more closely Friedrichs[4] and Moses.[14]

It is readily seen that $|1,E_p,j,m,\beta)$ satisfies required eigenvalue equation

$$(E-H_0)|1,E_p,j,m,\beta) = H_1|1,E_p,j,m,\beta)\,, \tag{20}$$

where

$$E = E_1 + E_p\,. \tag{20a}$$

We require these eigenfunctions to satisfy Eq. (18) because they are particularly useful in solving the initial-value problem in which we are interested. From Eq. (18) it follows that

$$\lim_{t\to-\infty}\exp\left(\frac{i}{\hbar}(H_0-E)t\right)|1,E_p,j,m,\beta) = |1,E_p,j,m,\beta\rangle\,, \tag{21}$$

$$\lim_{t\to+\infty}\exp\left(\frac{i}{\hbar}(H_0-E)t\right)|1,E_p,j,m,\beta) = |1,E_p,j,m,\beta\rangle - 2\pi i\delta(E-H_0)H_I|1,E_p,j,m,\beta)\,. \tag{22}$$

It should be noted that the right-hand side of Eq. (22) is an eigenstate of H_0 with the eigenvalue E. It can be shown that the eigenfunctions $|1,E_p,j,m,\beta)$ satisfy the orthonormality relations

$$(1,E_p,j,m,\beta\,|\,1,E_p',j',m',\beta') = E_p\delta(E_p-E_p')\delta_{jj'}\delta_{mm'}\delta_{\beta\beta'}\,. \quad (23)$$

Let us require that the solution $|\Phi(t)\rangle$ of the perturbed time-dependent Schrödinger equation approach, as $t\to-\infty$, the solution of the unperturbed time-dependent equation which corresponds to the state in which the atom is in the ground state and in which a photon is in an energy, angular-momentum state. The state of the system is the direct product of the ground state of the atom, which we take to be normalized to unity, and the wave function of the photon $g(E_p,j,m,\beta)$ whose norm is

$$\left(\sum_{j,m,\beta}\int_0^\infty |g(E_p,j,m,\beta)|^2\frac{dE_p}{E_p}\right)^{1/2}.$$

Then for $t\to-\infty$

$$|\Phi(t)\rangle = \exp\left(-\frac{i}{\hbar}H_0t\right)\sum_{j,m,\beta}\int_0^\infty |1,E_p,j,m,\beta\rangle \times g(E_p,j,m,\beta)\frac{dE_p}{E_p}$$
$$=\sum_{j,m,\beta}\int_0^\infty |1,E_p,j,m,\beta\rangle \exp\left(-\frac{i}{\hbar}(E_1+E_p)t\right)\times g(E_p,j,m,\beta)\frac{dE_p}{E_p}\,. \quad (24)$$

For t finite the state is given by

$$|\Phi(t)\rangle = \exp\left(-\frac{i}{\hbar}Ht\right)\sum_{j,m,\beta}\int_0^\infty |1,E_p,j,m,\beta) \times g(E_p,j,m,\beta)\frac{dE_p}{E_p}$$
$$=\sum_{j,m,\beta}\int_0^\infty |1,E_p,j,m,\beta) \exp\left(-\frac{i}{\hbar}(E_1+E_p)t\right)\times g(E_p,j,m,\beta)\frac{dE_p}{E_p}\,. \quad (25)$$

For $t\to+\infty$

$$|\Phi(t)\rangle = \exp\left(-\frac{i}{\hbar}H_0t\right)\times\left(\sum_{j,m,\beta}\int_0^\infty |1,E_p,j,m,\beta\rangle g(E_p,j,m,\beta)\frac{dE_p}{E_p} -2\pi i\sum_{j,m,\beta}\int_0^\infty \delta(E-H_0)H_I\,|1,E_p,j,m,\beta)\times g(E_p,j,m,\beta)\frac{dE_p}{E_p}\right), \quad (26)$$

where $E=E_p+E_1$, as before. By evaluating $\langle 1,E_p,j,m,\beta\,|\,\Phi(t)\rangle$ using Eq. (26), it is seen that the scattered part of the photon wave function in the energy, angular-momentum representation is

$$g_{sc}(E_p,j,m,\beta;t) = -2\pi i\sum_{j',m',\beta'}\langle 1,E_p,j,m,\beta\,|H_I|\,1,E_p,j',m',\beta')\times(E_p)^{-1}g(E_p,j',m',\beta')\times\exp\left(-\frac{i}{\hbar}E_pt\right)\,. \quad (27)$$

In terms of the linear momentum representation, the scattered part of the photon wave function is given by

$$f_{sc}(\vec{p},\beta;t)=\frac{c}{p}^{1/2}\sum_j\sum_m Y_j^{m\beta}(\theta,\phi)g_{sc}(cp,j,m,\beta;t)\,. \quad (28)$$

[See Eq. (31a').] The angles θ and ϕ are the usual angles which give the direction of $\vec{p}$ in spherical coordinates.

At finite times t let the wave function $h(\vec{p},\beta;t)$ be defined by

$$h(\vec{p},\beta;t) = \frac{c}{p}^{1/2}\sum_j\sum_m Y_j^{m\beta}(\theta,\phi)\langle 1,E_p,j,m,\beta\,|\,\Phi(t)\rangle,\quad (E_p=cp)\,. \quad (29)$$

Let $\hat{\eta}=(\vec{p}/p)$ and define $v(\hat{\eta},\beta;t)$ and $w(\hat{\eta},\beta,t)$ by

$$v(\hat{\eta},\beta;t)=\frac{d}{dt}\int_0^\infty |h(\vec{p},\beta;t)|^2p^2\frac{dp}{cp},$$
$$w(\hat{\eta},\beta;t)=\frac{d}{dt}\int_0^\infty |h(\vec{p},\beta;t)|^2p^2\,dp\,. \quad (30)$$

Then $v(\hat{\eta},\beta;t)d\Omega$, where $d\Omega=\sin\theta\,d\theta\,d\phi$ represents the number of photons with polarization described by β passing, per unit time, through the solid angle $d\Omega$. Likewise, $w(\hat{\eta},\beta;t)d\Omega$ gives the energy of radiation per unit time passing through the solid angle $d\Omega$ when the radiation is polarized in the manner given by β. The atom is in the ground state. When the wave function of the incident photon $g(E_p,j,m,\beta)$ is chosen to correspond in the limit to the case in which the photon is monochromatic and when its incident path is a prescribed straight line, $v(\hat{\eta},\beta;t)$ and $w(\hat{\eta},\beta;t)$ are independent of time. One can then use these quantities to obtain the cross sections. Our treatment will correspond to the discussion of time-proportional transition probabilities,[15,16] which in turn are more careful treatments of the theory discussed by Lippmann and Schwinger.[13]

It is seen that to solve the scattering problem, one must solve Eq. (18) for the eigenstates $|1,E_p,j,m,\beta)$. Usually, these eigenstates are obtained by perturbation theory or, equivalently, by iteration. On the right-hand side of Eq. (18), one replaces $|1,E_p,j,m,\beta)$ by $|1,E_p,j,m,\beta\rangle$ and continues this iterative process in an obvious way. The second-order iteration yields results which are of the Kramers-Heisenberg dispersion formula-type and gives infinite results when the incoming photon has its energy equal to the difference in energies of two atomic states. For this reason Dirac[3] proposed a different type of approximation which is more accurate near resonance. What follows is our version of the Dirac resonance theory. Our version is a generalization in which degeneracy of the atomic state is taken into account. Normally, one would need to use analogs of "stabilized eigenfunctions" of H_0. However because we are working in an angular-momentum representation and because both H_0 and the two level H commute with the angular momentum (as does the exact H, of course), there is a considerable simplification. Indeed, the use of the correct angular-momentum representations for photons makes this comparatively simple calculation possible.

In our approximation we assume that the only nonzero matrix elements of H_1 are those given in Eq. (17). These are all the one-photon state which connect the ground state and the first excited states with each other. The effect of this assumption is that we have replaced the interaction H_I by another interaction which is also Hermitian. This interacting enables us to solve Eq. (18) *exactly*.

From Eq. (18)

$$\langle 1,E_p',j',m',\beta'|1,E_p,j,m,\beta)=E_p\delta(E_p-E_p')\delta_{jj'}\delta_{mm'}\delta_{\beta\beta'}+\gamma_-(E_p-E_p')\sum_M\langle 1,E_p',j',m',\beta'|H_I|2,M\rangle \times\langle 2,M|1,E_p,j,m,\beta). \tag{31}$$

On using Eq. (17a)

$$\langle 1,E_p',j',m',\beta'|1,E_p,j,m,\beta)=k\delta(k-k')\delta_{jj'}\delta_{mm'}\delta_{\beta\beta'}-i(\alpha^3/\pi)^{1/2}a^{-1}\beta'\gamma_-(k-k')\delta_{j',1}G_1(k'a)\langle 2,m'|1,E_p,j,m,\beta). \tag{32}$$

In Eq. (32) and later, $k=E_p/\hbar c$ and $k'=E_p'/\hbar c$ and $k'=E_p'/\hbar c$.

From Eq. (20) we have, on multiplying through by $\langle 2,M|$

$$\begin{aligned}[E_p-(E_2-E_1)]\langle 2,M|1,E_p,j,m,\beta)=&\sum_{j',m',\beta'}\int_0^\infty\langle 2,M|H_1|1,E_p',j',m',\beta'\rangle\langle 1,E_p',j',m',\beta'|1,E_p,j,m,\beta)\frac{dE_p'}{E_p'}\\&+\sum_{j',m',\beta'}\int_0^\infty\langle 2,M|H_I|2,E_p',j',m',\beta'\rangle\langle 2,E_p',j',m',\beta'|1,E_p,j,m,\beta)\frac{dE_p'}{E_p'}\\&+\sum_{j',m',\beta'M'}\int_0^\infty\langle 2,M|H_I|2,M',E_p',j',m',\beta'\rangle\langle 2,M',E_p',j',m',\beta'|1,E_p,j,m,\beta)\\&\times\frac{dE_p'}{E_p'}.\end{aligned}\tag{33}$$

On using the expressions Eq. (17) for the matrix elements

$$\begin{aligned}(k-\kappa)\langle 2,M|1,E_p,j,m,\beta)=&\,i\left(\frac{\alpha^3}{\pi}\right)^{1/2}a^{-1}\sum_{\beta'}\beta'\int_0^\infty G_1(k'a)\langle 1,E_p',1,M,\beta'|1,E_p,j,m,\beta)\frac{dk'}{k'}\\&+i\left(\frac{\alpha^3}{\pi}\right)^{1/2}a^{-1}\sum_{\beta'}\beta'\int_0^\infty G_2(k'a)\langle 2,E_p',1,M,\beta'|1,E_p,j,m,\beta)\frac{dk'}{k'}\\&+(-1)^{M+1}\left(\frac{\alpha^3}{\pi}\right)^{1/2}a^{-1}\sum_{m',\beta'}\begin{pmatrix}1&1&1\\m'&-M&M-m'\end{pmatrix}\\&\times\int_0^\infty A(k'a)\langle 2,M-m',E_p',1,m',\beta'|1,E_p,j,m,\beta)\frac{dk'}{k'},\end{aligned}\tag{34}$$

where we have used $\kappa=(E_2-E_1)/\hbar c$.

From Eq. (18) one obtains in a similar fashion the following:

$$\langle 2,E_p',j',m',\beta'|1,E_p,j,m,\beta)=-i\delta_{j',1}\beta'(\alpha^3/\pi)^{1/2}a^{-1}\gamma_-(k-k'-\kappa)G_2(k'a)\langle 2,m'|1,E_p,j,m,\beta), \tag{35}$$

$$\begin{aligned}&\langle 2,M',E_p',j',m',\beta'|1,E_p,j,m,\beta)\\&=\delta_{j',1}\left(\frac{\alpha^3}{\pi}\right)^{1/2}a^{-1}\gamma_-(k-k'-\kappa)\Big[i\beta'(-1)^{m'}\delta_{m',-M'}G_1(k'a)\langle 1|1,E_p,j,m,\beta)\\&\qquad+i\beta'(-1)^{m'}\delta_{m',-M'}G_2(k'a)\langle 2|1,E_p,j,m,\beta)\\&\qquad-\begin{pmatrix}1&1&1\\m'&-(m'+M')&M'\end{pmatrix}(-1)^{M'+m'}A(k'a)\langle 2,m'+M'|1,E_p,j,m,\beta)\Big],\end{aligned}\tag{36}$$

$$\langle 1|1,E_p,jm,\beta\rangle=-i\left(\frac{\alpha^3}{\pi}\right)^{1/2}a^{-1}\gamma_-(k)\sum_{m',\beta'}\beta'(-1)^{m'}\int_0^\infty G_1(k'a)\langle 2,-m',E_p',1,m',\beta'|1,E_p,j,m,\beta\rangle\frac{dk'}{k'}, \tag{37}$$

$$\langle 2|1,E_p,j,m,\beta\rangle=-i\left(\frac{\alpha^3}{\pi}\right)^{1/2}a^{-1}\gamma_-(k-\kappa)\sum_{m',\beta'}\beta'(-1)^{m'}\int_0^\infty G_2(k'a)\langle 2,-m',\beta'|1,E_p,j,m,\beta\rangle\frac{dk'}{k'}. \tag{38}$$

Equations (32), (34), (35), (36), (37), and (38) are a set of equations for the quantities $\langle 1,E_p',j',m'\beta'|1,E_p,j,m,\beta\rangle$; $\langle 2,M|1,E_p,j,m,\beta\rangle$; $\langle 2,E_p',j',m',\beta'|1,E_p,j,m,\beta\rangle$; $\langle 2,M',j',m',\beta'|1,E_p,j,m,\beta\rangle$; $\langle 1|1,E_p,j,m,\beta\rangle$; and $\langle 2|1,E_p,j,m,\beta\rangle$. It is to be noted that these are the only components of $|1,E_p,j,m,\beta\rangle$ in the H_0 representation which have the possibility of being nonzero.

We shall now solve the set of equations. On substituting Eq. (36) into Eqs. (37) and (38), one obtains a pair of homogeneous linear equations for $\langle 1|1,E_p,j,m,\beta\rangle$ and $\langle 2|1,E_p,j,m,\beta\rangle$. Since the determinant of the coefficients is not zero it follows that

$$\langle 1|1,E_p,j,m,\beta\rangle=\langle 2|1,E_p,j,m,\beta\rangle=0. \tag{39}$$

Equation (36) now simplifies considerably. On substituting Eqs. (36), (32), and (35) into Eq. (34), one obtains an equation for $\langle 2,M|1,E_p,j,m,\beta\rangle$ which one can solve easily. On substituting $\langle 2,M|1,E_p,j,m,\beta\rangle$ so obtained into Eqs. (32), (35), and (36), one finds

$$\langle 1,E_p',j',m',\beta'|1,E_p,jm,\beta\rangle,$$

$$\langle 2,E_p',j',m',\beta'|1,E_p,j,m,\beta\rangle,$$

and

$$\langle 2,M',E_p',j',m'\beta'|1,E_p,j,m,\beta\rangle,$$

respectively. In carrying out the substitutions, one should note that summations over β yield factors of 2. Furthermore, one uses

$$\sum_{m'}\begin{pmatrix}1 & 1 & 1\\ m' & -M & M-m'\end{pmatrix}=\frac{1}{3}, \tag{40}$$

for $M=0,\pm 1$.

In order to give the solution, it is convenient to make some definitions. Let the functions $I_i(x)$ be defined for $i=2,3$ by

$$I_i(x)=\int_0^\infty [G_i(\xi)]^2\gamma_-(x-\xi)\frac{d\xi}{\xi}\quad\text{for } i=1,2, \tag{41}$$

$$I_3(x)=\int_0^\infty [A(\xi)]^2\gamma_-(x-\xi)\frac{d\xi}{\xi}. \tag{42}$$

The functions $I_i(x)$ are given in the appendix. Indeed, the imaginary parts can be obtained immediately using the δ function in Eq. (19).

Let us further define

$$\delta_1(k)=(2\alpha^3/\pi a)\,\mathrm{Re}I_i(ka),\ \delta_2(k)=\frac{2\alpha^3}{\pi a}\mathrm{Re}I_2(ka-\kappa a),$$
$$\delta_3(k)=(2\alpha^3/3\pi a)\,\mathrm{Re}I_3(ka-\kappa a). \tag{43}$$

Let $H(k)=1$ for $k\geq 0$ and $H(k)=0$ for $k<0$. Then also

$$\gamma_1(k)=(2\alpha^3/\pi a)\,\mathrm{Im}I_i(ka)=-(2\alpha^3/ka^2)[G_1(ka)]^2H(k),$$
$$\gamma_2(k)=(2\alpha^3/\pi a)\,\mathrm{Im}I_2(ka-\kappa a)$$
$$=-[2\alpha^3/(k-\kappa)a^2][G_2(ka-\kappa a)]^2H(k-\kappa), \tag{44}$$
$$\gamma_3(k)=(2\alpha^3/3\pi a)\,\mathrm{Im}I_3(ka-\kappa a)$$
$$=[2\alpha^3/3(k-\kappa)a^2][A(ka-\kappa a)]^2H(k-\kappa).$$

Also,

$$\delta(k)=\sum_{i=1}^3\delta_1(k),\ \gamma(k)=\sum_{i=1}^3\gamma_i(k). \tag{45}$$

[$\delta(k)$ of Eq. (45) should not be confused with usual δ function.] Then

$$\langle 1,E_p',j',m',\beta'|1,E_p,j,m,\beta\rangle=k\delta(k-k')\delta_{j,j'}\delta_{m,m'}\delta_{\beta,\beta'}+\frac{1}{2\pi}\delta_{j,1}\delta_{j,j'}\delta_{m,m'}\gamma_-(k-k')\frac{\beta\beta'}{k-\kappa-\delta(k)-i\gamma(k)}[kk'\gamma_1(k)\gamma_1(k')]^{1/2}, \tag{46}$$

$$\langle 2,M|,E_p,j,E_p,j,m,\beta\rangle=-i\delta_{j,1}\delta_{M,m}\frac{\beta[-(k/2\pi)\gamma_1(k)]^{1/2}}{k-\kappa-\delta(k)-i\gamma(k)}, \tag{47}$$

$$\langle 2,E_p',j',m',\beta'|1,E_p,j,m,\beta\rangle=\frac{1}{2\pi}\delta_{j,1}\delta_{j,j'}\delta_{m,m'}\beta\beta'\gamma_-(k-k'-\kappa)\frac{[kk'\gamma_1(k)\gamma_2(k'+\kappa)]^{1/2}}{k-\kappa-\delta(k)-i\gamma(k)}, \tag{48}$$

$$\langle 2,M',E_p',j',m',\beta'|1,E_p,j,m,\beta\rangle=\frac{i}{2\pi}(-1)^m\delta_{j,1}\delta_{j,j'}\delta_{m,M'+m'}\beta\gamma_-(k-k'-\kappa)\begin{pmatrix}1 & 1 & 1\\ m' & -m & M'\end{pmatrix}\times\frac{[3kk'\gamma_1(k)\gamma_3(k'+\kappa)]^{1/2}}{k-\kappa-\delta(k)-i\gamma(k)}. \tag{49}$$

A quantity which is important for finding the scattered portion of the wave function [see Eq. (27)] is given by

$$\frac{-2\pi i}{E_p}\langle 1,E_p,j,m,\beta|H_I|1,E_p,j',m',\beta'\rangle=\frac{-2\pi i}{\hbar ck}\sum_M\langle 1,E_p,j,m,\beta|H_I|2,M\rangle\langle 2,M|1,E_p',j',m',\beta'\rangle$$
$$=i\delta_{j,1}\delta_{j,j'}\delta_{mm'}\beta\beta'\gamma_1(k)\frac{1}{k-\kappa-\delta(k)-i\gamma(k)}. \qquad (50)$$

It is to be noted that angular momentum is conserved, as indicated by the presence of factors as $\delta_{j,j'}\ \delta_{m,m'}$. Equation (39) is another consequence of the conservation of angular momentum.

V. THE LINE BREADTH AND THE SHIFT IN POSITION OF RESONANCE

It is obvious that the square of the absolute value of $k-\kappa-\delta(k)-i\gamma(k)^{-1}$, that is, $\{[k-\kappa-\delta(k)]^2+[\gamma(k)]^2\}^{-1}$, is the resonance denominator in the scattering calculations. Since we are considering values of k near κ, and since $\delta(k)$ and $\gamma(k)$ are slowly varying functions of k, we may replace k by κ in these functions as is customary. We define δ and γ by

$$\delta=\delta(\kappa),\gamma=\gamma(\kappa)\equiv\gamma_1(\kappa). \qquad (51)$$

The resonance denominator then becomes $[(k-\kappa-\delta)^2+\gamma^2]^{-1}$. The values δ and γ given by Eq. (5a) are those obtained from Eq. (51). It is seen that while the matrix elements corresponding to the "forbidden" transitions contribute nothing to γ, they give a substantial contribution to δ. The value of δ in (6) and (7), which ignores the effect of the forbidden transitions, is the principal contribution of δ_1, which is seen to be $\delta_1(0)$. The value of γ of 6 is in error and should have the value given in Eq. (5a). To be more specific $\delta_1(\kappa)$ is the contribution due to the permitted transitions between the ground state 1S and the excited states 2P, while $\delta_2(\kappa)$ is the contribution due to the transitions between the 2S state and the 2P states and $\delta_3(\kappa)$ is that due to transitions of the 2P states among themselves.

Explicitly in terms of frequencies (in MHz)

$$\frac{c\delta_1(\kappa)}{2\pi}=-4358,\quad \frac{c\delta_2(\kappa)}{2\pi}=-342,\quad \frac{c\delta_3(\kappa)}{2\pi}=-1597.$$

VI. CALCULATION OF THE CROSS SECTIONS

We shall now derive Eqs. (4) and (6) for $\sigma_1(\theta)$ and $\sigma_2(\theta)$, respectively. Our procedure will be to obtain the transitions per unit time $w(\hat{\eta},\beta;t)$ of Eq. (30), taking as the initial photon state $g(E_p,j,m,\beta)$ that one which gives rise to a circularly polarized electromagnetic wave of a given wavelength, traveling along the positive z axis. One then divides $w(\hat{\eta},\beta;t)$ by the flux of energy of the incoming radiation, that is, the Poynting vector.

We shall now proceed. It is convenient to specify the initial photon state in the linear-momentum representation instead of the angular-momentum representation. Let the initial state in the linear-momentum representation be denoted by $f(\vec{p},\beta)$. Then from Eq. (31b′)

$$g(E_p,j,m,\beta)=\frac{E_p}{c^{3/2}}\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\sin\theta Y_j^{m,\beta*}(\theta,\phi)f(\vec{p},\beta),$$
$$\vec{p}=(E_p/c)(\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta). \qquad (52)$$

On using Eqs. (29), (46), and (52) we obtain the wave function of the photon at finite times in the linear-momentum representation as

$$h(\vec{p},\beta;t)=e^{-ickt}f(\vec{p},\beta)+\frac{1}{p}\sum_{m',\beta'}\int\frac{d\vec{p}'}{p'^2}Y_1^{m',\beta}(\theta,\phi)\times Y_1^{m',\beta'*}(\theta',\phi')\beta\beta'G(k',k)e^{-ick't}\gamma_-(k'-k)f(\vec{p},\beta'), \qquad (53)$$

where θ',ϕ' are the polar angles of $\vec{p}'$, and $G(k',k)$ is given by

$$G(k',k)=\frac{1}{2\pi}\frac{[kk'\gamma_1(k)\gamma_1(k')]^{1/2}}{k'-\kappa-\delta(k')-i\gamma(k')}, \qquad (53a)$$

and where here and later

$$E_p=cp=c\hbar k,\quad E_p'=cp'=c\hbar k',\quad E_p''=c\hbar k''. \qquad (53b)$$

In deriving Eq. (53), we have used the completeness relation for $Y_1^{m,m'}(\theta,\phi)$, Eq. (A12).[17]

For the wave function $f(\vec{p},\beta)$ let us take

$$f(\vec{p},\beta)=\delta_{\beta,\bar{\beta}}f(\vec{p}), \qquad (54)$$

where $f(\vec{p})$ is a real function of $\vec{p}$ which has a very sharp peak at $\vec{p}=\vec{p}_0$, where

$$\vec{p}_0=\hbar K(0,0,1). \qquad (54a)$$

The incoming electromagnetic field corresponding to this wave function can be obtained from Eq. (34′). Because of the sharpness of the peak in the wave function

$$\vec{E}(\bar{x},t) = -\frac{iA}{2\pi\hbar^{3/2}}[\tilde{\beta}\vec{Q}_\beta(\bar{p}_0)e^{iK(z-ct)} - \beta\vec{Q}^*_{\tilde{\beta}}(\bar{p}_0)e^{-iK(z-ct)}],$$

$$\vec{H}(\bar{x},t) = -\frac{A}{2\pi\hbar^{3/2}}\vec{Q}_{\tilde{\beta}}(\bar{p}_0)e^{iK(z-ct)} + \vec{Q}^*_{\tilde{\beta}}(\bar{p}_0)e^{-iK(z-ct)},$$

$$A = \int f(\bar{p})d\bar{p}. \tag{55}$$

In terms of the Cartesian components

$$E_x(\bar{x},t) = H_y(\bar{x},t) = \frac{A}{2^{1/2}\pi\hbar^{3/2}}\sin[K(z-ct)],$$

$$E_y(\bar{x},t) = H_x(\bar{x},t) = \frac{A\beta}{2^{1/2}\pi\hbar^{3/2}}\cos[K(z-ct)],$$

$$E_z(\bar{x},t) = H_z(\bar{x},t) = 0. \tag{56}$$

Only the z component of the Poynting vector is not zero. The z component, denoted by S, is given by

$$S = (E_xH_y - E_yH_x)\frac{c}{4\pi} = cA^2/(2\pi\hbar)^3. \tag{57}$$

We shall calculate $w(\hat{\eta},\beta;t)$ for $\hat{\eta}$ which does not coincide with the z axis. For this reason, and because $f(\bar{p})$ is so sharply peaked at $\bar{p}=\bar{p}_0$, the first term on the right of Eq. (53) is zero. Thus one has

$$\frac{d}{dt}|h(\bar{p},\beta;t|^2 = -\frac{ic}{p^2}\sum_{m'}\sum_{m''}\int\frac{d\bar{p}'}{p'^2}\int\frac{d\bar{p}''}{p''^2}Y_1^{m',\beta}(\theta,\phi)\times Y_1^{m'',\beta*}(\theta,\phi)Y_1^{m',\tilde{\beta}*}(\theta',\phi')G(k',k)Y_1^{m'',\tilde{\beta}}(\theta'',\phi'')G^*(k'',k)$$
$$\times(k'-k'')e^{-ic(k'-k)t}\gamma_-(k'-k)\gamma_-^*(k''-k)f(\bar{p}')f(\bar{p}''), \tag{58}$$

where p', θ', ϕ' and p'', θ'', ϕ'' are the spherical coordinates of $\bar{p}'$ and $\bar{p}''$, respectively. In Eq. (58) we make the substitution

$$(k'-k'')\gamma_-(k'-k)\gamma_-^*(k''-k) = [(k'-k)-(k''-k)]\gamma_-(k'-k)\gamma_-^*(k''-k) = \gamma_-^*(k''-k) - \gamma_-(k'-k) \tag{59}$$

and obtain two terms on the right of Eq. (58). On interchanging the primed and double-primed dummy variables in one of the terms

$$\frac{d}{dt}|h(\bar{p},\beta;t)|^2 = -\frac{2c}{p^2}\,\mathrm{Im}\sum_{m'}\sum_{m''}\int\frac{d\bar{p}'}{p'^2}\int\frac{d\bar{p}''}{p''^2}Y_1^{m',\beta}(\theta,\phi)Y^{m'',\beta*}(\theta,\phi)Y^{m',\tilde{\beta}*}(\theta',\phi')G(k',k)Y^{m'',\tilde{\beta}}(\theta'',\phi'')$$
$$\times G^*(k'',k)\,e^{-ic(k'-k'')t}\gamma_-(k'-k)f(\bar{p}')f(\bar{p}''). \tag{60}$$

We now use the fact that $f(\bar{p})$ is sharply peaked at $\bar{p}=\bar{p}_0$ to make the following approximations under the integrand which become increasingly good with increasing sharpness of the peak:

$$e^{-ic(k'-k'')t} \sim e^{-ic(K-K)t} = 1,$$
$$Y^{m',\tilde{\beta}*}(\theta',\phi') \sim Y_1^{m',\tilde{\beta}*}(0,\phi') = (\tfrac{3}{4}\pi)^{1/2}\delta_{m',\tilde{\beta}},$$
$$Y_1^{m'',\tilde{\beta}}(\theta'',\phi'') \sim Y_1^{m'',\tilde{\beta}}(0,\phi'') = (\tfrac{3}{4}\pi)^{1/2}\delta_{m'',\tilde{\beta}},$$
$$p' \sim \hbar K, \quad p'' \sim \hbar K, \tag{61}$$
$$G(k',k) \sim G(K,k), \quad G(k'',k) \sim G(K,k),$$
$$\gamma_-(k'-k) \sim \gamma_-(K-k).$$

Then, on using $\mathrm{Im}\gamma_-(x) = -\pi\delta(x)$

$$\frac{d}{dt}|h(\bar{p},\beta;t|^2 = \frac{3cA^2}{2p^2(\hbar K)^4}|G(K,k)|^2 \times|Y_1^{\tilde{\beta},\beta}(\theta,\phi)|^2\delta(K-k). \tag{62}$$

Finally, from Eq. (30) and the fact that $\delta(K-k) = \delta(p-K)$

$$w(\hat{\eta},\beta;t) = \int_0^\infty\frac{d}{dt}|h(\bar{p},\beta;t)|^2p^2dp$$
$$= \frac{3cA^2}{K^2 8\pi^2\hbar^3}\frac{[\gamma_1(K)]^2}{[K-\kappa-\delta(K)]^2+[\gamma(K)]^2}\times|Y_1^{\tilde{\beta},\beta}(\theta,\phi)|^2, \tag{63}$$

where θ,ϕ are, of courese, the polar angles of $\hat{\eta}$.

Now from Appendix D of Ref. 17

$$Y_1^{\beta,\beta}(\theta,\phi) = (3/16\pi)^{1/2}(1+\cos\theta),$$
$$Y^{\beta,-\beta}(\theta,\phi) = (3/16\pi)^{1/2}e^{2i\beta\phi}(1-\cos\theta),$$
$$\beta = \pm 1. \tag{64}$$

Now the cross section for the case that the circular polarization of the scattered photon is the same as that of the incident photon is given by

$$\sigma_1(\theta) = w(\hat{\eta},\beta;t)/S$$
$$= \frac{9}{4K^2}\frac{[\gamma_1(K)]^2}{[K-\kappa-\delta(K)]^2+[\gamma(K)]^2}\cos^4(\tfrac{1}{2}\theta). \tag{65}$$

Similarly, the cross section for the case that the circular polarization of the scattered photon is opposite to that of the incident photon is

$$\sigma_2(\theta)=w(\hat{\eta},-\beta;t)/S = \frac{9}{4K^2}\,\frac{[\gamma_1(K)]^2}{[K-\kappa-\delta(K)]^2+[\gamma(K)]^2}\sin^4(\tfrac{1}{2}\theta). \qquad (66)$$

The expressions Eqs. (4) and (6) are obtained from Eqs. (65) and (66), respectively, by replacing K in the functions K^2, $\delta(K)$, $\gamma(K)$, and $\gamma_1(K)$ by κ, and by using Eq. (51).

VII. CALCULATION OF THE SCATTERED ELECTROMAGNETIC FIELD

We shall now derive Eq. (14) for the scattered electromagnetic field. As before the wave function of the incident photon in the linear momentum, helicity representation will be denoted by the complex function $f(\vec{p},\beta)$. On using Eqs. (27), (28), (50), and (52), the wave function of the scattered photon in the linear momentum representation is

$$f_{sc}(\vec{p},\beta;t)=i\,\frac{\beta\gamma_1(k)}{k-\kappa-\delta(k)-i\gamma(k)}\,e^{-ickt}\sum_m\sum_{\beta'}\beta' Y_1^{m,\beta}(\theta,\phi)\int_0^{2\pi}d\phi'\int_0^{\pi}\sin\theta'\,Y_1^{m,\beta'*}(\theta',\phi')f(\vec{p}\,',\beta')d\theta', \qquad (67)$$

where θ,ϕ and θ',ϕ' are the polar angles of $\vec{p}$ and $\vec{p}\,'$, respectively, and $|\vec{p}|=|\vec{p}\,'|=p=\hbar k$.

The incident wave function will be taken as

$$f(\vec{p},\beta)=f(\vec{p}) \qquad (68)$$

and is independent of β. The function $f(\vec{p})$ is real and has a sharp peak at $\vec{p}\sim\vec{p}_0$, where $\vec{p}_0=\hbar K(0,0,1)$, as before. It is readily shown that the incident electromagnetic field is given by Eq. (13) where

$$C=\frac{2^{1/2}}{\pi\hbar^{3/2}}\int f(\vec{p})d\vec{p}. \qquad (69)$$

The proof is close to that for Eqs. (55) and (56).

The electromagnetic field of the scattered radiation is obtained by substituting $f_{sc}(\vec{p},\beta;t)$ for $g(\vec{p},\lambda)\exp[-(i/\hbar)cpt]$ in Eq. (24′). The scattered electromagnetic field can be written

$$\vec{E}(\vec{x},t)=\int\vec{E}(\vec{x},t;\hat{\eta})d\Omega,$$
$$\vec{H}(\vec{x},t)=\int\vec{H}(\vec{x},t;\hat{\eta})d\Omega, \qquad (70)$$

where in Eq. (24′) we have written $d\vec{p}=p^2dp\,d\Omega$, with $d\Omega=\sin\theta d\theta d\phi$ being the element of solid angle and $\hat{\eta}=\vec{p}/p$ as before. The vectors $\vec{E}(\vec{x},t;\hat{\eta})$ and $\vec{H}(\vec{x},t;\hat{\eta})$ are the components of the electrofield propagating in the direction $\hat{\eta}$. The quantities $\vec{E}(\vec{x},t;\hat{\eta})d\Omega$ and $\vec{H}(\vec{x},t;\hat{\eta})d\Omega$ are portions of the electromagnetic field which would be intercepted by an antenna of aperture $d\Omega$. In fact, $\vec{E}(\vec{x},t;\hat{\eta})$ and $\vec{H}(\vec{x},t;\hat{\eta})$ are $\vec{E}_{sc}(\vec{x},t)$ and $\vec{H}_{sc}(\vec{x},t)$ of Eq. (14). The evaluation of $\vec{E}(\vec{x},t;\hat{\eta})$ and $\vec{H}(\vec{x},t;\hat{\eta})$ involves an integration over the variable p. Because of the sharpness of $f(\vec{p})$ at $\vec{p}$ near $\vec{p}_0$, the following approximations are made:

$$e^{ik(\hat{\eta}\cdot\vec{x}-ct)}\sim e^{iK(\hat{\eta}\cdot\vec{x}-ct)}, \qquad (71)$$
$$\frac{\gamma_1}{k-\kappa-\delta(k)-i\gamma(k)}\sim\frac{\gamma_1(K)}{K-\kappa-\delta(K)-i\gamma(K)}\sim\frac{\gamma}{K-\kappa-\delta-i\gamma}=-[F(K)]^{1/2}e^{i\Phi(K)}.$$

In Eq. (71) we have used the fact that K is near κ. Eqs. (14a) and (51) have also been used.

The sharpness of $f(\vec{p})$ also permits the approximation given by the second of Eq. (61) where $\bar{\beta}$ is replaced by β'. Finally, one has

$$\vec{E}(\vec{x},t;\eta)=-(3/8\pi)^{1/2}C[F(K)]^{1/2}\,\mathrm{Re}\,e^{i[K(\hat{\eta}\cdot\vec{x}-ct+\Phi(K)}\times\sum_{\beta=\pm1}\sum_{\beta'=\pm1}\beta'\vec{Q}_\beta(\hat{\eta})Y_1^{\beta',\beta}(\theta,\phi). \qquad (72)$$

But by explicit calculation

$$\sum_{\beta=\pm1}\sum_{\beta'=\pm1}\beta'\vec{Q}_\beta(\hat{\eta})Y_1^{\beta',\beta}(\theta,\phi)=-(3/2\pi)^{1/2}[(\hat{i}_1\times\hat{\eta})\times\hat{\eta}]. \qquad (73)$$

The first of Eq. (14) then follows. The second of Eq. (14) is obtained in a similar fashion.

VIII. COMPLETENESS OF THE EIGENSTATES. HIGHER-ORDER PERTURBATION THEORY

By eliminating all but the two-level matrix elements of the interaction, we have constructed an approximate Hamiltonian H'. One can ask the question whether the eigenfunctions of Sec. IV are a complete set of eigenstates. That this set is complete can be proved by using the techniques of Ref. 4. When we have such a complete set, we may get a better approximation by considering the exact Hamiltonian H to be a sum of the approximate Hamiltonian H', whose eigenstates are known, and a perturbation consisting of the interaction which has been ignored so far. One can set up integral equations for the "outgoing" eigenfunctions of H in terms of the outgoing eigenfunctions of H'.[18] This integral equation can be solved, formally at least, in terms of a Born expansion about the outgoing eigenfunctions of H'. We believe that the expressions for these Born approximation terms will converge if the exact matrix elements of the electromagnetic interaction are used to prevent ultraviolet catastrophes. One of the principal causes of divergence in the usual Born expansion of the problem is that it is not recognized that H_0 has point eigenvalues embedded in the continuum which the interaction may cause to disappear. Even when one uses H', the Born expansion about H_0 would yield divergences. This matter is discussed in great detail for a simpler model.[4] Thus a more careful study of the nature of the changes of the spectrum is needed to prevent some of the divergences.

ACKNOWLEDGMENT

This research was sponsored by the Air Force Office of Scientific Research, Air Force Systems Command, United States Air Force, under Grant No. AFOSR-77-3169.

APPENDIX: EVALUATION OF THE INTEGRALS $I_i(x)$

We shall first give the integrals $I_i(x)$ and then sketch the derivation of $I_2(x)$ which is the most complicated of them, the derivation of $I_1(x)$ and $I_3(x)$ being a simpler version of that for $I_2(x)$. We need give only the real parts of $I_i(x)$, since the imaginary parts are given in Eq. (44):

$$\mathrm{Re}I_1(x) = -(\tfrac{2}{3})^8\left[\frac{5\pi}{32} - y\left(\frac{\pi y}{2}\sum_{q=1}^{4}\frac{(2q-2)!}{2^{2(q-1)}[(q-1)!]^2}\frac{1}{(1+y^2)^{5-q}} + \tfrac{1}{2}\sum_{q=2}^{4}\frac{1}{q-1}\frac{1}{(1+y^2)^{5-q}} + \frac{1}{(1+y^2)^4}\log|y|\right)\right],$$

where $y=(2x/3)$, (A1)

$$\mathrm{Re}I_2(x) = -\frac{1}{12}\left[\frac{3\pi}{512} - x\left(\frac{\pi x}{2}\sum_{q=1}\frac{(2q-2)!}{2^{2(q-1)}[(q-1)!]^2}\frac{1}{(1+x^2)^{5-q}} - \pi x\sum_{q=1}^{5}\frac{(2q-2)!}{2^{2(q-1)}[(q-1)!]^2}\frac{1}{(1+x^2)^{6-q}}\right.\right.$$
$$+\frac{\pi x}{2}\sum_{q=1}^{6}\frac{(2q-2)!}{2^{2(q-1)}[(q-1)]^2}\frac{1}{(1+x^2)^{7-q}} + \tfrac{1}{2}\sum_{q=2}^{4}\frac{1}{q-1}\frac{1}{(1+x^2)^{5-q}} - \sum_{q=2}^{5}\frac{1}{q-1}\frac{1}{(1+x^2)^{6-q}}$$
$$\left.\left.+\tfrac{1}{2}\sum_{q=2}^{6}\frac{1}{q-1}\frac{1}{(1+x^2)^{7-q}} + \frac{x^4}{(1+x^2)^6}\log|x|\right)\right], \qquad \text{(A2)}$$

$$\mathrm{Re}I_3(x) = -\frac{1}{2}\left[\frac{7\pi}{512} - x\left(\frac{\pi x}{2}\sum_{q=1}^{5}\frac{(2q-2)!}{2^{2(q-1)}[(q-1)!]^2}\frac{1}{(1+x^2)^{6-q}} - \frac{\pi x}{2}\sum_{q=1}^{6}\frac{(2q-2)!}{2^{2(q-1)}[(q-1)!]^2}\frac{1}{(1+x^2)^{7-q}}\right.\right.$$
$$\left.\left.+\tfrac{1}{2}\sum_{q=2}^{5} q-1\,\frac{1}{(1+x^2)^{6-q}} - \tfrac{1}{2}\sum_{q=2}^{6}\frac{1}{q-1}\frac{1}{(1+x^2)^{7-q}} + \frac{x^2}{(1+x^2)^6}\log|x|\right)\right]. \qquad \text{(A3)}$$

It should be noted that only the first terms on the right of Eqs. (A2) and (A3) contribute to δ, since $x=0$ in the computation.

To derive the expressions for $I_i(x)$ the following integrals are used:

$$\int_0^\infty \frac{d\xi}{(1+\xi^2)^q} = \frac{\pi}{2}\frac{(2q-2)!}{2^{2(q-1)}[(q-1)!]^2}, \qquad \text{(A4)}$$

$$\int_0^\infty \frac{d\xi}{(1+\xi^2)^p(\xi-z)} = -z\sum_{q=1}^{p}\int_0^\infty\frac{d\xi}{(1+\xi^2)^q} - \tfrac{1}{2}\sum_{q=2}^{p}\frac{1}{q-1}\frac{1}{(1+z^2)^{p-q+1}} - \frac{1}{(1+z^2)^p}\log(-z), \qquad \text{(A5)}$$

where z is a complex number.

Now, from Eq. (41)

$$I_2(x) = -\frac{1}{12}\int_0^\infty \frac{\xi^5 d\xi}{(1+\xi^2)^6(\xi-z)}, \qquad \text{(A6)}$$

where $z=x+i\epsilon$. After evaluating the integral we take $\epsilon\to 0$. But

$$\frac{\xi^5}{\xi-z}=(1+\xi^2)^2-2(1+\xi^2)+1+z\,\frac{(1+\xi^2)^2}{\xi-z}-2z\,\frac{(1+\xi^2)}{\xi-z}+z\,\frac{1}{\xi-z}\,. \tag{A7}$$

On substituting Eq. (A7) into (A6) we have integrals of the form (A4) and (A5), which give us our answer.

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