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Compton Scattering by *K*-Shell Electrons. I. Nonrelativistic Theory with Retardation

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An exact analytic calculation is presented for the cross section of the nonrelativistic Compton-type inelastic scattering of photons by electrons bound in the ground state of a hydrogen-like atom. The matrix element of the process was taken to be of the Kramers-Heisenberg-Waller form. It was integrated by the Coulomb-Green's-function method, developed previously by the author in connection with Rayleigh scattering. This is based on replacing the sum over intermediate states by the Green's function which is expressed in terms of the integral representation in momentum space given by Schwinger. The final continuum-state wave function was also described by an integral representation. Thus the evaluation of the matrix element requires the carrying out of momentum-space integrations, followed by two contour integrations. Its final form was expressed in terms of hypergeometric functions of four variables of Lauricella's type F_D . At small photon energies, where the dipole approximation is valid, the result simplifies considerably. The low-energy end of the scattered-photon spectrum is considered in detail in connection with the infrared divergence problem. The shape of the spectrum is discussed and a comparison with previous results is given.

I. INTRODUCTION

When a photon undergoes inelastic scattering by an atomic system, the latter may be excited or ionized. In the case of inelastic scattering accompanied by excitation, which we shall call Raman scattering, the final energy of the photon is diminished by a discrete amount determined by energy conservation. In the central-field model of the atom the process is due to the transition of an electron from its initial state to one of the unoccupied discrete states.

The process of inelastic scattering accompanied by ionization can be considered to be a Compton scattering. Whereas in the conventional case the electron is taken to be free, in the present case it is initially bound in the atom and then ejected into the continuum by the impact of the photon.¹ If the atomic nucleus is considered to be fixed, only energy is conserved in the process but not momentum. Consequently there is no longer a connection between the directions of the momenta of the final photon and of the ejected electron. Also, for every scattering angle the energy of the final photon varies continuously from zero to a maximum value

determined by the conservation of energy, in contrast to the sharp value it has when the electron is considered to be initially free. In the case of an isolated atom, on the high-energy side of the edge of the continuous spectrum, the discrete lines of the Raman transitions are expected to appear.¹

The differential cross section for Compton scattering by a bound electron may be written²

$$d^3\sigma = r_0^2 (\kappa_2/\kappa_1) |\mathfrak{M}|^2 d\kappa_2 d\Omega_2 d\Omega, \quad (1)$$

where $r_0 = e^2/m$ and \mathfrak{M} is the matrix element of the process. In the nonrelativistic case including retardation \mathfrak{M} is of the Kramers-Heisenberg-Waller type, given by³

$$\begin{aligned} \mathfrak{M} = & (\vec{s}_1 \cdot \vec{s}_2) (e^{i(\vec{\kappa}_1 - \vec{\kappa}_2) \cdot \vec{r}})_{c_0} \\ & - \frac{1}{m} \sum_n \frac{[e^{-i\vec{\kappa}_2 \cdot \vec{r}} (\vec{s}_2 \cdot \vec{P})]_{cn} [e^{i\vec{\kappa}_1 \cdot \vec{r}} (\vec{s}_1 \cdot \vec{P})]_{n0}}{E_n - (E_0 + \kappa_1 + i\epsilon)} \\ & - \frac{1}{m} \sum_n \frac{[e^{i\vec{\kappa}_1 \cdot \vec{r}} (\vec{s}_1 \cdot \vec{P})]_{cn} [e^{-i\vec{\kappa}_2 \cdot \vec{r}} (\vec{s}_2 \cdot \vec{P})]_{n0}}{E_n - (E_0 - \kappa_2)}. \end{aligned} \quad (2)$$

We denote by $\vec{\kappa}_1$ and $\vec{\kappa}_2$ the momenta of the initial and final photons, \vec{s}_1 and \vec{s}_2 their respective polarizations, \vec{p} the asymptotic momentum of the

ejected electron; \vec{p} and $\vec{\kappa}_2$ point in $d\Omega$ and $d\Omega_2$, respectively. \vec{P} is the momentum operator. Subscript 0 denotes the initial atomic state (energy E_0) and subscript c denotes its final ionized state (energy E_c). The infinitesimal positive quantity ϵ appearing in the denominator of the first sum prevents the occurrence of a singularity when integrating over the continuum. Energy conservation requires that

$$E_0 + \kappa_1 = E_c + \kappa_2. \quad (3)$$

The expression of \mathfrak{M} in Eq. (2) refers to the case of a hydrogenlike atom. The extension of Eq. (2) to a many-electron atom is straightforward. However, in the approximation of the central self-consistent-field model, when the scattering process involves a one-electron transition, the matrix element is again given by Eq. (2).⁴

The matrix element \mathfrak{M} can be derived in the framework of nonrelativistic quantum mechanics by considering the interaction of the atom with the radiation field as a perturbation. In order to describe the desired transition to lowest order, a first-order calculation has to be carried out for the \vec{A}^2 term of the interaction Hamiltonian, whereas the $\vec{A} \cdot \vec{P}$ term has to be treated to second order. The contribution of \vec{A}^2 is given by the first term of Eq. (2), the sums over intermediate states representing the contribution of the $\vec{A} \cdot \vec{P}$ term.

One can also derive the one-electron-atom result of Eq. (2) by starting from the exact relativistic matrix element for a bound electron. By appropriately taking the nonrelativistic limit and ignoring spin effects one ends up with Eq. (2).^{5,6}

All nonrelativistic treatments of Compton scattering by bound electrons which have been given so far are based on the \vec{A}^2 approximation of the matrix element \mathfrak{M} , that is

$$\mathfrak{M} \simeq (\vec{s}_1 \cdot \vec{s}_2) (e^{i(\vec{\kappa}_1 - \vec{\kappa}_2) \cdot \vec{r}})_{c0}. \quad (4)$$

Indeed, it was recognized that for $\kappa_1 \gg |E_0|$ the contribution of the $\vec{A} \cdot \vec{P}$ term to the matrix element is small in comparison to that of \vec{A}^2 .⁷ This circumstance concurred happily with the fact that the sums over intermediate states were difficult to handle. However, at low energies the situation is reversed, since the \vec{A}^2 approximation of Eq. (4) vanishes in the dipole approximation ($|\vec{\kappa}_1 - \vec{\kappa}_2| / \alpha Z m \ll 1$), whereas the $\vec{A} \cdot \vec{P}$ contribution does not.

For reasons of simplicity the first case to be considered was that of a hydrogenlike atom. It was Wentzel⁸ who first approached the problem and derived some general results starting from Eq. (4), but eventually considered only the case when $(\alpha Z m / p) \ll 1$. Schnaidt⁹ and Bloch¹⁰ gave exact evaluations of Eq. (4) and analyzed their consequences from various points of view. It was then shown that the effect of the binding of the initial

electron is that of broadening the Compton line for a free electron and of shifting its maximum towards smaller wavelengths.

By ingenious semiclassical arguments DuMond derived a formula for the spectral distribution of the Compton line, relating it to the momentum distribution of the electron in the bound state.^{11,12} His result was rederived and refined in the framework of quantum mechanics by Eisenberger and Platzman,¹³ by starting from Eq. (4) and applying the impulse approximation.

Considerable attention has been given to the probability of the inelastic scattering of the photon into an elementary solid angle $d\Omega_2$, regardless of what happens to the electron involved. If one does not distinguish between inelastic scattering with excitation or ionization, both Raman and Compton scattering will contribute to the cross section $d\sigma/d\Omega_2$. Starting from Eq. (4) and making some more approximations, which are plausible at nonrelativistic energies, the result for $d\sigma/d\Omega_2$ can be expressed simply, in terms of the "incoherent-scattering function."¹⁴

The experiments done in the range of validity of the nonrelativistic theory have been carried out with x rays and light elements. The efforts have been concentrated mainly in two directions. One of them was of studying the detailed profile of the Compton line and its relation to the electronic momentum distribution of the scatterer. Such studies were persistently followed in the thirties by DuMond, Kirkpatrick, and Ross.¹ However, it is only the global electronic structure of the scatterer which was revealed by these experiments, as one could not distinguish the contributions to the Compton line of the individual atomic shells. These studies were resumed in recent years with high accuracy.¹⁵

The other experimental direction pursued was of trying to isolate the contribution of the K-shell electrons by using favorable experimental setups. For the light elements considered ($Z \leq 6$), the $n = 2$ atomic electrons are valence electrons and quasifree in the polycrystal. They will yield a rather sharp Compton line which, for sufficiently small scattering angles, will lie almost entirely in the interval between κ_1 and $\kappa_1 - E_K$ (E_K is the binding energy of the K shell). Besides, the situation was such that $(\vec{\kappa}_1 - \vec{\kappa}_2)^2 \lesssim (\alpha Z m)^2$ and in this case one can show on the basis of Eq. (4) that the K-shell spectral distribution has a maximum at its high-energy edge $\kappa_1 - E_K$.¹⁶ This maximum will appear as a secondary peak in the global Compton profile. The existence of such a peak has been reported and investigated by several authors.¹⁷

At high photon energies (κ_1 comparable to m) and for high- Z atoms a relativistic calculation is necessary. The complexity of the problem is con-

siderably higher than in the nonrelativistic case. Therefore rather uncertain approximations have been developed for the relativistic matrix element⁵ (free intermediate and final electronic states, the "form-factor" approximation, the "incoherent-scattering-function" approximation). However, Whittingham¹⁸ has recently carried out an exact computation for the case of a purely Coulomb atomic field.

In this work we shall give an exact analytic evaluation of the nonrelativistic Kramers-Heisenberg-Waller matrix element of Eq. (2) for the Compton scattering by an electron bound initially in the ground state of a hydrogenlike atom.¹⁹ In fact our problem is that of evaluating the sums over intermediate states. To this end we shall follow a method used in previous works on the elastic scattering of photons by atomic hydrogen.^{20,21} It consists in expressing the sums over intermediate states in terms of momentum-space integrals involving the Green's function for the Coulomb field and of using for the latter the integral representation of Schwinger.²² An integral representation is used also for the final, continuum wave function of the electron. Hence, \mathfrak{M} contains terms involving momentum-space integrals followed by two contour integrals. All but one of these integrals can be carried out explicitly. The remaining one is a contour integral which can be expressed in terms of generalized hypergeometric functions of the Lauricella type F_D . Therefore, the matrix element \mathfrak{M} appears as a linear combination of such functions. A discussion of the result is given. It is shown that for vanishing energy of the final photon an infrared divergence occurs. This is considered in connection with the problem of photon attenuation. It is also shown that in the dipole approximation the analytic results simplify considerably. In a subsequent paper we present a detailed description of the dipole approximation together with its numerical computation.²³

II. MATRIX ELEMENT

We shall first rewrite the Kramers-Heisenberg-Waller matrix element in an alternative form involving the Green's function for the atomic field considered. The Green's function can be characterized by its eigenfunction expansion

$$G(\vec{r}_2, \vec{r}_1; \Omega) = \sum_n \frac{u_n(\vec{r}_2) u_n^*(\vec{r}_1)}{E_n - \Omega}. \quad (5)$$

It is an analytic function of Ω , except for points E_n belonging to the spectrum of the Hamiltonian.

Taking into account Eq. (5), \mathfrak{M} can be written

$$\mathfrak{M} = (\vec{s}_1 \cdot \vec{s}_2) \mathcal{O} - \sum_{i,j} s_{1i} s_{2j} [\Pi_{ij}(\Omega_1) + \tilde{\Pi}_{ij}(\Omega_2)], \quad (6)$$

where

$$\mathcal{O} = \int u_c^*(\vec{r}) u_0(\vec{r}) e^{i(\vec{\kappa}_1 - \vec{\kappa}_2) \cdot \vec{r}} d\vec{r}, \quad (7)$$

$$\begin{aligned} \Pi_{ij}(\Omega) = \frac{1}{m} \iint u_c^*(\vec{r}_2) e^{-i\vec{\kappa}_2 \cdot \vec{r}_2} P_{2j} G(\vec{r}_2, \vec{r}_1; \Omega) \\ \times P_{1i} e^{i\vec{\kappa}_1 \cdot \vec{r}_1} u_0(\vec{r}_1) d\vec{r}_1 d\vec{r}_2, \end{aligned} \quad (8)$$

and $\tilde{\Pi}_{ij}(\Omega)$ is obtained from $\Pi_{ij}(\Omega)$ by interchanging i with j and $\vec{\kappa}_1$ with $-\vec{\kappa}_2$. The quantities Ω_1 and Ω_2 are given by

$$\Omega_1 = E_0 + \kappa_1 + i\epsilon = -|E_0| + \kappa_1 + i\epsilon, \quad (9)$$

$$\Omega_2 = E_0 - \kappa_2 = -|E_0| - \kappa_2.$$

In the following we shall work in momentum space. Taking the Fourier transforms of the quantities involved, \mathcal{O} and Π_{ij} become

$$\mathcal{O} = \int u_c^*(\vec{p} - \vec{\kappa}_2) u_0(\vec{p} - \vec{\kappa}_1) d\vec{p}, \quad (10)$$

$$\begin{aligned} \Pi_{ij}(\Omega) = \frac{1}{m} \iint p_{1i} p_{2j} u_c^*(\vec{p}_2 - \vec{\kappa}_2) G(\vec{p}_2, \vec{p}_1; \Omega) \\ \times u_0(\vec{p}_1 - \vec{\kappa}_1) d\vec{p}_1 d\vec{p}_2. \end{aligned} \quad (11)$$

Let us denote by $\vec{\nu}_1$, $\vec{\nu}_2$, \vec{n} the unit vectors of $\vec{\kappa}_1$, $\vec{\kappa}_2$, \vec{p} , respectively. Rotational invariance arguments indicate that one can write

$$\begin{aligned} \sum_{i,j} s_{1i} s_{2j} \Pi_{ij}(\Omega) = (\vec{s}_1 \cdot \vec{s}_2) \mathcal{O}(\Omega) + (\vec{s}_1 \cdot \vec{\nu}_2)(\vec{s}_2 \cdot \vec{\nu}_1) \mathcal{Q}(\Omega) \\ + (\vec{s}_1 \cdot \vec{n})(\vec{s}_2 \cdot \vec{\nu}_1) \mathcal{R}(\Omega) + (\vec{s}_1 \cdot \vec{\nu}_2)(\vec{s}_2 \cdot \vec{n}) \mathcal{S}(\Omega) \\ + (\vec{s}_1 \cdot \vec{n})(\vec{s}_2 \cdot \vec{n}) \mathcal{T}(\Omega), \end{aligned} \quad (12)$$

where \mathcal{O} , \mathcal{Q} , \mathcal{R} , \mathcal{S} , \mathcal{T} are functions of Ω and of scalars constructed from $\vec{\kappa}_1$, $\vec{\kappa}_2$, \vec{p} . Applying the prescription given above for obtaining $\tilde{\Pi}_{ij}$, one gets

$$\begin{aligned} \sum_{i,j} s_{1i} s_{2j} \tilde{\Pi}_{ij}(\Omega) = (\vec{s}_1 \cdot \vec{s}_2) \tilde{\mathcal{O}}(\Omega) + (\vec{s}_2 \cdot \vec{\nu}_1)(\vec{s}_1 \cdot \vec{\nu}_2) \tilde{\mathcal{Q}}(\Omega) \\ - (\vec{s}_2 \cdot \vec{n})(\vec{s}_1 \cdot \vec{\nu}_2) \tilde{\mathcal{R}}(\Omega) - (\vec{s}_2 \cdot \vec{\nu}_1)(\vec{s}_1 \cdot \vec{n}) \tilde{\mathcal{S}}(\Omega) \\ + (\vec{s}_1 \cdot \vec{n})(\vec{s}_2 \cdot \vec{n}) \tilde{\mathcal{T}}(\Omega), \end{aligned} \quad (13)$$

The quantities $\tilde{\mathcal{O}}$, $\tilde{\mathcal{Q}}$, etc., are obtained from \mathcal{O} , \mathcal{Q} , etc., by changing $\vec{\kappa}_1$ into $-\vec{\kappa}_2$ and $\vec{\kappa}_2$ into $-\vec{\kappa}_1$.

The matrix element \mathfrak{M} can therefore be written

$$\begin{aligned} \mathfrak{M} = \mathcal{A}(\vec{s}_1 \cdot \vec{s}_2) + \mathcal{B}(\vec{s}_1 \cdot \vec{\nu}_2)(\vec{s}_2 \cdot \vec{\nu}_1) + \mathcal{C}(\vec{s}_1 \cdot \vec{n})(\vec{s}_2 \cdot \vec{\nu}_1) \\ + \mathcal{D}(\vec{s}_1 \cdot \vec{\nu}_2)(\vec{s}_2 \cdot \vec{n}) + \mathcal{E}(\vec{s}_1 \cdot \vec{n})(\vec{s}_2 \cdot \vec{n}). \end{aligned} \quad (14)$$

The five scattering amplitudes occurring here have the following expressions:

$$\begin{aligned} \mathcal{A} &= \mathcal{O} - \mathcal{O}(\Omega_1) - \tilde{\mathcal{O}}(\Omega_2), \\ \mathcal{B} &= -[\mathcal{Q}(\Omega_1) + \tilde{\mathcal{Q}}(\Omega_2)], \quad \mathcal{C} = -\mathcal{R}(\Omega_1) + \tilde{\mathcal{S}}(\Omega_2), \\ \mathcal{D} &= -\mathcal{S}(\Omega_1) + \tilde{\mathcal{R}}(\Omega_2), \quad \mathcal{E} = -[\mathcal{T}(\Omega_1) + \tilde{\mathcal{T}}(\Omega_2)]. \end{aligned} \quad (15)$$

From now on we shall specialize to the case of a Coulomb atomic field. The ground-state energy eigenfunction is

$$u_0(p) = (8\lambda^5/\pi^2)^{1/2} (p^2 + \lambda^2)^{-2}, \quad (16)$$

where $\lambda = \alpha Zm$. The final, continuum-state eigenfunction should have the asymptotic behavior of a (distorted) plane wave plus an incoming spherical wave, like in the case of the photoeffect. The expressions of the cross section Eq. (1) and of the matrix element Eq. (2) have been written assuming that it is normalized per energy interval and element of solid angle. Although it can be expressed in closed form, it is convenient to use the following integral representation:

$$G(\vec{p}_2, \vec{p}_1; \Omega) = \frac{m}{2\pi^2} X^3 \left(\frac{ie^{i\pi\tau}}{2 \sin\pi\tau} \right) \int_1^{(0+)} \rho^{-\tau} \frac{d}{d\rho} \left(\frac{1-\rho^2}{\rho} \frac{1}{[X^2(\vec{p}_1 - \vec{p}_2)^2 + (p_1^2 + X^2)(p_2^2 + X^2)(1-\rho)^2/4\rho]^2} \right) d\rho, \quad (18)$$

where

$$\tau = \lambda/X, \quad X^2 = -2m\Omega, \quad (19)$$

and X is chosen so that

$$\text{Re}X > 0. \quad (20)$$

The contour integration in Eq. (18) starts at $\rho = 1$ (where one should take $\rho^{-\tau} = 1$), encircles the origin $\rho = 0$ in the counter-clockwise sense and returns to 1. The form of $G(\vec{p}_2, \vec{p}_1; \Omega)$ given in Eq. (18) is valid for any Ω .

The parameters of the problem are related by the energy-conservation equation (3). Since we are dealing with a purely Coulomb field, $E_0 = -\lambda^2/2m$, and

$$p^2 + \lambda^2 = 2m(\kappa_1 - \kappa_2). \quad (21)$$

$G(\vec{p}_2, \vec{p}_1; \Omega)$ appears in $\Pi_{ij}(\Omega_1)$, $\bar{\Pi}_{ij}(\Omega_2)$ with values of Ω given by Eq. (9). Taking into account Eqs. (19) and (20) one finds for the corresponding values of X

$$u_c^{(-)}(\vec{p}_2) = -\frac{4pe^{(\pi/2)|n|}\Gamma(1+i|n|)}{(2\pi)^3} (pm)^{1/2} \times \oint \left(\frac{\xi-1}{\xi} \right)^n \frac{1}{\{(\vec{p}_2 - \vec{p}\xi)^2 + [\epsilon + ip(1-\xi)]^2\}^2} d\xi, \quad (17)$$

where \vec{p} is the asymptotic momentum, \vec{p}_2 is the momentum-space variable, $n = \lambda/ip$, and ϵ is an infinitesimal positive quantity. The principal value of the power n occurring in the integrand should be taken ($-\pi < \arg \xi/(\xi-1) < \pi$). The contour of integration is a closed loop encircling in the counter-clockwise sense the branch points $\xi = 0$ and $\xi = 1$ but leaving out the pole of the integrand.

For the Coulomb Green's function $G(\vec{p}_2, \vec{p}_1; \Omega)$ we use the integral representation derived by Schwinger²²:

$$X_1 = -i(2m\kappa_1 - \lambda^2)^{1/2}, \quad X_2 = (2m\kappa_2 + \lambda^2)^{1/2}. \quad (22)$$

III. CALCULATION OF SCATTERING AMPLITUDES

As discussed in the Introduction in connection with Eq. (4), the integral Θ of Eqs. (7) and (10) was evaluated exactly a long time ago.⁹ By inserting Eqs. (16) and (17) into (10) one finds

$$\Theta = \frac{1}{8}N[(\vec{\kappa}_1 - \vec{\kappa}_2)^2 + (n-1)\vec{p} \cdot (\vec{\kappa}_1 - \vec{\kappa}_2)] \times [(\vec{\kappa}_1 - \vec{\kappa}_2)^2 + (\lambda - ip)^2]^{n-1} [(\vec{\kappa}_1 - \vec{\kappa}_2 - \vec{p})^2 + \lambda^2]^{-n-2}, \quad (23)$$

where

$$N = (32/\pi)(2\lambda^5 pm)^{1/2} e^{(\pi/2)|n|} \Gamma(1-i|n|). \quad (24)$$

Our problem is that of evaluating the sums over intermediate states, which have been expressed in Eq. (6) in terms of Π_{ij} of Eq. (11). Introducing Eqs. (16)–(18) into Eq. (11) and interchanging the order of integrations, one finds

$$\Pi_{ij}(\Omega) = \frac{NpX^3}{64\pi^5} \left(\frac{ie^{i\pi\tau}}{2 \sin\pi\tau} \right) \int_1^{(0+)} d\rho \rho^{-\tau} \oint d\xi \left(\frac{\xi}{\xi-1} \right)^n \frac{d}{d\rho} \left(\frac{1-\rho^2}{\rho} T_{ij} \right), \quad (25)$$

where

$$T_{ij} = \iint \frac{p_{1i} p_{2j}}{[(\vec{p}_2 - \vec{\kappa}'_2)^2 + \mu^2]^2 [X^2(\vec{p}_1 - \vec{p}_2)^2 + \alpha(p_1^2 + X^2)(p_2^2 + X^2)]^2 [(\vec{p}_1 - \vec{\kappa}_1)^2 + \lambda^2]^2} d\vec{p}_1 d\vec{p}_2. \quad (26)$$

We have abbreviated

$$\alpha = (1-\rho)^2/4\rho, \quad (27)$$

$$\vec{\kappa}'_2 = \vec{\kappa}_2 + \vec{p}\xi, \quad \mu = \epsilon - ip(1-\xi). \quad (28)$$

The integration contour in the ξ plane can be de-

formed so that it lies very close to the real axis and hence, for any fixed ϵ , one can satisfy the condition

$$\text{Re } \mu > 0. \tag{29}$$

The momentum-space integral Eq. (26) can be expressed in terms of the following one:

$$J(X^2; \lambda, \mu) = \iint \frac{1}{[(\vec{p}_2 - \vec{\kappa}_2)^2 + \mu^2][X^2(\vec{p}_1 - \vec{p}_2)^2 + \alpha(\rho_1^2 + X^2)(\rho_2^2 + X^2)]^2[(\vec{p}_1 - \vec{\kappa}_1)^2 + \lambda^2]} d\vec{p}_1 d\vec{p}_2. \tag{30}$$

Indeed, denoting by $J'(X^2; \lambda, \mu)$ its value when $\vec{\kappa}_2$ is replaced by $\vec{\kappa}'_2$ of Eq. (28), one can easily establish the equality

$$\sum_{i,j} s_{1i} s_{2j} T_{ij} = \frac{1}{4} \sum_{i,j} s_{1i} s_{2j} \frac{\partial^2 J'}{\partial \kappa_{1i} \partial \kappa'_{2j}} - \frac{\zeta}{4\mu} (\vec{s}_2 \cdot \vec{p}) \sum_i s_{1i} \frac{\partial^2 J'}{\partial \kappa_{1i} \partial \mu}. \tag{31}$$

Use has been made here of the fact that $\vec{\kappa}_1 \cdot \vec{s}_1 = \vec{\kappa}_2 \cdot \vec{s}_2 = 0$.

Combining Eqs. (25) and (31) we may write

$$\begin{aligned} \sum_{i,j} s_{1i} s_{2j} \Pi_{ij}(\Omega) &= \frac{N\beta X^3}{256\pi^5} \left(\frac{ie^{i\pi\tau}}{2 \sin\pi\tau} \right) \int_1^{(0+)} d\rho \rho^{-\tau} \oint d\zeta \left(\frac{\zeta}{\zeta-1} \right)^n \\ &\times \left[\sum_{i,j} s_{1i} s_{2j} \frac{\partial^2}{\partial \kappa_{1i} \partial \kappa'_{2j}} \frac{d}{d\rho} \left(\frac{1-\rho^2}{\rho} J' \right) - \frac{\zeta}{\mu} (\vec{s}_2 \cdot \vec{p}) \sum_i s_{1i} \frac{\partial^2}{\partial \kappa_{1i} \partial \mu} \frac{d}{d\rho} \left(\frac{1-\rho^2}{\rho} J' \right) \right]. \end{aligned} \tag{32}$$

The integral $J(X^2; \lambda, \mu)$ was encountered and calculated in a previous work.²⁴ We have given there [Ref. 21(a), Eq. (23)] also an expression for the derivative

$$\frac{d}{d\rho} \left(\frac{1-\rho^2}{\rho} J(X^2; \lambda, \mu) \right).$$

This can be written in the following form:

$$\frac{d}{d\rho} \left(\frac{1-\rho^2}{\rho} J(X^2; \lambda, \mu) \right) = \frac{16\pi^4}{X^2} \frac{1}{c}, \tag{33}$$

where

$$\begin{aligned} c &= [(X+\lambda)^2 + \kappa_1^2][(X+\mu)^2 + \kappa_2^2] \\ &- 2\rho[4(\vec{\kappa}_1 \cdot \vec{\kappa}_2)X^2 + (\lambda^2 + \kappa_1^2 - X^2)(\mu^2 + \kappa_2^2 - X^2)] \\ &+ \rho^2[(X-\lambda)^2 + \kappa_1^2][(X-\mu)^2 + \kappa_2^2]. \end{aligned} \tag{34}$$

From these equations it follows that

$$\begin{aligned} \sum_{i,j} s_{1i} s_{2j} \frac{\partial^2}{\partial \kappa_{1i} \partial \kappa'_{2j}} \frac{d}{d\rho} \left(\frac{1-\rho^2}{\rho} J' \right) &= 128\pi^4 \left((\vec{s}_1 \cdot \vec{s}_2) \rho(c')^{-2} + 16(\vec{s}_1 \cdot \vec{\kappa}'_2)(\vec{s}_2 \cdot \vec{\kappa}_1) X^2 \rho^2(c')^{-3} \right. \\ &\left. - 4(\vec{s}_1 \cdot \vec{\kappa}'_2)(\vec{s}_2 \cdot \vec{\kappa}'_2) \rho(c')^{-3} \{ \rho^2[(X-\lambda)^2 + \kappa_1^2] - 2\rho(\kappa_1^2 + \lambda^2 - X^2) + [(X+\lambda)^2 + \kappa_1^2] \} \right), \end{aligned} \tag{35}$$

$$\begin{aligned} \sum_i s_{1i} \frac{\partial^2}{\partial \kappa_{1i} \partial \mu} \frac{d}{d\rho} \left(\frac{1-\rho^2}{\rho} J' \right) &= 512\pi^4 (\vec{s}_1 \cdot \vec{\kappa}'_2) \rho(c')^{-3} \left(X \{ \rho^2[(X-\lambda)^2 + \kappa_1^2] - [(X+\lambda)^2 + \kappa_1^2] \} \right. \\ &\left. - \mu \{ \rho^2[(X-\lambda)^2 + \kappa_1^2] - 2\rho(\lambda^2 + \kappa_1^2 - X^2) + [(X+\lambda)^2 + \kappa_1^2] \} \right), \end{aligned} \tag{36}$$

where c' is obtained from c by replacing $\vec{\kappa}_2$ with $\vec{\kappa}'_2$. In deriving Eqs. (35) and (36) we have used the equality $\vec{\kappa}_1 \cdot \vec{s}_1 = 0$.

We have thus obtained the derivatives needed in Eq. (32). If one takes into account also the definition Eq. (28) of $\vec{\kappa}'_2$ and μ , Eq. (32) becomes

$$\begin{aligned} \sum_{i,j} s_{1i} s_{2j} \Pi_{ij}(\Omega) &= \frac{N\beta X^3}{2\pi} \left(\frac{ie^{i\pi\tau}}{2 \sin\pi\tau} \right) \int_1^{(0+)} d\rho \rho^{-\tau} \oint d\zeta \left(\frac{\zeta}{\zeta-1} \right)^n \\ &\times \left\{ (\vec{s}_1 \cdot \vec{s}_2) \rho(c')^{-2} + 16X^2 [(\vec{s}_1 \cdot \vec{\kappa}'_2) + \zeta(\vec{s}_1 \cdot \vec{p})] (\vec{s}_2 \cdot \vec{\kappa}_1) \rho^2(c')^{-3} \right. \end{aligned}$$

$$-\frac{4X\xi}{ip(\xi-1)} \left\{ (\vec{s}_1 \cdot \vec{\kappa}_2 + \xi(\vec{s}_1 \cdot \vec{p})) (\vec{s}_2 \cdot \vec{p}) \left\{ \rho^2[(X-\lambda)^2 + \kappa_1^2] - [(X+\lambda)^2 + \kappa_1^2] \right\} \rho(c')^{-3} \right\}, \quad (37)$$

and c' can be written

$$c' = \beta + \gamma\xi, \quad (38)$$

$$\begin{aligned} \beta = & [(X+\lambda)^2 + \kappa_1^2] [(X-ip)^2 + \kappa_2^2] \\ & - 2\rho[4(\vec{\kappa}_1 \cdot \vec{\kappa}_2)X^2 + (\lambda^2 + \kappa_1^2 - X^2)(\kappa_2^2 - p^2 - X^2)] \\ & + \rho^2[(X-\lambda)^2 + \kappa_1^2] [(X+ip)^2 + \kappa_2^2], \quad (39) \end{aligned}$$

$$\begin{aligned} \gamma = & 2 \left\{ [(X+\lambda)^2 + \kappa_1^2] [(\vec{p} \cdot \vec{\kappa}_2) + p^2 + ipX] \right. \\ & - 2\rho[2(\vec{\kappa}_1 \cdot \vec{p})X^2 + (\lambda^2 + \kappa_1^2 - X^2)[(\vec{p} \cdot \vec{\kappa}_2) + p^2]] \\ & \left. + \rho^2[(X-\lambda)^2 + \kappa_1^2] [(\vec{p} \cdot \vec{\kappa}_2) + p^2 - ipX] \right\}. \quad (40) \end{aligned}$$

In Eqs. (37)–(40) we have ignored the ϵ contained

in the definition of μ because, from now on, this will give rise to no difficulties.

So far we have dealt with the momentum-space integrals. We next turn to the integral over ξ .

This is a closed-contour integral and it can be evaluated by the residue theorem. Indeed, it is a sum of terms of the following form:

$$\oint \xi^{n+p} (\xi-1)^{-n-q} (\beta+\gamma\xi)^{-r} d\xi,$$

where $p=0, 1, 2$; $q=0, 1$; and $r=2, 3$. In the domain situated outside the integration contour and extending to infinity, the integrand is analytic except for a pole at $\xi = -\beta/\gamma$, and vanishes at least as fast as $1/\xi^2$ for $|\xi| \rightarrow \infty$. The residue theorem can therefore be applied and leads to

$$\begin{aligned} \sum_{i,j} s_{1i} s_{2j} \Pi_{ij}(\Omega) = & \frac{1}{2} i N p X^3 \left(\frac{i e^{i\pi\tau}}{2 \sin\pi\tau} \right) \int_1^{(0+)} \rho^{-\tau} \left((\vec{s}_1 \cdot \vec{s}_2) 2\rho n \beta^{n-1} (\beta+\gamma)^{-n-1} \right. \\ & + (\vec{s}_1 \cdot \vec{\kappa}_2)(\vec{s}_2 \cdot \vec{\kappa}_1) 16X^2 \rho^2 n [2\beta - \gamma(n-1)] \beta^{n-2} (\beta+\gamma)^{-n-2} + (\vec{s}_1 \cdot \vec{p})(\vec{s}_2 \cdot \vec{\kappa}_1) 16X^2 \rho^2 n(n+1) \beta^{n-1} (\beta+\gamma)^{-n-2} \\ & + (\vec{s}_1 \cdot \vec{\kappa}_2)(\vec{s}_2 \cdot \vec{p}) \frac{4X}{ip} \rho \left\{ [(X+\lambda)^2 + \kappa_1^2] - \rho^2[(X-\lambda)^2 + \kappa_1^2] \right\} (n+1)(2\beta - \gamma n) \beta^{n-1} (\beta+\gamma)^{-n-3} \\ & \left. + (\vec{s}_1 \cdot \vec{p})(\vec{s}_2 \cdot \vec{p}) \frac{4X}{ip} \rho \left\{ [(X+\lambda)^2 + \kappa_1^2] - \rho^2[(X-\lambda)^2 + \kappa_1^2] \right\} (n+1)(n+2) \beta^n (\beta+\gamma)^{-n-3} \right) d\rho. \quad (41) \end{aligned}$$

Taking into account Eqs. (39) and (40), β and $\beta+\gamma$ can be written

$$\beta = [(X+\lambda)^2 + \kappa_1^2] [(X-ip)^2 + \kappa_2^2] (1 - \xi\rho) (1 - \eta\rho), \quad \beta + \gamma = [(X+\lambda)^2 + \kappa_1^2] [X^2 + (\vec{p} + \vec{\kappa}_2)^2] (1 - \xi'\rho) (1 - \eta'\rho),$$

where

$$\xi + \eta = 2[4(\vec{\kappa}_1 \cdot \vec{\kappa}_2)X^2 + (\lambda^2 + \kappa_1^2 - X^2)(\kappa_2^2 - p^2 - X^2)] [(X+\lambda)^2 + \kappa_1^2]^{-1} [(X-ip)^2 + \kappa_2^2]^{-1}, \quad (42)$$

$$\xi\eta = [(X-\lambda)^2 + \kappa_1^2] [(X+ip)^2 + \kappa_2^2] [(X+\lambda)^2 + \kappa_1^2]^{-1} [(X-ip)^2 + \kappa_2^2]^{-1}, \quad (43)$$

$$\xi' + \eta' = 2\{4\vec{\kappa}_1 \cdot (\vec{p} + \vec{\kappa}_2)X^2 + (\lambda^2 + \kappa_1^2 - X^2)[(\vec{p} + \vec{\kappa}_2)^2 - X^2]\} [(X+\lambda)^2 + \kappa_1^2]^{-1} [X^2 + (\vec{p} + \vec{\kappa}_2)^2]^{-1}, \quad (44)$$

$$\xi'\eta' = [(X-\lambda)^2 + \kappa_1^2] [(X+\lambda)^2 + \kappa_1^2]^{-1}. \quad (45)$$

Thus, Eq. (41) becomes a linear combination of integrals of the following form:

$$\int_1^{(0+)} \rho^{-\tau+a} [(1 - \xi\rho) (1 - \eta\rho)]^{n-b} \times [(1 - \xi'\rho) (1 - \eta'\rho)]^{-n-c} d\rho, \quad (46)$$

where $a=1, 2, 3$; $b=0, 1, 2$; $c=1, 2, 3$. These integrals cannot be expressed in terms of elementary functions. Nevertheless, they are expressible in terms of known transcendentals, namely the hypergeometric functions of several variables of Lauri-

cella's type F_D .²⁵ In the general case these depend on a number of complex variables x_1, \dots, x_n and parameters a, b_1, \dots, b_n, c , and admit the following integral representation²⁶:

$$\begin{aligned} F_D(a; b_1, \dots, b_n; c; x_1, \dots, x_n) \\ = -\frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \left(\frac{i e^{-i\pi a}}{2 \sin\pi a} \right) \int_1^{(0+)} \rho^{a-1} (1-\rho)^{c-a-1} \\ \times (1-x_1\rho)^{-b_1} \dots (1-x_n\rho)^{-b_n} d\rho, \quad (47) \end{aligned}$$

valid provided that $\text{Re}c > \text{Re}a$. The integral equation (46) can obviously be written in terms of Eq. (47).

Equation (41) is thus expressible as a linear combination of F_D functions. Comparing it with Eq. (12) one finds

$$\mathcal{P}(\Omega) = \mathfrak{N} \frac{\lambda}{2-\tau} \frac{F_D(2-\tau; 1-n, 1-n, 1+n, 1+n; 3-\tau; \xi, \eta, \xi', \eta')}{[(X+\lambda)^2 + \kappa_1^2]^2 [(X-ip)^2 + \kappa_2^2] [X^2 + (\vec{p} + \vec{\kappa}_2)^2]}, \quad (48)$$

$$\mathcal{Q}(\Omega) = 8 \mathfrak{N} \frac{\kappa_1 \kappa_2 X^2 \lambda}{[(X+\lambda)^2 + \kappa_1^2]^3 [(X-ip)^2 + \kappa_2^2] [X^2 + (\vec{p} + \vec{\kappa}_2)^2]} \left\{ \frac{n+1}{3-\tau} \frac{F_D(3-\tau; 1-n, 1-n, 2+n, 2+n; 4-\tau; \xi, \eta, \xi', \eta')}{X^2 + (\vec{p} + \vec{\kappa}_2)^2} - \frac{n-1}{3-\tau} \frac{F_D(3-\tau; 2-n, 2-n, 1+n, 1+n; 4-\tau; \xi, \eta, \xi', \eta')}{(X-ip)^2 + \kappa_2^2} \right\}, \quad (49)$$

$$\mathcal{R}(\Omega) = 8 \mathfrak{N} p \kappa_1 \lambda X^2 \frac{n+1}{3-\tau} \frac{F_D(3-\tau; 1-n, 1-n, 2+n, 2+n; 4-\tau; \xi, \eta, \xi', \eta')}{[(X+\lambda)^2 + \kappa_1^2]^3 [(X-ip)^2 + \kappa_2^2] [X^2 + (\vec{p} + \vec{\kappa}_2)^2]}, \quad (50)$$

$$\begin{aligned} \mathcal{S}(\Omega) = & -2 \mathfrak{N} \frac{\kappa_2 p X}{[(X+\lambda)^2 + \kappa_1^2]^2 [X^2 + (\vec{p} + \vec{\kappa}_2)^2]} \left\{ \frac{(X-\lambda)^2 + \kappa_1^2}{X^2 + (\vec{p} + \vec{\kappa}_2)^2} \frac{(n+1)(n+2)}{4-\tau} F_D(4-\tau; -n, -n, 3+n, 3+n; 5-\tau; \xi, \eta, \xi', \eta') \right. \\ & - \frac{(X+\lambda)^2 + \kappa_1^2}{X^2 + (\vec{p} + \vec{\kappa}_2)^2} \frac{(n+1)(n+2)}{2-\tau} F_D(2-\tau; -n, -n, 3+n, 3+n; 3-\tau; \xi, \eta, \xi', \eta') \\ & \left. - \frac{(X-\lambda)^2 + \kappa_1^2}{(X-ip)^2 + \kappa_2^2} \frac{n(n+1)}{4-\tau} F_D(4-\tau; 1-n, 1-n, 2+n, 2+n; 5-\tau; \xi, \eta, \xi', \eta') \right. \\ & \left. + \frac{(X+\lambda)^2 + \kappa_1^2}{(X-ip)^2 + \kappa_2^2} \frac{n(n+1)}{2-\tau} F_D(2-\tau; 1-n, 1-n, 2+n, 2+n; 3-\tau; \xi, \eta, \xi', \eta') \right\}, \quad (51) \end{aligned}$$

$$\begin{aligned} \mathcal{T}(\Omega) = & -2 \mathfrak{N} \frac{p^2 X(n+1)(n+2)}{[(X+\lambda)^2 + \kappa_1^2]^3 [X^2 + (\vec{p} + \vec{\kappa}_2)^2]^3} \left\{ \frac{(X-\lambda)^2 + \kappa_1^2}{4-\tau} F_D(4-\tau; -n, -n, 3+n, 3+n; 5-\tau; \xi, \eta, \xi', \eta') \right. \\ & \left. - \frac{(X+\lambda)^2 + \kappa_1^2}{2-\tau} F_D(2-\tau; -n, -n, 3+n, 3+n; 3-\tau; \xi, \eta, \xi', \eta') \right\}. \quad (52) \end{aligned}$$

The number of F_D functions occurring here is ten; however, only seven are distinct. Their variables are determined by Eqs. (42)–(45); their explicit form is rather complicated and we shall not write it down. The quantity \mathfrak{N} appearing above is given by

$$\mathfrak{N} = NX^3 \left(\frac{(X-ip)^2 + \kappa_2^2}{X^2 + (\vec{p} + \vec{\kappa}_2)^2} \right)^n; \quad (53)$$

the principal branch of the power n should be taken (of argument in the interval $-\pi, +\pi$).

Equations (48)–(53) combined with Eqs. (42)–(45) contain our main result. From this, one can obtain the quantities $\mathcal{P}(\Omega)$, $\mathcal{Q}(\Omega)$, etc., as indicated in Sec. II, by changing $\vec{\kappa}_1$ into $-\vec{\kappa}_2$, κ_2 into $-\kappa_1$, and interchanging κ_1, κ_2 . For $\mathcal{P}(\Omega_1)$, $\mathcal{Q}(\Omega_1)$, etc., X should be taken equal to X_1 of Eq. (22), whereas for $\mathcal{P}(\Omega_2)$, $\mathcal{Q}(\Omega_2)$, etc., X should take the value X_2 . We have thus obtained an exact analytic result for the scattering amplitudes \mathcal{A} , \mathcal{B} , \mathcal{C} , \mathcal{D} , \mathcal{E} of the process, Eqs. (14) and (15).²⁷

IV. LOW-ENERGY LIMIT OF SPECTRUM

We shall now consider what becomes of our formulas when the scattered photon has vanishing energy, $\kappa_2 \rightarrow 0$. This limit can be handled analytically and will yield a noteworthy result.

In the following, only the dominant terms of the amplitudes will be given. Therefore, in general, we can set from the beginning $\kappa_2 = 0$ in the energy-conservation equation (21), which thus becomes

$$p^2 + \lambda^2 = 2m\kappa_1. \quad (54)$$

Now, this is precisely the energy-conservation equation for the photoeffect from the ground state. We shall assume in the rest of this section that p and $n = \lambda/ip$ are fixed by Eq. (54).

One has to deal separately with the amplitudes depending on X_1 and those depending on X_2 . Beginning with the case of X_1 , from Eqs. (22) and (54) we get

$$X_1 \simeq -ip, \quad \tau_1 \simeq -n. \quad (55)$$

Consequently, by eliminating X_1 and τ_1 from $\mathcal{P}(\Omega_1)$, $\mathcal{Q}(\Omega_1)$, etc., one can express these only in terms of p and κ_1 . However, special care must be given to the quantity $[X^2 + (\vec{p} + \vec{\kappa}_2)^2]$ occurring in the denominators, since this vanishes when setting $\vec{\kappa}_2 = 0$ and using Eq. (55). If one uses Eq. (22) and the complete energy-conservation equation [Eq. (21)], one gets to lowest order

$$X_1^2 + (\vec{p} + \vec{\kappa}_2)^2 \simeq -2m\kappa_2[1 - (\vec{v}_2 \cdot \vec{p}/m)].$$

The behavior of the variables ξ , η , ξ' , η' for $\kappa_2 \rightarrow 0$ can easily be obtained from Eqs. (42)–(45).

Since $\xi + \eta \simeq 0$, $\xi\eta \simeq 0$, it follows that $\xi \simeq 0$, $\eta \simeq 0$. On the other hand, $\xi' + \eta'$ is of order $1/\kappa_2$ and tends to infinity, whereas $\xi'\eta'$ remains finite. Therefore $\xi' \simeq 0$, $\eta' \simeq \xi' + \eta'$ (tending to infinity).²⁸ More precisely, to lowest order

$$\eta' \simeq 4p_1^2 [(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2] [(\lambda - ip)^2 + \kappa_1^2]^{-1} \times \{-2m\kappa_2[1 - (\vec{v}_2 \cdot \vec{p}/m)]\}^{-1}. \quad (56)$$

We shall now take advantage of the fact that the three variables ξ , η , ξ' vanish in the limit $\kappa_2 \rightarrow 0$. Consider the general expansion formula²⁹

$$F_D(a; b_1, \dots, b_4; c; x_1, \dots, x_4) = \sum_{m_1 m_2 m_3} \frac{(a)_{m_1 + m_2 + m_3}}{(c)_{m_1 + m_2 + m_3}} \frac{(b_1)_{m_1} (b_2)_{m_2} (b_3)_{m_3}}{m_1! m_2! m_3!} x_1^{m_1} x_2^{m_2} x_3^{m_3} \times {}_2F_1(a + m_1 + m_2 + m_3, b_4, c + m_1 + m_2 + m_3; x_4), \quad (57)$$

where $(a)_p = a(a+1)\dots(a+p-1)$. This is valid for $|x_1|, |x_2|, |x_3| < 1$, whatever the value of x_4 . By transforming adequately the ${}_2F_1$ functions involved³⁰ and noting that we are interested in the case when the parameters have the form: $a = \alpha + n$, $b_1 = b_2 = \beta - n$, $b_3 = b_4 = \beta' + n$, $c = \alpha + 1 + n$ with $\alpha, \beta, \beta' = 0, 1, 2, \dots$, one can write further

$$F_D(\alpha + n; \beta - n, \beta - n, \beta' + n, \beta' + n; \alpha + 1 + n; \xi, \eta, \xi', \eta') = (1 - \eta')^{-\beta' - n} \sum_{m_1 m_2 m_3} \frac{(\alpha + n)_{m_1 + m_2 + m_3}}{(\alpha + n + 1)_{m_1 + m_2 + m_3}} \times \frac{(\beta - n)_{m_1} (\beta - n)_{m_2} (\beta' + n)_{m_3}}{m_1! m_2! m_3!} \xi^{m_1} \eta^{m_2} \xi'^{m_3} {}_2F_1(1, \beta' + n, \alpha + 1 + n + m_1 + m_2 + m_3; \eta'/(\eta' - 1)). \quad (58)$$

The variable $\eta'/(\eta' - 1)$ of the functions ${}_2F_1$ in Eq. (58) tends to 1 as $\kappa_2 \rightarrow 0$. The dominant behavior of ${}_2F_1$ is given for this case by known general formulas (see Ref. 30, p. 110). From these it follows that, whatever α and β' , the order of magnitude of ${}_2F_1$ with respect to κ_2 does not increase when the sum $m_1 + m_2 + m_3$ increases. This means that in all cases the leading term of F_D corresponds to $m_1 = m_2 = m_3 = 0$ and therefore

$$F_D \simeq (-\eta')^{-\beta' - n} {}_2F_1(1, \beta' + n, \alpha + 1 + n; \eta'/(\eta' - 1)) \quad (59)$$

Taking into account the dominant behavior of ${}_2F_1$ when the variable approaches 1 (see Ref. 30, p. 110), we get the following results: If $\beta' < \alpha$,

$$F_D \simeq (-\eta')^{-\beta' - n} (\alpha + n) / (\alpha - \beta'); \quad (60)$$

if $\beta' = \alpha$,

$$F_D \simeq (\alpha + n) (-\eta')^{-\alpha - n} \ln(-\eta'); \quad (61)$$

if $\beta' > \alpha$,

$$F_D \simeq (-\eta')^{-\alpha - n} \frac{\Gamma(\beta' - \alpha) \Gamma(\alpha + 1 + n)}{\Gamma(\beta' + n)}. \quad (62)$$

By specializing the values of the parameters α , β , β' , and taking into account Eq. (56), Eqs. (60)–

(62) yield the dominant behavior of all the F_D functions occurring in $\mathcal{P}(\Omega_1)$, $\mathcal{Q}(\Omega_1)$, etc. For the dominant behavior of these quantities themselves in the limit $\kappa_2 \rightarrow 0$, one finds

$$\mathcal{O}_0(\Omega_1) \simeq -\frac{1}{16} N n [(\lambda - ip)^2 + \kappa_1^2]^{-1} [(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2]^{-1} f, \quad (63)$$

$$\mathcal{R}_0(\Omega_1) \simeq i \frac{1}{8} N \lambda \kappa_1 (n + 1) [(\lambda - ip)^2 + \kappa_1^2]^{-1} \times [(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2]^{-2} f, \quad (64)$$

$$\mathcal{S}_0(\Omega_1) \simeq -\frac{1}{16} N (n + 1) \frac{p}{m} \left(1 - \frac{\vec{v}_2 \cdot \vec{p}}{m}\right)^{-1} \times [(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2]^{-2} f, \quad (65)$$

$$\mathcal{T}_0(\Omega_1) \simeq -\frac{1}{16} N (n + 1) \frac{p^2}{m\kappa_2} \left(1 - \frac{\vec{v}_2 \cdot \vec{p}}{m}\right)^{-1} \times [(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2]^{-2} f, \quad (66)$$

with

$$f = \left(\frac{(\lambda - ip)^2 + \kappa_1^2}{(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2}\right)^n. \quad (67)$$

$\mathcal{T}_0(\Omega_1)$ behaves like $1/\kappa_2$, whereas $\mathcal{O}_0(\Omega_1)$, $\mathcal{R}_0(\Omega_1)$, $\mathcal{S}_0(\Omega_1)$ are independent of κ_2 . $\mathcal{Q}_0(\Omega_1)$ turns out to be of order κ_2 and is not given.

Let us now consider the case of X_2 . From Eq. (22) we get

$$X_2 \approx \lambda, \quad \tau_2 \approx 1. \quad (68)$$

Consequently, Eqs. (42)–(45) modified so as to give $\xi + \eta$, $\xi \bar{\eta}$, $\xi' + \bar{\eta}'$, $\xi' \bar{\eta}'$ (see end of Sec. II), yield $\xi + \eta \approx 0$, $\xi \bar{\eta} \approx 0$, $\xi' + \bar{\eta}' \approx 0$, $\xi' \bar{\eta}' \approx 0$. From here it follows that $\xi \approx 0$, $\bar{\eta} \approx 0$, $\xi' \approx 0$, $\bar{\eta}' \approx 0$, and therefore in all cases $F_D \approx 1$.

We get thus the dominant behavior

$$\bar{\varphi}_0(\Omega_2) \approx \frac{1}{16} N [(\lambda - ip)^2 + \kappa_1^2]^{-1} [(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2]^{-1} f, \quad (69)$$

$$\begin{aligned} \bar{s}_0(\Omega_2) \approx & \frac{1}{8} N \kappa_1 p (n+1) [(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2]^{-2} f \\ & \times \{ (n+2) [(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2]^{-1} - n [(\lambda - ip)^2 + \kappa_1^2]^{-1} \}, \end{aligned} \quad (70)$$

$$\mathcal{T}_0(\Omega_2) \approx \frac{1}{8} N p^2 (n+1) (n+2) [(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2]^{-3} f, \quad (71)$$

with f given by Eq. (67). These quantities are independent of κ_2 , whereas $\bar{\varphi}_0(\Omega_2)$ and $\bar{\mathcal{R}}_0(\Omega_2)$ are of order κ_2 and have been omitted.

In what concerns the quantity \mathcal{O} , it is finite for $\kappa_2 \rightarrow 0$ and its value can be easily obtained from Eq. (23).

Summing up, we see that for $\kappa_2 \rightarrow 0$ the dominant term of the amplitudes is $\mathcal{T}_0(\Omega_1)$ of Eq. (66), which behaves like $1/\kappa_2$. Hence, from Eqs. (14) and (15) we get

$$\mathfrak{M}_0 \approx -\mathcal{T}_0(\Omega_1) (\vec{s}_1 \cdot \vec{n}) (\vec{s}_2 \cdot \vec{n}). \quad (72)$$

\mathfrak{M}_0 can be expressed in terms of the matrix element of the photoeffect from the ground state. Indeed, in our notation this is given by³¹

$$[e^{i\vec{\kappa}_1 \cdot \vec{r}} (\vec{s}_1 \cdot \vec{P})]_{co} = \frac{1}{16} N (n+1) (\vec{p} \cdot \vec{s}_1) [(\vec{p} - \vec{\kappa}_1)^2 + \lambda^2]^{-2} f, \quad (73)$$

where the quantities involved are related by the energy-conservation equation (54). Comparing with Eqs. (66) and (72) we get

$$\mathfrak{M}_0 \approx \frac{1}{\kappa_2 m} (\vec{s}_2 \cdot \vec{p}) \left(1 - \frac{\vec{v}_2 \cdot \vec{p}}{m} \right)^{-1} [e^{i\vec{\kappa}_1 \cdot \vec{r}} (\vec{s}_1 \cdot \vec{P})]_{co}. \quad (74)$$

Although this result was proved here for the case of a Coulomb field, it remains true for any atomic field. This can be shown by starting directly from Eqs. (2) and (6) and using some of the properties of the Green's function.

It is well known from the case of scattering processes involving free electrons that whenever a soft photon (energy $\kappa \rightarrow 0$) can be emitted, the matrix element behaves at low energies like $1/\kappa$ and is proportional to the matrix element of the process in which this photon is absent.³² Equation (74) represents an example of this situation for the case of a bound electron, the process in which the final photon is suppressed being here the photoeffect.

V. DIPOLE APPROXIMATION

We shall now consider the dipole approximation of our general nonrelativistic result, when the energies of the incident and outgoing photons are sufficiently small so that one can neglect κ_1/λ , κ_2/λ with respect to 1. This is equivalent to replacing by 1 the exponentials appearing in the Kramers-Heisenberg-Waller matrix element Eq. (2), or to setting $\vec{\kappa}_1 = \vec{\kappa}_2 = 0$ throughout the calculation.

As a result one finds that the quantities \mathcal{O} , \mathcal{Q} , \mathcal{R} , \mathcal{S} , given by Eqs. (7), (23) and (49)–(51) vanish in the dipole approximation and that $\bar{\varphi}(\Omega) = \mathcal{O}(\Omega)$, $\bar{\mathcal{T}}(\Omega) = \mathcal{T}(\Omega)$. Therefore, Eqs. (14) and (15) become

$$\mathfrak{M} = \alpha (\vec{s}_1 \cdot \vec{s}_2) + \mathcal{E} (\vec{s}_1 \cdot \vec{n}) (\vec{s}_2 \cdot \vec{n}), \quad (75)$$

$$\alpha = -[\mathcal{O}(\Omega_1) + \mathcal{O}(\Omega_2)], \quad (76)$$

$$\mathcal{E} = -[\mathcal{T}(\Omega_1) + \mathcal{T}(\Omega_2)]. \quad (77)$$

Setting $\vec{\kappa}_1 = \vec{\kappa}_2 = 0$ in Eqs. (42)–(45) one gets

$$\xi + \eta = \frac{2(X - \lambda)(X + ip)}{(X + \lambda)(X - ip)}, \quad (78)$$

$$\xi \eta = \frac{(X - \lambda)^2 (X + ip)^2}{(X + \lambda)^2 (X - ip)^2};$$

$$\xi' + \eta' = \frac{2(X - \lambda)(X^2 - p^2)}{(X + \lambda)(X^2 + p^2)}, \quad (79)$$

$$\xi' \eta' = \frac{(X - \lambda)^2}{(X + \lambda)^2}.$$

Equations (78) and (79) can be easily solved to determine ξ , η , ξ' , η' . One finds that three of the variables are equal; let x be their common value: $\xi = \eta = \xi' = x$. Let us also denote $\eta' = y$. The values of x and y are

$$\begin{aligned} x &= (X - \lambda)(X + ip)/(X + \lambda)(X - ip), \\ y &= (X - \lambda)(X - ip)/(X + \lambda)(X + ip). \end{aligned} \quad (80)$$

Now, from the integral representation Eq. (47) of the function F_D it follows that

$$\begin{aligned} F_D(a; b_1, b_2, b_3, b_4; c; x, x, x, y) \\ = F_1(a; b_1 + b_2 + b_3, b_4; c; x, y), \end{aligned}$$

where F_1 is the standard notation for the F_D function of two variables, called Appell function.

From Eqs. (48), (52), and (53) we finally get

$$\begin{aligned} \mathcal{O}(\Omega) &= N \left(\frac{X - ip}{X + ip} \right)^n \frac{1}{(X - ip)^2 (X^2 + p^2)} \frac{\tau}{(1 + \tau)^4 (2 - \tau)} \\ &\quad \times F_1(2 - \tau; 3 - n, 1 + n; 3 - \tau; x, y), \end{aligned} \quad (81)$$

$$\mathcal{T}(\Omega) = 2N \left(\frac{X - ip}{X + ip} \right)^n \frac{p^2 (n+1)(n+2)}{(X^2 + p^2)^3 (1 + \tau)^4}$$

$$\times \left[\frac{1}{2-\tau} F_1(2-\tau; 3-n, 3+n; 3-\tau; x, y) - \left(\frac{1-\tau}{1+\tau} \right)^2 \frac{1}{4-\tau} F_1(4-\tau; 3-n, 3+n; 5-\tau; x, y) \right], \quad (82)$$

where N is given by Eq. (24).²⁷

Thus, in the dipole approximation the matrix element \mathcal{M} reduces to a considerably simpler form. The scattering amplitudes α and \mathcal{E} are now angle independent, the whole angle dependence of Eq. (75) being concentrated in the scalar products.

VI. DISCUSSION

The exact formulas we have derived in Sec. III have a rather complicated analytic structure. Although the hypergeometric functions F_D involved have reasonably well-known properties and are eventually amenable to a form suited for numerical computation, this operation is by no means trivial. The situation is considerably complicated by the large number of parameters in the problem (for every Z , κ_1 there is a continuous variation of κ_2 , ν_2 , n).

On the other hand, there are limitations of a physical nature affecting the result. Since our starting point Eq. (2) is a nonrelativistic formula without spin, one would expect it to be valid for $\kappa_1 \ll m$ and $(\alpha Z)^2 \ll 1$. However, some arguments have been presented showing that already for $\kappa_1 \approx \alpha Z m$ relativistic corrections become important.⁶ This tends to show that the Kramers-Heisenberg-Waller matrix element can describe correctly only the lowest-order retardation corrections beyond the dipole approximation. Therefore, for the time being, we have attempted only the numerical computation of the dipole approximation, Eqs. (75)–(77), (81), and (82).²³

The basic cross section of the process is given by Eq. (1). However, if the outgoing electron is not recorded, the incident photon beam is unpolarized and no attention is given to the final photon polarization, the relevant cross section is

$$\frac{d^2\sigma}{d\kappa_2 d\Omega_2} = \frac{1}{2} \sum_{\mathbf{s}_1 \mathbf{s}_2} \int \frac{d^3\sigma}{d\kappa_2 d\Omega_2 d\Omega} d\Omega. \quad (83)$$

This yields the shape of the scattered photon spectrum for every scattering angle. A further integration will give the over-all spectral distribution of the photons scattered in all space

$$\frac{d\sigma}{d\kappa_2} = \int \frac{d^2\sigma}{d\kappa_2 d\Omega_2} d\Omega_2. \quad (84)$$

Let us now consider the shape of the spectrum as given by our general formulas. For low energies κ_1 , where the dipole approximation is valid, the quantity \mathcal{O} of Eq. (7) vanishes and the matrix

element reduces to that given by Eqs. (75)–(77). Then, for κ_2 increasing from zero, the matrix element Eq. (74) together with the cross section Eq. (83) decrease like $1/\kappa_2$. The numerical analysis²³ shows that the decrease is monotonic up to the end of the spectrum.

As the energy κ_1 increases, the term \mathcal{O} becomes more and more important and will eventually dominate the rest of the amplitudes. For not too small scattering angles, the term produces a maximum in the cross section Eq. (83), near the Compton frequency for the scattering by free electrons. This maximum moves towards lower frequencies as the angle increases.³³ Now, even though the term \mathcal{O} may give the dominant contribution for most of the spectrum, this is not true for the low-energy end (κ_2 approaching zero), where it is dominated by the $1/\kappa_2$ behavior of $\tau(\Omega_1)$. The $1/\kappa_2$ rise of the cross section for $\kappa_2 \rightarrow 0$ cannot be predicted from the approximation Eq. (4), hitherto considered.

For high, relativistic energies κ_1 , the process is no longer described by the matrix element of Eq. (2) but the spectrum retains essentially the same shape.^{18,34}

The total intensity of the photons scattered under a certain angle should be calculated from the cross section

$$\frac{d\sigma}{d\Omega_2} = \int_0^{\kappa_1 - E_0} \frac{d^2\sigma}{d\kappa_2 d\Omega_2} d\kappa_2. \quad (85)$$

This should yield the analog of the (nonrelativistic limit of the) Klein-Nishina cross section, for the case of bound electrons. However, taking into account the $1/\kappa_2$ behavior of Eq. (83) for $\kappa_2 \rightarrow 0$, $d\sigma/d\Omega_2$ cannot be evaluated because of the logarithmic divergence of the integral.³⁵ This is an aspect of the infrared divergence problem of quantum electrodynamics.^{32,36} It shows that when one wants to calculate the attenuation of a flux of photons passing through matter, the contribution of the Compton effect from bound electrons cannot be considered alone. Let us briefly discuss this point in the following.

At the nonrelativistic energies we are concerned with, the attenuation is due mainly to photoeffect and Compton scattering. The corresponding cross sections have to be added in the expression of the attenuation coefficient. The cross section of the photoeffect is of order $\alpha(\alpha Z)^5$ whereas that of Compton scattering by bound electrons is of order $\alpha^2(\alpha Z)^5$.³⁷ This indicates that if one wants to add consistently the two, one also needs to consider the first-order radiative corrections to the photoeffect, which are of order $\alpha^2(\alpha Z)^5$. Now, like other radiative corrections, these are divergent in the range of soft virtual photons. The diver-

gences can be eliminated by attributing a small mass μ to the photon. Let us denote by $d\sigma_{\text{ph}}/d\Omega$ the photoeffect cross section containing the radiative corrections.

Concerning the contribution of the Compton effect, consider the case when the outgoing electron is scattered in $d\Omega$, regardless of what happens to the final photon. The cross section describing this case is $d^2\sigma/d\kappa_2 d\Omega$ [defined in a manner similar to Eq. (83)] integrated over κ_2 . To prevent the occurrence of the divergence for $\kappa_2 \rightarrow 0$, let us provisionally integrate over κ_2 starting from an arbitrarily small value ϵ .

By adding the two cross sections one gets

$$\frac{d\sigma_{\text{tot}}}{d\Omega} = \frac{d\sigma_{\text{ph}}}{d\Omega} + \int_{\epsilon}^{\kappa_1 - E_0} \frac{d^2\sigma}{d\kappa_2 d\Omega} d\kappa_2. \quad (86)$$

The introduction of the cutoff ϵ is equivalent to at-

tributing a small mass μ to the photon; consequently there is a certain relation between these quantities. If one takes it into account, μ and ϵ will drop out of Eq. (86) and one will end up with a finite result.³⁸ One then can integrate over $d\Omega$ to obtain σ_{tot} which appears in the total attenuation coefficient. Thus, it is only by combining photoeffect and Compton effect that one can get a meaningful result. Also, notice that of the two terms contained in Eq. (86) it is the Compton term which gives the leading contribution for high κ_1 , even though it is of a higher order in α .

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¹A detailed description of the process and references to earlier literature can be found in A. Sommerfeld, *Atombau und Spektrallinien* (Vieweg, Braunschweig, 1939), Vol. 2, Chap. 8, Secs. 5 and 6; Phys. Rev. **50**, 38 (1936); and R. Evans, *Compton Effect*, in *Encyclopedia of Physics*, edited by S. Flügge (Springer, Berlin, 1958), Vol. 34, Part II, Chap. G.

²We are using natural units ($\hbar = c = 1$).

³H. A. Kramers and W. Heisenberg, Z. Physik **31**, 681 (1925); I. Waller, *ibid.* **51**, 213 (1928); **58**, 75 (1929).

⁴This procedure is approximate because in order to reduce the matrix element pertaining to the whole atom to the matrix element of Eq. (2), orthogonality properties of the individual electron orbitals are needed. These properties exist only if all the atomic electrons are considered to be under the influence of the *same* central field in the initial, intermediate and final states. Strictly speaking this is not the case in a self-consistent-field approximation and the error is expected to be larger the lower the Z .

⁵See A. I. Akhiezer and V. B. Berestetskii, *Quantum Electrodynamics*. (Interscience, New York, 1965), Chap. 5, Sec. 35.1.

⁶The relativistic limitations of Eq. (2) were considered by V. G. Gorshkov, A. I. Mikhailov, V. S. Polikanov, and S. G. Sherman, Phys. Letters **30A**, 455 (1969).

⁷In the limit $Z \rightarrow 0$ ($E_0 \rightarrow 0$), Eq. (4) becomes exact and yields the nonrelativistic version of the Klein-Nishina cross section; see A. Sommerfeld, Ref. 1, Chap. 8, Sec. 3.

⁸G. Wentzel, Z. Physik **43**, 1 (1927); **43**, 779 (1927); **58**, 348 (1929).

⁹F. Schnaidt, Ann. Physik **21**, 89 (1934).

¹⁰F. Bloch, Phys. Rev. **46**, 674 (1934).

¹¹J. DuMond, Rev. Mod. Phys. **5**, 19 (1933).

¹²The DuMond formula was applied by several authors to calculate the spectral distribution corresponding to various atomic subshells. See R. J. Weiss, A. Harvey, and W. C. Phillips, Phil. Mag. **17**, 241 (1968), and the

references quoted therein.

¹³P. Eisenberger and P. M. Platzman, Phys. Rev. A **2**, 415 (1970).

¹⁴References to this are contained in the report of J. H. Hubbell, *Photon Cross Sections, Attenuation Coefficients and Energy Absorption Coefficients*, NSRDS-NBS No. 29 (U.S. GPO, Washington, D.C., 1969). See also R. T. Brown, Phys. Rev. A **1**, 1342; **2**, 614 (1970); and M. Singh, Phys. Letters **31A**, 392 (1970).

¹⁵See, for example, R. J. Weiss, Phys. Rev. Letters **24**, 883 (1970); P. Eisenberger, Phys. Rev. A **2**, 1678 (1970), and the references quoted therein.

¹⁶For a free atom this follows from Schnaidt's evaluation of Eq. (4); see Ref. 9, Eq. (28) and the graphical representation given by Sommerfeld in Ref. 1, p. 620, Fig. 46(c). The corresponding cross section is proportional to $(1 + \cos^2\theta)(\vec{k}_1 - \vec{k}_2)^2/\lambda^2$; the same result was obtained by Y. Mizuno and Y. Ohmura [J. Phys. Soc. Japan **22**, 445 (1967)] for the case of an atom embedded in a crystal. Now, at these low energies an appreciable contribution would be expected from the sums over intermediate states, neglected in Eq. (4). However, it turns out that their contribution is rather small (see Sec. IV of Ref. 23).

¹⁷K. Das Gupta, Phys. Rev. Letters **3**, 38 (1959); **13**, 338 (1964); Phys. Rev. **128**, 2181 (1962); A. Faessler and P. Mühle, Phys. Rev. Letters **17**, 4 (1966); T. Suzuki *et al.*, J. Phys. Soc. Japan **22**, 1139 (1967); **29**, 730 (1970); N. G. Alexandropoulos and G. G. Cohen, Phys. Rev. **187**, 455 (1969). A rather varied terminology has been used to describe the occurrence of this peak: characteristic modified x-ray scattering, x-ray Raman scattering, modified Compton scattering, etc.

¹⁸I. B. Whittingham, J. Phys. A **4**, 21 (1971). This paper contains references to previous theoretical and experimental results in the relativistic domain.

¹⁹The results have been briefly reported in M. Gavrila, Nuovo Cimento Letters **2**, 180 (1969). Work on the same lines using somewhat different methods was done by V. G. Gorshkov and B. S. Polikanov, Zh. Eksperim. i Teor. Fiz. Pis'ma v Redaktsiyu **9**, 464 (1969) [Sov. Phys. JETP Letters **9**, 279 (1969)]; S. Klarsfeld, Nuovo Cimento Letters **2**, 548 (1969).

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- ²²J. Schwinger, J. Math. Phys. **5**, 1606 (1964), Eq. (3'). Equivalent results were obtained by the authors quoted in Ref. 9 of our paper Ref. 20. Our Green's function differs in sign from the one of Schwinger.
- ²³M. Gavrila, following paper, Phys. Rev. A **6**, 1360 (1972).
- ²⁴Reference 21(a), Appendix A, Eqs. (A1) and (A6)–(A8). [The misprints contained in Eq. (A1) were corrected in Ref. 21(b) and in Eq. (30) above.] The conditions given in Eq. (A9) for the validity of the formulas are satisfied in the present case if one takes into account Eqs. (20) and (29) above and the fact that λ is positive.
- ²⁵The basic monograph on hypergeometric functions of several variables remains P. Appell and J. Kampé de Fériet, *Fonctions Hypergéométriques et Hypersphériques* (Gauthier-Villars, Paris, 1926).
- ²⁶This is a slight generalization of Ref. 25, p. 116, Eq. (8).
- ²⁷Our results agree with the ones of Gorshkov *et al.* and Klarsfeld (see Ref. 19), as far as these go. While Gorshkov *et al.* only outline their method, Klarsfeld also gives the complete result for the dipole approximation, in agreement with our Eqs. (81) and (82).
- ²⁸It is irrelevant which of the variables ξ' , η' is considered to become infinite, because our F_D functions are symmetric with respect to ξ' , η' .
- ²⁹This is derived from Ref. 25, p. 114, Eq. (4).
- ³⁰A. Erdélyi, W. Magnus, F. Oberhettinger, and F. Tricomi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. I, p. 105, Eq. (4).
- ³¹Equation (73) can be derived from Sommerfeld's book, Ref. 1, Chap. 6, Sec. 4, Eqs. (4b), (5), and (20) and Sec. 5, Eq. (5b).
- ³²See J. M. Jauch and F. Rohrlich, *The Theory of Photons and Electrons* (Addison-Wesley, Reading, Mass., 1955), Sec. 16-1.
- ³³A detailed description of the situation from the standpoint of Eq. (4) is given by Sommerfeld, Ref. 1; see also Ref. 10.
- ³⁴One can show that there exists a relativistic analogue of Eq. (74). The occurrence of the divergence for $\kappa_2 \rightarrow 0$ was already apparent in the early relativistic formula for $d\sigma/d\kappa_2$ derived by H. Casimir, Helv. Phys. Acta **6**, 287 (1933)—the final equation for $Q_{\nu'}$; see also Ref. 5, Chap. 5, Sec. 35.3. The approximations involved (free intermediate and final states) are not of the nature to interfere with this feature. A numerical calculation of Eq. (83) proceeding essentially on the same lines, done by M. Di Lazzaro and G. Missoni [Lab. Fis., Istituto Sup. Sanità Report No. ISS 66/8, Part III, 1966 (unpublished)], also indicates this behavior. This was not realized in the numerical work of Whittingham (Ref. 18), which even gives values for $d\sigma/d\Omega_2$. (These were probably obtained on the basis of a "natural" extrapolation to $\kappa_2 = 0$ of the spectral distribution computed for $\kappa_2 \geq 0.2m$, followed by an integration over κ_2 , thereby ignoring the existence of the infrared divergence.)
- ³⁵This difficulty does not exist in the approximation of Eq. (4) or those derived from it (incoherent-scattering function; impulse approximation), because Eq. (4) remains finite for $\kappa_2 \rightarrow 0$. From the experimental point of view the recorded spectra always start from some finite value of κ_2 on, so that what one actually measures is not the $d\sigma/d\Omega_2$ of Eq. (85), but rather its analog with a low-energy cutoff.
- ³⁶For a more detailed discussion see D. R. Yennie, S. C. Frautschi, and H. Suura, Ann. Phys. (N.Y.) **13**, 379 (1961).
- ³⁷See Eqs. (1), (14), (15), and (48)–(53) and the value given by Eq. (24) for small αZ .
- ³⁸The situation is similar to that of the attenuation of a flux of electrons by elastic scattering and bremsstrahlung. An equation similar to Eq. (86) holds also in that case, the first term representing the contribution of elastic scattering (including radiative corrections) and the second term the contribution of bremsstrahlung; see, for example, J. W. Motz, H. Olsen, and H. W. Koch, Rev. Mod. Phys. **36**, 881 (1964).