Soft-photon approximation for bound-state Compton scattering

Leonard Rosenberg and Fei Zhou

Department of Physics, New York University, New York, New York, 10003

(Received 3 June 1991)

The transition amplitude for the inelastic scattering of a photon from a system of bound charged particles, with a single charge ejected, behaves at low-energy end of the scattered-photon spectrum as the inverse of the energy and is proportional to the on-shell matrix element corresponding to the process in which the soft photon is absent. The next term in the expansion in powers of the energy of the soft photon is derived here, and is expressed in terms of the same single-photon absorption amplitude. The correction takes the form of first-order momentum shifts in the arguments of the absorption amplitude; they enter in such a way as to leave this amplitude on the energy shell. This result is precisely what would be expected by analogy with Low's theorem [Phys. Rev. 110, 974 (1958)] on spontaneous bremsstrahlung. A nonrelativistic version of the theorem on bound-state Compton scattering is obtained through an asymptotic analysis of the configuration-space matrix element for this process, with the effect of a long-range Coulomb tail accounted for. Relativistic versions are derived as well, appropriate to particles of zero spin, and with spin effects included, based on the same type of gauge-invariance argument employed by Low. Analogous results are obtained from an external-field formulation in the weak-field limit.

PACS number(s): 32.80.Cy, 32.80.Fb, 03.80.+^r

I. INTRODUCTION

An exact analytic calculation of the cross section for nonrelativistic Compton-type inelastic scattering of photons by electrons bound in the ground state of a hydrogenlike atom was performed some years ago by Gavrila [1]. One of the results of this calculation was a verification that (as expected on general grounds) the transition amplitude behaves for low energies of the scattered photon as the inverse of the energy and is proportional to the matrix element in which the soft photon is absent —in the case considered the radiationless process is that of photoionization. Numerical computations [2] appropriate to a wider class of potentials (as required for the interpretation of several recent experiments [3]) have confirmed this infrared behavior. For potentials of finite range, such as that experienced by an electron originally bound to a neutral atom, one would expect that the next term in the expansion, of zeroth order in the energy of the scattered photon, could be determined as well, in terms of the physical (on-shell) photodetachment amplitude. This expectation is based on the analogy with the single-photon bremsstrahlung process and the very general 'type of argument used by Low [4] in his derivation of a soft-photon approximation for radiation accompanying the scattering of a charged particle by a neutral particle. If the target atom is neutral the ejected electron moves in a Coulomb potential asymptotically. This results in a modification of the soft-photon energy dependence and here too one can anticipate the form of this modification since the analogous low-frequency approximation for brernsstrahlung in a potential with a long-range Coulomb tail has been derived [5]. Here we derive two versions of the soft-photon approximation for bound-state Compton scattering. One approach, closely related to the treatment of the bremsstrahlung problem employed in Ref. [5], is based on an asymptotic evaluation of the nonrelativistic configuration-space matrix element. The inclusion of long-range Coulomb effects is straightforward in this method since the modification of the asymptotic form of the continuum-wave function in the presence of a Coulomb tail is known. The second derivation is more in line with Low's approach, in that it makes use of gauge invariance in the context of a relativistic formulation, with long-range Coulomb effects ignored.

It may be of interest to point out the relationship between the treatment of this problem in terms of inelastic photon scattering and an alternative picture based on an analysis of photodetachment in the presence of a lowfrequency external field. The connection can be made by taking the weak-field limit of the low-frequency approximation obtained [6] (nonrelativistically) for the externalfield problem. A relativistic version of this connection is derived in Sec. IV, below.

II. NQNRELATIVISTIC TREATMENT

We consider the scattering of a photon from an atomic system, initially in state $|\phi\rangle$ with energy E_0 , leading to the ejection of an electron into the continuum state $|p^{(-)}\rangle$ characterized by the energy E_p , asymptotic momentum p, and incoming-wave boundary conditions. The frequency, momentum, and polarization of the incident and scattered photons are represented as $\omega_1, \mathbf{k}_1, \lambda_1,$ and $\omega_2, \mathbf{k}_2, \lambda_2$, respectively. The matrix element for this process, in lowest nonvanishing order of perturbation theory, may be expressed, in units with $h=1$, as

7284 LEONARD ROSENBERG AND FEI ZHOU

$$
T(\mathbf{p}, \omega_2, \mathbf{k}_2, \lambda_2; \omega_1, \mathbf{k}_1, \lambda_1) = \langle \mathbf{p}^{(-)} | I(\omega_2, -\mathbf{k}_2, \lambda_2) G_0(E_0 + \omega_1) I(\omega_1, \mathbf{k}_1, \lambda_1) | \phi \rangle
$$

+ $\langle \mathbf{p}^{(-)} | I(\omega_1, \mathbf{k}_1, \lambda_1) G_0(E_0 - \omega_2) I(\omega_2, -\mathbf{k}_2, \lambda_2) | \phi \rangle$
+ $\frac{e^2}{2mc^2} \left[\frac{2\pi c^2}{\omega_1 \omega_2 V} \right] \lambda_1 \cdot \lambda_2 \langle \mathbf{p}^{(-)} | \exp[i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{R}] | \phi \rangle$ (2.1)

The Green's function $G_0(E)$ for the atomic system in the

absence of the field satisfies the resolvent equation
\n
$$
(E - H_0)G_0(E) = 1,
$$
\n(2.2)

along with outgoing-wave boundary conditions. To keep notation reasonably condensed we have introduced, in Eq. (2.1), the interaction operator

$$
I(\omega, \mathbf{k}, \lambda) \equiv -\frac{e}{mc} \left(\frac{2\pi c^2}{\omega V} \right)^{1/2} \lambda \cdot \mathbf{P} \exp(i\mathbf{k} \cdot \mathbf{R}) , \quad (2.3)
$$

where V is the quantization volume. **P** and **R** represent the momentum and position operators, respectively, of the electron. (For simplicity we assume that only a single electron is active.) The energy conservation condition is $E_0 + \omega_1 = E_p + \omega_2.$

We now make the substitution

$$
\mathbf{P} = -im[\mathbf{R}, H_0] \tag{2.4}
$$

in Eq. (2.1). The action of the Hamiltonian is taken into account with the aid of Eq. (2.2) along with the eigenvalue equations

$$
(H_0 - E_0)|\phi\rangle = 0, \quad (H_0 - E_p)|p^{(-)}\rangle = 0.
$$
 (2.5)

After some algebra one finds that Eq. (2.1) may be put in the alternative form

$$
T = \langle \mathbf{p}^{(-)} | \tilde{I}(\omega_2, -\mathbf{k}_2, \lambda_2) G_0(E_0 + \omega_1) \tilde{I}(\omega_1, \mathbf{k}_1, \lambda_1) | \phi \rangle + \langle \mathbf{p}^{(-)} | \tilde{I}(\omega_1, \mathbf{k}_1, \lambda_1) G_0(E_0 - \omega_2) \tilde{I}(\omega_2, -\mathbf{k}_2, \lambda_2) | \phi \rangle .
$$
\n(2.6)

The transformed interaction operator is defined as

$$
\widetilde{I}(\omega, \mathbf{k}, \lambda) \equiv -\frac{e}{mc} \left(\frac{2\pi c^2}{\omega V} \right)^{1/2} \times (-im) (\omega e^{i\mathbf{k} \cdot \mathbf{R}} \lambda \cdot \mathbf{R} + \lambda \cdot \mathbf{R} [H_0, e^{i\mathbf{k} \cdot \mathbf{R}}])
$$
 (2.7)

Note that the last term in Eq. (2.1), arising from the A^2 contribution to the interaction, has canceled in the passage to Eq. (2.6). It should also be noted that a similar transformation can be performed on the single-photon bound-free and free-free transition amplitudes. Thus the amplitude for ionization with the absorption of a single photon is given by

$$
t(\mathbf{p};\omega,\mathbf{k},\lambda) = \langle \mathbf{p}^{(-)}|I(\omega,\mathbf{k},\lambda)|\phi\rangle = \langle \mathbf{p}^{(-)}|\tilde{I}(\omega,\mathbf{k},\lambda)|\phi\rangle,
$$
\n(2.8)

with $E_p = E_0 + \omega$; the second form is obtained from the first by making the replacement (2.4) and using the Schrödinger equations (2.5).

Equation (2.6) provides a convenient starting point for the derivation of a low-frequency approximation in which

terms of order ω_2 and higher are ignored. We begin by observing that the second term in Eq. (2.6) makes no contribution to such an approximation since it is proportional to the soft-photon frequency, with a coefficient in the form of an integral that is finite in the zero-frequency limit. Indeed, a divergence in that limit could only arise from the asymptotic domain in the six-dimensional configuration space. The presence of the bound-state wave function $\phi(\mathbf{r}')$ ensures convergence in three of these variables. Convergence in the remaining variables is guaranteed by the fact that the Green's function $\langle \mathbf{r} | G_0(E_0 - \omega_2) | \mathbf{r}' \rangle$ decays exponentially in r since the energy $E_0 - \omega_2$ lies below the ionization threshold. An extension of this type of analysis is useful in evaluating the first term in Eq. (2.6) to the required accuracy. The integral appearing there is singular in the limit $\omega_2 \rightarrow 0$, and the singular contribution may be determined by inserting the asymptotic forms of both the Green's function and of the final-state continuum-wave function $\langle \mathbf{p}^{(-)} | \mathbf{r} \rangle$ for $r \rightarrow \infty$. Assuming for the moment that the potential is of short range, the integral of interest will contain terms behaving as $(\omega_2)^{-2}$ and $(\omega_2)^{-1}$. To correctly evaluate these contributions one must include the first two terms in the asymptotic expansions of both the wave function and Green's function. The effect of a Coulomb tail is simply to modify the asymptotic behavior of the two functions in a known manner, with the result that terms appear that depend logarithmically on the frequency and are explicitly calculable. The integral to be evaluated by this asymptotic procedure is of the form that appears as part of the bremsstrahlung matrix element. We will therefore be able to make use of an earlier derivation of a soft-photon approximation for nonrelativistic Coulomb bremsstrahlung [5], and this simplifies the present task considerably.

We suppose that the potential experienced by the electron at great distances is of the form $V(r) \sim Ze^2/r$. The partial-wave continuum function for scattering in such a potential may be expressed as a superposition of incoming- and outgoing-wave components; the first two terms in the asymptotic expansions of each of these components are known [7]. The asymptotic form of the Green's function for each partial wave is then determined, and a formal summation over partial waves leads to the form

$$
\lim_{r \to \infty} \langle \mathbf{r} | G_0(E_q) | \mathbf{r}' \rangle = - \left[\frac{2m}{4\pi} \right] (2\pi)^{3/2} r^{-1} e^{iqr} (2qr)^{-in}
$$

$$
\times \left[1 + \frac{n}{2qr} - \frac{L^2 + n^2}{2iqr} \right] \langle q^{(-)} | \mathbf{r}' \rangle .
$$
\n(2.9)

Here $n = Ze^{2}m/q$ is the Sommerfeld parameter, q is a vector in the direction of r, with $q^2/2m = \omega_2 + p^2/2m$, and $L = R \times P$ is the angular momentum.

The asymptotic form of the final-state wave function may be determined in a similar way. Actually, it is only the incoming-wave component that is required here since the component behaving as an outgoing wave at infinity gives rise to an integral that is not singular in the zerofrequency limit and may therefore be ignored according to the calculational procedure outlined above. [Near singularities arise when the integrand is very slowly varying at infinity and this requires a near cancellation of exponential phase factors. For this to occur the outgoing wave shown in Eq. (2.9) must be combined with an incoming wave.] The incoming wave behaves asymptotically as

$$
\lim_{r \to \infty} \langle \mathbf{p}^{(-)} | \mathbf{r} \rangle_{in} = (2\pi)^{-3/2} \frac{2\pi i}{pr} e^{-ipr} (2pr)^{in'}
$$

$$
\times \delta(\Omega_{\hat{r}} - \Omega_{\hat{p}}) \left[1 - \frac{n'}{2pr} + \frac{L^2 + n'^2}{2ipr} \right],
$$
\n(2.10)

with $n' = Ze^2m/p$. The presence of the two-dimensional 5 function simplifies the evaluation of the matrix element; the angular integration may be carried out immediately, fixing the direction of r to lie along the vector p.

The evaluation of the integral appearing in the first term of Eq. (2.6) is facilitated by the introduction of a multipole expansion for the interaction operator $I(\omega_2, -\mathbf{k}_2, \lambda_2)$, with only the electric-dipole, magneticdipole, and electric-quadrupole terms retained; omission of higher-order multipoles is justified since they give rise to corrections of order $(v/c)^2$. In this approximation the interaction operator becomes

$$
\widetilde{I}(\omega, -\mathbf{k}, \lambda) = \left[\frac{2\pi c^2}{\omega V}\right]^{1/2} \left[\frac{ie}{c}\omega\lambda \cdot \mathbf{R} + i\mathbf{k} \times \lambda \cdot \left(\frac{e}{2mc}\mathbf{L}\right) + \frac{e}{2c}\omega(\mathbf{k} \cdot \mathbf{R})(\lambda \cdot \mathbf{R})\right].
$$
\n(2.11)

Radial integrations extend over a domain $r > r_0$, with r_0 taken to be large enough to justify the neglect of the short-range component of the scattering potential in the construction of the asymptotic solutions shown in Eqs. (2.9) and (2.10). In practice we may extend the integration down to the origin since the contribution from the domain $r < r_0$ is nonsingular in the zero-frequency limit and, as explained above, such contributions are of higher order than those to be retained in the low-frequency approximation. All of the radial integrals which appear may then be evaluated in terms of the Γ function. For example, one of the integrals [8] is of the form

$$
\int_0^{\infty} e^{i(q-p)r} (2qr)^{-in} (2pr)^{in'} dr = [-i(q-p)]^{-1} B(p,q) ,
$$
\n(2.12)

$$
B(p,q) = e^{-|n-n'| \pi/2} \left[\frac{|p-q|}{2q} \right]^{i(n-n')} \left[\frac{p}{q} \right]^{in'}
$$

× $\Gamma(1-i(n-n'))$. (2.13)

Since at this point the details of the calculation are identical to those summarized in Ref. [5], we do not enter into them here. We state the final result, for the case of linear polarization where the expression takes on a relatively simple form, as

$$
T(\mathbf{p}, \omega_2, \mathbf{k}_2, \lambda_2; \omega_1 \mathbf{k}_1, \lambda_1)
$$

= $-\frac{e}{mc} \left[\frac{2\pi c^2}{\omega_2 V} \right]^{1/2} B(p, q) (1 + in' \mathbf{p} \cdot \mathbf{k}_2 / p^2)$
 $\times \frac{\lambda_2 \cdot \mathbf{p}}{\omega_2 - \mathbf{k}_2 \cdot \mathbf{p} / m} t(\mathbf{p}_s; \omega_1 \mathbf{k}_1, \lambda_1)$
+ $O(\omega_2 \ln \omega_2)$. (2.14)

Here t is the photoionization amplitude defined in Eq. (2.8), and $q = p_s$, with the shifted momentum p_s given by

$$
\mathbf{p}_s = \mathbf{p} + \mathbf{k}_2 + \lambda_2 \frac{m \omega_2 - \mathbf{k}_2 \cdot \mathbf{p}}{\lambda_2 \cdot \mathbf{p}} \tag{2.15}
$$

The relation $(p_s)^2/2m = p^2/2m+\omega_2$, correct to first order, places the t matrix on the energy shell. The factor $B(p,q)$ contains modifications associated with the Coulomb tail. Thus for a short-range potential the approximation contains terms of order $(\omega_2)^{-1}$ and $(\omega_2)^0$, whereas the low-frequency limit of the approximation (2.14) includes, in addition, terms of order $ln\omega_2$ and $\omega_2 \ln^2 \omega_2$. The form of Eq. (2.14) in the zero-frequency limit is consistent with that obtained by Gavrila [1], in the same limit, for the pure Coulomb potential.

III. RELATIVISTIC TREATMENT

A. Spin-zero particles

To account for relativistic effects one could modify the calculation of Sec. II through the use of (single-electron) relativistic wave functions and propagators. Here we describe a quite different procedure, introduced by Low [4] in a slightly different connection, based on the very general considerations of gauge invariance and analyticity. We first consider the inelastic scattering of a photon of 4-momentum k_1 and polarization λ_1 from a composite system of spin zero, mass m_1 , and charge e, with initial momentum q_1 . This system dissociates into a spin-zero "electron" of mass m , charge e , and momentum p , along with a neutral, spin-zero particle of momentum q_2 and mass m_2 . (Spin effects are treated in Sec. III B.) In the process a soft photon of momentum k_2 and polarization λ_2 is emitted. The conditions $\lambda_2 \cdot k_2 = \lambda_1 \cdot k_1 = 0$ are assumed to hold, and each particle is taken to be on its mass shell. (Here $a \cdot b \equiv a_0 b_0 - a \cdot b$.) We denote the amplitude for this inelastic photon scattering process as λ_2 *M* and we wish to relate it to the on-shell amplitude $t(p, q_2; q_1, k_1, \lambda_1)$ for the process in which no soft photon

with

is radiated. During the course of the derivation we will treat this amplitude as a function of the scalar variables

$$
v=p \cdot q_2
$$
, $\eta = (q_2-q_1)^2$, $\xi' = \lambda_1 \cdot p$, $\xi = \lambda_1 \cdot q_1$

In this way the mass-shell constraints on the momentum variables are easily accounted for.

Let M_a represent the contribution to M in which the soft photon has been emitted either before or after the dissociation process, so that it contains the correct singular behavior in the zero-frequency limit. This leaves some freedom in the manner in which it is continued away from the singularity. The most convenient choice [9] is to express M_a in terms of the on-shell matrix $t(\nu, \eta, \xi', \xi)$ as

$$
M_{a} = \frac{(2p + k_{2})}{2p \cdot k_{2}} t(\nu + k_{2} \cdot q_{2}, \eta, \xi' + \lambda_{1} \cdot k_{2}, \xi)
$$

- $t(\nu, \eta + 2(q_{2} - q_{1}) \cdot k_{2}, \xi', \xi - \lambda_{1} \cdot k_{2}) \frac{(2q_{1} - k_{2})}{2q_{1} \cdot k_{2}}$. (3.1)

We introduce a series expansion of the t matrix about k_2 =0, discarding terms that contribute to M to first order in k_2 . We then add a term M_b , independent of k_2 , chosen in such a way that gauge invariance, in the form $k_2 \cdot (M_a + M_b) = 0$, is satisfied. It follows [4] that the remainder $R \equiv M - M_a - M_b$ is of order k_2 . With derivatives of the t matrix evaluated at $k_2 = 0$, this construction provides us with the soft-photon approximation

$$
M_a + M_b = \left[\frac{(2p + k_2)}{2p \cdot k_2} - \frac{(2q_1 - k_2)}{2q_1 \cdot k_2} \right] t(\nu, \eta, \xi', \xi)
$$

+
$$
\left[p \frac{q_2 \cdot k_2}{p \cdot k_2} - q_2 \right] \frac{\partial t}{\partial \nu} - \left[2q_1 \frac{q_2 \cdot k_2}{q_1 \cdot k_2} - 2q_2 \right] \frac{\partial t}{\partial \eta}
$$

+
$$
p \frac{\lambda_1 \cdot k_2}{p \cdot k_2} \frac{\partial t}{\partial \xi'} + q_1 \frac{\lambda_1 \cdot k_2}{q_1 \cdot k_2} \frac{\partial t}{\partial \xi} - \lambda_1 \left[\frac{\partial t}{\partial \xi} + \frac{\partial t}{\partial \xi'} \right].
$$

(3.2)

This result may be expressed in a more compact form in terms of the shifted momenta

$$
p_s = p + k_2 - \lambda_2 \frac{p \cdot k_2}{p \cdot \lambda_2}, \quad q_{1s} = q_1 - k_2 + \lambda_2 \frac{q_1 \cdot k_2}{q_1 \cdot \lambda_2} \tag{3.3}
$$

Each of these momenta is on its mass shell to first order in the soft-photon energy. Reverting to the original notation in which the t matrix is written in terms of the momenta rather than the scalar variables, but with the understanding that it is actually defined by the values of these scalar variables, we have, assuming the polarization vectors to be real,

$$
\lambda_2 \cdot (M_a + M_b) = \frac{p \cdot \lambda_2}{p \cdot k_2} t(p_s, q_2; q_1, k_1, \lambda_1) - t(p, q_2; q_{1s}, k_1, \lambda_1) \frac{q_1 \cdot \lambda_2}{q_1 \cdot k_2} .
$$
 (3.4)

(The second term accounts for radiation by the recoiling target.) The correspondence between this result and the approximation (2.14), appropriate to the case where there is no Coulomb tail, is easily established by taking the nonrelativistic limit of the expression shown in Eq. (3.4), adopting the Coulomb gauge, and working in the laboratory reference frame with target recoil ignored.

B. Spin- $\frac{1}{2}$ charged particles

We now consider the case in which the charged particles have spin $\frac{1}{2}$. Following the procedure established above we begin by identifying the component of the transition amplitude containing the infrared singularity as

$$
M_a = \overline{w}(p)\gamma(p+k_2-m)^{-1}F(\nu+k_2\cdot q_2, \eta, \xi' + \lambda_1\cdot k_2, \xi)
$$

× $u(q_1) + \overline{w}(p)F(\nu, \eta + 2(q_2-q_1)\cdot k_2, \xi', \xi - \lambda_1\cdot k_2)$
× $(q_1 - k_2 - m_1)^{-1}\gamma u(q_1)$. (3.5)

Here we use the notation [10] $p = \gamma \cdot p$, where γ is the 4 vector of Dirac matrices, and (setting $c = 1$) we have introduced spinors satisfying

$$
\overline{w}(p)(p-m)=0, \quad (q_1-m_1)u(q_1)=0 \ . \tag{3.6}
$$

The photodissociation amplitude has been expressed as

$$
t(p,q_2;q_1,k_1,\lambda_1) = \overline{w}(p)F(p \cdot q_2,(q_2-q_1)^2,p \cdot \lambda_1,q_1 \cdot \lambda_1)u(q_1) . \qquad (3.7)
$$

To the singular contribution shown in Eq. (3.5) we add the amplitude

$$
M_b = \overline{w}(p) \left[-q_2 \frac{\partial F}{\partial v} - \lambda_1 \left(\frac{\partial F}{\partial \xi} + \frac{\partial F}{\partial \xi'} \right) + 2(q_2 - q_1) \frac{\partial F}{\partial \eta} \right] u(q_1) .
$$
 (3.8)

With the aid of the relations

$$
\overline{w}(p)k_2(p-k_2-m)^{-1} = \overline{w}(p),(q_1-k_2-m_1)^{-1}k_2u(q_1) = -u(q_1),
$$
\n(3.9)

one readily verifies that gauge invariance, in the form $k_2 \cdot (M_a + M_b) = 0$, is satisfied by the approximate amplitude $M_a + M_b$; it follows that the remainder is of first order in k_2 .

The soft-photon approximation is conveniently expressed in terms of the shifted momenta introduced in Eq. (3.3). Further simplification is obtained by rationalizing the propagators in Eq. (3.5) and using the Dirac equation to write

$$
\overline{w}(p) \chi_2 \frac{p + k_2 + m}{2p \cdot k_2} = \frac{p \cdot \lambda_2}{p \cdot k_2} \overline{w}(p) \left[1 + \frac{\chi_2 k_2}{2p \cdot \lambda_2}\right].
$$
 (3.10)

We may now make the identification

$$
\overline{w}(p)\left|1+\frac{\chi_2k_2}{2p\cdot\lambda_2}\right|=\overline{w}(p_s),\qquad(3.11)
$$

since both spinors satisfy the same Dirac equation —the

first of Eqs. (3.6)—and, by virtue of the relation $\lambda_2 \cdot k_2 = 0$, the same normalization condition. Similarly, we have

$$
\frac{q_1 - k_2 + m_1}{2q_1 \cdot k_2} \chi_2 u(q_1) = \left[1 - \frac{k_2 \chi_2}{2q_1 \cdot \lambda_2} \right] u(q_1) \frac{q_1 \cdot \lambda_2}{q_1 \cdot k_2}
$$

$$
= u(q_{1s}) \frac{q_1 \cdot \lambda_2}{q_1 \cdot k_2}, \qquad (3.12)
$$

where we used

$$
(\boldsymbol{q}_{1s} - m_1) \left[1 - \frac{k_2 \lambda_2}{2q_1 \cdot \lambda_2} \right] u(q_1) = 0 , \qquad (3.13)
$$

and the equality of normalizations to establish the second equality in Eq. (3.12). In this notation the soft-photon approximation takes on the same form as that shown in Eq. (3.4) for the spin-zero case, with the dissociation amplitude reinterpreted according to the defining relation $(3.7).$

IV. EXTERNAL-FIELD APPROACH

A variational method has been applied [6] to the study of a bound-free transition in an external (classical) field consisting of two components, one weak and of frequency well above that required for ionization, and the other intense and of low frequency. Here we outline a relativistic extension of that method and show that the variational approximation reduces, in the weak-coupling limit of the low-frequency field, to the soft-photon approximation obtained above for the bound-state Compton amplitude. This is the expected result since the effect of the intense field on the ejected electron is accounted for by a distorted (Volkov $[11]$) wave which may be thought of as arising from the summation of the perturbation expansion of the propagator of the electron in the field. The result provides a connection between spontaneous and stimulated radiative processes which may be of some interest and for this reason we have included the following alternative derivation of the soft-photon approximation.

Consider a Dirac electron described by the Hamiltonian

$$
H = \boldsymbol{\alpha} \cdot (-i \nabla - e \mathbf{A}) + \beta m + V , \qquad (4.1)
$$

with the potential V assumed here to be of short range for simplicity. The 4-vector potential (in the Coulomb gauge) is $(0, A)$ with

$$
\mathbf{A}(x) = \mathbf{A}_1 \cos(k_1 \cdot x) + \mathbf{A}_2 \cos(k_2 \cdot x) , \qquad (4.2)
$$

where the subscripts ¹ and 2 refer, respectively, to the high- and low-frequency fields, and x is the 4 vector (t, r) . The electron makes a transition from an initial (field-free) bound state $\phi(\mathbf{r})$ with energy E_0 to a final state $u_{\mathbf{p}}^{(-)}(\mathbf{r})$ with momentum **p** and energy E_p . A variational expression for the S matrix element for this transition is given by

$$
S \simeq i \int d^4x \left[\Psi_p^{(-)}(x) \right]^\dagger \left[H - i \frac{\partial}{\partial t} \right] \Psi_0(x) \ . \tag{4.3}
$$

The trial functions are chosen in close analogy with the functions introduced in Ref. [6]. Thus we take

$$
\Psi_0(x) = \exp(-iE_0 t + ie \mathbf{A} \cdot \mathbf{r})\phi(\mathbf{r}) .
$$
 (4.4)

In the approximation that terms of second order in A_1 and of first order in ω_2 are ignored we find that, with $\tau \equiv k_2 \cdot x$,

$$
(3.13) \qquad \left[H - i \frac{\partial}{\partial t} \right] \Psi_0(x) = \exp(-iE_0 t + ie \mathbf{A}_2 \cdot \mathbf{r} \cos \tau)
$$
\n
$$
\times [-e(\omega_1 - \alpha \cdot \mathbf{k}_1) \mathbf{A}_1 \cdot \mathbf{r} \sin k_1 \cdot x] \phi(\mathbf{r}).
$$
\n
$$
(4.5)
$$

Since the weak-field amplitude A_1 enters linearly in this expression the effect of this field may be ignored in the construction of the final-state trial function. This function is chosen as a relativistic generalization [12] of that introduced some time ago by Kroll and Watson [13] in their (nonvariational) treatment of scattering in a lowfrequency field. It has the form

$$
\Psi_p^{(-)}(x) = \exp[-iE_p t + ie \mathbf{A}_2 \cdot \mathbf{r} \cos \tau - i \Phi(x)] u_{p(\tau)}^{(-)}(\mathbf{r}).
$$
\n(4.6)

Here we have defined the shifted momentum

$$
\mathbf{p}(\tau) = \mathbf{p} - e \mathbf{A}_2 \cos \tau + \mathbf{k}_2 I_p , \qquad (4.7)
$$

with

$$
I_p(\tau) = \frac{1}{2k_2 \cdot p} \left[-2e \mathbf{p} \cdot \mathbf{A}_2 \cos \tau + e^2 A_2^2 \cos^2(\tau) \right]. \tag{4.8}
$$

The phase function in Eq. (4.6) is

$$
\Phi(x) = \int_0^{\tau} I_p(\tau') d\tau' + \mathbf{k}_2 \cdot \mathbf{r} I_p(\tau) . \qquad (4.9)
$$

The term in Eq. (4.8) that is quadratic in the vector potential will be ignored since it contributes to two-photon processes (and to the ponderomotive level shift) and we are ultimately concerned with the transition in which a single soft photon is emitted in the weak-coupling limit. With this simplification the phase function reduces to

$$
\Phi(x) = -\rho(\sin \tau + \mathbf{k}_2 \cdot \mathbf{r} \cos \tau) , \qquad (4.10)
$$

with

$$
\rho = \frac{e \mathbf{p} \cdot \mathbf{A}_2}{p \cdot k_2} \tag{4.11}
$$

and the shifted momentum becomes $p(\tau) = p - e A_2 cos \tau - k_2 \rho cos \tau$. An examination of the formal expression for the error in the variational approximation shows that with the above choice of trial functions it is of first order in ω_2 . (An estimate of the coefficient of ω_2 in this error term can be obtained following the procedure of Ref. [6]; however, this is unnecessary for our present purposes and we shall not pursue it further.)

The scalar product $k_2 \cdot r$ may be treated as a quantity of first order since it appears in the convergent spatial integral shown in Eq. (4.3). Accordingly, we may replace the factor sin $\tau + \mathbf{k}_2 \cdot \mathbf{r}$ cos τ in Eq. (4.10) by sin $\omega_2 t$. Similar reasoning allows us to replace the shifted momentum $p(\tau)$ by $p(\omega_2 t)$. In calculating the time integral in Eq. (4.3) we encounter terms corresponding to both the absorption and emission of a photon of frequency ω_1 . Since we are interested in the former term we may replace $\sin k_1 \cdot x$ by $(i/2) \exp(-ik_1 \cdot x)$. The variational approximation then becomes

$$
S \cong i \int_{-\infty}^{\infty} dt \, \exp[i(E_{\mathbf{p}} - E_0 - \omega_1)t]
$$

× $\exp(-i\rho \sin \omega_2 t)D(\mathbf{p}(\omega_2 t))$, (4.12)

where (with notation altered to avoid confusion with the time variable t)

$$
D(\mathbf{p}) \equiv \int d\mathbf{r} \left[u_{\mathbf{p}}^{(-)}(\mathbf{r}) \right]^{\dagger} \frac{e}{2i} (\omega_1 - \alpha \cdot \mathbf{k}_1) \mathbf{A}_1 \cdot \mathbf{r} \exp(i \mathbf{k}_1 \cdot \mathbf{r}) \phi(\mathbf{r})
$$
\n(4.13)

represents the (off-shell) photodetachment amplitude. [It is a simple matter to identify this amplitude with the matrix element of the interaction $-e\alpha \cdot A_1 \exp(i k_1 \cdot r)$ that arises in standard first-order perturbation theory.] The time integration in Eq. (4.12) may be carried out by first introducing the expansions, valid in the weak-coupling limit,

$$
\exp(-i\rho\sin\omega_2 t) \approx 1 - i\rho\sin\omega_2 t \quad , \tag{4.14a}
$$

$$
D(\mathbf{p}(\omega_2 t)) \cong D(\mathbf{p}) + (-e \mathbf{A}_2 - \mathbf{k}_2 \rho) \cos \omega_2 t \cdot \nabla_{\mathbf{p}} D(\mathbf{p})
$$
\n(4.14b)

Since we are interested in the emission of a soft photon we may make the replacements

$$
\cos \omega_2 t \rightarrow \frac{1}{2} \exp i \omega_2 t, \quad \sin \omega_2 t \rightarrow \frac{1}{2i} \exp i \omega_2 t.
$$

Gathering terms of the appropriate order we arrive at the soft-photon approximation [14]

$$
S \cong -2\pi i \delta (E_{\mathbf{p}} - E_0 - \omega_1 + \omega_2) \frac{e_{\mathbf{p}} \cdot \mathbf{A}_2}{2p \cdot k_2} D(\mathbf{p}_s) \quad (4.15)
$$

The shifted momentum is

$$
\mathbf{p}_s = \mathbf{p} + \mathbf{k}_2 + \mathbf{A}_2 \frac{p \cdot k_2}{\mathbf{p} \cdot \mathbf{A}_2} , \qquad (4.16)
$$

which places the photodetachment amplitude D on the energy shell. The result shown in Eq. (4.15) provides the sought-for relationship between the external-field treatment of the bound-state Compton process and that obtained earlier in terms of the standard photon scattering picture. A nonrelativistic version of this relationship follows from the weak-field limit of the low-frequency approximtion given in Eq. (2.22) of Ref. [6].

V. DISCUSSION

The soft-photon approximation, first derived by Low [4] for bremsstrahlung and then extended by others to treat a number of different processes involving lowfrequency radiation, provides an accurate representation of the transition amplitude, in analytic form. It is essentially model independent, requiring as input the physical amplitude for the transition taking place with no softphoton emission. The fact that only the on-shell amplitude is required is rather remarkable since it is not only the dominant, nearly singular, term in the low-frequency expansion that is obtained but the next term as well. While applicable to only a limited portion of the spectrum, its predictions can provide useful reference points for more extensive calculations based on specific models $[1,2]$.

We have outlined three quite different methods for the development of soft-photon approximations for inelastic photon scattering from bound electrons, each with its own advantages and limitations. In the procedure of Sec. II the calculation was reduced to the evaluation of an integral of the same form that arises in the analysis of lowfrequency bremsstrahlung. This enables us to make use of a method developed earlier for treatment of that process [5], based on the fact that for small energy transfer to the field the main contribution to the integral comes from the asymptotic domain of configuration space. This method has the advantage that long-range Coulomb effects can be accounted for by introducing the known Coulomb modifications of the asymptotic forms of the continuum wave function and Green's function. In Sec. III a variant of Low's treatment of bremsstrahlung, based on gauge invariance and analyticity in the context of a relativistic formulation, was applied to the photon scattering problem. While otherwise impressive in its generality, the method cannot be applied to the ionization of a neutral target; the analyticity assumption breaks down in such cases as evidenced by the appearance of terms in the low-frequency approximation derived in Sec. II (see also Ref. $[1]$) which depend logarithmically on the frequency. A third method, described in Sec. IV, is based on the assumption that the spontaneous emission process of interest here may be obtained from the amplitude for ionization in the presence of an external low-frequency field by taking the weak-field limit. This turns out to be the case, as seen by comparison of the result with those derived earlier, in Secs. II and III, from the photon scattering picture. A variational procedure, a relativistic extension of a method described in much greater detail elsewhere [6], was used to derive the low-frequency approximation for ionization in the presence of an external field. We remark, in conclusion, that the different techniques used here in the derivation of the soft-photon approximation are united by the concept of gauge invariance. This concept is used most directly in Low's method as applied in Sec. III. It should be noted, however, that an essential feature of each of the other two calculations is a transformation of the electron-field interaction from the "velocity" gauge to the "length" gauge, and this is justified, ultimately, by the invariance of the theory under such transformations.

ACKNOWLEDGMENTS

This work was supported in part by the National Science Foundation under Grant No. PHY-9019745.

- [1] M. Gavrila, Phys. Rev. A 6, 1348 (1972).
- [2] T. Surić, P. M. Bergstrom, K. Pisk, and R. H. Pratt, Phys. Rev. Lett. 67, 189 (1991).
- [3] See the papers cited in Ref. [2].
- [4] F. E. Low, Phys. Rev. 110, 974 (1958).
- [5] L. Rosenberg, Phys. Rev. A 27, 1879 (1983).
- [6] F. Zhou and L. Rosenberg, Phys. Rev. A 44, 3270 (1991).
- [7] See, for example, L. Schiff, Quantum Mechanics (McGraw-Hill, New York, 1968), Sec. 21.
- [8] Integrals with a factor of r^s in the integrand, with $s=1$ and 2, appear, and these too are calculable. A contribution with $s = -1$ has been neglected. As shown in Ref.

[5], this introduces an error of order $\omega_2 \ln \omega_2$, as reflected in the error estimate in Eq. (2.14).

- [9] L. S. Brown and R. G. Goble, Phys. Rev. 173, 1505 (1968).
- [10] J. D. Bjorken and S. D. Drell, Relativistic Quantum Mechanics (McGraw-Hill, New York, 1964).
- [11] D. M. Volkov, Z. Phys. 94, 250, 1935.
- [12] L. Rosenberg and F. Zhou, J. Phys. A 24, 631 (1991).
- [13] N. M. Kroll and K. M. Watson, Phys. Rev. A 8, 804 (1973).
- [14]The origin of the factor of 2 in the denominator of Eq. {4.15) may be traced to the choice of the space-time dependence of the vector potential as $\frac{1}{2}(e^{i\tau}+e^{-i\tau}).$