

## Variational formulation and low-frequency approximation for Coulomb scattering in a laser field

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The theory of scattering of a charged particle in the presence of a laser field is formulated variationally. If the field is slowly varying, its dominant effect over a wide range of field intensities will be to modify the asymptotic motion of the projectile. A trial function is chosen which correctly accounts for the projectile-field interaction in asymptotic states. It leads to a variational approximation for the transition amplitude which generalizes earlier versions of the low-frequency approximation in two respects. Firstly, the field is not restricted to be of the form of a monochromatic plane wave but, more realistically, is taken to be a pulse of finite length. Secondly, the target may carry a net charge. The dependence of the transition amplitude on the variable  $\Delta E$ , which represents the energy transferred to the field, is modified by the presence of the long-range Coulomb interaction; additional terms which depend logarithmically on  $\Delta E$  are found. The variational expression for the transition amplitude consists of two factors, one depending only on the external field and the other representing the amplitude for single-photon spontaneous bremsstrahlung. The present analysis of this bremsstrahlung amplitude is based on the assumption that  $\Delta E$  is sufficiently small so that the dominant contribution to the spatial integration comes from the asymptotic domain. The low-energy approximation obtained in this way provides a generalization of Low's theorem on spontaneous bremsstrahlung to include the effect of the Coulomb tail.

### I. INTRODUCTION

Variational methods have provided a powerful tool in electron-atom scattering calculations. It seems reasonable to expect that they will also prove useful in dealing with situations, currently of some interest, in which the collision takes place in the presence of an external radiation field. If one adopts the simplest representation of the field—a monochromatic plane wave of infinite extent—the scattering problem takes on a form which closely resembles the usual time-independent version of the theory and variational principles for the transition amplitude of the Kohn or Schwinger type are easily derived.<sup>1</sup> In more realistic models the field is represented as a traveling pulse of radiation and stationary-state methods are inapplicable. Rather, one may apply the variational principle for the time-evolution operator given by Lippmann and Schwinger<sup>2</sup> to this time-dependent scattering problem. Here we indicate the utility of the variational approach by using it in the Lippmann-Schwinger version to derive an approximation applicable to scattering in an intense, slowly varying external field. The variational principle is well suited for

this study since the basic physical approximation, namely, that over a wide range of intensities a slowly varying field has its dominant effect on the asymptotic motion of the system,<sup>3</sup> is easily incorporated by an appropriate choice of trial function. Furthermore, the first-order correction term in the approximation for the transition amplitude appears automatically in the variational approach. As will be seen in this paper, the derivations are simpler and the results are of a more general character than those reported previously.<sup>3-6</sup> One would also expect this method to provide the basis for systematic improvements in the approximation procedure.

We shall be particularly concerned here with the case where both the target and projectile carry a net charge (electron-ion scattering). Effects of the long-range Coulomb tail can be accounted for by suitable modification of the asymptotic form of trial functions. The small parameter in the problem is the energy  $\Delta E$  which is transferred from the atomic system to the field. As will be shown, the expansion of the transition amplitude in powers of  $\Delta E$ , previously derived for scattering by a short-range potential in a monochromatic field,<sup>4</sup> is modified in the Coulomb case by the presence of terms which

depend logarithmically on  $\Delta E$ . This is seen to be a direct consequence of the logarithmic phase factor which appears in the asymptotic form of the Coulomb wave function. The matrix element analyzed here is precisely the one which determines the spontaneous single-photon bremsstrahlung amplitude. [The influence of the external field is contained in a multiplicative factor, as shown in Eq. (2.28) below.] Our result therefore provides a generalization, to include the effect of the Coulomb tail, of the well-known soft-photon approximation obtained by Low.<sup>7</sup> The appearance, in the modified Low formula given in Eq. (3.28) below, of a function containing a logarithmic singularity could have been anticipated from an examination of Sommerfeld's exact expression for the bremsstrahlung matrix element for scattering in a pure Coulomb potential.<sup>8</sup> Terms which depend logarithmically on the photon frequency appear in classical treatments as well.<sup>9</sup> Here the problem is done quantum mechanically and allows for a potential which contains a short-range component in addition to the Coulomb term.

The fact that the present treatment allows for laser pulses of finite length is significant since it enables us to develop a proper physical picture of the interaction based on wave packets which spend only a finite amount of time in the field.<sup>10</sup> Effectively,

$$\chi_{\vec{p}}^{(+)}(\vec{r}, t; 0) = (2\pi\hbar)^{-3/2} \exp(i/\hbar) \left[ -E_{\vec{p}} t + \vec{p} \cdot \vec{r} + \frac{gm}{p} \ln[(pr - \vec{p} \cdot \vec{r})/\hbar] \right]. \quad (2.1)$$

Here  $E_{\vec{p}} = p^2/2m$  and  $r$  is the distance of the electron from the target, the latter being taken to be fixed. Effects of the internal structure and the target are ignored here to simplify the discussion. Wave packets are to be constructed by taking a superposition of functions of the form (2.1) corresponding to different values of the momentum  $\vec{p}$ . As is readily demonstrated,<sup>16</sup> the packets are concentrated about the classical trajectories corresponding to motion in the Coulomb potential. In the following the asymptotic states will be interpreted according to the wave-packet picture, although, to avoid an excessively cumbersome notation, we shall not explicitly carry out the wave-packet construction.

Suppose now that the electron has entered the field but is sufficiently far from the target so that the scattering potential is still well approximated by the Coulomb tail  $g/r$ . The wave function

the electron-field interaction is cut off asymptotically. As observed previously,<sup>11</sup> the cutoff is necessary in treating the limiting case of a static field; without it the asymptotic electron momenta would be unbounded. The cutoff is also of particular significance in Coulomb scattering since one would otherwise be obliged to build into the trial function the distortion by the field of the asymptotic form of the Coulomb wave function, thereby complicating the calculation considerably. The omission of such distortion effects in earlier treatments of Coulomb scattering in a monochromatic laser field<sup>12-15</sup> could perhaps be justified by appealing to the wave-packet picture and treating the monochromatic wave as a limiting case of a finite pulse, but we make no attempt to do so here.

## II. VARIATIONAL PRINCIPLE

### A. Formulation

The laser field is taken to be a pulse of radiation traveling in the  $z$  direction and described by the classical vector potential  $\vec{A}(\tau)$ , where  $\tau = t - z/c$ , with  $\vec{A}(\tau) = 0$  for  $|\tau| > \tau_0$ . The incident electron, in the period before it enters the field, moves under the influence of the Coulomb potential  $g/r$ ; its wave function is assumed to be of the form

$\chi_{\vec{p}}^{(+)}(\vec{r}, t; \vec{A})$  satisfies the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \chi_{\vec{p}}^{(+)}}{\partial t} = \left[ \frac{(-i\hbar \vec{\nabla} - e\vec{A}/c)^2}{2m} + \frac{g}{r} \right] \chi_{\vec{p}}^{(+)} \quad (2.2)$$

which has the approximate solution

$$\chi_{\vec{p}}^{(+)}(\vec{r}, t; \vec{A}) = \chi_{\vec{p}}^{(+)}(\vec{r}, t; 0) \exp[i\Phi_{\vec{p}}^{(+)}(\tau)/\hbar] \quad (2.3a)$$

with

$$\Phi_{\vec{p}}^{(+)}(\tau) = -(1 - p_z/mc)^{-1} \int_{-\tau_0}^{\tau} \left[ \frac{-e\vec{p} \cdot \vec{A}(\tau')}{mc} + \frac{e^2 A^2(\tau')}{2mc^2} \right] d\tau'. \quad (2.3b)$$

Corrections to this approximation are of two types. First, there are correction terms of order  $H_I/mc^2$ , where  $H_I$  is the electron-field interaction energy.<sup>11</sup> Such terms are properly neglected in the present nonrelativistic treatment of the problem. Second, there is a term in the Schrödinger equation of the form

$$\left[ -\frac{e\vec{A}(\tau)}{mc} \cdot (-i\hbar\vec{\nabla} - \vec{p}) \chi_{\vec{p}}^{(+)}(\vec{r}, t; 0) \right] \times \exp[i\Phi_{\vec{p}}^{(+)}(\tau)/\hbar]$$

$$\chi_{\vec{p}}^{(-)}(\vec{r}, t; \vec{A}) = (2\pi\hbar)^{-3/2} \exp(i/\hbar) \left[ -E_{\vec{p}} t + \vec{p}' \cdot \vec{r} - \frac{gm}{p'} \ln[(p'r + \vec{p}' \cdot \vec{r})/\hbar] + \Phi_{\vec{p}}^{(-)}(\tau) \right], \quad (2.4a)$$

with

$$\Phi_{\vec{p}}^{(-)}(\tau) = -(1 - p'_z/mc)^{-1} \int_{\tau_0}^{\tau} \left[ -\frac{e\vec{p}' \cdot \vec{A}(\tau')}{mc} + \frac{e^2 A^2(\tau')}{2mc^2} \right] d\tau'. \quad (2.4b)$$

It will be convenient in the following to introduce a constant shift in phase which allows us to replace  $\Phi_{\vec{p}}^{(-)}$  by  $\Phi_{\vec{p}'}^{(+)} \equiv \Phi_{\vec{p}'}$ .

The wave function  $\psi_{\vec{p}}^{(+)}$ , which evolves from the initial state  $\chi_{\vec{p}}^{(+)}$ , satisfies

$$\left[ i\hbar \frac{\partial}{\partial t} - H \right] \psi_{\vec{p}}^{(+)}(\vec{r}, t) = 0, \quad (2.5)$$

where  $H$  is the full Hamiltonian, including the short-range component of the projectile-target interaction. Formally, we have [writing  $\chi_{\vec{p}}^{(+)}(\vec{r}, t')$  rather than  $\chi_{\vec{p}}^{(+)}(\vec{r}, t'; \vec{A})$  to simplify notation]

$$\psi_{\vec{p}}^{(+)}(\vec{r}, t) = \lim_{t' \rightarrow -\infty} i \int G^{(+)}(\vec{r}, t; \vec{r}', t') \times \chi_{\vec{p}}^{(+)}(\vec{r}', t') d^3 r',$$

where  $G^{(+)}$  is the retarded Green's function satisfying

$$\left[ i \frac{\partial}{\partial t} - \frac{1}{\hbar} H \right] G^{(+)}(\vec{r}, t; \vec{r}', t') = \delta(\vec{r} - \vec{r}') \delta(t - t') \quad (2.7)$$

which is neglected in constructing the asymptotic solution. The error thus incurred is corrected variationally, as we shall see below. It is important to note that while the factor  $(-i\hbar\vec{\nabla} - \vec{p})\chi_{\vec{p}}^{(+)}$  vanishes only like  $\chi_{\vec{p}}^{(+)}/r$  for large  $r$ , the error term displayed above is proportional to  $\vec{A}(\tau)$  and this factor vanishes in the wave-packet picture in the very early stages before the electron has entered the field.

The asymptotic states appropriate to the post-collision stage are taken to be

with  $G^{(+)}(\vec{r}, t; \vec{r}', t') = 0$  for  $t < t'$ . The  $S$ -matrix element of interest may then be expressed as

$$\begin{aligned} S_{\vec{p}'\vec{p}} &= \lim_{t \rightarrow \infty} \int \chi_{\vec{p}}^{(-)*}(\vec{r}, t) \psi_{\vec{p}}^{(+)}(\vec{r}, t) d^3 r \\ &= \lim_{\substack{t \rightarrow \infty \\ t' \rightarrow -\infty}} i \int \chi_{\vec{p}}^{(-)*}(\vec{r}, t) G^{(+)}(\vec{r}, t; \vec{r}', t') \\ &\quad \times \chi_{\vec{p}}^{(+)}(\vec{r}', t') d^3 r d^3 r'. \end{aligned} \quad (2.8)$$

The defining relation (2.7) for the Green's function may be represented symbolically as

$$G^{(+)} = \left[ i \frac{\partial}{\partial t} - \frac{1}{\hbar} H \right]^{-1}.$$

Now a variational principle for any object  $O$  whose inverse  $O^{-1}$  is known follows directly from the identity

$$O = O_t - O(O^{-1}O_t - 1), \quad (2.9)$$

where  $O_t$  is an estimate of  $O$ ; replacing  $O$  on the right-hand side by a trial function  $\tilde{O}_t$  (which may be different from  $O_t$ ) introduces an error of second order. This procedure may now be applied to the calculation of the  $S$ -matrix element. (In the following the subscript  $t$  stands for "trial" and should not be confused with the time parameter.) We write

$$\begin{aligned} i \int G_t^{(+)}(\vec{r}, t; \vec{r}', t') \chi_{\vec{p}}^{(+)}(\vec{r}', t') d^3 r' \\ = \theta(t - t') \psi_{\vec{p}}^{(+)}(\vec{r}, t), \end{aligned} \quad (2.10)$$

and

$$i \int \chi_{\vec{p}}^{(-)*}(\vec{r}'', t'') G^{(+)}(\vec{r}'', t''; \vec{r}, t) d^3 r'' \\ = \theta(t'' - t) \psi_{\vec{p}}^{(-)*}(\vec{r}, t), \quad (2.11)$$

where  $\theta$  is the step function, and define the trial  $S$ -matrix element as

$$S_{\vec{p}' \vec{p}} = S_{\vec{p}' \vec{p} t} + \frac{1}{i\hbar} \int_{-\infty}^{\infty} dt \int d^3 r \psi_{\vec{p}}^{(-)*} \left[ H - i\hbar \frac{\partial}{\partial t} \right] \psi_{\vec{p} t}^{(+)}(\vec{r}, t). \quad (2.13)$$

Let us now establish the relationship between the  $S$ -matrix element and the amplitude of the outgoing-wave component of the wave function. Writing  $\psi_{\vec{p}}^{(+)} = \chi_{\vec{p}}^{(+)} + \tilde{\psi}_{\vec{p}}^{(+)}$  we have, from Eq. (2.8),

$$S_{\vec{p}' \vec{p}} = S_{\vec{p}' \vec{p}}^{(1)} + S_{\vec{p}' \vec{p}}^{(2)}. \quad (2.14a)$$

Here

$$S_{\vec{p}' \vec{p}}^{(1)} \equiv \lim_{t \rightarrow \infty} \int \chi_{\vec{p}}^{(-)*}(\vec{r}, t) \chi_{\vec{p}}^{(+)}(\vec{r}, t) d^3 r \quad (2.14b)$$

vanishes due to the presence of a rapidly oscillating logarithmic phase in the integrand.<sup>17</sup> We are then left with

$$\tilde{\psi}_{\vec{p}}^{(+)}(\vec{r}, t) \sim (2\pi\hbar)^{-3/2} \int_0^{\infty} dE_{\vec{q}} F^{(+)}(\vec{q}, \vec{p}) \exp \left[ (i/\hbar) \left( -E_{\vec{q}} t + q r - \frac{gm}{q} \ln(2qr/\hbar) + \Phi_{\vec{q}}(\tau) \right) \right] / r, \quad (2.15)$$

where  $\vec{q} = q\hat{r}$ , the caret denoting a unit vector. The angular integration in Eq. (2.14c) may now be performed using an integration by parts procedure, with only the dominant asymptotic contribution retained; this fixes  $\hat{r}$  in the direction of  $\vec{p}'$ .<sup>18</sup> To keep the radial integration well defined as  $E_{\vec{q}}$  varies in the neighborhood of  $E_{\vec{p}'}$ , a small positive imaginary part is temporarily added to  $E_{\vec{q}}$ . The radial integral, with only its most singular part retained, becomes

$$(2\pi) \frac{i\hbar}{p'} \int_0^{\infty} dr \exp[i(q - p')r/\hbar] \\ \rightarrow (-4\pi) \frac{\hbar^2}{2m} \frac{1}{E_{\vec{q}} - E_{\vec{p}'}}.$$

Here we have allowed the integration, which should have been cut off at some large radius  $r_0$ , to extend into the origin. The evaluation of the dominant singular contribution is unaffected by these approximations. After making use of the identity

$$S_{\vec{p}' \vec{p} t} = \lim_{t \rightarrow +\infty} \int \chi_{\vec{p}}^{(-)*}(\vec{r}, t) \psi_{\vec{p} t}^{(+)}(\vec{r}, t) d^3 r. \quad (2.12)$$

Applying the identity (2.9) to  $G^{(+)}$  and then forming the matrix element (2.8), we obtain the identity

$$S_{\vec{p}' \vec{p}}^{(2)} \equiv \lim_{t \rightarrow \infty} \int \chi_{\vec{p}}^{(-)*}(\vec{r}, t) \tilde{\psi}_{\vec{p}}^{(+)}(\vec{r}, t) d^3 r. \quad (2.14c)$$

This term is nonvanishing in spite of the rapid oscillations of the integrand as  $t \rightarrow \infty$  since the spatial integration is singular. Now the contribution from any finite spatial domain is nonsingular so that we may confine our attention to the asymptotic region. The scattered wave  $\tilde{\psi}_{\vec{p}}^{(+)}$  may be expressed as a superposition of outgoing-wave solutions of the Schrödinger equation corresponding to different values of the final-state energy; this accounts for the fact that energy may be transferred to or from the field. We therefore write, for  $r \rightarrow \infty$ ,

$$\lim_{t \rightarrow \infty} \frac{\exp[i(E_{\vec{p}'} - E_{\vec{q}})t/\hbar]}{E_{\vec{q}} - E_{\vec{p}'}} = -2\pi i \delta(E_{\vec{q}} - E_{\vec{p}'}), \quad (2.16)$$

we find

$$S_{\vec{p}' \vec{p}}^{(2)} = (-2\pi i)(-4\pi)(\hbar^2/2m)(2\pi\hbar)^{-3} F(\vec{p}', \vec{p}). \quad (2.17)$$

It is clear that, for consistency, this same connection between the  $S$ -matrix element and the amplitude of the outgoing wave must be maintained in choosing the trial function and trial  $S$ -matrix element in Eq. (2.13).

In the absence of the external field energy is conserved so that

$$F(\vec{p}', \vec{p}) = \delta(E_{\vec{p}'} - E_{\vec{p}}) f(\vec{p}', \vec{p}). \quad (2.18)$$

We then have the familiar result

$$S_{\vec{p}' \vec{p}}^{(2)} = -(2\pi i) \delta(E_{\vec{p}'} - E_{\vec{p}}) t(\vec{p}', \vec{p}) \quad (2.19)$$

with the  $t$ -matrix element related to the scattered-wave amplitude according to

$$t(\vec{p}', \vec{p}) = (-4\pi)(\hbar^2/2m)(2\pi\hbar)^{-3} f(\vec{p}', \vec{p}). \quad (2.20)$$

### B. Low-frequency approximation

We assume in the following that the external field is slowly varying relative to the collision time and that it is not strong enough to appreciably affect the

target system. The field will then have its dominant effect on the asymptotic motion of the projectile. This suggests the choice of trial function

$$\psi_{\vec{p}t}^{(+)}(\vec{r}, t) = \exp(i/\hbar)[-E_{\vec{p}}t + \Phi_{\vec{p}}(\tau)]u_{\vec{p}}^{(+)}(\vec{r}), \quad (2.21)$$

where  $u_{\vec{p}}^{(+)}$  is the outgoing-wave solution of the time-independent Schrödinger equation in the absence of the field. It has the asymptotic form

$$u_{\vec{p}}^{(+)}(\vec{r}) \sim (2\pi\hbar)^{-3/2} \left[ \exp(i/\hbar) \left[ \vec{p} \cdot \vec{r} + \frac{gm}{p} \ln[(pr - \vec{p} \cdot \vec{r})/\hbar] \right] + r^{-1} f(p\hat{r}, \vec{p}) \exp(i/\hbar) \left[ pr - \frac{gm}{p} \ln(2pr/\hbar) \right] \right] \quad (2.22)$$

for  $r \rightarrow \infty$ . To account for the structure of the target this form is to be multiplied by the wave function of the target system in the initial state, undistorted by the field in first approximation. (The variational approximation will then be correct to first order in the target-field interaction strength.) Associated with the trial function (2.21) we have, according to Eq. (2.12), the trial  $S$ -matrix element

$$S_{\vec{p}'\vec{p}t} = -(2\pi i)\delta(E_{\vec{p}'} - E_{\vec{p}})t(\vec{p}', \vec{p})\exp(i/\hbar)[\Phi_{\vec{p}'}(\tau_0) - \Phi_{\vec{p}}(\tau_0)], \quad (2.23)$$

so that the effect of the field is limited to the introduction of a phase factor in this first approximation.

The variational principle provides a convenient framework for generating an improved estimate of the transition amplitude. The replacement of the exact wave function  $\psi_{\vec{p}t}^{(-)}$  in the identity (2.13) by a trial function  $\psi_{\vec{p}t}^{(-)}$  which involves a first-order error leads to an estimate of  $S_{\vec{p}'\vec{p}t}$  which differs only in second order from the true value. In the low-frequency approximation we have

$$\psi_{\vec{p}t}^{(-)}(\vec{r}, t) = \exp(i/\hbar)[-E_{\vec{p}}t + \Phi_{\vec{p}}(\tau)]u_{\vec{p}}^{(-)}(\vec{r}). \quad (2.24)$$

The requirement that  $u_{\vec{p}}^{(-)}$  satisfy the Schrödinger equation with incoming-wave boundary conditions allows us to make the identification

$$u_{\vec{p}}^{(-)}(\vec{r}) = [u_{-\vec{p}}^{+}(\vec{r})]^*. \quad (2.25)$$

The variational estimate is

$$S_{\vec{p}'\vec{p}v} = S_{\vec{p}'\vec{p}t} + \frac{1}{i\hbar} \int_{-\infty}^{\infty} dt \int d^3r \psi_{\vec{p}t}^{(-)*} \times \left[ H - i\hbar \frac{\partial}{\partial t} \right] \psi_{\vec{p}t}^{(+)}. \quad (2.26)$$

To simplify the integral we transform from the set of variables  $\{t, x, y, z\}$  to the set  $\{\tau, x, y, z\}$ . The term  $(E_{\vec{p}'} - E_{\vec{p}})t$ , which appears in the exponent in the integrand, then becomes  $(E_{\vec{p}'} - E_{\vec{p}})\tau + \hbar\vec{k} \cdot \vec{r}$  with

$$\hbar\vec{k} = \frac{\hat{z}}{c}(E_{\vec{p}'} - E_{\vec{p}}). \quad (2.27)$$

In the following we consider the case where  $E_{\vec{p}'} - E_{\vec{p}}$  is nonvanishing, so that the term  $S_{\vec{p}'\vec{p}t}$  makes no contribution in Eq. (2.26). The variational expression then reduces to

$$S_{\vec{p}'\vec{p}v} = \frac{1}{i\hbar} \int_{-\infty}^{\infty} d\tau \exp(i/\hbar)[\Phi_{\vec{p}'}(\tau) - \Phi_{\vec{p}}(\tau) + (E_{\vec{p}'} - E_{\vec{p}})\tau] \left[ -\frac{e\vec{A}(\tau)}{mc} + \frac{\hat{z}}{mc} \left[ \frac{-e\vec{p} \cdot \vec{A}(\tau)}{mc} + \frac{e^2 A^2(\tau)}{2mc^2} \right] \right] \cdot \left[ \int d^3r u_{\vec{p}t}^{(-)*}(\vec{r}) e^{-i\vec{k} \cdot \vec{r}} (-i\hbar\vec{\nabla} - \vec{p}) u_{\vec{p}t}^{(+)}(\vec{r}) \right]. \quad (2.28)$$

The "free-free" matrix element which appears in Eq. (2.28) is similar in form to the amplitude for single-photon spontaneous bremsstrahlung with  $\omega \equiv (E_{\vec{p}} - E_{\vec{p}'})/\hbar$  playing the role of the photon frequency. If the scattering potential is of short range the Lippmann-Schwinger integral equation for the wave function<sup>2</sup> may be used to derive an expansion of the matrix element in powers of  $\omega$ . The coefficients of the first two terms can be expressed in terms of the on-shell  $t$  matrix and its first derivative with respect to the energy variable; this is Low's result,<sup>7</sup> reproduced in Eq. (3.26). When used in conjunction with Eq. (2.28) we obtain a soft-photon approximation for scattering in an external field which generalizes earlier versions based either on the assumption of a periodic field<sup>3-6</sup> or a constant crossed field.<sup>11</sup> In Sec. III we shall be concerned with the further generalization to include the case where the potential has a Coulomb tail. The analysis based on the Lippmann-Schwinger integral equation is inapplicable in that case. Instead, we base our treatment on an asymptotic expansion of the wave function in configuration space.<sup>19</sup> To simplify notation we shall continue to ignore the effects of the internal structure of the target. However, these effects are easily incorporated in the final result [Eq. (3.28)] by reinterpreting the field-free scattering amplitude which appears there as the amplitude for scattering from a composite target.

### III. ANALYSIS OF THE BREMSSTRAHLUNG MATRIX ELEMENT

If we ignore recoil corrections of order  $p/mc$  (dipole approximation) the matrix element in Eq. (2.28) takes the form

$$u_{\vec{p}}^{(+)}(\vec{r}) \underset{r \rightarrow \infty}{\sim} (2\pi)^{-3/2} (2pr)^{-1} \sum_{l=0}^{\infty} (2l+1) i^{l+1} [u_l^{(+)*}(p, r) - S_l(p) u_l^{+}(p, r)] P_l(\hat{r} \cdot \hat{p}), \quad (3.3)$$

with

$$S_l(p) = e^{2i(\delta_l + \eta_l)}. \quad (3.4)$$

The Coulomb phase is

$$\eta_l = \arg \Gamma(l+1+in) \quad (3.5a)$$

with

$$n = gm/p, \quad (3.5b)$$

and  $\delta_l$  represents the additional phase shift arising from the fact that the scattering potential is not

$$\begin{aligned} \mathcal{M}(\vec{p}', \vec{p}) = & -\frac{e}{mc} \vec{A}(\tau) \\ & \cdot \int u_{-\vec{p}'}^{(+)}(\vec{r}) (-i \vec{\nabla}) u_{\vec{p}}^{(+)}(\vec{r}) d^3r. \end{aligned} \quad (3.1)$$

Here we have set  $\hbar=1$  for simplicity; this factor will be reinstated at the end of this paper. We have also made use of the orthogonality property of the continuum wave functions along with the relation (2.25). A standard transformation leads to the alternative form

$$\begin{aligned} \mathcal{M}(\vec{p}', \vec{p}) = & -\frac{e}{ic} (E_{\vec{p}} - E_{\vec{p}'}) \vec{A} \\ & \cdot \int u_{-\vec{p}'}^{(+)}(\vec{r}) \vec{r} u_{\vec{p}}^{(+)}(\vec{r}) d^3r, \end{aligned} \quad (3.2)$$

more convenient for our present purposes. We seek an evaluation of  $\mathcal{M}$  for small values of  $E_{\vec{p}} - E_{\vec{p}'}$ . The integral in Eq. (3.2) is singular in the limit  $E_{\vec{p}} - E_{\vec{p}'} \rightarrow 0$ . Such a singular behavior can only come from the asymptotic domain of integration. We retain the dominant contribution, then, by replacing the wave functions in Eq. (3.2) by their asymptotic forms. The integral can then be expressed in terms of the on-shell amplitude for scattering in the absence of radiation. Contributions to the integral which remain finite in the limit  $E_{\vec{p}} - E_{\vec{p}'} \rightarrow 0$  are ignored in our approximation.

To proceed, we gather together some well-known results<sup>20</sup> and write the asymptotic wave function as

purely Coulombic for small values of  $r$ . The spherical Coulomb function  $u_l^{(+)}$  satisfies the radial Schrödinger equation in the presence of the Coulomb potential and has the asymptotic form

$$\begin{aligned} u_l^{(+)}(p, r) \underset{r \rightarrow \infty}{\sim} & e^{i(pr - l\pi/2)} (2pr)^{-in} \\ & \times \left[ 1 - \frac{(l+1+in)(l-in)}{2ipr} + \dots \right]. \end{aligned} \quad (3.6)$$

If we keep only the leading term in this expansion,

and insert it into the right-hand side of Eq. (3.3), we recover the asymptotic form shown in Eq. (2.22) with the scattering amplitude replaced by its partial-wave expansion<sup>20</sup>

$$f(p\hat{r}, \vec{p}) = (2ip)^{-1} \sum_{l=0}^{\infty} (2l+1) S_l(p) P_l(\hat{r} \cdot \hat{p}). \quad (3.7)$$

By including the  $r^{-1}$  correction term in Eq. (3.6) we gain a more accurate evaluation of the matrix element (3.2) while requiring only the physical (measurable) field-free scattering parameters as input data. Terms of order  $r^{-2}$  and higher in the expansion will not be retained here. Note that if the target is a polarizable system the effective potential will contain, in addition to the Coulomb tail, a component which behaves as  $r^{-4}$  for large  $r$ . An asymptotic expansion of the radial wave function for a potential of the form  $g/r + g'/r^4$  is easily generated by an iterative procedure. One finds (for positive scattering energies) that the first two terms are correctly given by Eq. (3.6). It follows that the approximation for the bremsstrahlung matrix element to be derived below will be valid, to the stated accuracy, for scattering by a target which is both polarizable and charged.

In evaluating the radial integral in Eq. (3.2) we

make the usual assumption that the energy of the incident electron contains a small positive imaginary part which is allowed to vanish at the end of the calculation. The domain of integration should be taken to be the region outside a large sphere. Since, in the integrals encountered here, the additional contribution coming from the interior of the sphere is finite even in the limit  $E_{\vec{p}} - E_{\vec{p}'} \rightarrow 0$  and since we do not retain terms of this order in our approximation, we may simply continue the radial integration down to the origin. The integrals can be evaluated using the relation

$$\lim_{\epsilon \rightarrow 0^+} \int_0^{\infty} e^{-(\epsilon+ia)r} r^b dr = (ia)^{-1-b} \Gamma(1+b). \quad (3.8)$$

Now for  $a = \pm(p+p')$  this integral is nonsingular in the limit  $p-p' \rightarrow 0$  and therefore, according to the scheme outlined above, it is to be neglected; we retain only those terms corresponding to  $a = \pm(p-p')$  and  $\text{Re} b > -1$ . In this approximation, then, the matrix element of interest may be expressed as

$$\int u_{-\vec{p}'}^{(+)}(\vec{r}) \vec{A} \cdot \vec{r} u_{\vec{p}}^{(+)}(\vec{r}) d^3r = M(\vec{p}', \vec{p}) + M(-\vec{p}, -\vec{p}') \quad (3.9)$$

with

$$M(\vec{p}', \vec{p}) = - \int \left[ (2p'r)^{-1} \sum_{l'=0}^{\infty} (2l'+1) i^{l'+1} u_{l'}^{(+)*}(p', r) P_{l'}(-\hat{p}' \cdot \hat{r}) \right] \times \vec{A} \cdot \vec{r} \left[ (2pr)^{-1} \sum_{l=0}^{\infty} (2l+1) i^{l+1} S_l(p) u_l^{(+)}(p, r) P_l(\hat{r} \cdot \hat{p}) \right] d^3r. \quad (3.10)$$

The product of radial wave functions appearing here may be replaced, to the required accuracy, by

$$u_{l'}^{(+)*}(p', r) u_l^{(+)}(p, r) \sim e^{i(p-p')r} i^{l'-l} (2pr)^{-in} (2p'r)^{in'} [1 - (2ipr)^{-1}(l+1+in)(l-in) + (2ip'r)^{-1}(l'+1-in')(l'+in')], \quad (3.11)$$

where  $n' = (gm/p')$ . We now write

$$M(\vec{p}', \vec{p}) = M_0(\vec{p}', \vec{p}) + M_{-1}(\vec{p}', \vec{p}),$$

where  $M_0$  is obtained by keeping only the first term in square brackets on the right-hand side of Eq. (3.11);  $M_{-1}$  represents the correction arising from the second and third terms. The evaluation of  $M_0$  is straightforward. The angular integrations are performed by writing

$$\vec{A} \cdot \vec{r} = \left[ \frac{2\pi}{3} \right]^{1/2} r [(-A_x + iA_y) Y_{11}(\hat{r}) + (A_x + iA_y) Y_{1-1}(\hat{r})]. \quad (3.12)$$

(The transversality condition  $A_z = 0$  has been used here.) The addition formula

$$P_l(\hat{r} \cdot \hat{p}) = \frac{4\pi}{2l+1} \sum_{m=-l}^l Y_{lm}(\hat{r}) Y_{lm}^*(\hat{p}) \quad (3.13)$$

and the expansion<sup>21</sup>

$$Y_{1\nu}(\hat{r})Y_{lm}(\hat{r}) = \sum_{l'=l-1}^{l+1} \left[ \frac{3(2l+1)}{4\pi(2l'+1)} \right]^{1/2} \langle l'0 | 00 \rangle \langle l'm + \nu | \nu m \rangle Y_{l'm+\nu}(\hat{r}) \quad (3.14)$$

are then employed, along with the orthonormality property of the spherical harmonics. The result is

$$M_0(\vec{p}', \vec{p}) = (2m)(-2ip')^{-1} \vec{A} \cdot \hat{p}' (p-p')^{-2+i(n-n')} e^{(n-n')\pi/2} (2p)^{-in} (2p')^{in} \Gamma[2-i(n-n')] t(p\hat{p}', \vec{p}), \quad (3.15)$$

where, in introducing the physical field-free  $t$ -matrix element we have made use of Eqs. (2.20) and (3.7).

The evaluation of the correction term  $M_{-1}(\vec{p}', \vec{p})$  may be simplified by recognizing that to the required accuracy the distinction between  $p$  and  $p'$  may be ignored in the second and third terms in the square brackets in Eq. (3.11). The sum of those terms may then be rewritten as

$$(2ipr)^{-1} [l'(l'+1) - l(l+1) + 2in].$$

The contribution to the matrix element arising from the term proportional to  $2in$  can be evaluated, following the procedure outlined above for  $M_0$ , as  $[-in(p-p')/p]M_0(\vec{p}', \vec{p})$ . The remaining contribution to  $M_{-1}$  involves the angular integration (with  $\nu = \pm 1$ )

$$[l'(l'+1) - l(l+1)] \int d\Omega_{\hat{r}} Y_{l'm}^*(\hat{r}) Y_{1\nu}(\hat{r}) Y_{lm}(\hat{r}) = \int d\Omega_{\hat{r}} Y_{l'm}^*(\hat{r}) [L^2, Y_{1\nu}(\hat{r})] Y_{lm}(\hat{r}). \quad (3.16)$$

Here  $L^2$  is the square of the angular momentum operator. If we write  $L^2 = L_+L_- + L_z^2 - L_z$  and make use of some well-known properties of the operators  $L_{\pm}$  and  $L_z$ ,<sup>22</sup> the commutator may be evaluated as

$$[L^2, Y_{1\nu}] = 2Y_{1\nu} + [2 - \nu(\nu-1)]^{1/2} Y_{1\nu-1} L_+ + [2 - \nu(\nu+1)]^{1/2} Y_{1\nu+1} L_- + 2\nu Y_{1\nu} L_z. \quad (3.17)$$

The contribution to the matrix element arising from the first term on the right-hand side of Eq. (3.17) is readily determined to be  $-[(p-p')/p]M_0(\vec{p}', \vec{p})$ . Collecting contributions to  $M(\vec{p}', \vec{p})$  obtained thus far we have

$$M_0(\vec{p}', \vec{p}) [1 - (p-p')/p - in(p-p')/p] = 2m(-2ipp')^{-1} (p-p')^{-2} B(p', p) \vec{A} \cdot \vec{p}' t(p\hat{p}', \vec{p}), \quad (3.18)$$

where we have defined

$$B(p', p) \equiv e^{-|n-n'|\pi/2} \left[ \frac{|p-p'|}{2p} \right]^{i(n-n')} \left[ \frac{p'}{p} \right]^{in'} [1 + i(n-n')\gamma]. \quad (3.19)$$

In arriving at this form for  $B$  we have used the relations

$$e^{(n-n')\pi/2} (p-p')^{i(n-n')} = e^{-|n-n'|\pi/2} |p-p'|^{i(n-n')}$$

and

$$\Gamma[2-i(n-n')] = [1-i(n-n')][1+i(n-n')\gamma],$$

where  $\gamma = 0.5772157 \dots$  is the Euler-Mascheroni constant. We have also replaced  $[1-i(n-n')][1-in(p-p')/p]$  by unity, ignoring corrections of second order.

To obtain the remaining contribution to  $M_{-1}(\vec{p}', \vec{p})$  we must take into account the last three terms on the right-hand side of Eq. (3.17). The calculation, which is straightforward, will not be reproduced in detail here. The only point which deserves emphasis is that use of the relations

$$[l(l+1) - m(m \pm 1)]^{1/2} Y_{lm \pm 1}(\hat{p}') = L'_{\pm} Y_{lm}(\hat{p}')$$

and

$$m Y_{lm}(\hat{p}') = L'_z Y_{lm}(\hat{p}')$$

allows one to express the result in terms of the angular momentum operator  $\vec{L}' = -i\vec{p}' \times \vec{\nabla}_{\vec{p}'}$ , which acts on the polar angles defining the unit vector  $\hat{p}'$ . When this contribution to  $M(\vec{p}', \vec{p})$  is added to that shown on the right-hand side of Eq. (3.18) we obtain



$$M(\vec{p}', \vec{p}) = 2m(-2ipp')^{-1}(p-p')^{-2}B(p', p)\{\vec{A} \cdot \vec{p}' t(p\hat{p}', \vec{p}) + (p-p')[\hat{p}' \times (\vec{A} \times \vec{p}')] \cdot \vec{\nabla}_{\vec{p}'} t(\vec{p}', \vec{p})\}. \quad (3.20)$$

According to Eqs. (3.2) and (3.9) we have

$$\mathcal{M}(\vec{p}', \vec{p}) = -\frac{e}{ic}(E_{\vec{p}} - E_{\vec{p}'})[M(\vec{p}', \vec{p}) + M(-\vec{p}, -\vec{p}')] . \quad (3.21)$$

When combined with Eqs. (3.19) and (3.20) we obtain a generalization, taking into account the presence of the Coulomb tail, of the version of the soft-photon approximation derived by Feshbach and Yennie.<sup>23</sup> Equivalently, we may rewrite the expression in curly brackets in Eq. (3.20) as  $\vec{A} \cdot \vec{p}' t(\vec{p}', \vec{p})$ , with

$$\vec{p}'_A = \vec{p}' + m(E_{\vec{p}} - E_{\vec{p}'})\vec{A}/\vec{A} \cdot \vec{p}' . \quad (3.22)$$

Note that under the interchange  $\vec{p}' \leftrightarrow -\vec{p}$  we have  $\vec{p}'_A \leftrightarrow -\vec{p}_A$  with

$$\vec{p}_A = \vec{p} - m(E_{\vec{p}} - E_{\vec{p}'})\vec{A}/\vec{A} \cdot \vec{p} . \quad (3.23)$$

The free-free matrix element then takes the form

$$\mathcal{M}(\vec{p}', \vec{p}) = -\frac{e}{mc}(E_{\vec{p}} - E_{\vec{p}'})^{-1}[B(p', p)\vec{A} \cdot \vec{p}' t(\vec{p}'_A, \vec{p}) - B(p, p')\vec{A} \cdot \vec{p} t(\vec{p}', \vec{p}_A)] . \quad (3.24)$$

Here we have made use of the relation  $t(-\vec{p}_A, -\vec{p}') = t(\vec{p}', \vec{p}_A)$  and have replaced a factor  $(p+p')^2/4pp'$  by unity, ignoring an error of order  $(E_p - E_{p'})^2$ . Since, to the accuracy of the present calculation, we have  $p'_A = p$  and  $p_A = p'$ , the  $t$ -matrix elements appearing in Eq. (3.24) are on the energy shell.

Let us consider, as a special case, the problem of scattering by a short-range potential. The soft-photon approximation is obtained from the general form (3.24) by setting  $n = n' = 0$  so that the function  $B$  is replaced by unity, and the Feshbach-Yennie version<sup>23</sup> is regained. Low's original version of the soft-photon approximation<sup>7</sup> is obtained as follows. The amplitude  $t(\vec{q}', \vec{q})$  is expressed as a function of the scalar variables  $E = q^2/2m$  and  $\Delta^2 = (\vec{q}' - \vec{q})^2$ , i.e.,  $t(\vec{q}', \vec{q}) \rightarrow t[q^2/2m, (\vec{q}' - \vec{q})^2]$ . Thus, in Eq. (3.24), we have

$$t(\vec{p}', \vec{p}_A) \rightarrow t[E_{\vec{p}'}, \Delta_0^2 + 2(\vec{p}' - \vec{p}) \cdot \vec{A} m(E_{\vec{p}} - E_{\vec{p}'})/\vec{A} \cdot \vec{p}] .$$

This latter form is now replaced by its Taylor-series expansion about the average energy variable  $\bar{E} = (E_{\vec{p}} + E_{\vec{p}'})/2$  and the momentum-transfer-squared variable  $\Delta_0^2 = (\vec{p}' - \vec{p})^2$ . Dropping correction terms of second and higher order in  $E_{\vec{p}} - E_{\vec{p}'}$ , we have

$$t(\vec{p}', \vec{p}_A) \cong t - \frac{1}{2}(E_{\vec{p}} - E_{\vec{p}'}) \frac{\partial t}{\partial E} + 2(\vec{p}' - \vec{p}) \cdot \frac{\vec{A}}{\vec{A} \cdot \vec{p}} m(E_{\vec{p}} - E_{\vec{p}'}) \frac{\partial t}{\partial \Delta^2} , \quad (3.25a)$$

where  $t$  and its derivatives are evaluated at  $E = \bar{E}$  and  $\Delta^2 = \Delta_0^2$ . Similarly, we have

$$t(\vec{p}_A, \vec{p}) \rightarrow t + \frac{1}{2}(E_{\vec{p}} - E_{\vec{p}'}) \frac{\partial t}{\partial E} + 2(\vec{p}' - \vec{p}) \cdot \frac{\vec{A}}{\vec{A} \cdot \vec{p}'} m(E_{\vec{p}} - E_{\vec{p}'}) \frac{\partial t}{\partial \Delta^2} . \quad (3.25b)$$

Setting  $B(p', p) = B(p, p') = 1$  in Eq. (3.24) we obtain Low's formula,

$$\mathcal{M}(\vec{p}', \vec{p}) \cong -\frac{e}{mc}(E_{\vec{p}} - E_{\vec{p}'})^{-1} \vec{A} \cdot \left\{ (\vec{p}' - \vec{p}) t + (\vec{p}' + \vec{p}) \frac{1}{2} (E_{\vec{p}} - E_{\vec{p}'}) \frac{\partial t}{\partial E} \right\} . \quad (3.26)$$

If the scattering energy is close to a resonance value the  $t$  matrix will be a rapidly varying function of the energy. The Taylor-series expansion will then be inappropriate and the Feshbach-Yennie version should be used.

Returning now to the more general case we note that it is a simple matter to obtain from Eq. (3.24), with  $B$  given by Eq. (3.19), a generalization of Low's version of the soft-photon approximation. The field-free scattering is assumed to be nonresonant, and includes the effect of the Coulomb tail. A convenient expansion parameter is

$$\beta(p', p) = (p - p')/p . \quad (3.27)$$

It may be seen that the omission of higher-order terms in the asymptotic expansion (3.6) introduces errors of order  $\beta \ln \beta$ . For consistency we omit terms of this order in the expansion and obtain the approximation

$$\mathcal{M}(\vec{p}', \vec{p}) \cong -\frac{e}{mc} (E_{\vec{p}} - E_{\vec{p}'})^{-1} \vec{A} \cdot \left[ [B(p', p) \vec{p}' - B(p, p') \vec{p}] t + (\vec{p}' + \vec{p}) \frac{1}{2} (E_{\vec{p}} - E_{\vec{p}'}) \frac{\partial t}{\partial E} \right]. \quad (3.28)$$

Here  $B$  may be replaced, to the required accuracy, by the expansion<sup>24</sup>

$$B(p', p) = 1 - in\beta \ln\left(\frac{1}{2} |\beta|\right) - (n\pi/2) |\beta| - in\beta(1 + \gamma) - n^2 \beta^2 \ln^2\left(\frac{1}{2} |\beta|\right) + O(\beta^2 \ln \beta). \quad (3.29)$$

As a check on this result we have examined the low-frequency limit of Sommerfeld's<sup>8</sup> exact expression for the bremsstrahlung matrix element for scattering by a pure Coulomb potential. With terms of order  $\beta \ln \beta$  ignored we find that the result is precisely the form (3.28), with the  $t$  matrix of course being that appropriate to scattering in the potential  $g/r$ . From Eqs. (3.28) and (3.29) we see that the matrix element contains terms of order  $\beta^{-1}$ ,  $\ln \beta$ ,  $\beta^0$ , and  $\beta \ln^2 \beta$ , where  $\beta$  is a measure of the energy transferred to the field. The logarithmic terms, not present in Low's original version of the soft-photon approximation, appear as a consequence of the long-range Coulomb interaction.

When the expression (3.28) for the bremsstrahlung matrix element is combined with Eq. (2.28), the latter simplified by neglect of recoil corrections of order  $p/mc$ , we obtain a low-frequency approximation for the  $S$ -matrix element of the form

$$S_{\vec{p}' \vec{p}} \cong \frac{1}{i\hbar} \int_{-\infty}^{\infty} d\tau \exp(i/\hbar) [\Phi_{\vec{p}}(\tau) - \Phi_{\vec{p}'}(\tau) + (E_{\vec{p}'} - E_{\vec{p}})\tau] \left[ -\frac{e}{mc} \vec{A}(\tau) \cdot (E_{\vec{p}} - E_{\vec{p}'})^{-1} \right. \\ \left. \times \left[ [B(p', p) \vec{p}' - B(p, p') \vec{p}] t + (\vec{p}' + \vec{p}) \frac{1}{2} (E_{\vec{p}} - E_{\vec{p}'}) \frac{\partial t}{\partial E} \right] \right]. \quad (3.30)$$

We recall that  $t$  and its derivative are evaluated at energy  $\bar{E} = (E_{\vec{p}} + E_{\vec{p}'})/2$  and momentum-transfer-squared  $\Delta_0^2 = (\vec{p}' - \vec{p})^2$ . The  $t$  matrix which appears here is on the energy shell. The origin of this useful and interesting property is easily traced in the present derivation. The matrix element has been evaluated by replacing the wave functions by their asymptotic forms (a replacement which is valid for sufficiently small values of the energy

transferred to the field) and only on-shell scattering parameters appear in these asymptotic wave functions.

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