Photon Scattering from Bound Atomic Systems at Very High Energy*

M. L. GOLDBERGER
Palmer Physical Laboratory, Princeton, New Jersey 08540

AND

F. E. LOW
Institute for Advanced Study, Princeton, New Jersey† 08540

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The elastic scattering of photons from bound atomic systems is studied in the limit of infinitely high energy. It is found that the amplitude differs significantly from the free-particle value when the binding is strong. Explicit formulas for a spin-0 particle bound in a $1/r$ potential (both world-scalar and Coulomb) are obtained as well as power series in the coupling strength for a spin-$\frac{1}{2}$ target. The general result in the latter case is reduced to quadratures.

I. INTRODUCTION

THE elastic scattering of photons by bound atomic systems has been the subject of considerable interest from the earliest days of quantum mechanics. Recently, an exact nonrelativistic treatment (dipole approximation) for the scattering from hydrogen has been given by Gavrila.[1] No corresponding result has been obtained for high-energy photons, taking into account retardation and treating the bound electron relativistically.

We have found, in fact, that it is also quite simple to treat the relativistic case in the limit of infinite energy. Our interest in this problem stems from early work on the Kramers-Kronig dispersion relation[2] in which there was a conjecture that the limiting value of the forward amplitude was simply that of a free electron—namely, $-(e^2/m)\boldsymbol{\varepsilon}_f\cdot\boldsymbol{\varepsilon}_i$, with $\boldsymbol{\varepsilon}$ the electron charge, m its mass, and ϵ_f and $\boldsymbol{\varepsilon}_i$ the final and initial photon polarization vectors. This conjecture is wrong, and we have obtained the exact result in the form of a quadrature involving the ground-state wave function.

It is necessary to be quite explicit about what one means by photon scattering from a bound electron in the relativistic regime.[3] The point here is that the nucleus itself, treated as a fixed force center, can scatter photons because of virtual pair production, and this is of the same order in the coupling constant $\alpha=e^2/\hbar c$ as the normal scattering from the electron. (We must differentiate between α and $Z\alpha$ here; the latter is not regarded as small.) Strictly speaking, we should also consider the scattering by the Coulomb field of the electron, but this is smaller than the normal scattering by a factor of α (for a one-electron atom) and will be neglected.

We call the bound-electron scattering the scattering by the atom minus the scattering by the nuclear Coulomb field in the absence of the electron. Thus (for $a=0$, for example), the imaginary part of our bound-electron scattering amplitude f is related to total cross sections as follows:

$$(4\pi/k)\,\mathrm{Im}f=\sigma_p(k)-\sigma_c(k)\,,$$

where k is the photon frequency ($c=1$), σ_p is the total photoelectric cross section, and σ_c is the total cross section for the process of pair production where the electron is produced in the initial bound state. The contribution from pair production by the atom with the electron going to any state other than the initial bound state is precisely cancelled by the pair production in the absence of the initial electron, as long as electron-electron interactions are neglected. Technically, the desired bound-electron scattering amplitude is obtained by using the usual Feynman computational rules but taking the electron propagator as given by the exact solutions of the electron in the Coulomb field.

It is known[3] that $\sigma_p(k)\sim 1/k$ for large k and that $\sigma_p(k)=\sigma_c(k)$ for large k and thus $\mathrm{Im}f\to 0$. If this were not the case, there would be no possibility of $f(k)$ approaching a limit for large k, as may be seen from the Kramers-Kronig dispersion relation

$$f(k)=\frac{k^2}{2\pi^2}\int_0^\infty dk'\frac{\sigma_p(k')-\sigma_c(k')}{k'^2-k^2-i\eta}\,.$$

Our calculations show that $\sigma_p-\sigma_c$ goes to zero at least as fast as $1/k$, to within a factor of $\ln k$, and that $f(\infty)$ is a constant.

In Sec. II we discuss the scattering amplitude for a system consisting of a spin-$\frac{1}{2}$ particle bound to an infinitely massive force center by either a world-scalar or fourth-component four-vector potential. The general structure of the amplitude in the forward direction is

$$f=f_1\boldsymbol{\varepsilon}_f\cdot\boldsymbol{\varepsilon}_i+f_2 i\boldsymbol{\sigma}\cdot\boldsymbol{\varepsilon}_f\times\boldsymbol{\varepsilon}_i\,,$$

and we obtain formulas for both f_1 and f_2. In addition, we consider the scattering from a bound spin-0 particle. These general results are illustrated in Sec. III for the special case of a $1/r$ potential. For the spin-0 target they

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† Permanent address: Department of Physics, Massachusetts Institute of Technology, Cambridge, Mass.

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are given exactly for any potential strength, and for the spin-$\frac{1}{2}$ target we treat the potential as weak. Finally, in Sec. IV we indicate how the exact result for spin-$\frac{1}{2}$ targets may be reduced to quadratures and evaluated explicitly for a particular (large) value of the coupling strength for a scalar potential.

II. DERIVATION

A. Spin-$\frac{1}{2}$ Target

We start from the well-known expression for the scattering amplitude

$$f^{(1/2)}=e^2\{\psi_{s'},\ e^{i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{r}}\ \boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}_f[H(\mathbf{p}+\mathbf{k}_i)-k-E]^{-1}\times\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}_i\psi_s\}+\{\mathbf{k}_i\to-\mathbf{k}_f,\ k\to-k,\ \boldsymbol{\varepsilon}_f\to\boldsymbol{\varepsilon}_i\},\quad(2.1)$$

where $e^2=1/137$, ψ_s is the bound-electron wave function of spin s, $\boldsymbol{\varepsilon}_f$ and $\boldsymbol{\varepsilon}_i$ are the final and initial photon polarization vectors, and H is the Dirac Hamiltonian

$$H=\boldsymbol{\alpha}\cdot(\mathbf{p}+\mathbf{k})+\beta m+V\,,\quad(2.2)$$

with $\mathbf{p}=-i\nabla$ and V representing a fourth-component vector potential. Any world-scalar potential would be included in m. The second term in (2.1) is the usual crossed term. We are interested in the limit of high k at fixed momentum transfer $\Delta\mathbf{k}$. In this limit [since $(\Delta\mathbf{k})^2=2k^2(1-\cos\theta)$ and $(\mathbf{k}_i-\mathbf{k}_f)\cdot\hat{k}_i=-(\mathbf{k}_i-\mathbf{k}_f)\cdot\hat{k}_f=k(1-\cos\theta)$], $\mathbf{k}_i-\mathbf{k}_f$ may be taken to be essentially transverse to either $\mathbf{k}_i$ or $\mathbf{k}_f$, which may be taken in the same direction.

In order to evaluate (2.1), we study the differential equation satisfied by the function

$$g=[H(\mathbf{p}+\mathbf{k})-k-E]^{-1}X$$

in the limit $k\to\infty$:

$$[H(\mathbf{p}+\mathbf{k})-k-E]g=X\,.\quad(2.3)$$

We write $g=g_1+g_2$, where

$$g_1=\tfrac{1}{2}(1+\boldsymbol{\alpha}\cdot\hat{k})g\,,\qquad g_2=\tfrac{1}{2}(1-\alpha\cdot\hat{k})g\,,\quad(2.4)$$

and we note for later reference that $\hat{k}\equiv\mathbf{k}/k$ does not change sign for $\mathbf{k}\to-\mathbf{k}$, $k\to-k$. Multiplying Eq. (2.3) successively by $\frac{1}{2}(1\pm\alpha\cdot\hat{k})$, with the Hamiltonian given by (2.2), we obtain

$$\begin{aligned}&(E-V-\hat{k}\cdot\mathbf{p})g_1-(\boldsymbol{\alpha}\cdot\mathbf{p}+\beta m+\hat{k}\cdot\mathbf{p})g^2=-\tfrac{1}{2}(1+\boldsymbol{\alpha}\cdot\hat{k})X\,,\\&(E+2k-V+\hat{k}\cdot\mathbf{p})g_2-(\boldsymbol{\alpha}\cdot\mathbf{p}+\beta m-\hat{k}\cdot\mathbf{p})g_1=-\tfrac{1}{2}(1-\boldsymbol{\alpha}\cdot\hat{k})X\,.\end{aligned}\quad(2.5)$$

Clearly, as $k\to\infty$, g_1 stays finite, whereas $g_2\sim1/k$. The operator $E-V-\hat{k}\cdot\mathbf{p}$ has zero eigenvalues, however, and we must be a little more accurate in evaluating g_1. We remember that m^2 has an infinitesimal negative imaginary part according to the Feynman rules, $m^2\to m^2-i\eta$. To a sufficient accuracy, we may write the equation for g_1 as

$$(E-V-\hat{k}\cdot\mathbf{p}-m^2/2k)g_1=-\tfrac{1}{2}(1+\boldsymbol{\alpha}\cdot\hat{k})X\,.\quad(2.6)$$

(This is not quite correct if part of m contains a world-scalar potential, because $[\mathbf{p},m]\neq0$; however, we are concerned here with avoiding the zeros of $E-V-\hat{k}\cdot\mathbf{p}$ and hence only with the imaginary part of m^2.)

In terms of this g_1, we have for the scattering amplitude $f^{(1/2)}$

$$\frac{-f^{(1/2)}}{e^2}=\left(\psi_{s'},e^{i\Delta\mathbf{k}\cdot\mathbf{r}}\left[\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}_f\frac{\frac{1}{2}(1+\boldsymbol{\alpha}\cdot\hat{k})}{E-V-\hat{k}\cdot\mathbf{p}+i\eta}\,\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}_i+\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}_i\frac{\frac{1}{2}(1+\boldsymbol{\alpha}\cdot\hat{k})}{E-V-\hat{k}\cdot\mathbf{p}-i\eta}\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}_f\right]\psi_s\right).\quad(2.7)$$

This is our main result and is exact to zeroth order in $1/k$. It is possible to evaluate the first-order terms quite easily, but we shall not do so here. In Sec. III we shall use Eq. (2.7) for numerical calculations. Note that the dispersive part of $f^{(1/2)}$ goes like $\boldsymbol{\varepsilon}_f\cdot\boldsymbol{\varepsilon}_i$ and is thus spin-independent in the forward direction, whereas the absorptive part goes like $\boldsymbol{\sigma}\cdot\boldsymbol{\varepsilon}_f\times\boldsymbol{\varepsilon}_i$ and is pure spin-flip in the forward direction.

In the forward direction it is customary[2] to write the amplitude as

$$f^{(1/2)}=\boldsymbol{\varepsilon}_f\cdot\boldsymbol{\varepsilon}_if_i+i\boldsymbol{\sigma}\cdot\boldsymbol{\varepsilon}_f\times\boldsymbol{\varepsilon}_f\times\boldsymbol{\varepsilon}_if_2\,,\quad(2.8)$$

and we see from Eq. (2.7) the following results:

$$\begin{aligned}&\mathrm{Re}f_1\to\text{const},\quad\mathrm{Im}f_i\sim1/k;\\&\mathrm{Re}f_2\sim1/k\,,\quad\mathrm{Im}f_2\to\text{const}.\end{aligned}\quad(2.9)$$

The dispersion relation satisfied by f_1 may be written

$$f_1(k)=f_1(\infty)+\frac{2}{\pi}\int_0^\infty\frac{k'dk'}{k'^2-k^2-i\eta}\,\mathrm{Im}f_1(k')\,.\quad(2.10)$$

Since $f_1(0)=0$, we also have the sum rule

$$\begin{aligned}f_1(\infty)&=-\frac{2}{\pi}\int_0^\infty\frac{dk}{k}\,\mathrm{Im}f_1(k)\\&=-\frac{1}{2\pi^2}\int_0^\infty dk\,[\sigma_p(k)-\sigma_c(k)]\,,\end{aligned}\quad(2.11)$$

where σ_p is the total photoelectric cross section and σ_c is the cross section for pair production with the electron produced into the initial bound state. As discussed in the Introduction, the total atom-scattering amplitude is obtained by adding the Delbrück scattering of light by the potential in the absence of an atomic electron. Finally, we note that since $\mathrm{Re}f_2(k)\to0$ as $k\to\infty$, the dispersion relation for f_2 may be written

$$f_2(k)=\frac{2k}{\pi}\int_0^\infty\frac{dk'}{k'^2-k^2-i\eta}\,\mathrm{Im}f_2(k')\,;\quad(2.12)$$

using the well-known low-energy theorem, we obtain in the limit $k \to 0$ the Drell-Hearn sum rule.[4]

B. Spin-0 Target

Here the formula equivalent to Eq. (2.7) is exceedingly simple:

$$f^{(0)} = -2e^2 \boldsymbol{\varepsilon}_f \cdot \boldsymbol{\varepsilon}_i \int d^3r |\varphi(\mathbf{r})|^2 e^{i\Delta\mathbf{k}\cdot\mathbf{r}}, \qquad (2.13)$$

where φ is the target wave function. The terms in the full scattering amplitude involving energy denominators as in Eq. (2.1) go in this case like $1/k$ and may be neglected; only the so-called "sea-gull" term survives, leading to Eq. (2.13).

The normalization of φ depends on the interaction. In the case of a world-scalar potential it is

$$\varphi = \psi/(2E)^{1/2}, \qquad (2.14)$$

where $\int d^3r|\psi|^2 = 1$ and E is the energy of the bound state. Thus, for $\Delta\mathbf{k} = 0$,

$$f_s^{(0)} = -\boldsymbol{\varepsilon}_f \cdot \boldsymbol{\varepsilon}_i e^2/E. \qquad (2.15)$$

In the case of a fourth-component vector potential (as, for example, the Coulomb potential), it is

$$\varphi = \psi/[2(E-\langle V\rangle)]^{1/2}, \qquad (2.16)$$

where again $\int d^3r|\psi|^2 = 1$ and

$$\langle V\rangle = \int d^3r \psi^* V \psi. \qquad (2.17)$$

Thus, for $\Delta\mathbf{k} = 0$,

$$f_V^{(0)} = [-e^2/(E-\langle V\rangle)] \boldsymbol{\varepsilon}_f \cdot \boldsymbol{\varepsilon}_i. \qquad (2.18)$$

It is obvious from Eqs. (2.7), (2.15), and (2.18) that the nonrelativistic (i.e., small binding) limit is the same for all four cases (spin-$\frac{1}{2}$ or spin-0, scalar or vector potential), namely, the Thomson formula

$$f_{\text{N.R.}} \underset{\lambda\to\infty}{=} -(e^2/m) \boldsymbol{\varepsilon}_f \cdot \boldsymbol{\varepsilon}_i p(\Delta\mathbf{k}), \qquad (2.19)$$

where

$$p(\Delta\mathbf{k}) = \int d^3r |\psi(\mathbf{r})|^2 e^{i\Delta\mathbf{k}\cdot\mathbf{r}}. \qquad (2.20)$$

Note, however, that for $\langle V\rangle/m$ and/or $\langle p^2\rangle/m^2$ not small, the high-k limit will be far from the Thomson value even for nonsingular potentials. We also see from Eqs. (2.15) and (2.18) that the first-order binding corrections for a spin-0 particle in a Coulomb field are equal and opposite for the vector and scalar potentials, since $E \cong m + \frac{1}{2}\langle V\rangle$ and $E - \langle V\rangle \cong m - \frac{1}{2}\langle V\rangle$. We shall see in Sec. III that to first order in $\langle V\rangle/m$ the non-spin-flip amplitude for a spin-$\frac{1}{2}$ particle is equal to that of a spin-0 particle, but in the next order they are different.

[4] S. Drell and A. Hearn, Phys. Rev. Letters **16**, 908 (1966).

III. NUMERICAL EVALUATION

In this section we shall carry out explicit calculations for the four cases under consideration for the special case of a $1/r$ potential and for forward scattering.

A. Spin-$\frac{1}{2}$ World-Scalar Potential

We proceed from Eq. (2.7) by setting $V=0$. The states ψ_s are the ground-state solutions of the Dirac equation

$$E\psi_s = [\boldsymbol{\alpha}\cdot\mathbf{p} + \beta(m - \lambda/r)]\psi_s; \qquad (3.1)$$

the value of E is $m/(1+\lambda^4)^{1/2}$. We shall give in Sec. IV the exact result for a special value of λ, but content ourselves here with the first few terms in a power series. Strictly speaking, we cannot evaluate Eq. (2.7) in a series about $\lambda = 0$, since there is a logarithmic singularity in the term of order $(e^2/m)\lambda^6$. The first few terms, however, can be readily calculated and we give only the result

$$\frac{-f_S^{(1/2)}}{e^2} = \boldsymbol{\varepsilon}_f \cdot \boldsymbol{\varepsilon}_i \frac{1}{m}\left(1 + \tfrac{1}{2}\lambda^2 + \frac{5}{24}\lambda^4 + \cdots\right) - i\boldsymbol{\sigma}\cdot\boldsymbol{\varepsilon}_f \times \boldsymbol{\varepsilon}_i \frac{35i}{38m}(\lambda^5 + \cdots). \qquad (3.2)$$

B. Spin-$\frac{1}{2}$ Fourth-Component Vector Potential

Here the states ψ_s are the gound-state solutions of

$$E\psi_s = (\boldsymbol{\alpha}\cdot\mathbf{p} + \beta m - Ze^2/r)\psi_s \qquad (3.3)$$

and $E = m(1 - Z^2e^2)^{1/2}$. The power-series expansion corresponding to (3.2) is

$$\frac{-f_V^{(1/2)}}{e^2} = \boldsymbol{\varepsilon}_f \cdot \boldsymbol{\varepsilon}_i \frac{1}{m}\left(1 - \tfrac{1}{2}Z^2e^4 + \frac{5}{24}Z^4e^8 + \cdots\right) - i\boldsymbol{\sigma}\cdot\boldsymbol{\varepsilon}_f \times \boldsymbol{\varepsilon}_i \frac{11i}{48m}(Z^5e^{10} + \cdots). \qquad (3.4)$$

C. Spin-0 World-Scalar Potential

We define the potential as an addition to the mass as in (3.1):

$$E^2 = \mathbf{p}^2 + (m - \lambda/r)^2. \qquad (3.5)$$

The ground-state energy is

$$E = m\left(1 - \frac{4\lambda^2}{[1 + (1+4\lambda^2)^{1/2}]^2}\right)^{1/2}, \qquad (3.6)$$

and thus the scattering amplitude from Eq. (2.15) is simply

$$f_S^{(0)} = -\frac{e^2}{m}\left(1 - \frac{4\lambda^2}{[1 + (1+4\lambda^2)^{1/2}]^2}\right)^{-1/2} \boldsymbol{\varepsilon}_f \cdot \boldsymbol{\varepsilon}_i. \qquad (3.7)$$

The first three terms in an expansion about $\lambda^2=0$ are

$$f_s^{(0)}\cong-(e^2/m)(1+\tfrac{1}{2}\lambda^2-\tfrac{1}{2}\lambda^4+\cdots)\boldsymbol{\varepsilon}_f\cdot\boldsymbol{\varepsilon}_i. \quad (3.8)$$

Comparison of (3.2) and (3.8) shows how the coefficients of $\boldsymbol{\varepsilon}_f\cdot\boldsymbol{\varepsilon}_i$ agree to order λ^2 but deviate in order λ^4.

D. Spin-0 Fourth-Component Vector Potential

Here we choose $V=-Ze^2/r$ and

$$(E+Ze^2/r)^2=\mathbf{p}^2+m^2. \quad (3.9)$$

The ground-state energy is

$$E=m\{1+4Z^2e^4/[1+(1-4Z^2e^4)^{1/2}]^2\}^{-1/2} \quad (3.10)$$

and

$$\langle V\rangle=\frac{-4Z^2e^4}{[1+(1-4Z^2e^4)^{1/2}]^2}E, \quad (3.11)$$

so that from Eq. (2.18) we have

$$f_V^{(0)}=-\frac{e^2}{m}\left(1+\frac{4Z^2e^4}{[1+(1-4Z^2e^4)^{1/2}]^2}\right)^{-1/2}\boldsymbol{\varepsilon}_f\cdot\boldsymbol{\varepsilon}_i. \quad (3.12)$$

The first three terms in an expansion about $Z^2e^4=0$ are

$$f_V^{(0)}=-(e^2/m)(1-\tfrac{1}{2}Z^2e^4-\tfrac{1}{8}Z^4e^8+\cdots)\boldsymbol{\varepsilon}_f\cdot\boldsymbol{\varepsilon}_i, \quad (3.13)$$

which again shows the agreement to order Z^2e^4 with the coefficient of $\boldsymbol{\varepsilon}_f\cdot\boldsymbol{\varepsilon}_i$ in Eq. (3.4).

IV. REDUCTION TO QUADRATURES

It is quite simple to express our general result for a spin-$\frac{1}{2}$ target, Eq. (2.7), in terms of quadratures that could be quite easily carried out numerically. To this end we note the following relation:

$$\frac{1}{E-p_z-V\pm i\eta}\psi(\mathbf{r})=\frac{1}{2i}\int_{-\infty}^{\infty}dz'\,[\epsilon(z'-z)\pm1]\times\left[\exp\left(i\int_{z'}^{z}dz''(E-V)\right)\right]\psi(z',x,y). \quad (4.1)$$

For the case of a world-scalar potential, we set $V=0$. In the latter case it is evidently simpler to work directly in momentum space, and we find for the scattering amplitude

$$\frac{-f_S^{(1/2)}}{e^2}=\int\frac{d^3p}{(2\pi)^3}\left(\Phi_{s'}(\mathbf{p}+\Delta\mathbf{k}),\times\left[\frac{\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}_f\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}_i}{E-p_z+i\eta}+\frac{\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}_i\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}_f}{E-p_z-i\eta}\right]\tfrac{1}{2}(1-\boldsymbol{\alpha}\cdot\hat{k})\Phi_s(\mathbf{p})\right), \quad (4.2)$$

where $\Phi_s(\mathbf{p})$ is the Fourier transform of $\psi_s(\mathbf{r})$.

The special case of $\lambda=\sqrt{3}$ and forward scattering may be obtained in closed form. We use Eq. (4.2) with

$$\Phi_s(p)=N[g(p)-\tfrac{1}{3}\sqrt{3}\boldsymbol{\alpha}\cdot\nabla_p h(p)]X_s, \quad (4.3)$$

where

$$g(p)=-8\pi\left(\frac{1}{(p^2+\mu^2)^2}-\frac{2\mu^2}{(p^2+\mu^2)^3}\right),$$
$$h(p)=8\pi\mu/(p^2+\mu^2)^2, \quad (4.4)$$
$$\mu=\tfrac{3}{2}m,$$
$$N^2=9m^5\sqrt{3}/128\pi,$$

and X_s is a Pauli spinor.

The result (as a matrix in spin space) is

$$\frac{-f_S^{(1/2)}}{e^2}=\frac{1}{m}\left(\frac{13}{32}\boldsymbol{\varepsilon}_f\cdot\boldsymbol{\varepsilon}_i+\frac{9\sqrt{3}i}{240}i\boldsymbol{\sigma}\cdot\boldsymbol{\varepsilon}_f\times\boldsymbol{\varepsilon}_i\right). \quad (4.5)$$

It is clear by comparison of Eqs. (3.2) and (4.5) that the power series in λ gives no indication of the large-λ behavior.

We have not attempted to evaluate $f_V^{(1/2)}$ for special values of Ze^2, although we have noted that at least the spin-flip term can be done for $Ze^2=1$.

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