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Theory of High-Energy Potential Scattering*†

P. J. Lynch‡ and B. C. Carlson

Institute for Atomic Research and Department of Physics

Iowa State University, Ames, Iowa

The exact amplitude for scattering of a Schrödinger or Dirac particle by a static potential is rewritten in a two-potential form by splitting the potential into two parts, one of which contributes only to exactly forward scattering. Replacement of the exact wave function by a modified plane wave gives a high-energy approximation that is shown to be equivalent to the Saxon-Schiff approximation in the Schrödinger case. Corrections to the approximation are obtained in principle from a simplified series expansion of the exact wave function having the modified plane wave as leading term. The approximate amplitude reduces at small scattering angles to a well-known result; at large angles, it reduces to Schiff's stationary-phase approximation in the Dirac case but not, as shown by the example of a Gaussian potential, in the Schrödinger case.

DISCLAIMER

I. INTRODUCTION

Elastic scattering of a high-energy particle by a static potential can be calculated either by partial-wave analysis, if the potential has spherical symmetry; or by the Born approximation, if the potential is sufficiently weak; or by a less familiar high-energy approximation, if the scattering angle is sufficiently small. The last of these methods was initiated by Molière,[1] but has been developed and expounded primarily by Glauber.[2] Briefly, it consists in approximating the unknown exact wave function by a plane wave modified in phase to take account of the shift in de Broglie wavelength while the particle is passing through the potential. Its virtue is its applicability to potentials so strong that the Born approximation is useless. Its weakness is the restriction to small angles: although most of the scattering at high energies is nearly forward, the large-angle scattering is often crucial for the interpretation of an experiment.

An extension of the high-energy approximation to large angles was made by Schiff,[3] who summed the infinite Born series after approximating each term by the method of stationary phase. For both Schrödinger and Dirac particles, Schiff obtained a large-angle scattering amplitude that differs from the Born approximation by phase modification of both the initial and final plane waves. He also recovered by the same method the small-angle approximation (in which only the initial plane wave is modified in phase), but obtained no results for intermediate angles. This gap was remedied by Saxon and Schiff[4] in a paper dealing only with the Schrödinger equation. The exact scattering amplitude was recast in a form that reduces to the small-angle approximation if the exact wave function is replaced by a plane wave. The high-energy approximation consists in replacing it instead by a plane wave modified in phase. Beside providing a well-defined (although somewhat cumbersome) approximation for all angles, this new approach to the problem was used to rederive the simplified small-angle and large-angle formulas and to revise their estimated ranges of validity.

The present paper develops a two-potential formulation of the high-energy approximation for both the Schrödinger and Dirac equations. The scattering potential (assumed real, although this is not essential to the method) is split into two parts, one of which is chosen to be the potential occurring in the wave equation satisfied by a modified plane wave. Since this part contributes only to exactly forward scattering, the remaining part provides a compact rearrangement of the exact scattering amplitude for nonzero angles. The exact wave function is then replaced by a modified plane wave as a high-energy approximation.

Although an approximation of this kind for all angles has not been given previously in the Dirac case, our procedure is related to earlier work on the Schrödinger scattering problem in two ways. Lippmann[5] proposed a two-potential formalism and used it to obtain an integral equation for the wave function, but his splitting of the potential is different from ours. Secondly, our form of the high-energy approximation will be shown in Sec. III to be equivalent to Saxon and Schiff's, although the conclusions that we draw from it are at variance with theirs. Specifically, for 180° scattering from a Gaussian potential, we shall find in Sec. V the Schiff large-angle formula multiplied by $\frac{1}{2}$, plus additional terms that are small in a wide range of parameters (not including the range of validity of the Born approximation). The discrepancy is attributed to the method by which Saxon and Schiff estimate the size of discarded terms. For large-angle Dirac scattering, on the other hand, we recover the Schiff large-angle formula with no factor $\frac{1}{2}$, its absence being due to the linearity of the Dirac Hamiltonian in space derivatives.

II. TWO-POTENTIAL FORM OF THE SCATTERING AMPLITUDE

The exact amplitude for scattering of a Schrödinger particle by a scalar potential will first be rearranged in a form that is characteristic of two-potential theory and has certain advantages at high energies. In order to simplify the derivation, the potential $V(\underset{\sim}{r})$ will be assumed to vanish outside a bounded region. If the particle has energy $E = \hbar^2k^2/2m$, its wave function satisfies

$$\left[\nabla^2 + k^2 - U(\underset{\sim}{r})\right]\psi(\underset{\sim}{r}) = 0 \quad , \tag{2.1}$$

where $U(\underset{\sim}{r}) = (2m/\hbar^2)\, V(\underset{\sim}{r})$. Solutions having the asymptotic form of a plane wave plus outgoing or incoming spherical waves will be denoted by ψ^+ or ψ^-, respectively. The exact scattering amplitude f is given by the well-known expressions[6]

$$-4\pi f(\underset{\sim}{k}_f, \underset{\sim}{k}_o) = (\phi_f, U\psi_o^+) \tag{2.2a}$$

$$= (\psi_f^-, U\phi_o) \quad , \tag{2.2b}$$

where the plane waves ϕ satisfy

$$(\nabla^2 + k^2)\,\phi(\underset{\sim}{r}) = 0 \quad . \tag{2.3}$$

The subscripts on the wave functions specify whether the plane wave (or plane-wave part of the asymptotic form) has the initial wave vector $\underset{\sim}{k}_o$ or the final wave vector $\underset{\sim}{k}_f$. Each of these vectors has magnitude k and direction given by the unit vector $\hat{\underset{\sim}{k}}_o$ or $\hat{\underset{\sim}{k}}_f$. The momentum transfer $\underset{\sim}{q} = \underset{\sim}{k}_o - \underset{\sim}{k}_f$ has magnitude $q = 2k \sin(\theta/2)$, where θ is the scattering angle.

A high-energy approximation to ψ_o^+ is the modified plane wave[2]

$$\chi_o^+(\underset{\sim}{r}) = \phi_o(\underset{\sim}{r}) \exp i \delta_o(\underset{\sim}{r}) \quad , \tag{2.4}$$

where

$$\phi_o(\underset{\sim}{r}) = \exp i \underset{\sim}{k}_o \cdot \underset{\sim}{r} \quad , \tag{2.5}$$

$$\delta_o(\underset{\sim}{r}) = -(2k)^{-1} \int_0^\infty U(\underset{\sim}{r} - \hat{\underset{\sim}{k}}_o s)\, ds \quad . \tag{2.6}$$

The phase modification δ_o takes account, to first order in U/k^2, of the shift in de Broglie wavelength when the particle is inside the potential. By observing that

$$\hat{\underset{\sim}{k}}_o \cdot \underset{\sim}{\nabla}\, \delta_o(\underset{\sim}{r}) = -(2k)^{-1}\, U(\underset{\sim}{r}) \quad , \tag{2.7}$$

it is easily verified that the modified plane wave satisfies the differential equation

$$\left[\nabla^2 + k^2 - U_S(\underset{\sim}{r}) \right] \chi_o^+(\underset{\sim}{r}) = 0 \quad , \tag{2.8}$$

where

$$U_S = U - U_L \tag{2.9}$$

$$U_L = -\exp(-i\delta_o)\, \nabla^2 \exp i\delta_o \quad . \tag{2.10}$$

To express the scattering amplitude in terms of χ_o^+, we apply Green's theorem to $\chi_o^+ - \phi_o$ and $(\psi_f^- - \phi_f)^*$, the star denoting complex conjugation:

$$\int d\underset{\sim}{r}\left[(\psi_f^- - \phi_f)^* \nabla^2(\chi_0^+ - \phi_0) - (\chi_0^+ - \phi_0)\nabla^2(\psi_f^- - \phi_f)^*\right] \tag{2.11}$$

$$= \int d\underset{\sim}{S}\cdot\left[(\psi_f^- - \phi_f)^* \underset{\sim}{\nabla}(\chi_0^+ - \phi_0) - (\chi_0^+ - \phi_0)\underset{\sim}{\nabla}(\psi_f^- - \phi_f)^*\right].$$

The right side is proportional to a transition current through the surface of a large sphere; we shall first show that this current vanishes as the radius of the sphere becomes infinite. The quantities $\delta_0(\underset{\sim}{r})$ and $\chi_0^+(\underset{\sim}{r}) - \phi_0(\underset{\sim}{r})$ vanish unless $\underset{\sim}{r}$ lies either in the potential or in a semi-infinite cylinder such that a straight line proceeding from $\underset{\sim}{r}$ in the direction $-\hat{\underset{\sim}{k}}_0$ pierces the potential. This second region will be called the forward cylinder with axis in the direction $\hat{\underset{\sim}{k}}_0$. Thus the surface integral reduces to an integral over the area of intersection of the forward cylinder with the sphere. As the radius of the sphere tends to infinity, this area remains bounded because the potential vanishes outside a bounded region, but $(\psi_f^- - \phi_f)^*$ and its gradient decrease as the reciprocal radius; hence the surface integral tends to zero.

If Eqs. (2.1), (2.3), and (2.8) are substituted in the volume integral in Eq. (2.11), we obtain (for real U)

$$\left((\psi_f^- - \varphi_f),\, U_S\, \chi_0^+\right) = \left(\psi_f^-,\, U(\chi_0^+ - \varphi_0)\right) \tag{2.12}$$

By use of Eqs. (2.2b) and (2.9), this equation becomes

$$-4\pi f(\underline{k}_f, \underline{k}_0) = \left(\varphi_f,\, U_S\, \chi_0^+\right) + \left(\psi_f^-,\, U_L\, \chi_0^+\right). \tag{2.13}$$

Eq. (2.13) has a form characteristic of scattering by two potentials: the first term is the scattering by U_S alone and the second term is the scattering by U_L as modified by the presence of U_S. A similar division of the amplitude is familiar[7] in scattering problems where two physically distinct forces are acting, particularly when the scattering produced by one of them alone can be calculated exactly. In the present situation a single potential has been divided into two parts in a convenient but artificial way by introducing χ_0^+; the separate parts are not real, and they differ from zero throughout both the potential region and the forward cylinder. Because of these peculiarities, we shall have to discuss the existence of the separate terms of Eq. (2.13); also, we have felt it desirable to derive this equation by an elementary procedure for which the conditions of validity are more evident than for the operator method.[7] Our method can be used also when the two potentials both have finite range, for the surface integral in Eq. (2.11) then vanishes because of cancellation between the two terms in the integrand. With a different choice of outgoing or incoming spherical waves, the same procedure is convenient for deriving other identities between different forms of the scattering amplitude; for instance, replacement of $\chi_0^+ - \varphi_0$ by $\psi_0^+ - \varphi_0$ in Eq. (2.11) shows the equivalence of Eqs. (2.2a) and (2.2b).

As mentioned, both U_S and U_L are nonzero throughout the forward cylinder. This implies that each term of Eq. (2.13) is an integral that appears to oscillate rather than converge, although the sum of the two terms is well defined. For exactly forward or backward scattering, this appearance is illusory as each term can actually be shown to converge separately. At all other angles, it will be convenient to define the integrals separately by adding a small positive imaginary part to the component of momentum transfer along the direction $\hat{k}_0$. That is, if the z axis is chosen along this direction, we replace q_z by $q_z + i\epsilon$ and take the limit of each integral as ϵ goes to zero. The use of this Abelian definition of the integrals cannot change their sum, which is well defined in any case; from a physical point of view, one may like to think of the convergence factor $\exp(-\epsilon z)$ as a device for representing the attenuation of the geometrical shadow by diffraction effects.

Because χ_0^+ describes a particle whose direction of motion is unchanged as it passes through the potential, U_S may be expected to contribute only to exactly forward scattering, while U_L produces scattering through finite angles. The idea of splitting the potential into two parts of this kind has been discussed by Lippmann,[5] but his division of the potential is different and less explicit than the one given by Eqs. (2.9) and (2.10).

One's qualitative view of the contributions of U_S and U_L to the scattering process is confirmed by the following exact result:

$$(\varphi_f, U_S \chi_0^+) = \begin{cases} (\varphi_0, U \chi_0^+) , & \theta = 0 , \\ 0 , & \theta > 0 . \end{cases} \tag{2.14}$$

Since the scattering amplitude is a continuous function of θ, this discontinuity in the first term of Eq. (2.13) must of course be accompanied by a compensating discontinuity in the second term. In order to prove Eq. (2.14), we consider first the matrix element

$$(\varphi_f, U_L \chi_0^+) = -\int d\underline{r} \, (\exp i \underline{q} \cdot \underline{r}) \nabla^2 \exp i \delta_0(\underline{r}) . \tag{2.15}$$

When the scattering is forward, q vanishes and the volume integral can be rewritten as an integral over the surface of a large sphere:

$$(\varphi_0, U_L \chi_0^+) = -\int d\underline{S} \cdot \underline{\nabla} \exp i \delta_0(\underline{r}) = 0 , \quad \theta = 0 . \tag{2.16}$$

Because $\underset{\sim}{\nabla}$ exp i δ_0 is nonzero only on the intersection of the sphere with the forward cylinder, only its component along the axis of the cylinder contributes to the integral when the sphere has infinite radius. However, this axial component is proportional to $U(\underset{\sim}{r})$ by Eq. (2.7) and therefore vanishes at large distances.

For nonzero angles, it is convenient to integrate by parts with respect to z in Eq. (2.15):

$$(\varphi_f, U_L \chi_0^+) = i\,(q_z + i\epsilon)^{-1} \iint_{-\infty}^{\infty} dx\, dy \exp(i q_x x + i q_y y)$$

$$\times \left[\exp(i q_z z - \epsilon z)\, \nabla^2 \exp i\,\delta_0(\underset{\sim}{r})\right]_{z=-\infty}^{\infty} \tag{2.17}$$

$$-(2k)^{-1} (q_z + i\epsilon)^{-1} \int d\underset{\sim}{r} \exp(i\underset{\sim}{q}\cdot\underset{\sim}{r})\, \nabla^2 (U \exp i\,\delta_0) \quad .$$

The boundary term vanishes because the convergence factor is zero at the upper limit and the factor ∇^2exp i δ_0 is zero at the lower limit. In the second term, the quantity ϵ may be set equal to zero (when $\theta > 0$), for the integration is limited to the potential region. The Laplacian operator can be transferred to the factor exp $i\underset{\sim}{q}\cdot\underset{\sim}{r}$ by an application of Green's theorem, the surface integral vanishing because the potential is bounded in space. Since the quantity $q^2/2kq_z$ is unity, Eq. (2.17) becomes, in conjunction with Eq. (2.16),

$$(\varphi_f, U_L \chi_0^+) = \begin{cases} 0 & , \ \theta = 0 \ , \\ (\varphi_f, U \chi_0^+) & , \ \theta > 0 \ . \end{cases} \tag{2.18}$$

(A unified proof of both parts of Eq. (2.18) may be obtained by observing that the limit as $\epsilon \to 0$ of $(2k)^{-1}(q_z + i\epsilon)^{-1} q^2$ is 0 for $\theta = 0$ and 1 for $\theta > 0$.) Because $U = U_S + U_L$, Eq. (2.14) follows directly. Finally, we can rewrite Eq. (2.13) as

$$-4\pi f(\underset{\sim}{k}_f, \underset{\sim}{k}_0) = \begin{cases} (\varphi_0, U\chi_0^+) + (\psi_0^-, U_L\chi_0^+), & \theta = 0, \\ (\psi_f^-, U_L\chi_0^+), & \theta > 0. \end{cases} \tag{2.19}$$

Eq. (2.19) is a rearrangement (without approximation) of the exact scattering amplitude, Eq. (2.2b), in a form that is expected to be useful at high energies. This expectation is supported by a comparison of the results of replacing ψ_f^- by the plane wave ϕ_f in the two expressions. Eq. (2.2b) gives the Born approximation, while Eq. (2.19) becomes

$$-4\pi f(\underset{\sim}{k}_f, \underset{\sim}{k}_0) \approx (\varphi_f, U\chi_0^+) \tag{2.20}$$

by virtue of Eq. (2.18). The last equation is a well-known approximation for high-energy scattering valid at small angles.[2] The use of a better approximate wave function in Eq. (2.19) will be discussed in Sec. V.

III. DERIVATION OF THE SAXON-SCHIFF AMPLITUDE

Saxon and Schiff[4] have rewritten the exact scattering amplitude in another form that is useful for obtaining high-energy approximations. We shall now show that the two-potential form of the amplitude, Eq. (2.13), is closely related to the Saxon-Schiff form and incidentally provides a substantially simpler way of deriving it than that given originally by Saxon and Schiff. Secondly, we shall show the equivalence of the high-energy approximations obtained when ψ_f^- is replaced by a modified plane wave χ_f^- in these two forms of the amplitude.

The Saxon-Schiff amplitude is

$$-4\pi f(\underset{\sim}{k}_f, \underset{\sim}{k}_0) = (\varphi_f, U\chi_0^+) + \\ + (i/2k)\int d\underset{\sim}{r}\; U(\underset{\sim}{r})\left[\exp i\delta_0(\underset{\sim}{r})\right]\nabla^2 \int_z^\infty dz'\, \varphi_0(\underset{\sim}{r}')\,\psi_{sc}^*(\underset{\sim}{r}') \,, \tag{3.1}$$

where r' = (x, y, z') and

$$\psi_{sc}(\underset{\sim}{r}) = \psi_f^-(\underset{\sim}{r}) - \varphi_f(\underset{\sim}{r}) \,. \tag{3.2}$$

To obtain this result from Eq. (2.13), we first substitute $U_S = U - U_L$:

$$-4\pi f(\underset{\sim}{k}_f, \underset{\sim}{k}_0) = (\varphi_f, U\chi_0^+) - (\psi_{sc}, (\nabla^2 \exp i\delta_0)\varphi_0) \,. \tag{3.3}$$

With the z axis parallel to $\hat{\underset{\sim}{k}}_0$, integration by parts with respect to z and use of Eq. (2.7) change the second term of Eq. (3.3) to

$$+\iint dx\,dy\left[\nabla^2 \exp i\delta_0(\underset{\sim}{r})\right]\int_z^\infty dz'\,\varphi_0(\underset{\sim}{r}')\,\psi_{sc}^*(\underset{\sim}{r}')\Big|_{z=-\infty}^{z=+\infty} \\ + (i/2k)\int d\underset{\sim}{r}\left\{\nabla^2\left[U(\underset{\sim}{r})\exp i\delta_0(\underset{\sim}{r})\right]\right\}\int_z^\infty dz'\,\varphi_0(\underset{\sim}{r}')\,\psi_{sc}^*(\underset{\sim}{r}') \,. \tag{3.4}$$

Since the asymptotic form of ψ_{sc} is an incoming spherical wave, $\phi_o(\underline{r}') \; \psi_{sc}^{*}(\underline{r}')$ varies as $(1/z')\exp(2ikz')$ at large positive z' for fixed x and y. Hence the integral over z' exists and tends to zero as $z \to +\infty$. Since $\nabla^2 \exp(i\,\delta_o)$ vanishes at large negative z, the first term of Eq. (3.4) clearly vanishes at both limits. Green's theorem applied to the second term now yields Eq. (3.1), the surface integral in Green's theorem having a vanishing integrand because U vanishes at large distances.

If ψ_f^- is replaced by a modified plane wave χ_f^-, the only part of this demonstration that needs changing is the reason why the boundary term vanishes at the upper limit. When χ_f^- is defined in more detail in Sec. IV, it will be seen that $\chi_f^- - \phi_f$ vanishes at large positive z for fixed x and y unless the scattering angle is 180° . In this exceptional case, the integral over z' must be defined in the Abelian sense, and the convergence factor then causes the boundary term to vanish at the upper limit.

IV. ITERATION SCHEME

In order to make use of Eq. (2.19), the unknown exact wave function ψ_f^- must be replaced by an approximate wave function or, more systematically, by the leading term or terms of a series expansion. For example, Eq. (2.20) resulted from replacing ψ_f^- by the leading term of its Born series. At high energies, a better choice should be the modified plane wave χ_f^-, which is a good approximation to ψ_f^- in the potential region provided that $kR \gg 1$, $U \ll k^2$, and $(U/k^2)(UR/k) \ll 1$.[4] (The potential is assumed to be smooth and to occupy a region of dimension R.) Postponing until Sec. V a further discussion of this approximation, we consider here the problem of expanding ψ_f^- in a series having χ_f^- as its leading term.

For convenience of notation we shall actually work with ψ_0^+ instead of ψ_f^-; one can be obtained from the other by use of the relation[8]

$$\psi_f^-(\underline{r}) = [\psi_{-f}^+(\underline{r})]^*, \tag{4.1}$$

where $-f$ refers to the wave vector $-\underline{k}_f$. Similarly, χ^- and χ^+ are related by

$$\chi_f^-(\underline{r}) = [\chi_{-f}^+(\underline{r})]^* = \exp[i\underline{k}_f\cdot\underline{r} - i\,\delta_{-f}(\underline{r})], \tag{4.2}$$

$$\delta_{-f}(\underline{r}) = -(2k)^{-1}\int_0^\infty U(\underline{r}+\hat{\underline{k}}_f s)\,ds. \tag{4.3}$$

The phase modification is nonzero if $\underline{r}$ lies in the potential or in the backward cylinder with axis in the direction $-\hat{\underline{k}}_f$ (a semi-infinite cylinder such that a straight line proceeding from $\underline{r}$ in the direction $\hat{\underline{k}}_f$ pierces the potential).

Saxon and Schiff[4] obtained a series for ψ_0^+ with χ_0^+ as leading term by iterating an integral equation for ψ_0^+. We shall instead obtain an integral equation for the exact Green's function and substitute its iteration series in a suitable expression for ψ_0^+, to be derived in the next paragraph. Although our procedure is more complicated, the results are in one respect simpler.

Whereas Saxon and Schiff applied Green's theorem to ψ_0^+ and an approximate Green's function, we shall apply it to χ_0^+ and the exact Green's function, which satisfies

$$\left[\nabla^2 + k^2 - U(\underline{r})\right] G^+(\underline{r},\underline{r}') = -\delta(\underline{r}-\underline{r}') \quad . \tag{4.4}$$

From Green's theorem and Eq.(2.8), it follows that

$$\Omega(\underline{r}) \equiv \int d\underline{S}' \cdot \left[G^+(\underline{r}',\underline{r})\, \underline{\nabla}'\chi_0^+(\underline{r}') - \chi_0^+(\underline{r}')\, \underline{\nabla}'\, G^+(\underline{r}',\underline{r})\right] \tag{4.5}$$

$$= \chi_0^+(\underline{r}) - \int d\underline{r}'\; G^+(\underline{r}',\underline{r})\; U_L(\underline{r}')\; \chi_0^+(\underline{r}') \quad . \tag{4.6}$$

Eq. (4.6) shows that the surface integral Ω satisfies the same Schrödinger equation as ψ_0^+. However, it is not obvious that Ω has the asymptotic form of a plane wave plus outgoing spherical waves (the asymptotic form of the integral cannot be obtained by simply substituting for G^+ its asymptotic form, since the integration in Eq. (4.6) extends over both the potential region and the forward cylinder). To show that Ω is indeed ψ_0^+, we observe that the same procedure, applied to ϕ_0 instead of χ_0^+, leads to the Chew-Goldberger equation[9] for ψ_0^+, with no difficulties about the asymptotic form:

$$\psi_0^+(\underline{r}) = \int d\underline{S}' \cdot \left[G^+(\underline{r}',\underline{r})\, \underline{\nabla}' \varphi_0(\underline{r}') - \varphi_0(\underline{r}')\, \underline{\nabla}' G^+(\underline{r}',\underline{r}) \right] \tag{4.7}$$

$$= \varphi_0(\underline{r}) - \int d\underline{r}'\, G^+(\underline{r},\underline{r}')\, U(\underline{r}')\, \varphi_0(\underline{r}') \; . \tag{4.8}$$

But the surface integrals (4.5) and (4.7) are equal, for $\chi_0^+ - \phi_0$ and its gradient are zero on the surface of a large sphere except at its intersection with the forward cylinder, while $G^+(\underline{r}',\underline{r})$ decreases at large r' as 1/r'. Finally, by the reciprocity property of the Green's function, Eq. (4.6) becomes

$$\psi_0^+(\underline{r}) = \chi_0^+(\underline{r}) - \int d\underline{r}'\, G^+(\underline{r},\underline{r}')\, U_L(\underline{r}')\, \chi_0^+(\underline{r}') \; . \tag{4.9}$$

This equation bears the same relation to Saxon and Schiff's integral equation for ψ_0^+ as does the Chew-Goldberger equation to the Schwinger integral equation for ψ_0^+.

The iteration series to be substituted for G^+ in Eq. (4.9) is chosen to have as its first term the approximate high-energy Green's function proposed by Saxon and Schiff[4]:

$$F^+(\underline{r},\underline{r}') = G_0^+(\rho)\, \exp i\, \delta(\underline{r},\underline{r}') \; , \tag{4.10}$$

where

$$\begin{aligned} \underline{\rho} &= \underline{r} - \underline{r}' \\ G_0^+(\rho) &= (4\pi\rho)^{-1} \exp i k \rho \\ \delta(\underline{r},\underline{r}') &= -(2k)^{-1} \int_0^{\rho} U(\underline{r} - \hat{\underline{\rho}}\, s)\, ds \; . \end{aligned} \tag{4.11}$$

The approximate Green's function satisfies the differential equation

$$\left[\nabla^2 + k^2 - U(\mathbf{r}) + W(\mathbf{r},\mathbf{r}')\right] F^+(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}') , \tag{4.12}$$

with

$$W(\mathbf{r},\mathbf{r}') = -\exp\left[-i S(\mathbf{r},\mathbf{r}')\right] \nabla^2 \exp\left[i S(\mathbf{r},\mathbf{r}')\right] - (i/k\rho)\, U(\mathbf{r}) . \tag{4.13}$$

When Green's theorem is applied to G^+ and F^+, the surface integral vanishes and we obtain the integral equation

$$G^+(\mathbf{r},\mathbf{r}') = F^+(\mathbf{r},\mathbf{r}') - \int d\mathbf{r}''\, F^+(\mathbf{r},\mathbf{r}'')\, W(\mathbf{r}'',\mathbf{r})\, G^+(\mathbf{r}'',\mathbf{r}') . \tag{4.14}$$

Iteration of this equation gives a series for G^+ that can be substituted in Eq. (4.9) to yield the desired series expansion of ψ_0^+ :

$$\begin{aligned} \psi_0^+(\mathbf{r}) = {} & \chi_0^+(\mathbf{r}) - \int d\mathbf{r}'\, F^+(\mathbf{r},\mathbf{r}')\, U_L(\mathbf{r}')\, \chi_0^+(\mathbf{r}') \\ & + \int d\mathbf{r}'\, d\mathbf{r}''\, F^+(\mathbf{r},\mathbf{r}'')\, W(\mathbf{r}'',\mathbf{r})\, F^+(\mathbf{r}'',\mathbf{r}')\, U_L(\mathbf{r}')\, \chi_0^+(\mathbf{r}') + \cdots . \end{aligned} \tag{4.15}$$

The series obtained by iterating Saxon and Schiff's integral equation differs from this in only one respect: the factor $U_L(\mathbf{r}')$ that precedes $\chi_0^+(\mathbf{r}')$ in all terms but the first of Eq. (4.15) is replaced by the more complicated $W(\mathbf{r}', \mathbf{r}^{(n)})$ of Eq. (4.13). This replacement does not change the values of the individual terms of the series; by a proof that begins with the application of Green's theorem to F^+ and χ_0^+, one can show that

$$\int d\mathbf{r}'\, F^+(\mathbf{r},\mathbf{r}')\left[U_L(\mathbf{r}') - W(\mathbf{r}',\mathbf{r})\right]\chi_0^+(\mathbf{r}') = 0 . \tag{4.16}$$

Before turning to other questions, we should like to mention a further use for Eq. (4.9): it provides an alternative derivation of the exact scattering amplitude in the form of Eq. (3.3). We observe that the argument of ψ_0^+ in Eq. (4.9) occurs in the integrand only as an argument of the exact Green's function. As a result, a familiar integral occurs when Eq. (4.9) is substituted in Eq. (2.2a) and the order of integration is reversed in the second term:

$$-4\pi f(\underset{\sim}{k}_f, \underset{\sim}{k}_0) = (\phi_f, U\chi_0^+) - \int d\underset{\sim}{r}\, U_L(\underset{\sim}{r})\, \chi_0^+(\underset{\sim}{r}) \times \int d\underset{\sim}{r}'\, \phi_f^*(\underset{\sim}{r}')\, U(\underset{\sim}{r}')\, G^+(\underset{\sim}{r}', \underset{\sim}{r}) . \tag{4.17}$$

Now the solution of the Schrödinger equation having the asymptotic form of a plane wave ϕ_f plus incoming spherical waves is

$$\psi_f^-(\underset{\sim}{r}) = \phi_f(\underset{\sim}{r}) - \int d\underset{\sim}{r}'\, G^-(\underset{\sim}{r}, \underset{\sim}{r}')\, U(\underset{\sim}{r}')\, \phi_f(\underset{\sim}{r}') . \tag{4.18}$$

By Eq. (3.2) and the identity

$$[G^-(\underset{\sim}{r}, \underset{\sim}{r}')]^* = G^+(\underset{\sim}{r}', \underset{\sim}{r}) ,$$

it follows that

$$\psi_{sc}^*(\underset{\sim}{r}) = -\int d\underset{\sim}{r}'\, G^+(\underset{\sim}{r}', \underset{\sim}{r})\, U(\underset{\sim}{r}')\, \phi_f^*(\underset{\sim}{r}') . \tag{4.19}$$

This identification of the integral shows Eq. (4.17) to be the same as Eq. (3.3).

V. SMALL-ANGLE AND LARGE-ANGLE APPROXIMATIONS

When ψ_f^- is replaced in Eq. (2.19) by the approximate high-energy wave function χ_f^-, we obtain an approximate scattering amplitude

$$-4\pi f_1(\underline{k}_f, \underline{k}_0) = \begin{cases} (\varphi_0, U\chi_0^+) + (\chi_0^-, U_L \chi_0^+) , & \theta = 0 , \\ (\chi_f^-, U_L \chi_0^+) , & \theta > 0 . \end{cases} \tag{5.1}$$

In spite of its very different appearance, this expression is equivalent, as shown already in Sec. III, to the high-energy approximation given by Saxon and Schiff.[4] They have discussed its accuracy, as well as the ranges of energy and angle in which it reduces to the simplified small-angle approximation, Eq. (2.20), or to Schiff's large-angle formula, $(\chi_f^-, U\chi_0^+)$.[3]

To discuss these questions again would surely be superfluous if Saxon and Schiff had not found it necessary to make order-of-magnitude estimates (following their Eq. (32), for example) of some rather complicated integrals containing rapidly oscillating factors in their integrands. Such estimates are very difficult to make with certainty; for instance, the relative magnitudes of two functions are no guide to the relative magnitudes of their Fourier transforms, except for the low-frequency components. In view of this, we have thought it worthwhile to see what conditions of validity can be established by taking the form (5.1) of f_1 as an alternative starting point and abstaining from order-of-magnitude estimates of the kind just mentioned.

The conclusions that we have reached by this route are very limited. The first is that f_1 reduces to the small-angle approximation for scattering angles $\theta \lesssim 1/kR$; that is, for such small angles, it is immaterial whether ψ_f^- is approximated in Eq. (2.19) by a modified or unmodified plane wave. For reasons to be explained presently, we are not able to extend this conclusion to the wider range of angles, $\theta \ll (kR)^{-\frac{1}{2}}$, given by Saxon and Schiff. For angles near 180°, our attempt to recover the Schiff large-angle formula will serve only to underline the hazards of making order-of-magnitude estimates. An effort to avoid them in a particular case, by an approximate saddle-point integration, will be found to suggest that the Schiff large-angle formula should be multiplied by $\frac{1}{2}$ and its range of validity restricted to avoid overlap with that of the Born approximation. (For a Dirac particle, on the other hand, the Schiff large-angle formula will be obtained without difficulty in Sec. VI.)

For small scattering angles, it is convenient first to rearrange Eq. (5.1) in the form

$$-4\pi f_1(\underset{\sim}{k}_f, \underset{\sim}{k}_0) = (\varphi_f, U\chi_0^+) + (\chi_f^- - \varphi_f, U_L\chi_0^+) \quad . \tag{5.2}$$

The first term is the familiar small-angle formula of Eq. (2.20); the second term is a correction whose relative order of magnitude we wish to estimate. (The second term is well-defined, with one exception, because the integrand vanishes except in the potential region and in the intersection of the forward and backward cylinders; at $\theta = 180°$, these cylinders coincide, but convergence can be restored by adding a small positive imaginary part to q_z as in Sec. II.) We suppose that the potential is smooth and occupies a region of dimension R, that $kR \gg 1$ and $U \ll k^2$, and that UR/k is not large compared to unity. Then the only factor in either integrand that can oscillate rapidly in a distance R is $\exp(i\underline{q}\cdot\underline{r})$. If $\theta \lesssim 1/kR$, this factor too is slowly varying, and a straightforward estimate of orders of magnitude gives roughly UR^3 for the first term of Eq. (5.2) and U^2R^3/k^2 for the second term. Thus the second term is of relative order U/k^2 and can be neglected. But if $\theta \gg 1/kR$, the integrand of each term contains the rapidly oscillating factor $\exp(i\underline{q}\cdot\underline{r})$, and order-of-magnitude estimates, whether of the individual terms or of their ratio, become unreliable.

At large scattering angles, this difficulty of estimating high-frequency Fourier components is aggravated. Reflection from a one-dimensional barrier will illustrate how one can be deceived by apparent orders of magnitude; the same hazards will then be encountered in a discussion of 180° scattering from a Gaussian potential in three dimensions.

The reflection amplitude from a one-dimensional barrier is[10]

$$r = (2ik)^{-1}\,(\varphi_f\,, U\,\psi_0^+)\;. \tag{5.3}$$

This can be rewritten in the two-potential formalism as

$$2ikr = (\varphi_f\,, U_S\,\chi_0^+) + (\psi_f^-\,, U_L\,\chi_0^+)\;, \tag{5.4}$$

where

$$\varphi_f(z) = \exp(-ikz)\;, \tag{5.5}$$

$$\chi_0^+(z) = \exp[ikz + i\delta_0(z)] = [\chi_f^-(z)]^*\;, \tag{5.6}$$

$$\delta_0(z) = -(2k)^{-1}\int_{-\infty}^{z} U(z')\,dz' \quad , \tag{5.7}$$

$$U_L(z) = -\exp(-i\delta_0)\,\frac{d^2}{dz^2}\exp(i\delta_0) \quad . \tag{5.8}$$

As expected, the first term of Eq. (5.4) is easily shown to vanish. Replacement of ψ_f^- in the second term by χ_f^- gives a high-energy approximation analogous to Eq. (5.1):

$$2ikr_1 = (\chi_f^-, U_L\chi_0^+) = -\int_{-\infty}^{\infty} dz\,\exp(2ikz + i\delta_0)\,\frac{d^2}{dz^2}\exp i\delta_0 \quad . \tag{5.9}$$

The integral can be rewritten in two ways by substituting the identities

$$\exp(i\delta_0)\,\frac{d^2}{dz^2}\exp i\delta_0 = \frac{1}{2}\,\frac{d^2}{dz^2}\exp(2i\delta_0) + \left(\frac{d}{dz}\delta_0\right)^2\exp(2i\delta_0) \tag{5.10a}$$

$$= \frac{1}{4}\,\frac{d^2}{dz^2}\exp(2i\delta_0) + i\,\frac{1}{2}\left(\frac{d^2}{dz^2}\delta_0\right)\exp(2i\delta_0) \,. \tag{5.10b}$$

In each case, we integrate the first term by parts to obtain

$$2ikr_1 = \left(\chi_f^-,\,[U - (U^2/4k^2)]\,\chi_0^+\right) \tag{5.11a}$$

$$= \left(\chi_f^-,\,\left[\frac{1}{2}U + \frac{i}{4k}\,\frac{dU}{dz}\right]\chi_0^+\right) \quad . \tag{5.11b}$$

A glance at Eq. (5.11a) suggests that the second term is of order U_0/k^2 compared to the first and can be neglected at high energies, leaving $(\chi_f^-, U\chi_0^+)$ as expected by analogy with the Schiff large-angle formula in three dimensions. A fallacy in this argument is that U^2 usually varies more rapidly than U and consequently has larger high-frequency components. Moreover, a contradictory conclusion is reached by estimating the second term of Eq. (5.11b) to be of order 1/kR compared to the first.

We shall try to resolve this dilemma by considering a Gaussian potential, $U = U_0 \exp(-z^2/a^2)$. The integrand of Eq. (5.11a) has no singularities for finite complex z, but the quantity

$$\ln\left[(\chi_f^-)^* \chi_0^+\right] = 2ikz - i(U_0/k)\int_{-\infty}^{z} \exp(-z'^2/a^2)\, dz' \tag{5.12}$$

has a saddle point at

$$\begin{aligned} z &= ia\left[\ln(2k^2/U_0)\right]^{\frac{1}{2}} = iy_0 \quad , \\ U(iy_0) &= 2k^2 \quad . \end{aligned} \tag{5.13}$$

If the integration contour is shifted from the real axis to the line $z = x + iy_0$, then the real part of Eq. (5.12) has a sufficiently sharp maximum as x goes through zero that the variation of the remaining terms of the integrand can be neglected, provided that $y_0 \ll ka^2$. Instead of recording the rather cumbersome result of the saddle-point integration, we observe only that $U^2/4k^2$ has the same value as U/2 at the saddle point; thus, in this approximation, we simply recover the first term of Eq. (5.11b).

A better approximation should result from applying the same procedure to Eq. (5.11b), because $dU/dz = -2zU/a^2$ varies less rapidly than U^2. Indeed, only z need be replaced by its value at the saddle point to obtain a small correction term:

$$2ikr_1 \approx \frac{1}{2}(\chi_f^-, U\chi_0^+)\left[1 + (ka^2)^{-1} y_0\right] \quad . \tag{5.14}$$

If the saddle point is defined more carefully by adding ln U to Eq. (5.12), the algebra becomes more complicated but the saddle point is shifted by a negligible amount to approximately $iy_0 - i(2k)^{-1}$.

An objection to this saddle-point approximation is that the real part of Eq. (5.12) does not continue to decrease with further increase of $|x|$ but oscillates and reaches a local maximum (never as large as the one at the saddle point) whenever $|x|$ is an integral multiple of $\pi a^2/y_0$. However, if $y_0 \lesssim \pi a$, i.e. if $U_0/k^2 \gtrsim 10^{-4}$, the heights of these subsidiary maxima decrease rapidly from one to the next. Even at the first and largest of them, the exponential of the real part is small compared to its value at the saddle point, and the exponential of the imaginary part is oscillating rapidly. Consequently, we believe that the value of the integral comes almost entirely from the saddle point.

Since the high-energy approximation requires $ka \gg 1$ and $(U_0/k^2)(U_0 a/k) \ll 1$, we find that r_1 is half as large as the analogue of the Schiff large-angle formula in the range of parameters $10^{-4} \lesssim U_0/k^2 \ll (ka)^{-\frac{1}{2}}$. No inconsistency with the Born approximation arises from the factor $\frac{1}{2}$, because the second Born approximation for a Gaussian potential is large compared to the first in this range.

The factor $\frac{1}{2}$ does not seem to be a peculiarity of the one-dimensional case. In three dimensions, the approximate amplitude for 180° scattering is

$$-4\pi f_1(-\underset{\sim}{k}_0, \underset{\sim}{k}_0) = (\chi_f^-, U_L \chi_0^+) = -\int d\underset{\sim}{r}\, \exp(2ikz + i\delta_0)\, \nabla^2 \exp i\delta_0 \, . \tag{5.15}$$

As in one dimension, we avoid terms explicitly quadratic in U by substituting an identity similar to Eq. (5.10b):

$$\exp(i\delta_0)\nabla^2 \exp i\delta_0 = \frac{1}{4}\nabla^2 \exp 2i\delta_0 + \frac{1}{2}i(\nabla^2\delta_0)\exp 2i\delta_0 . \tag{5.16}$$

When the first term is integrated by parts, the surface integral vanishes by the reasoning applied earlier to Eq. (2.16), and the volume integral is just one-half the Schiff large-angle formula. If the second term is evaluated for a Gaussian potential, $U = U_0 \exp(-r^2/a^2)$, Eq. (5.15) becomes

$$-4\pi f_1 = \int d\underline{r}\ \exp(2ikz + 2i\delta_0) \times \left[\frac{1}{2}U - \frac{1}{2}i(ka^2)^{-1}zU - 2ia^{-4}(x^2+y^2-a^2)\delta_0\right] . \tag{5.17}$$

The integrations over x and y can be carried out exactly, a convenient variable being $t = \exp\left[-(x^2+y^2)/a^2\right]$. The first two terms present no difficulties; the third term, which is defined in the Abelian sense by the convergence factor $\exp(-\epsilon z)$, is first integrated by parts with respect to z and then with respect to t. The result is

$$-4\pi f_1 = \pi a^2 \int_{-\infty}^{\infty} dz\ \exp(2ikz + 2i\delta_0)\ \frac{1}{2}U(z) \times \left\{\left[1 - i(ka^2)^{-1}z - (ka)^{-2}\right](2i\delta_0)^{-1}\left[1 - \exp(-2i\delta_0)\right] + (ka)^{-2}\right\} . \tag{5.18}$$

In this last equation, but not in Eq. (5.17), U and δ_0 are functions of z alone: U(z) stands for $U_0 \exp(-z^2/a^2)$ and δ_0 is related to it by Eq. (5.7). The terms in $(ka)^{-2}$ come from the third term of Eq. (5.17).

As in the earlier discussion of the reflection amplitude, we estimate the relative importance of the slowly varying factors by evaluating them at the same saddle point, $z = iy_0$. Admittedly, the variation of $\left[1 - \exp(-2i\,\delta_0)\right]$ is not slow near the saddle point, but its value remains very close to unity. The term in $(ka^2)^{-1}z$ is then of relative order y_0/ka^2, and the square bracket containing this term is effectively unity. The last term in Eq. (5.18) is of relative order $(ka)^{-2}\ \delta_0 \approx (ky_0)^{-1} \ll 1$. We conclude that only the first term of Eq. (5.17) is important, again provided that $y_0 \lesssim \pi a$:

$$-4\pi f_1(-\underline{k}_0, \underline{k}_0) \approx \tfrac{1}{2}\left(\chi_f^-, U\chi_0^+\right) \quad . \tag{5.19}$$

One would like to know whether Eq. (5.19) is correct for potentials other than a Gaussian, in a suitable range of parameters, and whether it can be extended to scattering angles other than 180°. The assumption of a Gaussian potential was not used in obtaining this expression directly from the first term of Eq. (5.16), and we speculate that this term will in general have substantially larger high-frequency components than the second term because it contains the square of the z-derivative of the potential. As in the Gaussian case, the effect of its more rapid variation will be compensated by its quadratic dependence on U_0 when U_0 becomes sufficiently small that the Born approximation is valid. The first term leads directly to the right-hand side of Eq. (5.19) also at scattering angles other than 180° provided that χ_f^- is approximated by $\phi_f \exp(-i\,\delta_0)$. We have not been able to estimate reliably the range of angles about 180° in which no serious error is caused by this approximation.

VI. DIRAC SCATTERING

In order to describe high-energy potential scattering of physical electrons, one must use the Dirac equation to satisfy the requirements of special relativity. We shall find that the two-potential formalism developed earlier for the Schrödinger equation can be applied also to the single-particle Dirac equation with only minor changes. Aside from the complications of spin, the resulting high-energy approximation is in fact simpler in the Dirac case; for 180° scattering, in particular, we shall recover the Schiff large-angle formula[9] with no factor ½ and with no additive terms. These simplifications occur because the Dirac Hamiltonian is linear rather than quadratic in space derivatives.

The Dirac equation for a particle in a scalar potential $V(\underline{r})$ is[11]

$$[E - H_0 - V(\underline{r})]\,\psi(\underline{r}) = 0 , \tag{6.1}$$

where

$$H_0 = i\hbar c\, \underline{\alpha}\cdot\underline{\nabla} - \beta m c^2 . \tag{6.2}$$

If no potential is present, the plane-wave solutions with positive energy will be denoted by

$$\varphi_i(\underline{r}) = u_i(\underline{k}) \exp(i\,\underline{k}\cdot\underline{r}) , \quad i = \pm\tfrac{1}{2} , \tag{6.3}$$
$$k^2 = (E/\hbar c)^2 - k_c^2 ,$$
$$k_c = mc/\hbar .$$

The four-component spinors u_i satisfy the orthogonality relations

$$u_i^{+} u_j = (E/mc^2)\,\delta_{ij} = \gamma\,\delta_{ij} \quad , \tag{6.4}$$

$$u_i^{+} \beta\, u_j = -\,\delta_{ij} \quad . \tag{6.5}$$

The exact amplitude for scattering from an initial state with wave vector $\underline{k}_o$ and spin s_o (spinor u_i with $i = s_o$) to a final state with $\underline{k}_f$ and s_f is given by

$$-4\pi\, f(\underline{k}_f, s_f ; \underline{k}_o, s_o) = (\varphi_f, U\,\psi_o^{+}) = (\psi_f^{-}, U\,\varphi_o) , \tag{6.6}$$

$$U(\underline{r}) = (2m/\hbar^2)\; V(\underline{r}) \; .$$

The differential cross section $|f|^2$ must of course be averaged over initial spins if the beam is unpolarized and summed over final spins if the spin direction is not observed.

To split the potential into two parts, we again use a plane wave modified by a phase factor that corrects for the change of wavelength in the potential region:

$$\chi_o^{+}(\underline{r}) = \varphi_o(\underline{r}) \exp\,[i\,\delta_o(\underline{r})] \quad , \tag{6.7}$$

$$\delta_o(\underline{r}) = -\,\gamma\,(2k)^{-1} \int_0^\infty U(\underline{r} - \hat{\underline{k}}_o s)\, ds \quad .$$

The only differences from the Schrödinger case are that the plane waves are now spinors and that δ_o is now proportional to $\gamma = E/mc^2$. The origin of the factor γ becomes obvious when the relativistic expression for the wave number is expanded to first order in V. The Dirac equation satisfied by the modified plane wave is

$$[E - H_0 - V_S(\underline{r})]\, \chi_0^{+} = 0 \quad , \tag{6.8}$$

$$V_S(\underline{r}) = -i\hbar c \exp(-i\delta_0)\, \underline{\alpha}\cdot\underline{\nabla} \exp i\delta_0 = \hbar c\, \underline{\alpha}\cdot\underline{\nabla}\,\delta_0 \ . \tag{6.9}$$

To express the scattering amplitude in two-potential form, we again integrate the transition current between $(\psi_f^{-} - \phi_f)$ and $(\chi_0^{+} - \phi_0)$ over the surface of a large sphere:

$$\int d\underline{S}\cdot(\psi_f^{-} - \phi_f)^{\dagger}\underline{\alpha}\,(\chi_0^{+} - \phi_0) = \int d\underline{r}\ \underline{\nabla}\cdot\left[(\psi_f^{-} - \phi_f)^{\dagger}\underline{\alpha}\,(\chi_0^{+} - \phi_0)\right] . \tag{6.10}$$

The surface integral vanishes because the factor $(\chi_0^{+} - \phi_0)$ limits the integration to the intersection of the forward cylinder with the sphere, while $(\psi_f^{-} - \phi_f)$ decreases asymptotically as $1/r$. By substituting Eqs.(6.1) and (6.8) in the volume integral and using Eq.(6.6), we obtain

$$-4\pi f = (\phi_f, U_S\,\chi_0^{+}) + (\psi_f^{-}, U_L\,\chi_0^{+}) \quad , \tag{6.11}$$

where

$$U_S = (2m/\hbar^2)\, V_S = 2k_c\, \underline{\alpha}\cdot\underline{\nabla}\,\delta_0 \quad , \tag{6.12}$$

$$U_L = U - U_S \ . \tag{6.13}$$

As in Sec. II, the two terms of Eq. (6.11) can be defined separately in the Abelian sense. The first term again contributes only to exactly forward scattering:

$$(\varphi_f, U_s \chi_o^+) = \begin{cases} (\varphi_f, U \chi_o^+) & , \quad \theta = 0 , \\ 0 & , \quad \theta > 0 . \end{cases} \tag{6.14}$$

(Even at zero angle, it must be remembered that ϕ_f and ϕ_o may describe different spin states.) To prove Eq. (6.14), we first write out the matrix element in detail:

$$(\varphi_f, U_s \chi_o^+) = -2ik_c\, u_f^\dagger \underset{\sim}{\alpha}\, u_o \cdot \int d\underset{\sim}{r}\, (\exp i\underset{\sim}{q}\cdot\underset{\sim}{r})\, \underset{\sim}{\nabla} \exp i\delta_o . \tag{6.15}$$

In the case of forward scattering, the spinor product is proportional to the incident current density if the initial and final spin states are the same, and vanishes otherwise:

$$k_c\, u_f^\dagger(\underset{\sim}{k}_o)\, \underset{\sim}{\alpha}\, u_o(\underset{\sim}{k}_o) = -\underset{\sim}{k}_o\, \delta(s_f, s_o) . \tag{6.16}$$

Use of Eq. (6.4) and the second of Eqs. (6.7) leads at once to

$$\begin{aligned} (\varphi_f, U_s \chi_o^+) &= \gamma\, \delta(s_f, s_o) \int d\underset{\sim}{r}\; U \exp i\delta_o \\ &= (\varphi_f, U \chi_o^+) \quad , \quad \theta = 0 . \end{aligned} \tag{6.17}$$

Since this proof makes no demands on the spatial dependence of ϕ_f , we observe for future reference that also

$$(\chi_f^-, U_s \chi_o^+) = (\chi_f^-, U \chi_o^+) \quad , \quad \theta = 0 . \tag{6.18}$$

For nonzero angles, we perform an integration by parts with respect to z in Eq. (6.15):

$$(\varphi_f, U_S\, \chi_0^+) = -2k_c\,(q_z + i\epsilon)^{-1}\, \mu_f^\dagger \underset{\sim}{\alpha}\, \mu_0 \cdot \Big\{ \iint_{-\infty}^{+\infty} dx\,dy\, \exp(i q_x x + i q_y y) \Big[\exp(i q_z z - \epsilon z)\, \underset{\sim}{\nabla} \exp i\delta_0\Big]_{z=-\infty}^{+\infty} + i\gamma(2k)^{-1} \int d\underset{\sim}{r}\, \exp(i\underset{\sim}{q}\cdot\underset{\sim}{r})\, \underset{\sim}{\nabla}\,(U \exp i\delta_0) \Big\} . \tag{6.19}$$

The boundary term vanishes at the upper limit because of the convergence factor and at the lower limit because of the factor $\underset{\sim}{\nabla} \exp(i\ \delta_0)$. Integration of the second term by parts transfers the gradient operator to the factor $\exp(i\underset{\sim}{q}\cdot\underset{\sim}{r})$, the surface integral vanishing because the potential vanishes at large distances. The second half of Eq. (6.14) now follows from the identity

$$\mu_f^\dagger \underset{\sim}{\alpha}\, \mu_0 \cdot \underset{\sim}{q} = 0 \quad . \tag{6.20}$$

Alternatively, the two parts of Eq. (6.14) can be proved in a unified way by observing that

$$\lim_{\epsilon\to 0} \mu_f^\dagger \underset{\sim}{\alpha}\, \mu_0 \cdot (\underset{\sim}{q} + i\epsilon\, \hat{\underset{\sim}{z}})\,(q_z + i\epsilon)^{-1} = \begin{cases} -\delta(s_f, s_0)\,(k/k_c) , & \theta = 0, \\ 0 , & \theta > 0 . \end{cases} \tag{6.21}$$

The exact scattering amplitude can now be written as

$$-4\pi f = \begin{cases} (\varphi_f, U\chi_0^+) + (\psi_f^-, U_L\,\chi_0^+) , & \theta = 0 , \\ (\psi_f^-, U_L\,\chi_0^+) , & \theta > 0 . \end{cases} \tag{6.22}$$

As in the Schrödinger case, replacement of ψ_f^- by ϕ_f gives the familiar approximation

$$-4\pi f \approx (\varphi_f , U \chi_o^+) \quad , \tag{6.23}$$

where we have used Eq. (6.14). A better replacement for the exact wave function is the modified plane wave

$$\chi_f^-(\underline{r}) = \varphi_f(\underline{r}) \exp\left[-i\,\delta_{-f}(\underline{r})\right] \quad , \tag{6.24}$$

$$\delta_{-f}(\underline{r}) = -\gamma(2k)^{-1}\int_0^\infty U(\underline{r} + \hat{\underline{k}}_f s)\,ds \; . \tag{6.25}$$

The parameters are assumed to satisfy the same conditions as in the Schrödinger case, with U replaced by γU ; in addition, we assume that $\gamma >> 1$. Because of Eq. (6.18), the resulting high-energy approximation is simpler at 0° than in the Schrödinger case:

$$-4\pi f_1 = \begin{cases} (\varphi_f , U\chi_o^+) \quad , & \theta = 0 \; , \\ (\chi_f^- , U_L \chi_o^+) \quad , & \theta > 0 \; . \end{cases} \tag{6.26}$$

For small scattering angles $\theta \lesssim 1/kR$, it is again immaterial whether a modified or unmodified plane wave is used as the approximate wave function, and we are again unable to extend this conclusion to the wider range of angles $\theta << (kR)^{-\frac{1}{2}}$.[9] We first rearrange Eq. (6.26) in the form

$$-4\pi f_1 = (\varphi_f , U\chi_o^+) + (\chi_f^- - \varphi_f , U_L \chi_o^+) \; , \tag{6.27}$$

$$U_L = U - 2k_c\, \underline{\alpha} \cdot \underline{\nabla}\, \delta_o \quad .$$

If $\gamma UR/k$ is not large compared to unity, the integrals contain no rapidly oscillating factors, and their orders of magnitude can be safely estimated. On evaluating the matrix elements of $\underset{\sim}{\alpha}$, the terms in α_x and α_y are found to be at most of order θ relative to $(\phi_f, U\,\chi_o^{+})$. When the remaining terms of U_L are combined in the form $U(1 + c\,v^{-1}\,\alpha_z)$, where v is the speed of the particle, their contribution is at most of order $1/\gamma$ relative to $(\phi_f, U\,\chi_o^{+})$, and only of order θ^2/γ if the spin state is unchanged.

At a scattering angle of 180°, Eq. (6.26) will be shown to reduce to the Schiff large-angle formula[9] with no approximations:

$$-4\pi f_1 = (\chi_f^{-}, U\,\chi_o^{+}) \quad , \qquad \theta = 180^\circ . \tag{6.28}$$

We consider first the matrix element

$$(\chi_f^{-}, U_s\,\chi_o^{+}) = -2ik_c\,u_f^{\dagger}\underset{\sim}{\alpha}\,u_o \cdot \int d\underset{\sim}{r}\,\exp(i\underset{\sim}{q}\cdot\underset{\sim}{r} + i\delta_{-f})\,\underset{\sim}{\nabla}\exp i\delta_o . \tag{6.29}$$

The phase modification δ_{-f} is equal to δ_o for $\theta = 180^\circ$; in contrast with Eq. (5.16), we have

$$(\exp i\delta_o)\,\underset{\sim}{\nabla}\exp i\delta_o = \tfrac{1}{2}\,\underset{\sim}{\nabla}\exp(2i\delta_o) . \tag{6.30}$$

Thus, Eq. (6.29) has the same structure for 180° scattering as Eq. (6.15), and the same steps that were used earlier to prove the second half of Eq. (6.14) now lead to

$$(\chi_f^{-}, U_s\,\chi_o^{+}) = 0 \quad , \qquad \theta = 180^\circ . \tag{6.31}$$

Eq. (6.28) follows immediately, and its derivation clearly remains valid in a range of angles about 180° provided that χ_f^- is approximated by $\phi_f \exp(-i\delta_0)$. As in the Schrödinger case, we are unable to estimate reliably the accuracy of this approximation.

Footnotes

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[‡] Now at Space Technology Laboratories, Los Angeles, California.

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