Multiple-Scattering Analysis of the Three-Body Scattering Problem*

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CONTENTS

I. INTRODUCTION

A. Background

THE nucleon-nucleon, pion-nucleon, and kaon-nucleon interactions are at present imperfectly known. The structure of complex nuclei is also not completely understood. Information on both the two-body interaction and the structure of complex nuclei could be obtained from (say) nucleon-nucleus scattering, provided that a theoretical method exists for separating the nucleon-nucleon force effects from the structure effects. With a theoretical expression available for the nucleon-nucleus cross section in terms of the nucleon-nucleon cross section, the data from nucleon-nucleon and nucleon-nucleus scattering experiments could be used to gain information about the nuclear structure; inversely, data from nucleon-nucleus scattering experiments and independently obtained knowledge about the nuclear structure could be used to determine particulars of the nucleon-nucleon force. A relation between the nucleon-nucleus cross section and the (on-the-energy-shell) nucleon-nucleon scattering amplitude could be used in the same manner, but in this case there would be the additional complication of the determination of the relative phases of the nucleon-proton and nucleon-neutron amplitudes.

The simplest complex nucleus available as a target is the deuteron. The deuteron should be an advantageous target for the type of analysis just mentioned not only because of its relative simplicity of structure, but also because it is such a loosely bound system; i.e., the average separation of its constituents is large compared to the range of the two-body interaction and its binding energy per particle is small. It would be expected that each of the nucleons in the deuteron would scatter the incident particle in a manner not much different from the way a free nucleon would scatter the incident particle.

The problems of nucleon-deuteron, pion-deuteron, and kaon-deuteron scattering are three-body problems; they have not been solved exactly. Aside from this basic fact, many of the physical details involved contribute to their complexity. For example, in the nucleon-deuteron system the identity of two of the nucleons, the spin dependence of the nucleon-nucleon interaction, the presence of tensor forces and exchange forces in the nucleon-nucleon interaction, and the importance of P-wave and higher-order partial-wave scatterings must all be taken into account. Nevertheless, many varied and clever approximations (the resonating group structure method,[1] the Born approximation,[2] the high-energy approximation,[3] the impulse approximation,[4] several variational procedures[5]) have been applied to these problems.

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[1] See H. S. W. Massey, Progr. in Nuclear Physics **3**, 235 (1953), and references cited therein.

[2] For example, see T. Y. Wu and J. Ashkin, Phys. Rev. **73**, 986 (1948); G. F. Chew, *ibid.* **74**, 809 (1948); F. de Hoffman, *ibid.* **78**, 216 (1950); R. L. Gluckstern and H. A. Bethe, *ibid.* **81**, 761 (1951).

[3] See R. J. Glauber, "High Energy Collision Theory," in *Lectures in Theoretical Physics*, edited by Wesley E. Brittin and Lita G. Dunham (Interscience Publishers, Inc., New York, 1959), Vol. I, pp. 315–414, and references cited therein.

[4] For example, see G. F. Chew, Phys. Rev. **84**, 1057 (1951); S. Fernbach, T. A. Green, and K. M. Watson, *ibid.* **84**, 1084 (1951); L. Castillejo and L. S. Singh, Nuovo cimento **11**, 131 (1959); Y. Sakamoto and T. Sasawaka, Progr. Theoret. Phys. (Kyoto) **21**, 879 (1959); E. M. Ferreira, Phys. Rev. **115**, 1727 (1959).

[5] See, for example, E. Clementel, Nuovo cimento **8**, 185 (1951); L. Sartori and S. I. Rubinow, Phys. Rev. **112**, 214 (1958); B. H. Bransden and R. G. Moorhouse, Nuclear Phys. **6**, 310 (1958); L. Spruch and L. Rosenberg, *ibid.* **17**, 30 (1960).

One of the approximations that has been applied to all three of the problems is the impulse approximation.[6] In this, the incident particle is viewed as scattering from the deuteron by scattering once from either of the two nucleons in the deuteron; each of these scatterings is viewed as the scattering from a free nucleon whose momentum distribution is that of the actual bound nucleon. The only role played by the intradeuteron potential is the determination of this momentum distribution. This approximation does indeed lead to an expression (for example) for the elastic neutron-deuteron scattering cross section in terms of the nucleon-nucleon cross sections and a form factor for the deuteron structure. But this approximation neglects "potential" effects (those effects of the intradeuteron potential other than the passive role mentioned above) and multiple-scattering effects; i.e., effects due to the incident particle's scattering more than once from the individual target nucleons. This paper analyzes these multiple scatterings.

B. The Present Work

Inclusion of the multiple-scattering terms complicates the problem enormously. Because of this and the fact that it has been possible in the past to include the effects of spin, isospin, and the identity of particles once the basic problem has been solved, only the case of scalar particles interacting through scalar potentials is considered. As a further simplification the adiabatic approximation for the motion of the target nucleons is made. The basic problem then is just the scattering of a scalar particle by two scalar potentials; the latter are assumed to be spherically symmetric. Even with these restrictions the total scattering amplitude cannot be expressed in terms of the amplitudes for scattering from each target particle individually without further assumptions.

The problem treated here no longer describes the physical situation for nucleon-deuteron, pion-deuteron, or kaon-deuteron scattering. Direct application to nucleon-deuteron scattering is ruled out because the identity of two of the particles is not taken into account. However, with the addition of spin and isospin considerations, application has in fact been made to pion-deuteron[7–10] and kaon-deuteron[11] scattering for moderate energy of the incident particle; i.e., the energy of the incident particle is high enough to make the nucleons appear to be stationary, but yet not so high that it causes a nucleon, when struck, to recoil violently. Because the recoil of the nucleons is not taken into account, the application to scattering of the pion, whose mass is much smaller than that of the nucleon, is more justifiable than application to scattering of a kaon whose mass is approximately half that of a nucleon.

This discussion begins with the problem of the scattering of a scalar particle by one scalar, spherically symmetric potential with a finite radius. Several methods of obtaining the scattering amplitude for this problem are briefly reviewed; off-origin-centered and off-energy-shell amplitudes, as well as the separable potential approximation for the scattering amplitude, are given. Application of these methods is made to the square well potential.

With this as a background, methods developed previously by other authors for obtaining the total scattering amplitude in terms of the individual scattering amplitudes are applied to the problem of S-wave scattering by each of two spherically symmetric potentials of finite radius. A method for solving this problem using the total Green's function for scattering from one potential is also presented. After a test of the separable potential approximation for S-wave scattering by two completely overlapping identical square wells is made, the relationships among the various methods of solution are discussed.

In Appendix A the integrals needed to evaluate off-energy-shell scattering amplitudes for a square well potential are evaluated. In Appendix B one of the methods used to treat S-wave scattering by two potentials is generalized to include the scattering of all partial waves.

II. SCATTERING BY ONE POTENTIAL

The problem discussed in this section is that of the scattering of a particle of mass m and energy E by a potential $V(r)$. The Schrödinger equation for this problem is

$$(\hbar^2/2m)\{\nabla_{\mathbf{r}}^2+k^2-U(r)\}\psi(\mathbf{r})=0, \tag{1}$$

where $r=|\mathbf{r}|$ and

$$U(r)=(2m/\hbar^2)V(r),$$
$$k^2=(2m/\hbar^2)E.$$

The desired solution to Eq. (1) is the sum of an incident plane wave with wave vector $\mathbf{k}_i$ and a scattered wave which is finite at the origin and which, for large r, is an outgoing spherical wave:

$$\psi(\mathbf{r})=\psi_i(\mathbf{r})=|\mathbf{k}_i\rangle+\psi^{sc}(\mathbf{r}), \tag{2}$$

where

$$|\mathbf{k}_i\rangle=\exp(i\mathbf{k}_i\cdot\mathbf{r}),$$

$$\psi^{sc}(\mathbf{r})\longrightarrow\begin{cases}\text{finite as } r\longrightarrow 0\\ r^{-1}e^{ikr}f(\mathbf{k}_f,\mathbf{k}_i).\end{cases} \tag{3}$$

[6] G. F. Chew, Phys. Rev. **80**, 196 (1950); G. F. Chew and G. C. Wick, *ibid.* **85**, 636 (1952); G. F. Chew and M. L. Goldberger, *ibid.* **87**, 778 (1952).
[7] K. A. Brueckner, Phys. Rev. **89**, 834 (1953); **90**, 715 (1953).
[8] S. D. Drell and L. Verlet, Phys. Rev. **99**, 849 (1955).
[9] R. M. Rockmore, Phys. Rev. **105**, 256 (1957); **113**, 1696 (1959).
[10] V. DeAlfaro and R. Stroffolini, Nuovo cimento **11**, 447 (1959).
[11] T. B. Day, G. A. Snow, and J. Sucher, Nuovo cimento **11**, 637 (1959); Phys. Rev. **119**, 1100 (1960).

Equation (3) also serves to define the scattering amplitude $f(\mathbf{k}_f, \mathbf{k}_i)$ from the initial state with wave vector $\mathbf{k}_i$ to the final state with wave vector $\mathbf{k}_f$, in which energy conservation requires $|\mathbf{k}_f| = |\mathbf{k}_i| = k$.

Equation (1) can also be written as an integral equation which incorporates the boundary conditions of Eq. (3); i.e.,

$$\psi_i(\mathbf{r}) = |\mathbf{k}_i\rangle + \int d\mathbf{r}' g_k(\mathbf{r}, \mathbf{r}') V(r') \psi_i(\mathbf{r}'), \quad (4)$$

where the free-wave Green's function $g_k(\mathbf{r}, \mathbf{r}')$ is defined by

$$(\hbar^2/2m)\{\nabla_{\mathbf{r}}^2 + k^2\} g_k(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'), \quad (5)$$

and the requirement that $g_k(\mathbf{r}, \mathbf{r}')$ as a function of $\mathbf{r}$ have the same asymptotic behavior as $\psi^{sc}(\mathbf{r})$. The application of $(\hbar^2/2m)[\nabla_{\mathbf{r}}^2 + k^2]$ to both sides of Eq. (4) and the subsequent use of Eq. (5) yields Eq. (1).

It is well known that $g_k(\mathbf{r}, \mathbf{r}')$ is given by[12]

$$g_k(\mathbf{r}, \mathbf{r}') = -\frac{2m}{4\pi\hbar^2} \frac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}. \quad (6)$$

Substitution of Eq. (6) into Eq. (4), the taking of the limit $r \to \infty$, the use of

$$\lim_{r\to\infty} \frac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} = \exp(-i\mathbf{k}_f\cdot\mathbf{r}') r^{-1} \exp(ikr), \quad (7)$$

and comparison of the resultant expression with Eq. (3) gives

$$f(\mathbf{k}_f, \mathbf{k}_i) = -(2m/4\pi\hbar^2) \int d\mathbf{r}' \exp(-i\mathbf{k}_f\cdot\mathbf{r}') V(\mathbf{r}') \psi_i(\mathbf{r}'). \quad (8)$$

The following discussion is devoted to obtaining several alternative, but of course equivalent, explicit expressions for $f(\mathbf{k}_f, \mathbf{k}_i)$. This discussion is limited to potentials which not only are spherically symmetric but which also have a finite radius; i.e., $V(r) = 0$ for $r > a$.

A. Solution from Matching at the Potential Boundary

One method of solution is the usual partial wave analysis. Since this is a well-known method,[13] only the results are given here. These results are

$$\psi_i(\mathbf{r}) = \begin{cases} \sum_{l=0}^{\infty} (2l+1) i^l [\phi_{1l}^k(a)]^{-1} e^{i\delta_l} [\cos\delta_l j_l(ka) \\ \quad -\sin\delta_l n_l(ka)] \phi_{1l}^k(r) P_l(\mu_{k_i r}), \quad r \leqq a \\ \sum_{l=0}^{\infty} (2l+1) i^l e^{i\delta_l} [\cos\delta_l j_l(kr) \\ \quad -\sin\delta_l n_l(kr)] P_l(\mu_{k_i r}), \quad r \geqq a \end{cases} \quad (9)$$

$$\psi^{sc}(\mathbf{r}) = \begin{cases} \sum_{l=0}^{\infty} (2l+1) i^l \{[\phi_{1l}^k(a)]^{-1} e^{i\delta_l} [\cos\delta_l j_l(ka) \\ \quad -\sin\delta_l n_l(ka)] \phi_{1l}^k(r) - j_l(kr)\} P_l(\mu_{k_i r}), \\ \qquad\qquad r \leqq a \\ \sum_{l=0}^{\infty} (2l+1) i^{l+1} \eta_l h_l^{(1)}(kr) P_l(\mu_{k_i r}), \quad r \geqq a \end{cases} \quad (10)$$

$$f(\mathbf{k}_f, \mathbf{k}_i) = k^{-1} \sum_{l=0}^{\infty} (2l+1) \eta_l P_l(\mu_{k_f k_i}), \quad (11)$$

$$\eta_l = e^{i\delta_l} \sin\delta_l, \quad (12)$$

$$\tan\delta_l = \frac{kj_l'(ka)\phi_{1l}^k(a) - \phi_{1l}^{k\prime}(a) j_l(ka)}{kn_l'(ka)\phi_{1l}^k(a) - \phi_{1l}^{k\prime}(a) n_l(ka)}. \quad (13)$$

Here δ_l is the phase shift of the lth partial wave; $P_l(\mu_{xy})$ is the lth Legendre polynomial, μ_{xy} being the cosine of the angle between $\mathbf{x}$ and $\mathbf{y}$. The functions $j_l(x)$, $n_l(x)$, and $h_l^{(1)}(x)$, are respectively, the lth spherical Bessel function, the lth spherical Neumann function, and the lth spherical Hankel function of the first kind.[14] That solution to the lth radial Schrödinger equation for $r \leqq a$ which is finite at $r=0$ is denoted by $\phi_{1l}^k(r)$. In Eq. (13) "prime" denotes differentiation with respect to the argument of the function.

The coefficients in Eqs. (9) and (10), as well as the relation given by Eq. (13), were determined by matching at $r=a$ the value and first radial derivative of $\psi_i(\mathbf{r})$ for $r \leqq a$ to the value and first radial derivative, respectively, of $\psi_i(\mathbf{r})$ for $r \geqq a$.

B. Solution from the Total Green's Function

An alternative method involves the use of the total Green's function $G_k(\mathbf{r}, \mathbf{r}')$. This Green's function is defined by the equation

$$(\hbar^2/2m)\{\nabla_{\mathbf{r}}^2 + k^2 - U(r)\} G_k(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'), \quad (14)$$

and the requirement that $G_k(\mathbf{r}, \mathbf{r}')$ as a function of $\mathbf{r}$ have the same asymptotic behavior as $\psi^{sc}(\mathbf{r})$. With this Green's function, Eq. (1) and the boundary conditions of Eq. (3) can be combined into

$$\psi_i(\mathbf{r}) = |\mathbf{k}_i\rangle + \int d\mathbf{r}' G_k(\mathbf{r}, \mathbf{r}') V(r') \exp(i\mathbf{k}_i\cdot\mathbf{r}'); \quad (15)$$

i.e., application of $(\hbar^2/2m)[\nabla_{\mathbf{r}}^2 + k^2 - U(r)]$ to both sides of Eq. (15) and the subsequent use of Eq. (14) yields Eq. (1).

The total Green's function has the following explicit form[15]:

$$G_k(\mathbf{r}, \mathbf{r}') = (2m/4\pi\hbar^2) \sum_{l=0}^{\infty} (2l+1) P_l(\mu_{rr'}) G_k^{(l)}(r, r'), \quad (16)$$

$$G_k^{(l)}(r, r') = (r'^2\Delta)^{-1} \chi_{1l}^k(r_<) \chi_{2l}^k(r_>), \quad (17)$$

[12] See, for example, L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), 2nd ed., pp. 162–164.

[13] For example, see reference 12, pp. 100–107.

[14] See, for example, reference 12, pp. 77–79 for the definitions and properties of these functions.

[15] Phillip M. Morse and Herman Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. I, pp. 791–895.

where $r_<(r_>)$ is the lesser (greater) of r and r', $\chi_{1l}^k(r)$ and $\chi_{2l}^k(r)$ are linearly independent solutions of the radial Schrödinger equation

$$\left\{\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)-\frac{l(l+1)}{r^2}+k^2-U(r)\right\}\chi_l^k(r)=0, \quad r\leqq a, \tag{18a}$$

$$\left\{\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)-\frac{l(l+1)}{r^2}+k^2\right\}\chi_l^k(r)=0, \quad (r\geqq a), \tag{18b}$$

and Δ is the Wronskian of these two solutions evaluated at $r=r'$.

The particular solutions to be used are determined by the boundary conditions on $G_k^{(l)}(r, r')$; i.e., $G_k^{(l)}(r, r')$ is finite at $r=0$ and $G_k^{(l)}(r\to\infty, r')\sim r^{-1}e^{ikr}$. The solution $\chi_{1l}^k(r)$ is chosen to satisfy the first boundary condition, and $\chi_{2l}^k(r)$ is chosen to satisfy the second. It is assumed that $\phi_{1l}^k(r)$ and $\phi_{2l}^k(r)$ are linearly independent solutions to Eq. (18a) such that $\phi_{1l}^k(r)$ satisfies the first boundary condition. It is known[14] that $j_l(kr)$ and $n_l(kr)$ are linearly independent solutions to Eq. (18b) with $h_l^{(1)}(kr)=j_l(kr)+in_l(kr)$ satisfying the second boundary condition. This means the χ^k's can be written as

$$\chi_{1l}^k(r)=\begin{cases}A_l\phi_{1l}^k(r), & r\leqq a\\ B_l j_l(kr)+C_l n_l(kr), & r\geqq a\end{cases}, \tag{19a}$$

$$\chi_{2l}^k(r)=\begin{cases}D_l\phi_{1l}^k(r)+E_l\phi_{2l}^k(r), & r\leqq a\\ F_l h_l^{(1)}(kr), & r\geqq a\end{cases}, \tag{19b}$$

The coefficients B_l, C_l, D_l, and E_l can be eliminated from Eqs. (19) by the requirements that both χ_l^k's be continuous and have a continuous first derivative at $r=a$.

With the aid of[16]

$$j_l(x)n_l'(x)-n_l(x)j_l'(x)=x^{-2}, \tag{20}$$

$$\phi_{1l}^k(r)\phi_{2l}^{k\prime}(r)-\phi_{2l}^k(r)\phi_{1l}^{k\prime}(r)=\lambda^{-1}r^{-2}, \quad \lambda=\text{const}, \tag{21}$$

(where again "prime" denotes differentiation with respect to the argument) the Wronskian Δ can be evaluated. Substitution of the resulting expressions for χ_{1l}^k, χ_{2l}^k, and Δ into Eq. (17) yields

For $r'\leqq a\leqq r$

$$G_k^{(l)}(r, r')=[(c_l+ib_l)a^2]^{-1}\phi_{1l}^k(r')h_l^{(1)}(kr). \tag{22a}$$

For $r, r'\leqq a$

$$G_k^{(l)}(r, r')=[(c_l+ib_l)a^2]^{-1}\phi_{1l}^k(r_<)\times[d_l\phi_{1l}^k(r_>)+(c_l+ib_l)\phi_{2l}^k(r_>)]. \tag{22b}$$

In this result

$$b_l\equiv kn_l'(ka)\phi_{1l}^k(a)-\phi_{1l}^{k\prime}(a)n_l(ka)\equiv b_l(\alpha, k, a), \tag{23}$$

$$c_l\equiv kj_l'(ka)\phi_{1l}^k(a)-\phi_{1l}^{k\prime}(a)j_l(ka)\equiv c_l(\alpha, k, a), \tag{24}$$

$$d_l\equiv\phi_{2l}^{k\prime}(a)h_l^{(1)}(ka)-kh_l^{(1)\prime}(ka)\phi_{2l}^k(a)\equiv d_l(k, \alpha, a). \tag{25}$$

The left-hand side of Eq. (21) is the Wronskian of the ϕ_l^k's; these functions were chosen to be linearly independent, so that $\lambda^{-1}\neq 0$. Equations (22) give $G_k^{(l)}(r, r')$ only for $r'\leqq a$; this is the only region of interest, since in Eq. (15) $G_k^{(l)}(r, r')$ appears multiplied on the right by $V(r')$ which was assumed to be zero for $r'>a$.

The rest of the procedure for finding the scattering amplitude consists of the substitution of $G_k(\mathbf{r}, \mathbf{r}')$ as given by Eqs. (16) and (22a) into Eq. (15), the evaluation of the integral by standard techniques, the taking of the limit $r\to\infty$, and the comparison of the result with Eq. (3). The resulting expression for $f(\mathbf{k}_f, \mathbf{k}_i)$ is

$$f(\mathbf{k}_f, \mathbf{k}_i)=k^{-1}\sum_{l=0}^{\infty}(2l+1)P_l(\mu_{k_fk_i})\frac{(-i)}{(c_l+ib_l)a^2}\times\int_0^a r'^2\phi_{1l}^k(r')U(r')j_l(kr')dr' \tag{26}$$

With the aid of the differential equations satisfied by $\phi_{1l}^k(r)$ and $j_l(kr)$ the integral in Eq. (26) is found to be given by

$$\int_0^a r'^2\phi_{1l}^k(r')U(r')j_l(kr')dr'=-c_la^2, \tag{27}$$

so that $f(\mathbf{k}_f, \mathbf{k}_i)$ is given by Eq. (11) with

$$\eta_l=ic_l[c_l+ib_l]^{-1} \tag{28}$$

From Eqs. (13), (23), and (24) it follows that Eq. (28) is identical to Eq. (12).

C. Solution from the *t*-Matrix Formalism

A third method is the t-matrix formalism.[17] This begins with the writing of Eq. (4) in the symbolic form

$$\psi_i=|\mathbf{k}_i\rangle+g_kV\psi_i; \tag{29}$$

i.e., g_k is an integral operator with kernel $g_k(\mathbf{r}, \mathbf{r}')$. This equation is then solved for ψ_i,

$$\psi_i=[1-g_kV]^{-1}|\mathbf{k}_i\rangle. \tag{30}$$

This yields

$$f(\mathbf{k}_f, \mathbf{k}_i)=-(2m/4\pi\hbar^2)\int d\mathbf{r}'\times\exp(-i\mathbf{k}_f\cdot\mathbf{r}')V(r')[1-g_kV]^{-1}|\mathbf{k}_i\rangle \equiv-(2m/4\pi\hbar^2)\langle\mathbf{k}_f|V[1-g_kV]^{-1}|\mathbf{k}_i\rangle \tag{31}$$

[16] Equation (20) is given in reference 14, while Eq. (21) can be easily derived from the fact that the ϕ_l^k's satisfy Eq. (18a).

[17] B. A. Lippman and J. Schwinger, Phys. Rev. 79, 469 (1950).

With the t matrix t_k defined by

$$t_k = V[1-g_kV]^{-1}, \tag{32}$$

where it is understood that t_k operates to the right on $|\mathbf{k}_i\rangle$, Eq. (31) reduces to

$$f(\mathbf{k}_f, \mathbf{k}_i) = -(2m/4\pi\hbar^2)\langle \mathbf{k}_f | t_k | \mathbf{k}_i\rangle. \tag{33}$$

The matrix element in this last expression can be evaluated by expanding the operator in Eq. (32).

The operator t_k can also be found in terms of the total Green's function. In symbolic form Eq. (15) reads

$$\psi_i = |\mathbf{k}_i\rangle + G_kV|\mathbf{k}_i\rangle; \tag{34}$$

i.e., G_k is an integral operator with kernel $G_k(\mathbf{r}, \mathbf{r}')$. But from Eqs. (29), (30), and (32)

$$\psi_i = |\mathbf{k}_i\rangle + g_kt_k|\mathbf{k}_i\rangle, \tag{35}$$

so that

$$g_kt_k = G_kV,$$

where both sides of this equation operate on $|\mathbf{k}_i\rangle$. This equation, when combined with Eq. (32), yields

$$t_k = V[1-g_kV]^{-1} = V\{1+g_kV[1-g_kV]^{-1}\} = V[1+g_kt_k],$$

or

$$t_k = V[1+G_kV]. \tag{36}$$

It is now a relatively simple matter to evaluate the matrix element in Eq. (33).

D. Off-Energy-Shell and Off-Origin-Centered Amplitudes

The application of these methods to the problem of scattering from two potentials is complicated by two facts. In the first place, only over-all energy conservation can be required. If the incident particle scatters off the target by, for example, scattering from one potential into an intermediate state and then scattering from the other potential into its final state, the energy of the intermediate state need not be the same as that of the initial and final states. Such scatterings are called off-energy-shell scatterings. An expression for a general off-energy-shell scattering amplitude can be obtained by defining the operator t_k by Eq. (32) with the understanding that this equation now holds independently of the state upon which it operates.[18] The general off-energy-shell scattering amplitude is then given by

$$f(\mathbf{p}, \mathbf{q}) = -(2m/4\pi\hbar^2)\langle \mathbf{p} | t_k | \mathbf{q}\rangle, \tag{37}$$

where $p = |\mathbf{p}| \neq k$ and $q = |\mathbf{q}| \neq k$. This equation also holds when p and/or q are equal to k.

Secondly, although each potential is spherically symmetric about its own center, neither potential is in general centered at the origin. This complication is easily handled because the value of the matrix element in Eq. (37) is independent of origin. If t_j is the t matrix for scattering from the potential $V_j(\mathbf{r}-\mathbf{R}_j)$ centered at $\mathbf{r}=R_j$ (from here on the energy dependence of the t-matrix is suppressed), and $t_{j,0}$ is the t matrix for scattering from this same potential centered at $\mathbf{r}=0$, then

$$\langle \mathbf{p} | t_j | \mathbf{q}\rangle = \exp[i(\mathbf{q}-\mathbf{p})\cdot\mathbf{R}_j]\langle \mathbf{p} | t_{j,0} | \mathbf{q}\rangle.$$

With f_j and $f_{j,0}$ defined in an analogous manner, it follows that

$$\begin{aligned} f_j(\mathbf{p}, \mathbf{q}) &= -(2m/4\pi\hbar^2)\langle \mathbf{p} | t_j | \mathbf{q}\rangle \\ &= -(2m/4\pi\hbar^2)\langle \mathbf{p} | t_{j,0} | \mathbf{q}\rangle \exp[i(\mathbf{q}-\mathbf{p})\cdot\mathbf{R}_j] \\ &= f_{j,0}(\mathbf{p}, \mathbf{q}) \exp[i(\mathbf{q}-\mathbf{p})\cdot\mathbf{R}_j]. \end{aligned} \tag{38}$$

E. The Separable Potential Approximation

Because it has been proved applicable to nucleon-nucleon,[19] pion-nucleon,[20] and pion-deuteron[10] scattering, the separable potential approximation (SPA) is described briefly.

The first step in the SPA is the replacing of the local potential $V(\mathbf{r})$ with a nonlocal potential, or else the assumption is made that the two-body potential is nonlocal in the first place; i.e.,

$$V(\mathbf{r})\psi_i(\mathbf{r}) = \int d\mathbf{r}' V(\mathbf{r}, \mathbf{r}')\psi_i(\mathbf{r}'). \tag{39}$$

The second step in the SPA is the replacing of the kernel $V(\mathbf{r}, \mathbf{r}')$ by a separable kernel; i.e.,

$$V(\mathbf{r}, \mathbf{r}') = \lambda v(\mathbf{r})v(\mathbf{r}') \tag{40}$$

where λ is a normalizing constant. These last two equations yield

$$V(\mathbf{r})\psi_i(\mathbf{r}) = \lambda v(\mathbf{r})\bar{\psi}_i, \tag{41}$$

where

$$\bar{\psi}_i = \int d\mathbf{r}' v(\mathbf{r}')\psi_i(\mathbf{r}'). \tag{42}$$

Substitution of Eq. (41) in Eq. (4), multiplication of the result by $v(\mathbf{r})$ and integration over $\mathbf{r}$ gives

$$\bar{\psi}_i = [1-\lambda\bar{g}_k]^{-1}v(\mathbf{k}_i), \tag{43}$$

where

$$v(\mathbf{k}_i) \equiv \int d\mathbf{r} v(\mathbf{r}) \exp(i\mathbf{k}_i\cdot\mathbf{r}),$$

$$\bar{g}_k \equiv \int d\mathbf{r}d\mathbf{r}' v(\mathbf{r})g_k(\mathbf{r}, \mathbf{r}')v(\mathbf{r}').$$

But from Eq. (41) and Eq. (8)

$$f(\mathbf{k}_f, \mathbf{k}_i) = -(2m/4\pi\hbar^2)\lambda\bar{\psi}_i v(-\mathbf{k}_f),$$

so that with Eq. (43)

$$f(\mathbf{k}_f, \mathbf{k}_i) = -\frac{2m}{4\pi\hbar^2}\lambda\frac{v(-\mathbf{k}_f)v(\mathbf{k}_i)}{1-\lambda\bar{g}_k}. \tag{44}$$

[18] N. C. Francis and K. M. Watson, Phys. Rev. **92**, 291 (1953).

[19] S. Yamaguchi, Phys. Rev. **95**, 1628 (1954).

[20] A. Wentzel, Helv. Phys. Acta **15**, 111 (1942).

Equation (44) is also the result obtained for the scattering amplitude if $V(\mathbf{r})$ is a local potential with a shape $v(\mathbf{r})$ and normalizing constant λ; i.e., Eq. (41) is interpreted to mean

$$V(\mathbf{r})=\lambda v(\mathbf{r}), \tag{45}$$

where

$$\int d\mathbf{r} v(\mathbf{r})=1; \tag{46}$$

$\bar{\psi}_i$ is still given by Eq. (42), but it is now merely the average of the wave function over the shape of the local potential. In this case Eqs. (41) and (42) constitute an approximation which is only valid under certain conditions. From the physics of these two equations it is clear that these conditions should be roughly $ka\ll 1$ and $U_0a^2\ll 1$, where a is the range of $V(r)$ and $V_0=(\hbar^2/2m)U_0$ is in some sense the depth of $V(\mathbf{r})$.

F. Application: Square Well Potential

These techniques are applied here to the square well potential

$$U(r)=(2m/\hbar^2)V(r)=\begin{cases}-U_0=-(2m/\hbar^2)V_0, & r\leq a\\ 0, & r>a\end{cases}. \tag{47}$$

The solution to the lth radial Schrödinger equation with this potential which is finite at the origin is[14]

$$\phi_{1l}{}^k(r)=j_l(\alpha r), \tag{48}$$

where

$$\alpha=[U_0+k^2]^{\frac{1}{2}}. \tag{49}$$

Then

$$\phi_{1l}{}^{k\prime}(r)=\alpha j_l'(\alpha r). \tag{50}$$

Equations (48) and (50) are all that is needed to make the results of Sec. II(A) appropriate for the square well.

The results of Sec. II(B) can be applied to the square well by the use of Eqs. (48), (50), and

$$\phi_{2l}{}^k(r)=n_l(\alpha r), \qquad \phi_{2l}{}^{k\prime}(r)=\alpha n_l'(\alpha r); \tag{51}$$

i.e., $n_l(\alpha r)$ is a solution to Eq. (18a) which is linearly independent of $j_l(\alpha r)$.

An explicit expression can also be obtained for the off-energy-shell, square well scattering amplitudes. From Eqs. (36) and (37)

$$\begin{aligned}f(\mathbf{p},\mathbf{q})&=-(2m/4\pi\hbar^2)\langle\mathbf{p}\mid V+VG_kV\mid\mathbf{q}\rangle\\&=-(2m/4\pi\hbar^2)\Big\{\int d\mathbf{r}\exp(-i\mathbf{p}\cdot\mathbf{r})V(r)\exp(i\mathbf{q}\cdot\mathbf{r})\\&\quad+\int d\mathbf{r}d\mathbf{r}'\exp(-i\mathbf{p}\cdot\mathbf{r})V(r)G_k(\mathbf{r},\mathbf{r}')V(r')\\&\qquad\times\exp(i\mathbf{q}\cdot\mathbf{r}')\Big\}.\end{aligned} \tag{52}$$

Use of the results of Sec. II(B) applied to the square well, along with Eqs. (A4) and (A5) of Appendix A, gives

$$f(\mathbf{p},\mathbf{q})=k^{-1}\sum_{l=0}^{\infty}(2l+1)\eta_l(p,q)P_l(\mu_{pq}), \tag{53}$$

where

$$\begin{aligned}\eta_l(p,q)=\eta_l(q,p)=kU_0a^2\Big\{&\Big[1-\frac{U_0}{(\alpha^2-q^2)}\Big]\frac{c_l(\alpha,p,a)}{p^2-q^2}\\&+\frac{U_0[c_l(q,k,a)+ib_l(q,k,a)]}{(c_l+ib_l)(\alpha^2-q^2)(\alpha^2-p^2)}c_l(\alpha,p,a)\Big\}.\end{aligned} \tag{54}$$

It is easily seen that for $q=p=k$ Eq. (54) reduces to Eq. (28).

Finally, the SPA can be applied to the square well. From Eqs. (45), (46), and (47)

$$v(\mathbf{r})=\begin{cases}3/4\pi a^3, & r\leqq a\\ 0, & r>a,\end{cases} \tag{55}$$

$$\lambda=-(4\pi a^3/3)V_0. \tag{56}$$

These relations and Eq. (42) lead to

$$\psi_i(\mathbf{r})\approx\bar{\psi}_i=(3\eta_0/c_0k\alpha a^3)j_1(\alpha a), \qquad r\leqq a. \tag{57}$$

A numerical comparison of this result with Eq. (9) in the region $0\leqq r\leqq a$ shows that Eq. (57) is a good approximation when

$$ka\ll 1 \quad\text{and}\quad \alpha a\lesssim 1. \tag{58}$$

These restrictions merely mean that inside the potential the total wave function is approximately equal to its average over the shape of the potential provided that the wavelength outside the potential is large compared to the radius of the potential and that, inside the potential, the wavelength is at least as large as the radius; i.e., the wave function is a slowly varying function both inside and outside the potential.

III. SCATTERING FROM TWO POTENTIALS

The problem under consideration now is that of the scattering of a scalar particle by two spherically symmetric potentials. The Schrödinger equation for this problem is

$$\begin{aligned}(\hbar^2/2m)\{&\nabla_{\mathbf{r}}{}^2+k^2-U_1(|\mathbf{r}-\mathbf{R}_1|)\\&-U_2(|\mathbf{r}-\mathbf{R}_2|)\}\psi_i(\mathbf{r})=0.\end{aligned} \tag{59}$$

In this equation the origin is the midpoint of the vector $\mathbf{R}$ joining the centers of the two potentials, $\mathbf{r}$ is the position vector of the incident particle, $\mathbf{R}_j$ is the position vector of the center of the jth potential, and

$$\mathbf{R}=\mathbf{R}_2-\mathbf{R}_1=2\mathbf{R}_2=-2\mathbf{R}_1. \tag{60}$$

The desired solution to Eq. (59) has the form

$$\psi_i(r)=|\mathbf{k}_i\rangle+\psi^{\mathrm{sc}}(\mathbf{r}), \tag{61}$$

where

$$\psi^{\mathrm{sc}}(\mathbf{r})\xrightarrow[r\to\infty]{}F(\mathbf{k}_f,\mathbf{k}_i)r^{-1}e^{ikr}; \tag{62}$$

i.e., $F(\mathbf{k}_f, \mathbf{k}_i)$ is the scattering amplitude for this problem for scattering from the initial state $|\mathbf{k}_i\rangle$ to the final state $|\mathbf{k}_f\rangle$. The goal of the following calculations is to obtain an expression for $F(\mathbf{k}_f, \mathbf{k}_i)$ in terms of the $f_{j,0}(\mathbf{k}_f, \mathbf{k}_i)$, $j=1, 2$, the individual origin-centered scattering amplitudes for scattering from potentials one and two.

Several methods for solving this problem are presented for the case of S-wave scattering; i.e., each potential scatters only S waves relative to its own center. It is assumed that the two potentials are identical; this is not a necessary assumption, but it makes the form of the equations somewhat simpler than otherwise.

A. Point Potentials

The simplest case is that of S-wave scattering from two point potentials. Brueckner[7] discussed this problem in 1951; his derivation is given below.

The wave function outside the potentials is written as the sum of the incident plane wave, a wave scattered from potential one, and a wave scattered from potential two; i.e.,

$$\psi_i(\mathbf{r}) = \exp(i\mathbf{k}_i\cdot\mathbf{r}) + A_0\frac{\exp(ik\,|\,\mathbf{r}-\mathbf{R}_1\,|)}{|\,\mathbf{r}-\mathbf{R}_1\,|} + B_0\frac{\exp(ik\,|\,\mathbf{r}-\mathbf{R}_2\,|)}{|\,\mathbf{r}-\mathbf{R}_2\,|}, \quad (63)$$

this being the general solution to the wave equation outside the potentials for S-wave scattering by each potential. The outgoing amplitude A_0 is given in terms of the total wave amplitude at $\mathbf{R}_1$ by

$$A_0 = \frac{\eta_0}{k}\left\{\exp(i\mathbf{k}_i\cdot\mathbf{R}_1) + B_0\frac{\exp(ik\,|\,\mathbf{R}_1-\mathbf{R}_2\,|)}{|\,\mathbf{R}_1-\mathbf{R}_2\,|}\right\}, \quad (64)$$

where (η_0/k) is the S-wave scattering amplitude for potential one: from the assumption of identical potentials, (η_0/k) is also the S-wave scattering amplitude from potential two. Similarly

$$B_0 = \frac{\eta_0}{k}\left\{\exp(i\mathbf{k}_i\cdot\mathbf{R}_2) + A_0\frac{\exp(ik\,|\,\mathbf{R}_1-\mathbf{R}_2\,|)}{|\,\mathbf{R}_1-\mathbf{R}_2\,|}\right\}. \quad (65)$$

When Eqs. (63), (64), and (65) are solved for the scattering amplitude the result is

$$F(\mathbf{k}_f, \mathbf{k}_i) = \left[1-\frac{\eta_0^2\exp(2ikR)}{(kR)^2}\right]^{-1} \times\left\{\frac{\eta_0}{k}\{\exp[i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}_1]+\exp[i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}_2]\} + [\eta_0^2\exp(ikR)/k^2R][\exp[i(\mathbf{k}_i\cdot\mathbf{R}_1-\mathbf{k}_f\cdot\mathbf{R}_2)] + \exp[i(\mathbf{k}_i\cdot\mathbf{R}_2-\mathbf{k}_f\cdot\mathbf{R}_1)]]\right\}, \quad (66)$$

where $R=|\,\mathbf{R}\,|$.

From the discussion in Sec. II(A, B, and F) the details can be filled in. That Eq. (63) is the solution to the Schrödinger equation outside the potentials and for S-wave scattering by each potential, can be seen from Eq. (10) and the identity $h_0^{(1)}(x) = -ix\exp(ix)$.

Equation (64) states that the amplitude of the wave scattered by potential one is the S-wave scattering amplitude for this potential times the wave incident on this potential evaluated at the position of this potential. This also follows from the discussion in Sec. II: From Eqs. (2), (16), (22a), (28), and Sec. II(F), it follows that for a square well centered at $\rho=0$,

$$\psi^{sc}(\rho>a) = -(\eta_0/4\pi kc_0a^2)(e^{ik\rho}/\rho) \times\int d\varrho' j_0(\alpha\rho')U(\rho')\psi^{inc}(\varrho'), \quad (67)$$

where $\psi^{inc}(\varrho)$ is the wave incident upon the well; it is legitimate to use the entire incident wave in Eq. (67) since only its S wave part will survive the integration. It is assumed now that the range of $U(\rho')$ is small enough to allow the removal of the incident wave from the integrand. The remaining integration can be performed and the result is

$$\psi^{sc}(\rho>a) = (\eta_0/k)\psi^{inc}(0)[U_0 j_1(\alpha a)/c_0\alpha]\rho^{-1}\exp(ik\rho).$$

The taking of the limit of a point well, $a\to 0$, $U_0\to\infty$ (which means that the previous manipulation is exact), results in

$$U_0 j_1(\alpha a)/c_0\alpha \to 1,$$

so that

$$\psi^{sc}(\rho) = (\eta_0/k)\psi^{inc}(0)\rho^{-1}\exp(ik\rho),$$

or with $\varrho=\mathbf{r}-\mathbf{R}_j$,

$$\psi^{sc}(|\,\mathbf{r}-\mathbf{R}_j\,|) = (\eta_0/k)\psi^{inc}(\mathbf{r}=\mathbf{R}_j)\frac{\exp(ik\,|\,\mathbf{r}-\mathbf{R}_j\,|)}{|\,\mathbf{r}-\mathbf{R}_j\,|}. \quad (68)$$

The realization that the wave incident on one potential is just the original plane wave plus the wave scattered by the other potential gives an immediate explanation of Eqs. (64) and (65).

Finally, from Eq. (62) and Eq. (7), Eq. (63) implies

$$F(\mathbf{k}_f, \mathbf{k}_i) = \exp(-i\mathbf{k}_f\cdot\mathbf{R}_1)A_0 + \exp(-i\mathbf{k}_f\cdot\mathbf{R}_2)B_0. \quad (69)$$

Equation (66) follows directly from Eqs. (64), (65), and (69).

Bruckner's result for $F(\mathbf{k}_f, \mathbf{k}_i)$ can be interpreted as follows: The first two terms in the numerator of Eq. (66) are the single-scattering (or impulse approximation) terms; i.e., the incident particle scatters once from either potential, and the amplitude for each of these scatterings is shifted in phase because the potentials are centered at $\mathbf{r}=\mathbf{R}_1$ and $\mathbf{r}=\mathbf{R}_2$, rather than at $\mathbf{r}=0$. The next two terms in the numerator are the double-scattering terms; i.e., the incident particle scatters from potential one (two), propagates as an

outgoing spherical wave $R^{-1}\exp(ikR)$ until it scatters from potential two (one). The denominator represents all higher-order multiple scatterings; the four different phase factors in Eq. (66) come from the four different possibilities of the initial and final scatterings being from potentials one or two.

B. Solution from the *t*-Matrix Formalism

In 1955 Drell and Verlet[8] calculated the scattering amplitude $F(\mathbf{k}_f, \mathbf{k}_i)$ by using the t-matrix formalism. A somewhat expanded form of their derivation is given below.

For the case of scattering from two potentials $V_1(\mathbf{r}-\mathbf{R}_1)$ and $V_2(\mathbf{r}-\mathbf{R}_2)$, Eq. (4) has the symbolic form

$$\psi_i=|\,\mathbf{k}_i\rangle+\psi^{sc}=|\,\mathbf{k}_i\rangle+g_k(V_1+V_2)\psi_i. \tag{70}$$

The solution is

$$\psi_i=[1-g_k(V_1+V_2)]^{-1}\,|\,\mathbf{k}_i\rangle,$$

which gives for the scattered wave

$$\psi^{sc}=g_k(V_1+V_2)[1-g_k(V_1+V_2)]^{-1}\,|\,\mathbf{k}_i\rangle. \tag{71}$$

Use of the usual noncommutative algebra gives

$$\begin{aligned}
&g_kV_1[1-g_k(V_1+V_2)]^{-1}\\
&\quad=g_kV_1[(1-g_kV_2)(1-g_kV_1)-g_kV_2g_kV_1]^{-1}\\
&\quad=g_kV_1[(1-g_kV_1)-g_kt_2g_kV_1]^{-1}(1-g_kV_2)^{-1}\\
&\quad=g_kt_1[1-g_kt_2g_kt_1]^{-1}(1-g_kV_2)^{-1}\\
&\quad=g_kt_1[1-g_kt_2g_kt_1]^{-1}(1+g_kt_2),
\end{aligned} \tag{72}$$

where, independent of the state upon which it operates,

$$t_j=V_j[1-g_kV_j]^{-1},\qquad j=1,2, \tag{73}$$

is the off-origin-centered t matrix for scattering from $V_j(\mathbf{r}-\mathbf{R}_j)$. The last line of Eq. (72) follows from

$$(1-g_kV_2)^{-1}=1+g_kV_2(1-g_kV_2)^{-1}=1+g_kt_2.$$

Substitution of Eq. (72) as it stands, as well as with $1\leftrightarrow2$, into Eq. (71) yields[21]

$$\begin{aligned}
\psi^{sc}(\mathbf{r})=-(2m/4\pi\hbar^2)\int d\mathbf{r}'\frac{\exp(ik\,|\,\mathbf{r}-\mathbf{r}'\,|)}{|\,\mathbf{r}-\mathbf{r}'\,|}\\
\times\{[1-t_1g_kt_2g_k]^{-1}t_1(1+g_kt_2)\\
+[1-t_2g_kt_1g_k]^{-1}t_2(1+g_kt_1)\}\,|\,\mathbf{k}_i\rangle.
\end{aligned}$$

Use has been made of Eq. (6) and the operator identity $A[1-BA]^{-1}=[1-AB]^{-1}A$. The scattering amplitude obtained from this last equation is

$$\begin{aligned}
&F(\mathbf{k}_f,\mathbf{k}_i)\\
&\quad=-(2m/4\pi\hbar^2)\,\langle\mathbf{k}_f\,|\,[1-t_1g_kt_2g_k]^{-1}t_1(1+g_kt_2)\\
&\qquad+[1-t_2g_kt_1g_k]^{-1}t_2(1+g_kt_1)\,|\,\mathbf{k}_i\rangle.
\end{aligned} \tag{74}$$

[21] D. Park, Compt. rend. **245**, 291 (1957) also obtained this result.

The interpretation of this result in terms of single, double, and multiple scatterings is apparent.

The use of the closure property

$$\int d\boldsymbol{\gamma}\,|\,\boldsymbol{\gamma}\rangle\langle\boldsymbol{\gamma}\,|=\int d\boldsymbol{\gamma}\exp[i\boldsymbol{\gamma}\cdot(\mathbf{r}-\mathbf{r}')]=(2\pi)^3\delta(\mathbf{r}-\mathbf{r}'), \tag{75}$$

permits Eq. (75) to be written (through double-scattering terms) as

$$\begin{aligned}
&F^{(2)}(\mathbf{k}_f,\mathbf{k}_i)\\
&\quad=-(2m/4\pi\hbar^2)\{\langle\mathbf{k}_f\,|\,t_1\,|\,\mathbf{k}_i\rangle+\langle\mathbf{k}_f\,|\,t_2\,|\,\mathbf{k}_i\rangle\}\\
&\quad-(2m/4\pi\hbar^2)^2(2\pi)^{-6}\int d\boldsymbol{\gamma}d\boldsymbol{\lambda}\{\langle\mathbf{k}_f\,|\,t_1\,|\,\boldsymbol{\gamma}\rangle\langle\boldsymbol{\gamma}\,|\,g_k\,|\,\boldsymbol{\lambda}\rangle\\
&\quad\times\langle\boldsymbol{\lambda}\,|\,t_2\,|\,\mathbf{k}_i\rangle+\langle\mathbf{k}_f\,|\,t_2\,|\,\boldsymbol{\gamma}\rangle\langle\boldsymbol{\gamma}\,|\,g_k\,|\,\boldsymbol{\lambda}\rangle\langle\boldsymbol{\lambda}\,|\,t_1\,|\,\mathbf{k}_i\rangle\}.
\end{aligned} \tag{76}$$

The Green's function $g_k(\mathbf{r},\mathbf{r}')$ can be written as the Fourier integral[12]

$$g_k(\mathbf{r},\mathbf{r}')=-\frac{2m}{\hbar^2(2\pi)^3}\int\frac{d\mathbf{q}\exp[i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')]}{\mathbf{q}^2-(k+i\epsilon)^2},\quad\epsilon\to0^+ \tag{77}$$

i.e., $\epsilon>0$ and the limit $\epsilon\to0$ is taken after the integration is performed. This expression for $g_k(\mathbf{r},\mathbf{r}')$ leads to

$$\begin{aligned}
\langle\boldsymbol{\gamma}\,|\,g_k\,|\,\boldsymbol{\lambda}\rangle&=\int d\mathbf{r}d\mathbf{r}'\exp(-i\boldsymbol{\gamma}\cdot\mathbf{r})g_k(\mathbf{r},\mathbf{r}')\exp(i\boldsymbol{\lambda}\cdot\mathbf{r}')\\
&=-\frac{2m}{\hbar^2}(2\pi)^3\frac{\delta(\boldsymbol{\gamma}-\boldsymbol{\lambda})}{\lambda^2-(k+i\epsilon)^2}.
\end{aligned} \tag{78}$$

From this relation, Eq. (38), Eq. (60), and Eq. (76), it follows that

$$\begin{aligned}
F^{(2)}(\mathbf{k}_f,\mathbf{k}_i)&=\exp[-i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}/2]f_{1,0}(\mathbf{k}_f,\mathbf{k}_i)\\
&+\exp[i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}/2]f_{2,0}(\mathbf{k}_f,\mathbf{k}_i)\\
&+\exp[i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]\frac{4\pi}{(2\pi)^3}\int\frac{d\boldsymbol{\gamma}\exp(-i\boldsymbol{\gamma}\cdot\mathbf{R})}{\gamma^2-(k+i\epsilon)^2}\\
&\times f_{1,0}(\mathbf{k}_f,\boldsymbol{\gamma})f_{2,0}(\boldsymbol{\gamma},\mathbf{k}_i)\\
&+\exp[-i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]\frac{4\pi}{(2\pi)^3}\int\frac{d\boldsymbol{\gamma}\exp(i\boldsymbol{\gamma}\cdot\mathbf{R})}{\gamma^2-(k+i\epsilon)^2}\\
&\times f_{2,0}(\mathbf{k}_f,\boldsymbol{\gamma})f_{1,0}(\boldsymbol{\gamma},\mathbf{k}_i).
\end{aligned} \tag{79}$$

The first two terms are the single-scattering terms, while the integrand contains the double-scattering terms. For example, the first double-scattering term reads as follows: The incident particle with momentum $\mathbf{k}_i$ scatters from potential two into an intermediate state of momentum $\boldsymbol{\gamma}$; it then propagates in this intermediate state until it scatters from potential one. The total amplitude for this process is found by integration over all intermediate momenta. This last statement means that, even though the propagator in the integrand is peaked at $\gamma^2=k^2$, the scattering amplitudes in the integrand are off-energy-shell amplitudes.

The assumptions of S-wave scattering and identical potentials permit the reduction of Eq. (79) to the form

$$F^{(2)}(\mathbf{k}_f,\mathbf{k}_i)=\{\exp[i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}/2]+\exp[-i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}/2]\}(\eta_0/k)+\{\exp[i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]+\exp[-i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]\}\times\frac{2}{\pi}\int_0^\infty\frac{\gamma^2d\gamma}{\gamma^2-(k+i\epsilon)^2}j_0(\gamma R)f_0(k,\gamma)f_0(\gamma,k),\quad(80)$$

where $f_0=f_{1,0}=f_{2,0}$.

Drell and Verlet considered two approximations for the amplitudes in the integrand of Eq. (80):

$$\text{I.}\qquad f_0(k,\gamma)=f_0(\gamma,k)=f_0(k,k)=\eta_0/k,\quad(81)$$

$$\text{II.}\qquad f_0(k,\gamma)=f_0(\gamma,k)=0\quad\text{for}\quad\gamma\neq k.\quad(82)$$

The first form states that the off-energy-shell amplitudes are the same as the energy-conserving amplitudes, while Eq. (82) states that the off-energy-shell amplitudes vanish.

The substitution of I. into Eq. (80) leads to

$$\frac{2}{\pi}\int_0^\infty\frac{\gamma^2d\gamma}{\gamma^2-(k+i\epsilon)^2}j_0(\gamma R)f_0(k,\gamma)f_0(\gamma,k)=(\eta_0^2/k)I(kR),$$

where

$$I(kR)=-\frac{i}{2\pi kR}\int_{-\infty}^\infty\frac{\gamma d\gamma}{\gamma^2-(k+i\epsilon)^2}\times[\exp(i\gamma R)-\exp(-i\gamma R)]=(kR)^{-1}\exp(ikR).\quad(83)$$

Equation (80) can then be written

$$F_{\text{I}}^{(2)}(\mathbf{k}_f,\mathbf{k}_i)=(\eta_0/k)\times\{\exp[i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}/2]+\exp[-i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}/2]\}+(\eta_0/k)^2R^{-1}\exp(ikR)\{\exp[i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]+\exp[-i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]\}.\quad(84)$$

On the other hand, the form for the scattering amplitude given by Eq. (82) means that the factor $[\gamma^2-(k+i\epsilon)^2]^{-1}$ in the integrand can be replaced by[17] $(\pi i/2k)\delta(\gamma-k)$. This yields

$$F_{\text{II}}^{(2)}(\mathbf{k}_f,\mathbf{k}_i)=(\eta_0/k)\times\{\exp[i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}/2]+\exp[-i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}/2]\}+(\eta_0/k)^2\frac{i\sin kR}{R}\{\exp[i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]+\exp[-i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]\}.\quad(85)$$

All the higher-order multiple-scattering terms can be evaluated in the same manner as the double-scattering terms by using, in addition to Eqs. (81) and (82), the approximations

$$\text{I.}\qquad f_0(\gamma,\gamma')=f_0(k,k)=\eta_0/k,\quad(86)$$

$$\text{II.}\qquad f_0(\gamma,\gamma')=0\quad\text{for }\gamma\text{ or }\gamma'\neq k.\quad(87)$$

Summation of all the multiple-scattering terms leads to

$$F_{\text{I,II}}(\mathbf{k}_f,\mathbf{k}_i)=[1-(\eta_0/k)^2W_{\text{I,II}}^2]^{-1}\times(\eta_0/k)\{\{\exp[i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}/2]+\exp[-i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{R}/2]\}+(\eta_0/k)W_{\text{I,II}}\{\exp[i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]+\exp[-i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]\}\},\quad(88)$$

where the "propagators" $W_{\text{I,II}}$ are given by

$$W_{\text{I}}=e^{ikR}/R,\qquad W_{\text{II}}=i\sin kR/R.\quad(89)$$

Drell and Verlet pointed out the following features of Eq. (88). If the propagator W_{I} is used the resulting expression for $F(\mathbf{k}_f,\mathbf{k}_i)$ is the same as that obtained by Brueckner [Eq. (66)] and it has the same fault; i.e., in the limit $R\to0$, when the two wells collapse to a single well centered at the origin twice as deep as either of the original wells, Eq. (88) yields the incorrect result $F_{\text{I}}\to0$. If the region $kR<1$ is important, then Eq. (88) with W_{I} as the propagator is a poor approximation. If only terms through double scattering are included and W_{I} is used as the propagator, then, in this same limit, $F_{\text{I}}\to\infty$, which also is not correct. If, however, W_{II} is used in Eq. (88), then

$$F_{\text{II}}\xrightarrow[R\to0]{}2(\eta_0/k)[1+i\eta_0]/[1+\eta_0^2],$$

which at least reduces to the correct values for $\eta_0\ll1$.

A third approximation method, the SPA, was also used by Drell and Verlet to evaluate $F(\mathbf{k}_f,\mathbf{k}_i)$. This work is discussed later.

C. Solution from Matching at the Potential Boundaries

In 1957 Eyges[22] presented a method for solving nonseparable boundary value problems for those cases in which the nonseparable boundary is a sum of boundaries, each of which by itself constitutes a separable problem. This method is illustrated below for the problem of S-wave scattering from two identical, nonoverlapping, spherically symmetric potentials.

The Schrödinger equation is again Eq. (59) with the boundary condition given by Eqs. (61) and (62). Here, however, the additional restriction that $R>2a$ is imposed, where a is the radius of each of the potentials. The general procedure for the scattering of all partial waves is first to write the solution $\psi_i(\mathbf{r})$ in the region outside both potentials as the sum of the original plane wave and a scattered wave from each potential:

$$\psi_i(\mathbf{r})=|\,\mathbf{k}_i\rangle+\psi_i^{\text{sc}}(\mathbf{r}-\mathbf{R}_1)+\psi_2^{\text{sc}}(\mathbf{r}-\mathbf{R}_2).\quad(90)$$

The scattered wave from the jth potential ($j=1,2$) is

[22] L. Eyges, Ann. Phys. **2**, 101 (1957).

then written as a linear combination of the partial wave solutions for the scattered wave when only the jth potential is present. Next, the solution $\psi_i(\mathbf{r})$ inside each potential is written as a linear combination of the partial wave solutions for the problem when each potential is present by itself. Finally, the coefficients in these linear combinations are determined by the usual continuity requirements on the wave function and its first radial derivative at the boundary of each potential.

For S-wave scattering by each potential Eq. (90) is identical to Eq. (63):

$$\psi_i(\mathbf{r})=\exp(i\mathbf{k}_i\cdot\mathbf{r})+A_0\rho_1^{-1}\exp(ik\rho_1)+B_0\rho_2^{-1}\exp(ik\rho_2),\quad \rho_1,\ \rho_2>a, \tag{91}$$

where $\rho_j=|\,\boldsymbol{\varrho}_j\,|=|\,\mathbf{r}-\mathbf{R}_j\,|$, $j=1, 2$. Equation (9) can be used to write the wave function inside the jth potential as

$$\psi_i(\boldsymbol{\varrho}_j)=\sum_{l=0}^{\infty}D_{l,j}\phi_{1l}{}^{k}(\rho_j)\,P_l(\mu_{k_i\rho_j}),\quad \rho_j\leqq a,\ j=1, 2. \tag{92}$$

To determine the coefficients A_0 and B_0 the wave function inside and outside the jth potential must be expressed in terms of $\boldsymbol{\varrho}_j$ so that the continuity condition on ψ_i and its derivative with respect to ρ_j at the boundary $\rho_j=a$ can be easily applied. To accomplish this, Bauer's[23] formula is used in the form

$$\exp(i\mathbf{k}_i\cdot\mathbf{r})=\exp(i\mathbf{k}_i\cdot\mathbf{R}_j)\,\exp(i\mathbf{k}_i\cdot\boldsymbol{\varrho}_j)$$
$$=\exp(i\mathbf{k}_i\cdot\mathbf{R}_j)\sum_{l=0}^{\infty}(2l+1)i^l j_l(k\rho_j)\,P_l(\mu_{k_i\rho_j}), \tag{93}$$

and the relation[24]

$$\frac{\exp(ik\,|\,\boldsymbol{\varrho}_j\pm\mathbf{R}\,|)}{|\,\boldsymbol{\varrho}_j\pm\mathbf{R}\,|}$$
$$=ik\sum_{l=0}^{\infty}(2l+1)j_l(k\rho_j)\,h_l{}^{(1)}(kR)\,P_l(\mu_{\pm R,\rho_j}),\quad R>\rho_j \tag{94}$$

is also used. Substitution of Eq. (93) and Eq. (94) into Eq. (91) gives[25] for $j=1$

$$\psi_i(\boldsymbol{\varrho}_1)$$
$$=\exp(i\mathbf{k}_i\cdot\mathbf{R}_1)\sum_{l=0}^{\infty}(2l+1)i^l j_l(k\rho_1)\left(\frac{4\pi}{2l+1}\right)^{\frac{1}{2}}Y_{l,0}(L_{k_i\rho_1})$$
$$+(4\pi)^{\frac{1}{2}}A_0\rho_1^{-1}\exp(ik\rho_1)\,Y_{0,0}(L_{k_i\rho_1})$$
$$+ikB_0\sum_{l=0}^{\infty}\sum_{m=-l}^{l}j_l(k\rho_1)\,h_l{}^{(1)}(kR)$$
$$\times 4\pi Y_{l,m}{}^{*}(L_{Rk_i})\,Y_{l,m}(L_{k_i\rho_1}),\quad a\leqq\rho_1<R, \tag{95}$$

where the spherical harmonic addition formula

$$P_l(\mu_{R\rho_1})=\frac{4\pi}{(2l+1)}\sum_{m=-l}^{l}Y_{l,m}{}^{*}(L_{Rk_i})\,Y_{l,m}(L_{k_i\rho_1}) \tag{96}$$

also has been used.

The continuity conditions at $\rho_1=a$ can now be applied to Eq. (92) with $j=1$ and Eq. (95). A similar analysis can be performed for $j=2$. The resulting expressions connecting A_0 and B_0 are just those given in Eqs. (64) and (65). Consequently, $F(\mathbf{k}_f, \mathbf{k}_i)$ is given by Eq. (66).

The key point is that the potentials are nonoverlapping. This allowed the use of Eq. (92) for the wave function inside each potential. If the potentials overlapped, the region $\rho_j\leq a$ would not possess spherical symmetry about $\rho_j=0$, so that Eq. (92) would no longer be the correct expression for ψ_i in this region.

D. Solution from the One-Potential Total Green's Function

In this section a third method of solution is presented; one that also is applicable only for nonoverlapping potentials. The starting point is the Schrödinger equation (59) with the total wave function ψ_i given by Eq. (90). The boundary conditions are

$$\psi_j{}^{\mathrm{sc}}(\mathbf{r}-\mathbf{R}_j)\rightarrow\begin{cases}\text{finite at } |\,\mathbf{r}-\mathbf{R}_j\,|=0, & j=1, 2,\\ |\,\mathbf{r}-\mathbf{R}_j\,|^{-1}\exp(ik\,|\,\mathbf{r}-\mathbf{R}_j\,|) & \\ \qquad\text{as } |\,\mathbf{r}-\mathbf{R}_j\,|\rightarrow\infty & \end{cases} \tag{97}$$

and the no-overlap condition $R>2a$ is assumed to hold. The total wave function can also be written as

$$\psi_i(\mathbf{r})=\psi_j{}^{\mathrm{inc}}(\mathbf{r}-\mathbf{R}_j)+\psi_j{}^{\mathrm{sc}}(\mathbf{r}-\mathbf{R}_j),\quad j=1, 2, \tag{98}$$

where

$$\psi_j{}^{\mathrm{inc}}(\mathbf{r}-\mathbf{R}_j)=\exp(i\mathbf{k}_i\cdot\mathbf{R}_j)\,\exp[i\mathbf{k}_i\cdot(\mathbf{r}-\mathbf{R}_j)]$$
$$+\psi_n{}^{\mathrm{sc}}(\mathbf{r}-\mathbf{R}_j-[\mathbf{R}_n-\mathbf{R}_j]),\quad n\neq j, \tag{99}$$

is the wave incident on the jth potential; i.e., the wave incident on each potential is the original plane wave plus the wave scattered from the other potential.

Because the potentials do not overlap the Schrödinger equation in the region outside U_2 is

$$(\hbar^2/2m)\{\nabla_{\rho_1}{}^2+k^2-U_1(\rho_1)\}\psi_i(\boldsymbol{\varrho}_1)=0, \tag{100}$$

where the variable has been changed from $\mathbf{r}$ to $\boldsymbol{\varrho}_1=\mathbf{r}-\mathbf{R}_1$. From Eqs. (98) and (99), $\psi_i(\boldsymbol{\varrho}_1)$ is the sum of an incident wave

$$\psi_1{}^{\mathrm{inc}}(\boldsymbol{\varrho}_1)=\exp[i\mathbf{k}_i\cdot(\boldsymbol{\varrho}_1+\mathbf{R}_1)]+\psi_2{}^{\mathrm{sc}}(\boldsymbol{\varrho}_1-\mathbf{R}), \tag{101}$$

and a scattered wave. The first term on the right-hand side of Eq. (101) clearly satisfies the free-wave Schrödinger equation and, in fact, so does the second term. This last follows from the fact that $\psi_2{}^{\mathrm{sc}}(\boldsymbol{\varrho}_1-\mathbf{R})$ is the wave scattered by U_2; i.e., once $\psi_2{}^{\mathrm{sc}}$ is outside U_2 it is a free wave. This being the case, Eq. (100) can be

[23] See, for example, Gerald Goertzel and Nunzio Tralli, *Some Mathematical Methods of Physics* (McGraw-Hill Book Company, Inc., New York, 1960), p. 161.

[24] This relation can be derived easily from Eq. (77) with the help of Bauer's formula.

[25] For the definition and properties of the spherical harmonics $Y_{l,m}(L_{xy})$ used here see A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957). The notation L_{xy} means the angular coordinates of $\mathbf{y}$ with respect to $\mathbf{x}$ as polar axis.

written as

$$(\hbar^2/2m)\{\nabla_{\rho_1}{}^2+k^2-U_1(\rho_1)\}\psi_1{}^{sc}(\varrho_1)=V_1(\rho_1)\psi_1{}^{inc}(\varrho_1). \tag{102}$$

Equation (102) can be converted into an integral equation by using the total Green's function formalism of Sec. II(B). The result is

$$\psi_1{}^{sc}(\varrho_1)=\int d\varrho_1' G_k(\varrho_1,\varrho_1')V_1(\varrho_1') \times\{\exp[i\mathbf{k}_i\cdot(\varrho_1'+\mathbf{R}_1)]+\psi_2{}^{sc}(\varrho_1'-\mathbf{R})\}, \tag{103}$$

where $G_k(\varrho_1,\varrho_1')$ satisfies

$$(\hbar^2/2m)\{\nabla_{\rho_1}{}^2+k^2-U_1(\rho_1)\}G_k(\varrho_1,\varrho_1')=\delta(\varrho_1-\varrho_1'), \tag{104}$$

and the boundary conditions of Eq. (97); i.e., $G_k(\varrho_1,\varrho_1')$ is the same total Green's function as that used in Sec. II(B).

In analogous fashion $\psi_2{}^{sc}(\varrho_2)$ in the region outside U_1 is given by

$$\psi_2{}^{sc}(\varrho_2)=\int d\varrho_2' G_k(\varrho_2,\varrho_2')V_2(\varrho_2') \times\{\exp[i\mathbf{k}_1\cdot(\varrho_2'+\mathbf{R}_2)]+\psi_1{}^{sc}(\varrho_2'+\mathbf{R})\}, \tag{105}$$

where $\varrho_2=\mathbf{r}-\mathbf{R}_2$.

Equations (103) and (105) constitute a pair of coupled integral equations for the scattered waves $\psi_j{}^{sc}$, $j=1, 2$. Furthermore, the implicit restrictions on these equations, Eq. (103) valid only for $\rho_2>a$, and Eq. (105) valid only for $\rho_1>a$, can be dropped. This follows from the fact that, for example, once $\psi_2{}^{sc}$ is outside U_2 by its definition noting more can happen to it; it is true that $\psi_2{}^{sc}$ can be regarded as impinging on U_1 and being scattered by this potential, but this process is a contribution to $\psi_1{}^{sc}$ rather than a modification of $\psi_2{}^{sc}$. The result is that Eqs. (103) and (105) are valid even when the potentials overlap.[26] When, as has been assumed, the potentials are nonoverlapping, however, the form for each of the scattered waves is known, so that this pair of equations can be solved.

In both Eqs. (103) and (105), the plane-wave term on the right-hand side is just the single-scattering (impulse approximation) term; e.g., in Eq. (103) this is all that would appear inside the braces if potential two were not present. The other term in each of the integrals represents all of the multiple-scattering terms.

To illustrate the method of solution, the case of S-wave scattering is again considered. From the results presented in Sec. II(A) it is known that, for S-wave scattering from a spherically symmetric potential centered at $x=0$, the scattered wave is spherically symmetric and proportional to $x^{-1}e^{ikx}$. This means

$$\psi_1{}^{sc}(\varrho_1)=A_0\rho_1{}^{-1}\exp(ik\rho_1) =A_0\,|\,\varrho_2+\mathbf{R}\,|^{-1}\exp(ik\,|\,\varrho_2+\mathbf{R}\,|), \tag{106}$$

$$\psi_2{}^{sc}(\varrho_2)=B_0\rho_2{}^{-1}\exp(ik\rho_2) =B_0\,|\,\varrho_1-\mathbf{R}\,|^{-1}\exp(ik\,|\,\varrho_1-\mathbf{R}\,|), \tag{107}$$

where the coefficients A_0 and B_0 are to be determined. From Eqs. (16), (22a), (28), (103), and (107), $\psi_1{}^{sc}(\varrho_1)$ for $\rho_1>a$ is given by

$$\psi_1{}^{sc}(\varrho_1)=-\frac{i\eta_0}{4\pi c_0 a^2}\{\exp(i\mathbf{k}_i\cdot\mathbf{R}_1)I_1+B_0I_2\}, \tag{108}$$

where

$$I_1=\int d\varrho_1'\phi_{1_0}{}^k(\rho_1')U_1(\rho_1')\exp(i\mathbf{k}_i\cdot\varrho_1'), \tag{109}$$

$$I_2=\int d\varrho_1'\phi_{1_0}{}^k(\rho_1')U_1(\rho_1')\,|\,\varrho_1'-\mathbf{R}\,|^{-1}\exp(ik\,|\,\varrho_1'-\mathbf{R}\,|). \tag{110}$$

The use of Bauer's formula in Eq. (109), the performing of the angular integration, and comparison of the result with Eq. (27) gives

$$I_1=-4\pi c_0 a^2. \tag{111}$$

From Eq. (94), Bauer's formula, and Eq. (27), Eq. (110) reduces to[27]

$$I_2=-4\pi ikh_0{}^{(1)}(kR)c_0a^2. \tag{112}$$

The substitution of Eqs. (111), (112), and the definition of $h_0{}^{(1)}(k\rho_1)$ into Eq. (108) leads to Eq. (64). Equation (65) can be derived in a similar manner. The resulting expression for $F(\mathbf{k}_f,\mathbf{k}_i)$ is again that given in Eq. (66).

E. The Separable Potential Approximation

The third approximation used by Drell and Verlet[8] was the SPA. Their derivation of $F(\mathbf{k}_f,\mathbf{k}_i)$ for S-wave scattering from identical potentials proceeded in the following manner.

The use of Eq. (14) and the application of the SPA to each potential term individually leads to

$$\psi_i=|\,\mathbf{k}_i\rangle+\lambda_1\bar{\psi}_1g_kv_1+\lambda_2\bar{\psi}_2g_kv_2, \tag{113}$$

where

$$\bar{\psi}_j\equiv\int d\mathbf{r}v_j(\mathbf{r}-\mathbf{R}_j)\psi_i(\mathbf{r}),\quad j=1, 2, \tag{114}$$

and $v_j(\mathbf{r}-\mathbf{R}_j)$ is $V_j(\mathbf{r}-\mathbf{R}_j)$ normalized to unit volume integral with normalizing constant λ_j. From the averaging of Eq. (113) over v_1 there results

$$\bar{\psi}_1=\exp(i\mathbf{k}_i\cdot\mathbf{R}_1)v_1(\mathbf{k}_i)+\lambda_1\bar{\psi}_1g_k{}^{11}+\lambda_2\bar{\psi}_2g_k{}^{12}, \tag{115}$$

[26] See Sec. III(E).

[27] The use of Eq. (94) is restricted to S-wave scattering. A more general method, applicable to higher partial waves, is given in Appendix B.

where

$$v_j(\mathbf{q})\equiv\int d\boldsymbol{\varrho}_j v_j(\boldsymbol{\varrho}_j)\exp(i\mathbf{q}\cdot\boldsymbol{\varrho}_j),\quad j=1,2, \tag{116}$$

$$g_k{}^{ij}\equiv\int d\mathbf{r}d\mathbf{r}' v_i(\mathbf{r}-\mathbf{R}_i)g_k(\mathbf{r},\mathbf{r}')v_j(\mathbf{r}'-\mathbf{R}_j). \tag{117}$$

Similarly,

$$\bar{\psi}_2=\exp(i\mathbf{k}_i\cdot\mathbf{R}_2)v_2(\mathbf{k}_i)+\lambda_1\bar{\psi}_1 g_k{}^{21}+\lambda_2\bar{\psi}_2 g_k{}^{22}. \tag{118}$$

From the asymptotic form of Eq. (113) it follows that

$$F_{\mathrm{III}}(\mathbf{k}_f,\mathbf{k}_i)=-(2m/4\pi\hbar^2)[\lambda_1\bar{\psi}_1 v_1(-\mathbf{k}_f)$$
$$\times\exp(-i\mathbf{k}_f\cdot\mathbf{R}_1)+\lambda_2\bar{\psi}_2 v_2(-\mathbf{k}_f)\exp(-i\mathbf{k}_f\cdot\mathbf{R}_2)]. \tag{119}$$

Equations (115) and (118) can be solved for $\bar{\psi}_1$ and $\bar{\psi}_2$. Substitution of the results into Eq. (119) gives Eq. (88) with $W_{\mathrm{I,II}}$ replaced by W_{III},

$$W_{\mathrm{III}}\equiv-\frac{2m}{4\pi\hbar^2}\frac{g_k{}^{12}}{v_2(-\mathbf{k}_f)v_1(\mathbf{k}_i)}=\frac{2m}{4\pi\hbar^2}\frac{g_k{}^{21}}{v_1(-\mathbf{k}_f)v_2(\mathbf{k}_i)}, \tag{120}$$

and with

$$(\eta_0/k)=f_{j,0}(\mathbf{k}_f,\mathbf{k}_i)\equiv-\frac{2m}{4\pi\hbar^2}\lambda_j\frac{v_j(-\mathbf{k}_f)v_j(\mathbf{k}_i)}{1-\lambda_j g_k{}^{jj}}. \tag{121}$$

The accuracy with which the SPA result approximates the correct expression for $F(\mathbf{k}_f,\mathbf{k}_i)$ depends on whether or not the potentials overlap. For any two spherically symmetric potentials Eq. (94), Bauer's formula, and $v_1(\mathbf{q})=v_2(\mathbf{q})=v(q)=v(-q)$ can be used in Eq. (120) to obtain

$$W_{\mathrm{III}}=v^{-2}(k)\pi^{-1}\int_{-\infty}^{\infty}\frac{q^2dq}{q^2-(k+i\epsilon)^2}j_0(qR)v^2(q). \tag{122}$$

As Drell and Verlet pointed out, for nonoverlapping potentials W_{III} reduces to the exact value $R^{-1}\exp(ikR)$. This follows from the fact that $v^2(q)$ is an even, analytic, oscillatory function of $2qa$ so that, first, for q large and complex the R-dependent term in Eq. (122) determines the behavior of the integrand, and second, $v^2(q)$ can be removed from this integrand and evaluated at $q=k$.

The case $R<2a$ is much more complicated. Only the special case of low-energy ($ka\ll1$) S-wave scattering from two completely overlapping ($R=0$) identical square wells is investigated here. For this case $F(\mathbf{k}_f,\mathbf{k}_i)$ is calculated through double-scattering terms first using the SPA and then exactly.

The double-scattering terms in the SPA are given by

$$F_{\mathrm{III}}{}^{D}(\mathbf{k}_f,\mathbf{k}_i)=(\eta_0/k)^2W_{\mathrm{III}}\{\exp[i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]$$
$$+\exp[-i(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{R}/2]\}. \tag{123}$$

From Eq. (55), for a square well

$$v(q)=\int d\mathbf{r}v(\mathbf{r})\exp(i\mathbf{q}\cdot\mathbf{r})=3a^{-3}\int_0^a r^2j_0(qr)dr$$
$$=3(qa)^{-1}j_1(qa),$$

so that Eq. (122) becomes

$$W_{\mathrm{III}}=\frac{k^2}{\pi j_1{}^2(ka)}\int_{-\infty}^{\infty}\frac{j_0(qR)j_1{}^2(qa)}{q^2-(k+i\epsilon)^2}dq. \tag{124}$$

Evaluation of this integral for $R<2a$ and the taking of the limit $R\to0$ gives for the region $ka\ll1$[28]

$$W_{\mathrm{III}}k^{-1}\xrightarrow[x\ll1]{R\to0}\frac{6}{5x}+i+O(x)+\cdots, \tag{125}$$

where $x=ka$.

On the other hand from Eqs. (53), (54), and (80) the exact double-scattering terms are given by Eq. (123) with W_{III} replaced by W,

$$W=\frac{U_0{}^2}{\pi c_0{}^2}\int_{-\infty}^{\infty}\frac{j_0(qR)c_0{}^2(\alpha,q,a)}{[q^2-(k+i\epsilon)^2][q^2-\alpha]^2}q^2dq \tag{126}$$

where, from Eqs. (24), (48), and (50),

$$c_0(\alpha,q,a)=qj_0'(qa)j_0(\alpha a)-\alpha j_0'(\alpha a)j_0(qa). \tag{127}$$

Evaluation of the integral in Eq. (126) and the taking of the limit $R\to0$, gives for the region $x=ka\ll1$, $y=\alpha a\cong1$ (which, from Sec. II(F), is the region where the SPA is applicable to the square well)

$$Wk^{-1}\xrightarrow[x\ll1]{R\to0}\frac{y^2j_0(y)}{j_1(y)}x^{-4}-\left[\tfrac{1}{2}y+\frac{yj_0{}^2(y)}{6j_1{}^2(y)}\right]x^{-3}+O(x^{-2})+\cdots. \tag{128}$$

A direct comparison of Eq. (128) with Eq. (125) shows a marked disagreement. This indicates that the SPA as applied to two local potentials is not a good approximation when the potentials overlap.

F. Comparison of the Various Methods

The relationships among the various methods can be summarized as follows:

1. Brueckner's point potential calculation is merely a special case of the more general calculation of two spherically symmetric nonoverlapping potentials. The reason that the S-wave scattering amplitude from two nonoverlapping potentials has the same form as that from two point potentials is that, because the potentials do not overlap, each potential has incident upon it the scattered wave from the other potential in the region where the scattered wave is a function of the potential parameters only through the combination η_0.

2. The t-matrix formalism used by Drell and Verlet is the most general and the only method by which the case of overlapping potentials can be treated exactly. The reason why their approximation I (II) gives (does not give) the correct result for the scattering amplitude from nonoverlapping potentials can be found from a consideration of the integral in the double-scattering

[28] This result also is contained in reference 8.

term of Eq. (80). From Eqs. (34), (36), and (38),

$$f_0(\boldsymbol{\gamma}, \mathbf{k}_i) = -(2m/4\pi\hbar^2)\langle \boldsymbol{\gamma} \mid V+VGV \mid \mathbf{k}_i\rangle = -(1/4\pi)\langle \boldsymbol{\gamma} \mid U\psi_i\rangle, \quad (129)$$

which for S-wave scattering reduces to

$$f_0(\gamma, k) = -(4\pi)^{-1}\int d\mathbf{r} \exp(-i\boldsymbol{\gamma}\cdot\mathbf{r})\, U(r)\psi_{i,0}(r),$$

where $\psi_{i,0}(r)$ is the S-wave part of $\psi_i(\mathbf{r})$. The use of Bauer's formula and the performing of the angular integration gives

$$f_0(\gamma, k) = -\int_0^a r^2 j_0(\gamma r)\, U(r)\psi_{i,0}(r)\, dr. \quad (130)$$

From this it follows that $f_0(\gamma, k)$ is an analytic, oscillatory function of γa. From Eq. (129) it is clear that $f_0(\gamma, k) = f_0(k, \gamma)$ so that the product of these two functions is an analytic oscillatory function of $2\gamma a$. If $j_0(\gamma R)$ in the integral in Eq. (80) is written as a sum of exponentials, then from the above remark, so long as $R > 2a$, the R-dependent terms determine the behavior of the integrand for γ large and complex. These facts, along with the remark that $f_0(\gamma, k)$ is an even function of γ, imply that the $f_0(\gamma, k)f_0(k, \gamma)$ can be taken outside the integral in Eq. (80) and evaluated at $\gamma = k$. The remaining integral is easily evaluated, and the usual result for nonoverlapping potentials is obtained. A similar argument holds for the higher-order multiple-scattering terms. The key point is that all the integrals in these terms can be evaluated without decomposing the amplitudes $f_0(p, q)$ into their constituent parts. Under this condition $f_0(p, q)$ is an analytic function of p and q. It is because Drell and Verlet's approximation I (II) satisfies (does not satisfy) this analyticity condition, that their approximation I (II) gives (does not give) the correct scattering amplitude for nonoverlapping potentials. This leads to the conclusion that if an approximation is to be used for $f_0(p, q)$ such as to represent the case of overlapping potentials, then the approximate form of $f_0(p, q)$ must be nonanalytic with respect to p or q.

3. It follows from the preceding discussion that Brueckner's point potential calculation, as well as the calculations of Secs. III(C and D), include the contributions from off-energy-shell *t-matrix elements*. However, in the sense that for nonoverlapping potentials the incident particle propagates between collisions as an outgoing spherical wave with an energy equal to the incident energy, the multiple scatterings are on the energy shell *scatterings*. These two statements merely reflect the fact that it is necessary to use all momenta $\mathbf{p}$, including those with $p \neq k$, in the Fourier integral representation of $r^{-1}\exp(ikr)$.

4. The advantage of the total Green's function method over Eyges' method is that the former contains fewer undetermined coefficients at an intermediate stage. This is because part of the work of determining the coefficients has already been done in constructing the Green's function. Also, the physical picture of the multiple scatterings is somewhat clearer in the Green's function method than it is in Eyges' formalism.

5. The basic equations of the Green's function method are contained in the general formalism used by Drell and Verlet. This can be seen as follows: Eq. (70) can be written as

$$\psi_i = \mid \mathbf{k}_i\rangle + \psi_1^{sc} + \psi_2^{sc},$$

where

$$\psi_j^{sc} = g_k V_j \psi_i = g_k V_j[\mid \mathbf{k}_i\rangle + \psi_j^{sc} + \psi_n^{sc}], \qquad j = 1, 2 \neq n,$$

or

$$\psi_j^{sc} = g_k V_j[1 - g_k V_j]^{-1}[\mid \mathbf{k}_i\rangle + \psi_n^{sc}],$$

so that from Eq. (32) and the relation $g_k V_j = G_k t_k$ there results[29]

$$\psi_1^{sc} = G_k V_1[\mid \mathbf{k}_i\rangle + \psi_2^{sc}],$$
$$\psi_2^{sc} = G_k V_1[\mid \mathbf{k}_i\rangle + \psi_1^{sc}].$$

If these last two equations are expressed in explicit form, the first in terms of ϱ_1 and ϱ_1' and the second in terms of ϱ_2 and ϱ_2', the resulting expressions are just Eqs. (103) and (105).

6. From a physical viewpoint the reason why the SPA result reduces to the same form as the correct answer for the case of nonoverlapping potentials is that the SPA approximates the wave function only in the region inside each potential. When the potentials do not overlap, neither potential "knows" what is happening to the wave function inside the other potential. One potential "sees" the effect of the other potential only through the wave scattered by the other potential after it has left the interior of the other potential; in this region the SPA uses the exact wave function.

7. Each of the methods used in Secs. III(A–D) can be generalized to include the scattering of all partial waves. The calculations become rather involved; e.g., to find the scattering amplitude for the scattering of the first N partial waves, determinants of order $2N^2$ must be computed. Remarks 1 through 4, generalized in the appropriate manner, are valid even in this case.

APPENDIX A: SOME USEFUL INTEGRALS

The values for the integrals which occur in the evaluation of $f(\mathbf{p}, \mathbf{q})$ for a square well potential derived are derived below.

The derivation begins with the definition that $\phi_{p,l}(r)$ and $\phi_{q,l}(r)$ satisfy, respectively,

$$\left\{\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - l(l+1) + p^2r^2\right\}\phi_{p,l}(r) = 0, \quad (A1)$$

$$\left\{\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - l(l+1) + q^2r^2\right\}\phi_{,ql}(r) = 0, \quad (A2)$$

[29] The momentum-space equivalent of these equations for the case of N potentials was obtained by H. Ekstein, Phys. Rev. **88**, 721 (1951).

Multiplication of Eq. (A1) on the left by $\phi_{q,l}(r)$, Eq. (A2) on the left by $\phi_{p,l}(r)$, and the subtraction of one of the resultant expressions from the other gives

$$\phi_{q,l}\frac{d}{dr}\left(r^2\frac{d}{dr}\phi_{p,l}\right)-\phi_{p,l}\frac{d}{dr}\left(r^2\frac{d}{dr}\phi_{q,l}\right)=(q^2-p^2)\phi_{p,l}\phi_{q,l}r^2,$$

or

$$\frac{d}{dr}\left[r^2\phi_{q,l}\frac{d}{dr}\phi_{p,l}-r^2\phi_{p,l}\frac{d}{dr}\phi_{q,l}\right]=(q^2-p^2)\phi_{p,l}\phi_{q,l}r^2,$$

so that

$$\int_y^x r^2\phi_{p,l}(r)\phi_{q,l}(r)\,dr$$

$$=\left[\frac{r^2}{(q^2-p^2)}\left\{\phi_{q,l}(r)\frac{d}{dr}\phi_{p,l}(r)-\phi_{p,l}(r)\frac{d}{dr}\phi_{q,l}(r)\right\}\right]_{r=x}^{r=y}\quad\text{(A3)}$$

Application to the spherical Bessel and spherical Neumann functions yields

$$\int_y^x r^2 j_l(pr)j_l(qz)\,dz=\frac{y^2c_l(p,q,y)-x^2c_l(p,q,x)}{p^2-q^2}\quad\text{(A4)}$$

$$\int_y^x r^2 n_l(pr)j_l(qr)\,dr=\frac{-y^2b_l(q,p,y)+x^2b_l(q,p,x)}{p^2-q^2},\quad\text{(A5)}$$

where Eqs. (23) and (24), with

$$\phi_{1l}{}^k(r)=j_l(kr),\quad \phi_{2l}{}^k(r)=n_l(kr),\quad k=p,q,\quad r=x,y,$$

have all been applied in arriving at Eqs. (A4) and (A5).

APPENDIX B: EXTENSION OF III (D) TO ALL PARTIAL WAVES

Eyges has treated the generalization to all partial waves of the method described in Sec. III (C), for the problem of two hard spheres when the scattered wave is incident along the line joining the spheres,[22] and for the problem of a particle bound to two or more nonoverlapping spherically symmetric potentials of finite radius but otherwise arbitrary radial profile.[30] The derivation given here is the generalization to all partial waves of the method used in Sec. III (D) for the problem of scattering from two identical nonoverlapping spherically symmetric potentials of finite radius but otherwise arbitrary radial profile.

The derivation begins with the use of Eq. (10) to write Eq. (103) as

$$\psi_1{}^{sc}(\boldsymbol{\varrho}_1)=\psi_{1\text{I.A.}}{}^{sc}(\boldsymbol{\varrho}_1)+\int d\boldsymbol{\varrho}_1' G_k(\boldsymbol{\varrho}_1,\boldsymbol{\varrho}_1')V_1(\rho_1')\psi_2{}^{sc}(\boldsymbol{\varrho}_1'-\mathbf{R}),\quad\text{(B1)}$$

where the impulse approximation (single-scattering) term is given by

$$\psi_{1\text{I.A.}}{}^{sc}(\boldsymbol{\varrho}_1)=\exp(i\mathbf{k}_i\cdot\mathbf{R}_1)\sum_{l=0}^{\infty}(2l+1)i^{l+1}\eta_l h_l{}^{(1)}(k\rho_1)P_l(\mu_{k_i\rho_i}),\quad \rho_1>a.\quad\text{(B2)}$$

From Eqs. (16), (22a), and (28) it follows that Eq. (B1) can be written as

$$\psi_1{}^{sc}(\boldsymbol{\varrho}_1)=\psi_{1\text{I.A.}}{}^{sc}(\boldsymbol{\varrho}_1)-\frac{i}{4\pi a^2}\sum_{l=0}^{\infty}(2l+1)\eta_l c_l{}^{-1}h_l{}^{(1)}(k\rho_1)I_l,\quad\text{(B3)}$$

where for $\rho_1>a$

$$I_l=\int d\boldsymbol{\varrho}_1' P_l(\mu_{\rho_1\rho_1'})\phi_1{}^k(\boldsymbol{\varrho}_1')U_1(\rho_1')\psi_2{}^{sc}(\boldsymbol{\varrho}_1'-\mathbf{R}).\quad\text{(B4)}$$

To complete the preliminary work, the generalizations of Eqs. (106) and (107) are written. From the form of Eq. (10) these are

$$\psi_1{}^{sc}(\boldsymbol{\varrho}_1)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}A_{l,m}h_l{}^{(1)}(k\rho_1)Y_{l,m}(L_{k_i\rho_1}),\quad \rho_1>a,\quad\text{(B5)}$$

$$\psi_2{}^{sc}(\boldsymbol{\varrho}_2)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}B_{l,m}h_l{}^{(1)}(k\rho_2)Y_{l,m}(L_{k_i\rho_2}),\quad \rho_2>a,\quad\text{(B6)}$$

where, because the two-potential problem in general lacks azimuthal symmetry about the direction $\mathbf{k}_i$, spherical harmonics rather than Legendre polynomials must be used in these last two equations.

In order to evaluate I_l, the scattered wave $\psi_2{}^{sc}(\boldsymbol{\varrho}_1'-\mathbf{R})$ is represented by the Fourier integral

$$\psi_2{}^{sc}(\boldsymbol{\varrho}_1'-\mathbf{R})=(2\pi)^{-3}\int d\boldsymbol{\gamma}\, g_{\mathbf{k}_i}(\boldsymbol{\gamma})\exp(i\boldsymbol{\gamma}\cdot\boldsymbol{\varrho}_1'),\quad\text{(B7)}$$

where

$$g_{\mathbf{k}_i}(\boldsymbol{\gamma})=\int d\mathbf{t}_1\psi_2{}^{sc}(\mathbf{t}_1-\mathbf{R})\exp(-i\boldsymbol{\gamma}\cdot\mathbf{t}_1).\quad\text{(B8)}$$

From Eqs. (B7) and (B4) it follows that

$$I_l=(2\pi)^{-3}\int d\boldsymbol{\gamma}\, g_{\mathbf{k}_i}(\boldsymbol{\gamma})J_l,\quad\text{(B9)}$$

where

$$J_l=\int d\boldsymbol{\varrho}_1' P_l(\mu_{\rho_1\rho_1'})\phi_1{}^k(\rho_1')U_1(\rho_1')\exp(i\boldsymbol{\gamma}\cdot\boldsymbol{\varrho}_1'),$$

or, upon application of Bauer's formula and the spherical harmonic addition formula,

$$J_l=4\pi i^l P_l(\mu_{\gamma\rho_1})\int_0^a x^2\phi_1{}^k(x)U_1(x)j_l(\gamma x)\,dx.\quad\text{(B10)}$$

On the other hand, Eq. (B6) can be used in Eq. (B8), and, after the variable is changed from $\mathbf{t}_1$ to $\mathbf{t}_2=\mathbf{t}_1-\mathbf{R}$,

[30] L. Eyges, Phys. Rev. **111**, 683 (1959).

the angular integration can be performed to give

$$g_{\mathbf{k}_i}(\boldsymbol{\gamma}) = 4\pi \exp(-i\boldsymbol{\gamma}\cdot\mathbf{R}) \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} B_{l',m'} \times Y_{l',m'}(L_{k_i\gamma}) K_{l'}, \quad \text{(B11)}$$

where

$$K_{l'} \equiv \int_0^\infty h_{l'}^{(1)}(ky) j_{l'}(\gamma y) y^2 dy \quad \text{(B12)}$$

This last expression can be evaluated by using Eqs. (A4) and (A5) of Appendix A. If

$$K_{l'} = -\left(\frac{i}{k}\right) \frac{(\gamma/k)^{l'}}{\gamma^2 - (k+i\epsilon)^2}, \quad \epsilon \to 0^+ \quad \text{(B13)}$$

is used in Eq. (B11) and the resulting expression substituted into Eq. (B7), Eq. (B6) is regained. Equations (B13), (B11), and (B10) are now substituted into Eq. (B9), and Bauer's formula and the spherical harmonic addition formula are used to perform the angular integration. The resulting expression for I_l is

$$I_l = \frac{-16\pi a^2 i^l}{(2l+1)} \sum_{l',l''} \sum_{m,m',m''} (-i)^{l'+l''} B_{l',m'} \times J_{mm'm'',ll'l''} Y_{l,m}^*(L_{kj\rho_1}) Y_{l',m'}^*(L_{k_i R}) M_{ll'l''}, \quad \text{(B14)}$$

where

$$J_{mm'm'',ll'l''} = \int d\Omega Y_{l,m} Y_{l',m'} Y_{l'',m''} \quad \text{(B15)}$$

and

$$M_{ll'l''} = \frac{2i}{ka^2} \int_0^a x^2 dx \phi_{1l}^k(x) \int_0^\infty \frac{(\gamma/k)^{l'} j_l(\gamma x) j_{l'}(\gamma R)}{\gamma^2 - (k+i\epsilon)^2} \gamma^2 d\gamma.$$

Because[25]

$$J_{mm'm'',ll'l''} = 0 \text{ for } l+l'+l'' \neq \text{even integer},$$

and $j_l(z)$ has the parity $(-1)^l$, the γ integrand in this last equation can be replaced by one half the integral from $-\infty$ to ∞. Again for nonoverlapping potentials the R-dependent term determines the behavior of the γ integrand for γ large and complex. Evaluation of the γ integral yields

$$M_{ll'l''} = -\pi h_{l'}^{(1)}(kR) a^{-2} \int_0^a x^2 \phi_{1l}^k(x) U_1(x) j_l(kx) dx,$$

so that from Eq. (27)

$$M_{ll'l''} = \pi c_l h_{l'}^{(1)}(kR), \quad \text{(B16)}$$

where c_l is given by Eq. (24). Finally from Eqs. (B16) and (B14) it follows that

$$I_l = \frac{-16\pi^2 a^2 i^l c_l}{(2l+1)} \sum_{l',l''} \sum_{m,m',m''} (-i)^{l'+l''} B_{l',m'} \times J_{mm'm'',ll'l''} Y_{l,m}^*(L_{kj\rho_1}) Y_{l',m'}^*(L_{k_i R}) h_{l'}^{(1)}(kR). \quad \text{(B17)}$$

Equation (B17) is now substituted into Eq. (B3), Eqs. (B2) and (B5) are substituted in the resulting expression, and the coefficients of $Y_{l,m}(L_{kj\rho_1}) h_l^{(1)}(k\rho_1)$ are equated. The result of these manipulations is

$$A_{l,m} = [4\pi(2l+1)]^{\frac{1}{2}} i^{l+1} \eta_l \delta_{m,0} \exp(i\mathbf{k}_i\cdot\mathbf{R}_1) + 4\pi i^{l+1} (-1)^m \eta_l \sum_{l',l''} \sum_{m',m''} (-i)^{l+l'} J_{mm'm'',ll'l''} \times Y_{l',m'}^*(L_{k_i R}) h_{l'}^{(1)}(kR). \quad \text{(B18)}$$

The other half of the set of relations between the $A_{l,m}$ and the $B_{l,m}$ can be obtained from this result by the substitutions $A_{l,m} \leftrightarrow B_{l,m}$, $\mathbf{R}_1 \to \mathbf{R}_2$, $\mathbf{R} \to -\mathbf{R}$. In order to find the $A_{l,m}$ and the $B_{l,m}$ from these relations, determinants of infinite order would have to be calculated. If instead of using all partial waves only the first N partial waves are used, then the $A_{l,m}$ $B_{l,m}$ would constitute $2N^2$ unknowns with Eq. (B18) and its mate being $2N^2$ inhomogeneous equations among these unknowns; i.e., determinants of order $2N^2$ would have to be evaluated.

Once the $A_{l,m}$ and the $B_{l,m}$ are known, the scattering amplitude is determined: From Eqs. (B5) and (B6) $F(\mathbf{k}_f, \mathbf{k}_i)$ is given by

$$F(\mathbf{k}_f, \mathbf{k}_i) = \sum_{l=0}^{\infty} \sum_{m=-1}^{l} (-i)^{l+1} Y_{l,m}(L_{k_f k_i}) \times \{A_{l,m} \exp(-i\mathbf{k}_f\cdot\mathbf{R}_1) + B_{l,m} \exp(-i\mathbf{k}_f\cdot\mathbf{R}_2)\}.$$