PHYSICAL REVIEW VOLUME 179, NUMBER 1 5 MARCH 1969

Extension of the Integral Formulation of Scattering Theory to Coulomb Interactions*

P. L. Altick†
Physics Department, University of Chicago, Chicago, Illinois 60637
(Received 23 September 1968)

The integral formulation of scattering theory is extended to the treatment of a residual interaction with a Coulomb tail. The approach involves expanding the Green's function in a basis set and then finding the proper analytical treatment of the familiar pole as well as of other singularities in the kernel which are peculiar to long-range interactions. The pure Coulomb case is given as an example of the formulation. Methods of reducing the integral equations to an algebraic set are given for a residual interaction with arbitrary short-range form and a Coulomb tail. Finally, the extension of this procedure to many channels is described.

I. INTRODUCTION

Nonrelativistic scattering theory can be cast in either differential or integral forms. Although formally equivalent, each form has its distinct advantages for particular purposes. The integral formulation generally involves breaking off a residual interaction from the Hamiltonian and has been most used for perturbation-theory calculations and formal developments of the theory. However, recently, continuum wave functions for auto-ionization calculations, along the lines developed by Fano[1] and Fano and Prats,[2] have been found by expanding the Green's function in a basis set of functions.[3,4] This is not a perturbation procedure but is analogous to the configuration interaction approach to bound-state problems. It is applicable to systems with several open channels although the applications up to now have been limited to one open channel.

The present paper extends this integral equation technique to the situation where the residual interaction has a Coulomb tail. The extension is motivated by the desire to have the widest possible choice of basis functions for any particular problem and not be limited to functions with a certain asymptotic form. This flexibility becomes increasingly important, almost crucial, when complex systems are to be studied.

In scattering theory the Coulomb interaction requires special development essentially because plane or spherical waves are not asymptotic solutions to the wave equation in the presence of such a potential. For the simplest type of scattering – one particle potential scattering – expressions for scattering amplitudes from a potential which has an arbitrary (nonsingular) short-range form plus a Coulomb tail exist in standard references, e.g., Mott and Massey.[5] More general problems are frequently formulated in terms of integral equations which in their abstract form are the Lippmann-Schwinger equations. These equations contain a singular kernel, and the path of integration in the neighborhood of the singularity is chosen to yield the desired boundary conditions on the scattering function. If the residual interaction has a Coulomb tail, however, then its effect is not only to add a phase shift to the scattered wave but also to distort the waves by introducing an r-dependent logarithmic term in the phase; so the standard treatment of the singularity in the integral equations does not suffice in this instance. The Coulomb potential also causes a logarithmic divergence of the interaction matrix elements, a fact which has prevented a perturbation-theory treatment in the past.[6]

In the next section the modifications to the usual treatment of the integral equations are given which make their solution possible for long-range interactions. The pure Coulomb case, i.e., the expansion of a Coulomb wave with one charge in terms of Coulomb waves with another, is then given as an example in Sec. III. The integral equations for arbitrary short-range interactions with Coulomb tails are written down in Sec. IV and methods are given which reduce these equations to a linear algebraic set. Finally in Sec. V, the extension to several open channels is described.

II. THEORY

In this section and throughout the paper a partial-wave decomposition is assumed. Thus in the one channel case, we deal only with a radial function, which is a standing wave asymptotically, associated with a particular angular momentum. (To simplify notation the angular momentum label will not be carried.) The basis functions are solutions of

$$(H_0 - k^2/2)S(k, r) = 0. \tag{1}$$

The basis set may also include discrete states. These will play no direct role in the discussion so they will not be specifically noted but are implicitly included in any sum over states. We wish to find the solution of

$$(H - k^2/2)T(k, r) = (H_0 + V - k^2/2)T(k, r) = 0. \tag{2}$$

A formal expression for $T(k, r)$ is

$$T(k, r) = (k^2/2 - H_0)^{-1} VT(k, r), \tag{3}$$

and this is written as an integral equation by introducing the set $S(k, r)$ giving

$$T(k, r) = 2\int k'dk' S(k', r) K_{kk'}/(k^2 - k'^2) \tag{4}$$

with

$$K_{kk'} = \int dr S(k', r) VT(k, r). \tag{5}$$

For short-range interactions, $K_{kk'}$ is an element of the reaction matrix, but we consider it here just an expansion amplitude.

If the interaction V drops off faster than $1/r$, the effect of the integral on the right-hand side of Eq. (4) is just to add a phase shift to $S(k, r)$ as $r \to \infty$. This is accomplished by writing

$$(k - k')^{-1} = P(k - k')^{-1} + \beta\delta(k - k'), \tag{6}$$

where P indicates the principal part and β is a normalization constant. The singular kernel in Eq. (4) is defined by Eq. (6), and equations for $K_{kk'}$ can be found and solved. If the interaction has a Coulomb tail, however, then the asymptotic forms of $S(k, r)$ and $T(k, r)$ are given by

$$S(k, r) \sim (2/\pi k)^{1/2} r^{-1} \cos[kr + (Z'/k)\ln 2kr - \tfrac{1}{2}\pi(l + 1) - \arg\Gamma(l + 1 + iZ'/k) + \delta_S]$$

$$= (2/\pi k)^{1/2} r^{-1} \cos[\zeta(Z', k, r) + \delta_S], \tag{7a}$$

$$T(k, r) \sim (2/\pi k)^{1/2} r^{-1} \cos[kr + (Z/k)\ln 2kr - \tfrac{1}{2}\pi(l + 1) - \arg\Gamma(l + 1 + iZ/k) + \delta_T]$$

$$= (2/\pi k)^{1/2} r^{-1} \cos[\zeta(Z, k, r) + \delta_T], \tag{7b}$$

where δ_S and δ_T are phase shifts which arise from the departure of the potential from the Coulomb form at short distances, $\zeta(Z, k, r)$ is the Coulomb phase, and Z' and Z are the asymptotic charges. In this case the effect of the integral in Eq. (4) is to add a phase shift and also to correct the coefficient of the logarithmic term in the phase. Further, the integral in Eq. (5) fails to converge for $k = k'$. Thus the prescription given by Eq. (6) fails because neither term is defined when multiplied by $K_{kk'}$.

As will be seen explicitly in the next section, $K_{kk'}$ has a branch point at $k = k'$ for Coulomb potentials so the singularity in Eq. (4) is a pole plus a branch point. The proper contour around this singularity can be found by introducing a convergence factor $e^{-\eta r}$ for η arbitrarily small in the integrand of Eq. (5) thus defining $K_{kk'}$ for $k = k'$. This is equivalent to giving k a small positive imaginary part $i\eta$; thus the contour in Eq. (4) goes below the singularity and the branch cut must therefore be in the upper half plane. Introducing the symbol $\mathcal{P}$ to denote this contour (see Fig. 1) we have

$$T(k, r) = 2\mathcal{P}\int k'dk' S(k', r) K_{kk'}/(k^2 - k'^2). \tag{8}$$

To get an equation for $K_{kk'}$, Eq. (8) is multiplied by $S(k', r)V$ and integrated over r giving

$$K_{kk'} = 2\mathcal{P}\int k''dk'' V_{k'k''} K_{kk''}/(k^2 - k''^2) \tag{9}$$

where $V_{k'k''}$ is the matrix element of V within the basis set $S(k, r)$.

For the pure Coulomb case, $K_{kk'}$ is known exactly and Eq. (8) will be made explicit for this case in the next section. For an arbitrary interaction, methods of reducing Eq. (9) to a linear algebraic set which is suitable for numerical solution will be given in Sec. IV.

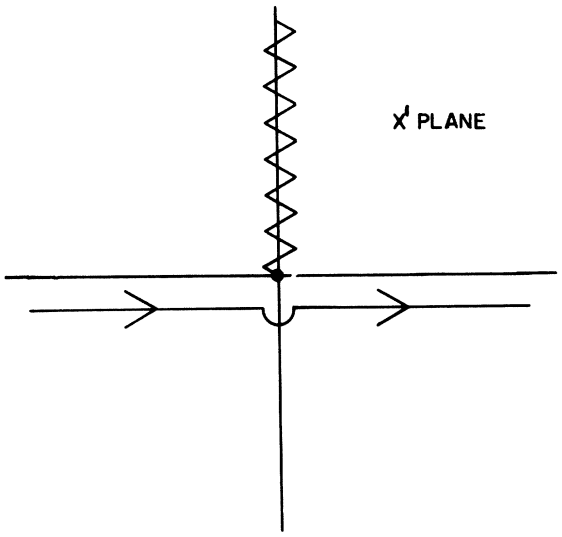

FIG. 1. The contour $\mathcal{P}$. There is a branch cut along the positive imaginary axis. The variable $x' = (k' - k)/2k$.

III. THE PURE COULOMB INTERACTION

We denote the Coulomb wave with charge Z' by $S_{Z'}(k, r)$ and the Coulomb wave with charge Z by $T_Z(k, r)$ to conform to our previous notation. Then

$$(H_{Z'}{}^{C} - k^2/2)S_{Z'}(k, r) = 0, \tag{10a}$$

$$\text{and } (H_Z{}^{C} - k^2/2)T_Z(k, r) = (H_{Z'}{}^{C} + V^{C} - k^2/2)T_Z(k, r) = 0, \tag{10b}$$

where $H_Z{}^{C}$ is the hydrogenic Hamiltonian and

$$V^{C} = (Z' - Z)/r = \Delta Z/r. \tag{11}$$

Equation (8) now reads

$$T_Z(k, r) = 2\mathcal{P}\int k'dk' S_{Z'}(k', r)K_{kk'}/(k^2 - k'^2) \tag{12}$$

or as $r \to \infty$,

$$(2/\pi k)^{1/2} r^{-1}\cos\zeta(Z, k, r) = 2\mathcal{P}\int k'dk'[K_{kk'}/(k^2 - k'^2)](2/\pi k')^{1/2} r^{-1}\cos\zeta\,(Z', k', r). \tag{13}$$

The integral expression for $K_{kk'}$ in Eq. (5) can be evaluated exactly in this instance giving[7]

$$K_{kk'} = \frac{2\Delta Z(4kk')^{l+\frac{1}{2}} e^{\frac{1}{2}\pi(Z'/k' - Z/k)}}{(k + k')^{2l+2}\pi} \operatorname{Re}\left[\left(\frac{k' - k}{k' + k}\right)^{i(Z'/k' - Z/k)}\right.$$

$$\left.\times\frac{\Gamma(-i(Z'/k' - Z/k))F(l + 1 - iZ/k, l + 1 + iZ'/k', 1 + i(Z'/k' - Z/k), [(k' - k)/(k' + k)]^2}{\exp i[\arg\Gamma(l + 1 + iZ/k) - \arg\Gamma(l + 1 + iZ'/k')]}\right], \tag{14}$$

where $F(a, b, c, x)$ is the hypergeometric function. Because the cosine term on the right-hand side of Eq. (13) oscillates rapidly for large r, the only region in the integration which will contribute is the neighborhood of $k' = k$. Thus we introduce the variable

$$x' = (k' - k)/2k, \tag{15}$$

and write Eq. (13) to the lowest order in x';

$$\cos\zeta(Z,k,r) = -(n' e^{-\frac{1}{2}\pi n'}/2\pi)$$

$$\times \mathrm{Re}\left(\frac{\Gamma(-in')\ \int dx'(x')^{in'-1}\left[e^{i[2krx'+\zeta(Z',k,r)]} + e^{-i[2krx'+\zeta(Z',k,r)]}\right]}{\exp i[\arg\Gamma(l+1+iZ/k) - \arg\Gamma(l+1+iZ'/k)]}\right), \tag{16}$$

where $n' = \Delta Z/k$. We now evaluate the integral over x' along the contour in Fig. 1. There is a branch cut from the origin along the positive imaginary axis. The limits are extended to $\pm\infty$ for convenience, but no contribution is added to the integral by so doing because of the oscillating cosine. In Eq. (16) the cosine has been written as a sum of exponentials; the integral over the first exponential gives

$$I = \mathcal{P}\int dx'(x')^{in'-1} e^{2ikrx'}. \tag{17}$$

With the variable change

$$t = -2ikrx', \tag{18}$$

the integral becomes

$$I = e^{\frac{1}{2}\pi n'} e^{-in'\ln 2kr} \int_{-i\infty}^{+i\infty} dt(-t)^{in'-1} e^{-t}. \tag{19}$$

Note that the variable change provided a scale factor which will correct the logarithmic term in the phase of the Coulomb wave. The remaining integral can be deformed into Hankels expression for a gamma function[8] giving finally

$$I = e^{\frac{1}{2}\pi n'} e^{-in'\ln 2kr}\Gamma(in')2\sinh\pi n'. \tag{20}$$

A similar treatment for the second exponential in Eq. (16) gives an expression like Eq. (19) except e^{+t} appears in the integrand rather than e^{-t}. This allows the contour to be closed on the left-hand side of the t plane over a region with no singularities; thus the integral is equal to zero, and this second term does not contribute to the right-hand side of Eq. (16). When Eq. (20) is inserted into Eq. (16), the phase factors just transform $e^{i\zeta(Z',k,r)}$ into $e^{i\zeta(Z,k,r)}$ while the other factors reduce to unity so the right side becomes just $\cos\zeta(Z,k,r)$.

By this exercise we have seen how the integral in Eq. (12) establishes the correct Coulomb phase. The important property of $K_{kk'}$ is its behavior as $k' \to k$, but this behavior is a direct consequence of the long range of V^C, so for any interaction with a Coulomb tail, we expect that

$$K_{kk'} \to \mathrm{Re}\{C[(k'-k)/2k]^{in'}\}, \quad \text{for } k' \to k, \tag{21}$$

where C is a complex function of k.

IV. TREATMENT OF AN ARBITRARY INTERACTION

We consider here the problem of finding the expansion amplitude $K_{kk'}$ for a function $T(k,r)$ where

$$(H_Z - k^2/2)T(k,r) = (H_{Z'} + V - k^2/2)T(k,r) = 0. \tag{22}$$

The Hamiltonians H_Z and $H_{Z'}$ contain arbitrary short-range potentials (different) with Coulomb tails $-Z/r$ and $-Z'/r$, respectively. The basis set $S(k,r)$ is given as solutions of

$$(H_{Z'} - k^2/2)S(k,r) = 0. \tag{23}$$

The asymptotic forms of $S(k,r)$ and $T(k,r)$ are given by Eqs. (7a) and (7b). We see from Eq. (8) and the last section that as $k' \to k$

$$K_{kk'} \to \frac{n' e^{-\frac{1}{2}\pi n'}}{\pi}\mathrm{Re}\left(\frac{\Gamma(-in')e^{i(\delta_T - \delta_S)}[(k'-k)/2k]^{in'}}{\exp i[\arg\Gamma(l+1+iZ/k) - \arg\Gamma(l+1+iZ'/k)]}\right). \tag{24}$$

This form of $K_{kk'}$ assures the asymptotic form in Eq. (7b). The factor containing δ_S and δ_T just adds δ_T and removes δ_S from the asymptotic form of $T(k,r)$ while the remaining factors correct the Coulomb phase.

Equation (9) is to be solved then with the boundary condition in Eq. (24). In general, $V_{k'k''}$ is known only numerically so the task is to treat only the singularities in Eq. (9) analytically, resulting in a set of equa-

tions which can be handled numerically. In fact we will outline a procedure which reduces Eq. (9) to a linear set of algebraic equations.

The singularities in Eq. (9) occur in $K_{kk'}$, $1/(k^2-k'^2)$, and $V_{k'k''}$ as their arguments become equal. By studying the long-range contribution to $V_{k'k''}$ which becomes dominant as $k''\to k'$, it is found that

$$V_{k'k''}\to -(\Delta Z/2\pi k')\ln[(k''-k')/2k']^2, \quad \text{for } k''\to k'. \tag{25}$$

Because of these singularities it is not possible to represent $K_{kk'}$ or $V_{k'k''}$ solely by their values at mesh points, which is the usual numerical treatment.[3,4] Rather, in the region $k'\to k$ which we imagine to be bounded by two mesh points such that $|x'|$ is small in the region, we represent $K_{kk'}$ by

$$K_{kk'}=K(x')=\mathrm{Re}\left((x')^{in'}\sum_{n=0}a_n(x')^n\right)+\sum_{n=1}b_n(x')^n. \tag{26}$$

This form contains the dominant singularity, $(x')^{in'}$ for x' in the neighborhood of zero. This is of course the factor which corrects the logarithmic term in the Coulomb phase of the basis set to that of the wave function $T(k,r)$. The function of the two power series then is to represent all the slowly varying factors some of which are associated with the Coulomb interaction, and some will arise from the short-range interaction; because the second series begins with x' it does not contribute to $T(k,r)$ asymptotically. An actual expansion around $x'=0$ of $K_{kk'}$ for the pure Coulomb interaction gives a series multiplying $(x')^{in}$ which contains powers of x' and $x'\ln x'$. These latter terms are not analytic as $x'\to 0$ but in that limit the ratio of their contribution to that of the first term in the series (which is $(x')^{in'}$) goes to zero. Thus for the sake of simplicity, only the power series is retained and the assumption is that it represents $K_{kk'}$ adequately. The number of terms in each series will be discussed below. The a_n are complex constants while the b_n are real. Similarly in the region $k''\to k'$, but neither close to k, we represent $V_{k'k''}$ by

$$V_{k'k''}=V(y)=-(\Delta Z/2\pi k')\ln y^2\sum_{n=0}c_n y^n, \tag{27}$$

where
$$y=(k''-k')/2k', \tag{28}$$

$c_0=1$, and enough terms are taken for an accurate representation. Finally we must consider the case when k, k', and k'' are all close together. In this region it is advantageous to introduce the variable

$$x''=(k''-k)/2k, \tag{29}$$

and write

$$V_{k'k''}=V(x',x'')=-(n'/2\pi)\ln(x''-x')^2\sum_{m,n=0}d_{nm}(x')^n(x'')^m \tag{30}$$

where $d_{00}=1$. Note that the c_n and d_{nm} are found from computation of the matrix elements and are part of the input data.

Altogether then the unknowns are the a_n and b_n and the value of $K_{kk'}$ at mesh points. By putting k' equal to each of the mesh points, the integral on the right-hand side of Eq. (9) can be evaluated by the same general techniques as used in Refs. (3) and (4). The procedure is not exactly the same because of the more complicated nature of $K_{kk'}$ and $V_{k'k''}$, but the net result will be one linear equation, involving the a_n, b_n, and $K_{kk'}$, for each mesh point. This is not a sufficient number of equations, however, and must be supplemented by two equations for each a_n retained (two because a_n is complex) and one equation for each b_n retained.

These additional relations are found by considering the region $|x''|$, $|x'|<\rho$ where ρ is small, and we assume that the region is bounded by mesh points. In this region we have power series representations of $K_{kk'}$ and $V_{k'k''}$, and Eq. (9) can be written

$$\mathrm{Re}\left((x')^{in'}\sum_{n=0}a_n(x')^n\right)+\sum_{n=1}b_n(x')^n=I_\rho(x')-\mathcal{P}\int_{-\rho}^{\rho}dx''V(x',x'')K(x'')\sum e_n(x'')^n/x'', \tag{31}$$

where $I_\rho(x')$ represents the integral over the remaining interval (and the sum over bound states) and may be expressed as

$$I_\rho(x')=\sum_{n=0}f_n(x')^n, \tag{32}$$

i.e., a Taylor series around $x'=0$. The series with coefficients e_n appears because the variable change

from k'' to x'' leaves a factor $2k''/(k+k'')$ which must then be expanded in terms of x''. Note that $e_0 = 1$.

The singularity in $V(x', x'')$ given by Eq. (30) is integrable. Thus in evaluating an integral containing $V(x', x'')$ the neighborhood of the singularity does not contribute so all paths of integration in this neighborhood give the same result. However, we are going to evaluate the integral in Eq. (31) by an integration by parts so a specification for the singularity is necessary, and we choose, for convenience, to treat it as a principal part.

The program is now (1) to substitute the expressions in Eqs. (26) and (30) into the integrand in Eq. (31); (2) perform the integration which will result in two power series in x', one beginning with $(x')^{in'}$ and one beginning with $(x')^0$; (3) equate coefficients of equal powers of x' on both sides thus obtaining new linear relations between the a_n, b_n, and $K_{kk'}$.[9] The procedure will be illustrated by evaluating the integral in Eq. (31) only to lowest order in x' and x''. This will reveal the method that can be used for each higher term. We have

$$J = (n'/2\pi)\,\mathrm{Re}[a_0 \mathcal{P} \textstyle\int_{-\rho}^{+\rho} dx'' \ln(x'' - x')^2 (x'')^{in'-1}]. \tag{33}$$

The path is below the branch point at $x'' = 0$ as in Fig. 1, and a principal part is taken at $x'' = x'$. The evaluation proceeds by a partial integration giving

$$J = \frac{n'}{2\pi}\,\mathrm{Re}\left(\frac{a_0 \ln(x'' - x')^2 (x'')^{in'}}{in'}\Big|_{-\rho}^{+\rho} - \frac{2a_0}{in'}\,\mathcal{P}\int_{-\rho}^{+\rho} \frac{dx''(x'')^{in'}}{(x'' - x')}\right). \tag{34}$$

In the first term the principal part has been taken. In the second term, writing the principal part integral as a sum of two contour integrals along S and S' as shown in Fig. 2 gives

$$-\frac{2}{in'}\,\mathcal{P}\int_{-\rho}^{+\rho} \frac{dx''(x'')^{in'}}{(x'' - x')} = \frac{2\pi}{n'}(x')^{in'} - \frac{2}{in'}\int_{S'} \frac{dx''(x'')^{in'}}{(x'' - x')}, \tag{35}$$

where the first term on the right is the contribution from the contour S, and the second integral is along S'. Finally

$$J = \mathrm{Re}\left(a_0 (x')^{in'} + a_0 \frac{\rho^{in'} \ln(\rho - x')^2 - (-\rho)^{in'} \ln(\rho + x')^2}{2\pi i}\right) - \frac{a_0}{i\pi}\int_{S'} \frac{dx''(x'')^{in'}}{(x'' - x')}. \tag{36}$$

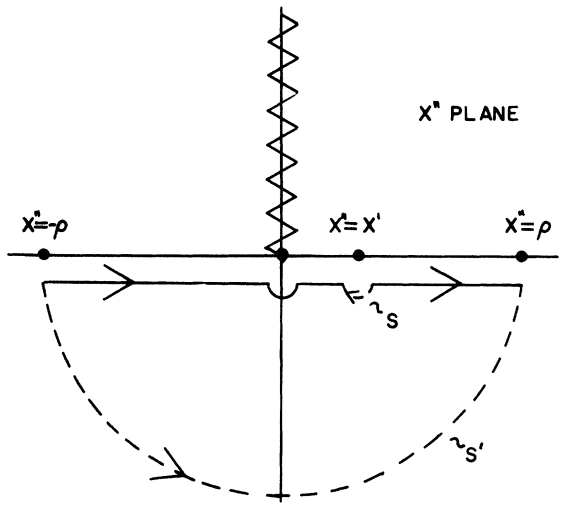

FIG. 2. The principal-part integral along the solid line is replaced by the contours S and S'.

Since we have specified $|x'| < \rho$, we use x'/ρ as an expansion parameter and express the second and third terms on the right-hand side of Eq. (36) as power series. This is possible for the third term because $|x''| = \rho$ all along S'. The final result for J, then is one term with $(x')^{in'}$ and a power series in x' beginning with $(x')^0$. The contributions to the integral in Eq. (31) of higher members of the series for $K(x'')$ or $V(x', x'')$ give other series beginning with $(x')^0$ as well as terms of the form $(x')^{in'+m}$.

In practice, of course, the series for $K(x'')$ must be truncated – say at N terms (including a_0) for the series beginning with $(x')^{in'}$ and N' terms for the series beginning with x'. Linear equations are then established by comparing coefficients of powers of x' up to $(x')^{in'+N-1}$ and $(x')^{N'}$ on both sides of Eq. (31). The number of relations then appears to be $2N+N'$, however, as we have seen above in Eq. (36), the equation for the coefficient of $(x')^{in'}$ is satisfied identially so the number of meaningful equations is reduced by 2. But there is a coefficient of $(x')^0$ on the right-hand side of Eq. (31) which must be zero because the series on the left begins with x', so this relation leaves the final number of equations obtained from the region $|x'|<\rho$ at $2N+N'-1$. Adding M equations found at M mesh points gives a total of $2N+N'-1+M$. On the other hand, the number of unknowns is

$$2N\ (a_0 \text{ to } a_{N-1}) + N'(b_1, \text{ to } b_{N'}) + M(K_{kk'} \text{ at the mesh points}).$$

Since there is one more unknown than there are equations, a solution exists and is unique except for normalization. After a solution has been found, the modulus and phase of a_0 are compared with Eq. (24) to find the phase shift and the correct normalization.

The detailed establishment of the algebraic equations follows directly from the above procedures, although there are a number of questions of numerical detail which will not be discussed here. Numerical applications are underway to demonstrate the feasibility of this approach.

V. EXTENSION TO MANY CHANNELS

In this section, the procedure for solving Eq. (9) for one channel is generalized to the many channel case. This extension appears to proceed without difficulty and will only be briefly described here. Recall that a partial-wave decomposition is assumed and for simplicity we will not write any angular factors.

In an N channel situation, N-degenerate wave functions must be found for each energy. If $T_i(Z,E)$ is one such function for an energy E, a convenient boundary condition to impose is

$$T_i(Z,E) \to \sum_{j=1}^{N} \chi_j (2/\pi k_j)^{1/2} [\delta_{ij} \cos\zeta(Z,k_j,r) + \mathcal{K}_{ij} \sin\zeta(Z,k_j,r)], \tag{37}$$

as $r\to\infty$ where r is the coordinate of the scattered particle, χ_j are the target eigenstates, k_j is the wave number of the particle scattered in the jth channel, and $\mathcal{K}_{ij}$ is an element of the reaction matrix.

To determine the $T_i(Z,E)$ by expanding in basis functions $S_i(Z',k_i)$ which have the asymptotic form.

$$S_i(Z',k_i) \to \chi_i (2/\pi k_i)^{1/2} r^{-1} \cos[\zeta(Z',k_i,r) + \delta_i], \tag{38}$$

Eqs. (8) and (9) are generalized to give

$$T_i(Z,E) = \sum_j 2\mathcal{P} \int k_j dk_j K_{ij}(E,k_j) S_j(Z',k_j)/(E-\epsilon_j - k_j^2/2), \tag{39}$$

and

$$K_{il}(E,k_l) = \sum_j 2\mathcal{P} \int k_j dk_j K_{ij}(E,k_j) V_{jl}(k_j,k_l)/(E-\epsilon_j - k_j^2/2), \tag{40}$$

where ϵ_j are the energies of the target states χ_j. Equation (40) must be solved subject to the boundary condition

$$K_{il}(E,k_l) \to \frac{n_l' e^{-\frac{1}{2}\pi n_l'}}{\pi} \mathrm{Re}\left\{ \frac{\Gamma(-in_l') e^{-i\delta_i} (x_l')^{in_l'} (\delta_{il} - i\mathcal{K}_{il})}{\exp i[\arg\Gamma(l+1+iZ/\kappa_l) - \arg\Gamma(l+1+iZ'/k_l)]} \right\} \tag{41}$$

as $k_l \to \kappa_l = [2(E-\epsilon_l)]^{1/2}$. Since $V_{jl}(k_j,k_l)$ has a singularity only for $j=l$ and $k_j\to\kappa_l$, Eq. (40) can be handled similarly to the one channel case. In the sum over target states, the term $j=l$ will have to be treated as in the last section while the other terms which do not contain a confluence of singularities raise no new problems.

After the reaction matrix is found, cross sections are computed by combining this matrix with the Coulomb scattering as shown, e.g., by Burke, McVicar, and Smith.[10]

ACKNOWLEDGMENT

I would like to thank Dr. U. Fano for numerous, extensive, and critical discussions of this work and for several suggestions which helped a great deal in reaching the main results of this paper. I would also like to acknowledge support from the National Aeronautics and Space Administration under Grant No. NGR-29-001-008 while the manuscript was being completed in Nevada.

---

*Supported by the Atomic Energy Commission, Contract No. COO-1674-14.

†Permanent address: Physics Department, University of Nevada, Reno, Nevada, 89507.

[1]U. Fano, Phys. Rev. 124, 1866 (1961).

[2]U. Fano and F. Prats, Proc. Natl. Acad. Sci. India A33, 553 (1963).

[3]P. L. Altick and E. N. Moore, Phys. Rev. 147, 49 (1966).

[4]P. L. Altick, Phys. Rev. 169, 21 (1968).

[5]N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Oxford University Press, New York, 1965), 3rd ed. Chapt. III,

[6]However, recently a formulation of the Born Series has been given which avoids divergences; see G. B. West, J. Math Phys. 8, 942 (1967).

[7]See, e.g., L. D. Landau and E. M. Lifshitz, Quantum Mechanics (Addison-Wesley Publishing Company, Inc., Reading, Mass., 1958), Appendix F. In addition an analytic continuation formula for the hypergeometric function has been used.

[8]E. T. Whittaker and G. M. Watson, A Course of Modern Analysis (Cambridge University Press, New York, 1965), 4th ed., p. 244.

[9]The complex series containing $(x')^{in'+m}$ reduces to two real series of the form $(x')^m \cos(n' \ln x')$ and $(x')^m \sin(n' \ln x')$ thus each term will give rise to two equations.

[10]P. G. Burke, D. D. McVicar, and K. Smith, Proc. Phys. Soc. (London), 83, 397 (1964).

PHYSICAL REVIEW VOLUME 179, NUMBER 1 5 MARCH 1969

Phase-Shift Calculation for Low-Energy Electron-Rb Scattering

Ludwig C. Balling
University of New Hampshire, Durham, New Hampshire 03824
(Received 4 November 1968)

Total elastic and total spin-exchange cross sections have been calculated numerically for low-energy electrons incident on rubidium atoms. The effects of electron exchange and of target distortion are treated through the use of the adiabatic exchange approximation and the method of polarized orbitals.

I. INTRODUCTION

Several authors have, in recent years, computed elastic scattering cross sections for electron-alkali atom collisions at low energies. Of these, the calculations by Garrett[1] for sodium and lithium appear to be the most successful. His calculated cross sections are in excellent agreement with the experimental data of Brode[2] and with that of Perel, *et al.*[3] in the energy range 0.25–16.0 eV. In addition, optical-pumping experiments[4,5] yield a spin-exchange cross section for electron-sodium collisions at thermal energies in good agreement with Garrett's results.

The optical-pumping data is useful because it gives information about the phase shifts at extremely low energies. At the lowest energies, the theoretical phase shifts are particularly sensitive to the approximations made in the calculation.

Recently, it has become feasible to carry out spin-exchange optical-pumping experiments over a wide range of thermal energies.[6] It appears reasonable that the energy dependence of alkali