Variational Principle for Potential Scattering*†

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Potential scattering is treated by a minimum variational principle. The method, known as the error method, is applicable to problems which can be cast as linear inhomogeneous equations. The method makes use of a non-negative functional which reduces to zero for the exact solution. The magnitude of the functional for approximate solutions provides an indication of the accuracy of the wave function. The method is illustrated by some examples, and compared with the Schwinger and Kohn principles.

I. INTRODUCTION

VARIATIONAL principles have come into extensive use for the calculation of phase shifts or scattering amplitudes in potential scattering problems.[1–8] A number of different principles have been formulated. The Hulthén[9] and Kohn[10] methods make use of differential operators and thus require trial wave functions of correct asymptotic form to satisfy boundary conditions. The Schwinger[11] method and several related ones[12,13] make use of associated integral operators which implicitly contain the boundary conditions, and do not restrict the choice of trial function. Kato[14] developed a generalized functional from which he obtained those of Hulthén, Schwinger, and Kohn; other workers have given different generalized functionals.[15]

Variational principles for the eigenvalue problem generally have the desirable feature that they give bounds on the eigenvalues. It has been noted that the aforementioned methods for scattering do not, in general, give bounds or an error indication.[13,16,17] Moe and Saxon[13] have looked for minimum functionals for the phase shifts or scattering amplitude with no success. Kato[14,16] has shown that upper and lower bounds on phase shifts can be obtained if certain conditions are fulfilled. In general the bounds are difficult to calculate, although Spruch[18] could obtain one of them quite readily for certain cases. Recently, Rosenberg and Spruch[19] have developed methods by which they can obtain rigorous lower bounds on the phase shifts for compound system scattering as well as for potential scattering.

In the present work use is made of an error functional, one which reduces to zero for the correct eigenfunction and is positive otherwise. Minimizing such a functional with respect to the parameters in a trial wave function yields an approximate state function which may then be used in calculating scattering cross sections. This application is a special case of a general error method for finding approximate solutions to linear inhomogeneous equations.[20]

The method is described in general outline in Sec. II. The inhomogeneous integral scattering equations are given in Sec. III. A generalized functional is introduced in Sec. IV, from which the error, Kohn, and Schwinger principles may be obtained. Some procedures for calculating approximate phase shifts or scattering amplitudes are described in Sec. V. In Sec. VI, two numerical problems are considered for illustrative purposes; one makes use of a spheroidal potential scatterer.

II. ERROR METHOD

We consider an arbitrary nonsingular linear operator L, and desire the solution f to the inhomogeneous equation $\mathsf{L}f=g$, where g is an arbitrary source function. Here, and in what follows, operators are indicated by sans serif.

Let $\tilde{f}_0$ represent a parametrized wave function (a trial solution) which is determined by minimizing the so-called error functional $\Lambda_E=\int|\mathsf{W}\epsilon_0|^2d\mathbf{r}$, where the function ϵ_0 is defined by $\epsilon_0=g-\mathsf{L}\tilde{f}_0$, and W is a suitably chosen nonsingular weighting operator. Here, and in what follows, trial solutions are indicated by a tilde. The error functional reduces to zero only when ϵ_0 vanishes, yielding the exact wave function for $\tilde{f}_0$. The precise nature of the operator W does not affect these

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considerations. If the function is itself of secondary importance, and is only required for the subsequent calculation of phase shifts or scattering amplitudes, it is desirable to pick a weighting function which yields the smallest error in the latter quantities. For example, in our case of potential scattering it is desirable to have the accuracy of the wave function greatest in the region where the potential is large. This suggests the potential itself as a multiplicative weighting operator. The effect of the multiplicative weighting operator in the error functional is treated in Sec. VI.

A procedure similar to that of Rayleigh-Ritz exists for systematic improvement of a trial wave function. Define $\epsilon_1=\epsilon_0-\mathbf{L}\tilde{f}_1$, where $\tilde{f}_1$ is a new parametrized function of adjustable amplitude. The error functional with ϵ_1 is smaller than that with ϵ_0 as long as $\tilde{f}_1$ is not zero. Thus the function $\tilde{f}_0+\tilde{f}_1$, which satisfies $\epsilon_1=g-\mathbf{L}(\tilde{f}_0+\tilde{f}_1)$, is by this criterion closer to the exact solution. By proceeding in this manner, using the error of an approximation as the source for the next approximation, we have a systematic procedure for improving the accuracy. Moreover, the size of the error functional, after minimization, can be used as a criterion for convergence. Unfortunately, this iteration procedure is only as good as the intuition of the investigator in choosing new trial functions $\tilde{f}_n$.

III. SCATTERING EQUATIONS

In this work we treat both spherical and spheroidal potential scattering by the method of partial waves. In both cases spherical harmonic expansions are used. The partial wave equations for a spheroidal potential are developed in Appendix A, and may be easily particularized to yield those for a spherical potential.

The method of partial waves for a spherical potential is treated in a number of standard texts.[21,22] Following in part the notations of Kato[16] and Kolsrud,[12] we may write the partial wave integral equations in the form

$$\mathbf{L}_l^R y_l(r)=u_l(r), \quad l=0, 1, \cdots, \infty, \tag{1}$$

where

$$u_l(r)\equiv rU^{\frac{1}{2}}(r)j_l(kr), \tag{2}$$

$$y_l(r)\equiv rU^{\frac{1}{2}}(r)S_l(r), \tag{3}$$

$$\mathbf{L}_l^R\equiv\mathbf{I}-krU^{\frac{1}{2}}(r)\int_0^\infty g_l(r,r')U^{\frac{1}{2}}(r')r'\cdots dr', \tag{4}$$

with $\mathbf{I}$ the identity operator, and $g_l(r,r')$ the radial Green's function

$$g_l(r,r')=n_l(kr_>)j_l(kr_<). \tag{5}$$

Here $r_>$ and $r_<$ denote the greater and lesser of (r,r'), respectively, and (n_l,j_l) are the spherical Neumann and Bessel functions of order l, respectively. The function $U(r)$ is the potential, in atomic units; in these units, the energy of the incident plane wave $\exp(i\mathbf{k}\cdot\mathbf{r})$ is k^2. The function u_l then represents the lth expansion coefficient in a spherical harmonic expansion of the plane wave; similarly, the y_l represent the wave function $\psi(\mathbf{r})$, which is the (unique) solution of the Schrödinger equation for scattering of the plane wave by a given potential $U(r)$. The function $S_l(r)$ is a real function proportional to the radial wave function $R_l(r)$ of the radial Schrödinger equation of order l.

In this notation, the phase shift δ_l is given by

$$\tan\delta_l=-k\int_0^\infty u_l y_l dr. \tag{6}$$

Once the $\tan\delta_l$ have been found, the scattering cross section is unambiguously determined.[21]

The radial wave function $R_l(r)$ must be everywhere bounded; it may be complex, but it must be of the form

$$R_l(r)=C_l S_l(r), \tag{7}$$

with C_l a complex constant. This follows because all the operators in the radial Schrödinger equation are real [we consider here only elastic scattering, so the potential $U(r)$ is real]. It is well known that there exists a "dispersion relation" connecting the ratio of imaginary to real parts of $R_l(r)$ to the phase shift.[23] This relation is

$$\mathrm{Im}(C_l)/R(C_l)\equiv\nu_l=\tan\delta_l. \tag{8}$$

In Appendix A we obtain the corresponding result in the partial wave treatment of a spheroidal potential.

IV. VARIATIONAL PRINCIPLES

In this section we formally discuss several variational principles. All of these may be applied with certain modifications to the partial wave equations for a spheroidal scatterer, or directly to the integral form of the three-dimensional Schrödinger equation. For simplicity we give a generalized variational function for the partial wave equations (1) for a spherical potential, which are rewritten here without the subscript l:

$$\mathbf{L}^R y-u=0. \tag{9}$$

As a generalized variational functional for this equation we write

$$\Lambda_G=\int_0^\infty[\mathbf{W}_1(\mathbf{L}^R\tilde{y}-u)][\mathbf{W}_2(\mathbf{L}^R\tilde{y}-u)]dr, \tag{10}$$

where $\mathbf{W}_1$ and $\mathbf{W}_2$ are nonsingular but otherwise arbitrary linear operators; different choices for these lead to different variational principles. For example, if we

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choose $\mathbf{W}_1=\mathbf{W}_2=\mathbf{W}$, we get

$$\Lambda_E=\int_0^\infty[\mathbf{W}(\mathbf{L}^R\tilde{y}-u)]^2dr, \tag{11}$$

which is the error functional for Eq. (1).

Another interesting choice for $\mathbf{W}_1$ and $\mathbf{W}_2$ is $\mathbf{W}_1=\mathbf{I}$, $\mathbf{W}_2=(\mathbf{L}^R)^{-1}-\mathbf{I}$. Inserting these in Eq. (10), we find

$$\Lambda'=-\int_0^\infty(\mathbf{L}^R\tilde{y}-u)^2dr + \int_0^\infty\tilde{y}(\mathbf{L}^R\tilde{y}-2u)dr+\int_0^\infty uydr. \tag{12}$$

The use of the operator $(\mathbf{L}^R)^{-1}$ here is purely formal, since we cannot evaluate it. (If we could, the problem would already be solved.) We notice that this functional does not provide an error indication because of the last term. This term cannot be evaluated without knowledge of the exact solution y. This fact has no effect on the use of this functional for variational purposes, since the last term is constant. The problem arose because of the nature of $\mathbf{W}_2$.

From the fact that $\mathbf{L}^R$ is symmetric, it follows that the first two terms of Eq. (12) are separately stationary for $\mathbf{L}^Ry=u$. The first is the error functional; the second is closely related to the Schwinger functional, as will be shown. These two terms taken together comprise the Kohn functional, as shown in Appendix B. In what follows we refer to the second term of Eq. (12) as Λ_K'.

The procedure for obtaining amplitude-independent functionals from those already given is illustrated for the case of Λ_K'. Let $\tilde{y}(r)=b\tilde{f}(r)$. Using the stationary property $\partial\Lambda_K'/\partial b=0$, we get

$$b=\int_0^\infty u\tilde{f}dr\Big/\int_0^\infty\tilde{f}\mathbf{L}^R\tilde{f}dr. \tag{13}$$

Substituting this in the expression for $\tilde{y}$ and inserting in Λ_K', we get

$$\Lambda_S=-\left(\int_0^\infty u\tilde{y}dr\right)^2\Big/\int_0^\infty\tilde{y}\mathbf{L}^R\tilde{y}dr, \tag{14}$$

which is easily recognized as the Schwinger functional. It is clearly immaterial whether we write $\tilde{f}$ or $\tilde{y}$ in the integrands.

By the same procedure, the following amplitude-independent form can be found for the error principle:

$$\Lambda_E'=-\left\{\left[\int_0^\infty(\mathbf{W}u)(\mathbf{W}\mathbf{L}^R\tilde{y})dr\right]^2\Big/\int_0^\infty(\mathbf{W}\mathbf{L}^R\tilde{y})^2dr\right\} + \int_0^\infty(\mathbf{W}u)^2dr. \tag{15}$$

In practice the amplitude-independent form of a given variational principle yields the same results as the amplitude-dependent form.

V. APPROXIMATE PHASE-SHIFT CALCULATIONS

As mentioned previously, the calculation of an approximate wave function is only an intermediate step in the scattering problem. We desire a functional of $\tilde{y}$ which yields the correct phase shift for the exact y and is insensitive to small errors in $\tilde{y}$. An expression of this character is one whose stationary value is an approximation to a particular phase shift. The Hulthén, Schwinger, and Kohn functionals are of this type; the error functional is not. Consider, for example, the previously discussed stationary functional Λ_K':

$$\Lambda_K'=-\int_0^\infty\tilde{y}(\mathbf{L}^R\tilde{y}-2u)dr. \tag{16}$$

The numerical value of this functional when $\tilde{y}=y$ is then $\Lambda_K'=-\int_0^\infty uydr=\tan\delta/k$. Thus the approximate value of the phase shift is quadratic in the error in $\tilde{y}$ if Λ_K' is used for its determination. This can be contrasted with the linear dependence when we determine the phase shift from the expression $-k\int u\tilde{y}dr$. The former expression is preferable as being less sensitive to small errors in $\tilde{y}$. There are an infinite number of such expressions to choose from which reduce to the correct phase shift when the exact wave function is used. No attempt is made here to optimize this choice. We merely compare the two already mentioned for a few numerical examples.

We wish to investigate the accuracy of the phase shifts determined by the error method in conjunction with each of the above-mentioned expressions. In particular we compare them with the Schwinger method for the case of s-wave scattering by a square well for two different incident energies. We pick a well of radius a and depth K^2. The trial function is chosen to be

$$\tilde{y}=b\sin(\lambda kr), \tag{17}$$

where b is to be determined variationally and λ is a parameter which is held fixed during the variation. For the choice $\lambda=\lambda_0\equiv k^{-1}(k^2+K^2)^{\frac{1}{2}}$, where k^2 is the incident energy, all methods lead to the exact answer.

The results are plotted in Fig. 1. The dashed curves are the Schwinger results for the phase shift. The dash-dot and solid curves are the corresponding results for the error method. The former are the results when the linear expression $-k\int_0^\infty u\tilde{y}dr$ for $\tan\delta$ is used while the latter are from the quadratic expression Λ_K', Eq. (16). The numerical values of the error functional are also plotted in units of k. Note that in the low-energy case, Fig. 1(b), the Schwinger functional has a singularity on each side of $\lambda=\lambda_0$; these merely correspond to phase shifts which are odd multiples of $\pi/2$.

As expected the linear expression is not as good as

the quadratic near $\lambda=\lambda_0$. The latter is similar to the Schwinger functional for the high-energy case and turns out better for the low-energy case in that it has no singularities and is flat over a relatively wide range of λ near λ_0. Calculations for energies intermediate between those quoted here were carried out. In general, the error method combined with the quadratic approximation gave the most reliable results for these test cases.

If the error functional is 1% or less of the source term $\int u^2 dr$, we find in all cases that the quadratic phase shift is within 1% of the exact value. Using the other expressions for $\tan\delta$, the corresponding errors came out as high as 50%.

These results support the view that it may be advantageous to first use the error method to determine an approximate wave function, and then use a stationary expression such as the Schwinger or Kohn functional to evaluate the approximate phase shift or scattering amplitude. Alternatively, the error functional can be used solely as an error indicator; for example, a wave function may be determined by the Kohn or Schwinger principles, and then an accuracy indication can be obtained by evaluating the error functional for this function.

VI. ILLUSTRATIVE PROBLEMS

In this section we consider two numerical problems which illustrate certain features of the error method. Part A is concerned with the effect of weighting operators in the error functional; part B, with the application of the error method to scattering from a spheroidal potential. All numerical calculations were done on the IBM type 650 digital computer at Rensselaer Polytechnic Institute.

A. Weighting Operators

We base the discussion here on the error functional for the real partial wave scattering equations (1). For these equations, the error functional is

$$\Lambda_E=\int_0^\infty [\mathbf{W}(\mathbf{L}^R\tilde{y}-u)]^2 dr, \tag{18}$$

where $\mathbf{W}$ is a nonsingular linear operator. Again we consider only the $l=0$ case for simplicity.

In order to decide what sort of weighting operator is likely to lead to the greatest accuracy in an approximate phase shift for a particular trial function, we look at the expression for the exact phase shift, Eq. (6):

$$\tan\delta=-k\int_0^\infty uy dr. \tag{19}$$

We remember that u and y both contain the square root of the potential as a factor, so the integrand contains the potential linearly. Referring to the definitions

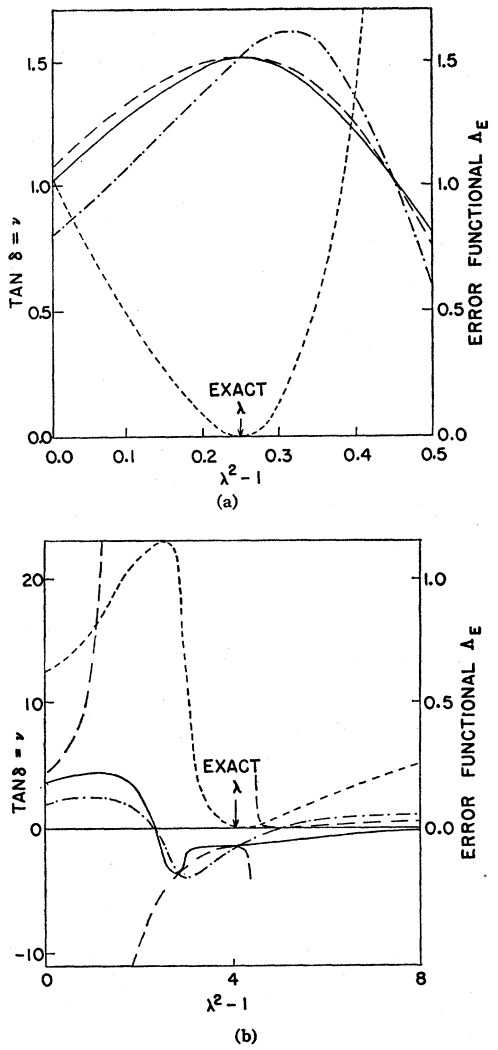

FIG. 1. Calculated s-wave phase shifts from spherical square well potential. Radius$=a$, depth$=K^2$, $Ka=4$. (a) $K^2/k^2=$well depth/incident energy$=\frac{1}{4}$. (b) $K^2/k^2=4$.

of u and y, Eqs. (2) and (3), we find that Eq. (19) may be written

$$\tan\delta_l=-k\int_0^\infty j_l(kr)U(r)S_l(r)r^2 dr, \tag{20}$$

where the real function S_l is defined by writing the complex radial wave function R_l as

$$R_l(r)=[(1+i\tan\delta_l)/(1+\tan^2\delta_l)]S_l(r).$$

From this we see that the greatest contribution to $\tan\delta_l$ comes from the region of r where $r^2U(r)$ is large, provided the rest of the integrand, (the product j_lS_l), is not relatively small there.

These considerations suggest the use of the identity for the weighting operator $\mathbf{W}$, inasmuch as this choice leaves the quantity $r^2U(r)$ in the integrand of the error functional (18).

TABLE I. Comparison of weighting operators for the error method in the s-wave scattering from the potential $U(r)=-U_0(a/r)\exp(-\alpha r)$, $r\leq a$; $=0$, $r>a$, with $U_0a^2=0.64$, $\alpha a=1.0$, and $ka=7.0$.

Method	Weighting operator	Trial radial wave function form	$\tan\delta_0$	Source term $k\int_0^\infty(\mathbf{W}u)^2dr$	$k\Lambda_E$
Error variational	$[rU^{\frac{1}{2}}(r)]^{-1}$	"Exact"	0.1107	3.252	0.00002
Error variational	$[rU^{\frac{1}{2}}(r)]^{-1}$	Parabola	0.1059	3.252	0.166
Error variational	$[rU^{\frac{1}{2}}(r)]^{-1}$	$bj_0(kr)$	0.1080	3.252	0.030
Error variational	unity	Parabola	0.1082	8.391	0.196
Error variational	unity	$bj_0(kr)$	0.1098	8.391	0.033
Born approximation	...	...	0.1096	...	...

We choose as an example a spherical shielded Coulomb potential which is set equal to zero outside a spherical surface of radius a. The potential is given in the heading of Table I. We compare two weighting operators: the identity, and the multiplicative one $[rU^{\frac{1}{2}}]^{-1}$, which causes the quantity $r^2U(r)$ to be removed from the error functional integrand. To find the "exact" value of $\tan\delta$, we first numerically integrate the $l=0$ radial Schrödinger equation to obtain the functional form of the exact radial wave function. Then we apply the error method to find the correct amplitude, and evaluate $\tan\delta=-k\int_0^\infty uydr$. This result is listed in the first row of Table I. The value of Λ_E for this case would be zero except for the inaccuracies inherent in numerical computation. The approximate phase shifts are evaluated from the linear expression $-k\int_0^\infty u\tilde{y}dr$. We see that for a given trial function, use of the identity operator leads to the more accurate phase shift.

For this relatively high energy problem we expect the Born approximation to be quite accurate. The Born approximation here consists of putting $\tilde{y}=rU^{\frac{1}{2}}j_0(kr)$ and evaluating $\tan\delta\approx-k\int_0^\infty j_0^2(kr)U(r)r^2dr$. It is interesting to note that a "quasi-Born" approximation, where we let the error method determine the amplitude b in a trial function $\tilde{y}=brU^{\frac{1}{2}}j_0(kr)$, is more accurate than the Born approximation only for the identity weighting operator. Also note that the ratio of the error functional to its "source" term $\int_0^\infty(\mathbf{W}u)^2dr$ is consistently smaller for the identity operator.

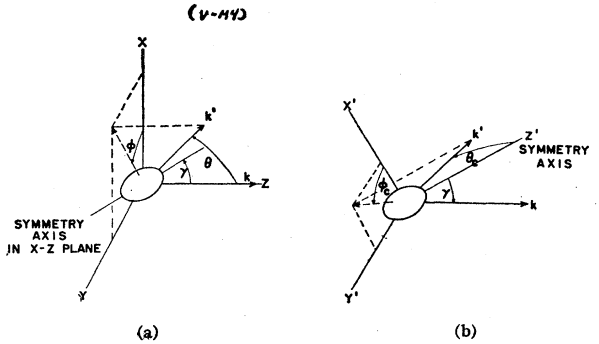

FIG. 2. Geometry for a spheroidal scatterer. The incident wave vector is $\mathbf{k}$; a particular scattering direction is indicated by $\mathbf{k}'=k\hat{r}$. (a) Conventional coordinates; θ=scattering angle. (b) Coordinates used in calculation.

B. Spheroidal Potential

In recent years a number of authors have employed spheroidal and other nonspherical potentials to represent the effect of the nucleus in scattering alpha particles, neutrons, and electrons.[24–31] It has also been shown that the general neutron transport equation reduces to a set of coupled one-dimensional Fredholm integral equations,[32] which have the same form as the spherical harmonic partial wave equations which we find in Appendix A for a spheroidal scatterer.

Although apparently excellently suited to these problems, variational methods have not been widely applied to them. The use of variational methods for nonspherical scattering problems seems to have been confined to the problem of scattering by simple tensor forces, a problem which can be represented by two or three coupled equations in one variable.[33–35]

In this subsection we make use of the error method to calculate the approximate scattering cross section for an oblate spheroidal Gaussian potential, in order to illustrate a procedure for using the error method in a relatively complicated problem. In addition, we are able to point out certain characteristics of the Kohn, Schwinger, and error principles which have not yet been noted.

As shown in Appendix A, the spherical harmonic partial wave equations for a spheroidal potential have the form

$$\sum_{l'=m}^{\infty}\mathbf{J}_{ll'}{}^mR_{l'}{}^m(r)-\Gamma_l{}^mj_l(kr)=0, \qquad (21)$$

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where the index m can take on integral values from zero to infinity, and l from m to infinity. The function $R_l^m(r)$ is the radial wave function. The parameter Γ_l^m is defined by

$$\Gamma_l^m = P_l^m(\cos\gamma), \tag{22}$$

with P_l^m the associated Legendre polynomial of order (l,m), and γ the angle between the incident direction $\mathbf{k}$ and the symmetry axis of the potential (see Fig. 2). The integral operator $\mathbf{J}_{ll'}^m$ is given by

$$\mathbf{J}_{ll'}^m = \delta_{ll'} - ik\int_{r'=0}^{\infty} g_l'(r,r')V_{ll'}^m(r')\cdots(r')^2dr', \tag{23}$$

with $g_l'(r,r')$ the radial Green's function,

$$g_l'(r,r') = [j_l(kr_>)+in_l(kr_>)]j_l(kr_<), \tag{24}$$

and

$$V_{ll'}^m(r) = \text{const}\times\int_0^{\pi} P_l^m(\cos\theta_c)P_{l'}^m(\cos\theta_c) \times U(r,\theta_c)\sin\theta_c d\theta_c. \tag{25}$$

Here $U(r,\theta_c)$ is the spheroidal potential, and θ_c is the colatitude of Fig. 2(b). $V_{ll'}^m$ is always real for a spheroidal potential; it would not be for a potential not having a plane of symmetry.

Just as in the spherical case, a phase shift δ_l^m may be defined here for each partial wave (l,m). It is shown in Appendix A that the $\tan\delta_l^m$ determine the scattering and are given by

$$\tfrac{1}{2}\Gamma_l^m \sin 2\delta_l^m = -k\sum_{l'=m}^{\infty}\int_0^{\infty} r^2dr\, j_l(kr)V_{ll'}^m(r)T_{l'}^m(r), \tag{26}$$

where $T_l^m(r)$ is a real function related to the radial wave function $R_l^m(r)$ by

$$R_l^m(r) = (1+i\tan\delta_l^m)T_l^m(r). \tag{27}$$

Kohn and Schwinger functionals may be easily formulated for Eqs. (21), but their stationary values do not provide approximations to the individual $\tan\delta_l^m$ or $\sin 2\delta_l^m$, which they do for the $\tan\delta_l$ in the spherical case.[36] In this formulation of the spheroidal problem, we have been unable to find any functionals whose stationary values do provide approximations to the individual phase shifts.

The potential used in this sample calculation is given in the heading of Table II. For convenience, we set the potential equal to zero outside a spherical surface of radius a. For the parameters chosen, the potential is an oblate spheroidal Gaussian with a major-minor axis ratio of $\sqrt{3}$, and is quite strongly screened. We have chosen a low energy, for which we expect the scattering to be primarily s-wave. With this in mind we limit m to the values (0,1,2), and, for each m, $m\leq l\leq 2$. We find later that these terminations of the summation indices provide sufficient accuracy, inasmuch as the quadratic terms in $\sin\theta_c$ and $\cos\theta_c$ in the scattering amplitude are already negligible.

[36] This limitation of the Schwinger, Kohn, and similar principles in the spheroidal potential problem is a result of the spherical harmonic expansion used here. An expansion in spheroidal harmonics is no better in this regard, except for a very limited class of potentials for which the Schrödinger equation separates completely in spheroidal coordinates. If we were to expand the wave function as $\psi(\mathbf{r})=\Sigma_m\epsilon_m\cos m\varphi_c F_m(r,\theta_c)$, and the other quantities similarly, these variational principles for the resulting equations in two variables would then have their usual property of directly approximating the quantities analogous to $\tan\delta_l^m$.

TABLE II. Error method results for the potential $U(r,\theta_c) = -U_0\exp[-(\alpha r)^2(1-\epsilon^2\cos^2\theta_c)]$, $r\leq a$; $=0$, $r>a$, with $\epsilon^2=-2$, $U_0a^2=4$, $\alpha a=2$, $ka=0.6$.

γ (degrees)	Differential cross section $10^3k^2\sigma(\theta,\varphi)$	Total cross section $(10^3k^2/4\pi)\sigma$
0	$7.254+0.186\cos\theta-0.180\cos^2\theta$	7.194
45	$7.323+0.356\cos\theta+0.170\sin\theta\cos\varphi$ $-0.092(\cos\theta-\sin\theta\cos\varphi)^2$	7.261
90	$7.384+0.527\cos\theta-0.189\sin^2\theta\cos^2\varphi$	7.321

We use the simple trial functions

$$\tilde{R}_l^m(r) = (b_l^m+ic_l^m)j_l(kr), \tag{28}$$

even though we expect for the low energy considered here that the full partial-wave Born approximation ($b_l^m=1$) would be quite inaccurate. Previous experience has led us to believe that this "quasi-Born" approximation (both b and c arbitrary) often works well where the full Born approximation is poor.

We use here the error functional,

$$\Lambda_E^m = \sum_{l=m}^{2}\int_0^a \Big|\sum_{l'=m}^{2}(\mathbf{J}_{ll'}^m\tilde{R}_{l'}^m) - \Gamma_l^m j_l\Big|^2 r^2dr. \tag{29}$$

The values we find for this functional for different choices of incident direction are given in Table III, along with the corresponding values of the source term $\sum_l(\Gamma_l^m)^2\int_0^a j_l^2(kr)r^2dr$. Note that for each m the ratio $\Lambda_E^m/(\text{source term})$ is quite small ($<10^{-2}$), indicating that the corresponding phase shifts are quite accurate.

In evaluating the (l,m) contribution to the scattering amplitude, we make use of a result obtained in Appendix A,

$$c_l^m/b_l^m \equiv \nu_l^m = \tan\delta_l^m. \tag{30}$$

The computed cross sections tabulated in Table II are

TABLE III. Values of the error functional and its corresponding source terms for scattering by the oblate spheroidal Gaussian potential.

γ (degrees)	m	Source term	$k\Lambda_E^m$
0	0	8.22×10^{-2}	2×10^{-4}
45	0	7.44×10^{-2}	2×10^{-4}
45	1	1.873×10^{-3}	4×10^{-7}
45	2	1.66757×10^{-6}	6×10^{-11}
90	0	6.71×10^{-2}	2×10^{-4}
90	1	3.6928×10^{-3}	8×10^{-7}
90	2	6.6702×10^{-6}	2×10^{-10}

in terms of the conventional coordinates (θ,φ) shown in Fig. 2(a).

VII. DISCUSSION

The error method may be regarded from a point of view which provides some additional insight. Minimization of the error functional leads to a wave function which may be regarded as the *exact* solution of the scattering function with an altered source function. We refer to the difference between this function and the correct source function as the difference function. The error functional is then the weighted mean-square value of the magnitude of the difference function. Minimization of this *tends* to reduce the scattering from this additional source. The size of this minimum functional relative to that of the corresponding one involving the correct source function, [the source term $\int_0^\infty(\mathbf{W}u)^2dr$], serves as a guide to the accuracy of the calculation. However, since the scattering is not completely determined by the *magnitude* of the wave function at the scatterer, this cannot be considered as a completely reliable guide to the accuracy of the scattering amplitude.

In general the method compares favorably with the Schwinger method over the limited range in which it has been tested. It may also be useful in connection with problems for which it is desirable to know the wave function close to the scatterer. A number of such problems exist in connection with the interaction of electrons with defects in solids.

APPENDIX A

Partial Waves for a Spheroidal Potential

We make use of spherical polar coordinates. The symmetry axis of the potential is chosen as polar axis, with the origin at the geometrical center of a spheroidal surface. This is the coordinate system (r,θ_c,φ_c) of Fig. 2(b). In these coordinates the spherical harmonic expansion of the wave function is

$$\psi(\mathbf{r})=\sum_{m=0}^{\infty}\sum_{l=m}^{\infty} i^l\epsilon_m\Omega_l{}^m P_l{}^m(\cos\theta_c)\cos m\varphi_c R_l{}^m(r), \quad \text{(A1)}$$

where $\epsilon_m=2-\delta_{m,0}$, with $\delta_{m,0}$ the Kronecker delta; $\Omega_l{}^m=(2l+1)(l-m)!/(l+m)!$; $P_l{}^m(\cos\theta_c)$ is an associated Legendre polynomial; $R_l{}^m(r)$ is an unknown radial wave function. The absence of $\sin m\varphi_c$ in the sum follows from the fact that the plane wave $\exp(i\mathbf{k}\cdot\mathbf{r})$ can be expanded in terms of the cosine only.[22] The double sum $\sum_{m=0}^{\infty}\sum_{l=m}^{\infty}$ is identical with the usual form $\sum_{l=0}^{\infty}\sum_{m=0}^{l}$.

In this coordinate system a spheroidal potential is a function of r and θ_c only; it may be written

$$U(r,\theta_c)=U[r(1-\epsilon^2\cos^2\theta_c)^{\frac{1}{2}}], \quad \text{(A2)}$$

with ϵ^2 the eccentricity.

Inserting the expansion (A1) for $\psi(\mathbf{r})$ into the three-dimensional Schrödinger equation, we obtain for each m a set of radial Schrödinger equations coupled over all values of $l\geq m$. These equations may be written

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+k^2-\frac{l(l+1)}{r^2}\right)R_l{}^m(r) - \sum_{l'=m}^{\infty} V_{ll'}{}^m(r)R_{l'}{}^m(r)=0, \quad \text{(A3)}$$

where

$$V_{ll'}{}^m(r)=\tfrac{1}{2}\Omega_{l'}{}^m[\exp\tfrac{1}{2}i\pi(l'-l)]\int_0^{\pi} P_l{}^m(\cos\theta_c) \times P_{l'}{}^m(\cos\theta_c)U(r,\theta_c)\sin\theta_c d\theta_c. \quad \text{(A4)}$$

From the facts: (1) that the potential $U(r,\theta_c)$ is an even function of $\cos\theta_c$, and (2) that the product $P_l{}^m(\cos\theta)P_{l'}{}^m(\cos\theta)$ is even in $\cos\theta$ if $l'-l$ is even, odd if $l'-l$ is odd, it follows that $V_{ll'}{}^m(r)$ is nonzero only for *even* $l'-l$. It is therefore real.

Since all the operators in Eq. (A3) are real, the solution $R_l{}^m(r)$ which is everywhere bounded must be of the form

$$R_l{}^m(r)=(1+i\nu_l{}^m)T_l{}^m(r), \quad \text{(A5)}$$

where $T_l{}^m(r)$ and $\nu_l{}^m$ are real. Substituting this in Eq. (A3), we find that the $T_l{}^m(r)$ must themselves satisfy this equation, and that

$$\sum_{l'}\nu_{l'}{}^m V_{ll'}{}^m(r)T_{l'}{}^m(r)=\nu_l{}^m\sum_{l'}V_{ll'}{}^m(r)T_{l'}{}^m(r). \quad \text{(A6)}$$

In the radial Schrödinger equation, the term involving $V_{ll'}{}^m(r)$ is negligible asymptotically for potentials which fall off faster than r^{-2}. In particular, it is zero for $r>a$ for potentials truncated at $r=a$. For such potentials, then, the equations decouple in the asymptotic region and are satisfied there by spherical Bessel and Neumann functions:

$$T_l{}^m(r)\sim C_l{}^m[j_l(kr)-\tan\delta_l{}^m n_l(kr)], \quad \text{(A7)}$$

with $C_l{}^m$ a constant, and $\delta_l{}^m$ the phase shift.

We could now write an integral equation for $T_l{}^m(r)$, using the Green's function for the radial Schrödinger equation. However, we would make an error in identifying $\tan\delta_l{}^m$ with the coefficient of $n_l(kr)$ in the asymptotic form of $T_l{}^m(r)$ obtained from this integral equation. We must first consider the integral equation for the complex radial wave function $R_l{}^m(r)$:

$$R_l{}^m(r)=\Gamma_l{}^m j_l(kr)-ik\int_{r'=0}^{\infty} g_l'(r,r') \times\sum_{l'} V_{ll'}{}^m(r')R_{l'}{}^m(r')(r')^2dr', \quad \text{(A8)}$$

where $g_l'(r,r')$ is the complex radial Green's function

$$g_l'(r,r')=[j_l(kr_>)+in_l(kr_>)]j_l(kr_<). \quad \text{(A9)}$$

If we now substitute $R_l{}^m(r)=(1+i\nu_l{}^m)T_l{}^m(r)$ in Eq.

(A8) and make use of Eqs. (A6) and (A9), we find

$$[1+(\nu_l^m)^2]\sum_{l'}(\mathbf{J}^R)_{ll'}^m T_{l'}^m(r)=\Gamma_l^m j_l(kr), \quad \text{(A10)}$$

and

$$\sum_{l'}\nu_{l'}^m(\mathbf{J}^R)_{ll'}^m T_{l'}^m(r)=-\sum_{l'}(\mathbf{J}^I)_{ll'}^m T_{l'}^m(r), \quad \text{(A11)}$$

where $(\mathbf{J}^R)_{ll'}^m$ and $(\mathbf{J}^I)_{ll'}^m$ are real integral operators given by

$$(\mathbf{J}^R)_{ll'}^m=\delta_{ll'}-k\left\{n_l(kr)\int_{r'=0}^{r} j_l(kr')V_{ll'}^m(r')\cdots(r')^2dr' + j_l(kr)\int_{r'=r}^{\infty} n_l(kr')V_{ll'}^m(r')\cdots(r')^2dr'\right\}; \quad \text{(A12)}$$

$$(\mathbf{J}^I)_{ll'}^m=kj_l(kr)\int_0^{\infty} j_l(kr')V_{ll'}^m(r')\cdots(r')^2dr'. \quad \text{(A13)}$$

Suppose we write

$$S_l^m(r)=[1+(\nu_l^m)^2]T_l^m(r). \quad \text{(A14)}$$

Substituting for the $T_l^m(r)$ in Eqs. (A10) does not permit cancellation of the $(1+\nu^2)$ factors. In fact, these equations are not very useful, since they contain the unknown quantities $(\nu_l^m)^2$, which apparently cannot be removed by any conceivable parametrization of trial functions $\tilde{T}_l^m(r)$. Therefore we work with the complex equations

$$\sum_{l'}\mathbf{J}_{ll'}^m R_{l'}^m=\Gamma_l^m j_l, \quad \text{(A15)}$$

where $\mathbf{J}_{ll'}^m=(\mathbf{J}^R)_{ll'}^m+i(\mathbf{J}^I)_{ll'}^m$.

In the spherical case, $\mathbf{J}$ is diagonal, and substitution of (A14) for $T_l(r)$ *does* eliminate the unknown factor $1+\nu_l^2$. It is this very process which leads to Eqs. (1) and (6) of the text for the spherical scattering problem.

We now write the asymptotic forms of Eqs. (A10), and (A11), using (A12) and (A13). The results are (we omit the m):

$$T_l(r)\sim\Gamma_l(1+\nu_l^2)^{-1}\left\{j_l-\left[-\Gamma_l^{-1}(1+\nu_l^2)\times\sum_{l'}k\int_0^{\infty} j_l V_{ll'}T_{l'}r^2dr\right]n_l\right\}; \quad \text{(A16)}$$

$$T_l(r)\sim-k\nu_l^{-1}\left(\sum_{l'}\int_0^{\infty} j_l V_{ll'}T_{l'}r^2dr\right)(j_l-\nu_l n_l). \quad \text{(A17)}$$

Equating coefficients of j_l in both equations, and comparing either (A16) or (A17) with Eq. (A6), we find

$$\nu_l^m=\tan\delta_l^m; \quad \text{(A18)}$$

$$\tfrac{1}{2}\Gamma_l^m\sin2\delta_l^m=-\sum_{l'}k\int_0^{\infty} j_l V_{ll'}^m T_{l'}^m r^2dr. \quad \text{(A19)}$$

The expression for the scattering amplitude $f(\theta_c,\varphi_c)$ is

$$f(\theta_c,\varphi_c)=\sum_m\sum_l\epsilon_m\Omega_l^m P_l^m(\cos\theta_c)\cos m\varphi_c\times\left[-\sum_{l'}\int_0^{\infty} j_l V_{ll'}^m R_{l'}^m r^2dr\right], \quad \text{(A20)}$$

where (θ_c,φ_c) are the coordinates of Fig. 2(b). Using Eqs. (A4), (A18), and (A19), we find for $f(\theta_c,\varphi_c)$ the expression

$$f(\theta_c,\varphi_c)=(2k)^{-1}\sum_m\sum_l\epsilon_m\Omega_l^m P_l^m(\cos\theta_c)\times\cos m\varphi_c\Gamma_l^m\sin2\delta_l^m(1+i\tan\delta_l^m). \quad \text{(A21)}$$

This expression has the same form as that for a spherical potential, and reduces directly to the latter if $\mathbf{k}$ is along the symmetry axis. In order to find $f(\theta,\varphi)$, where (θ,φ) are the conventional coordinates of Fig. 2(a), we perform a simple transformation of coordinates.

APPENDIX B

Kohn Principle

In this Appendix we show that the Kohn variational principle for the spherical scatterer partial wave equations $\mathbf{L}^R y-u=0$ may be written as the first two terms of Eq. (12) of the text, viz.,

$$\Lambda_K=-\int_0^{\infty}(\mathbf{L}^R\tilde{y}-u)^2dr+\int_0^{\infty}\tilde{y}(\mathbf{L}^R\tilde{y}-2u)dr, \quad \text{(B1)}$$

where the first term is the error functional, and the second is Λ_K', Eq. (16). Here, and in what follows, the subscript l is omitted. We shall work with the complex operator $\mathbf{L}$ and the complex radial function R.

In the development of his variational principle, Kohn[10] considers the functional

$$J=\int_0^{\infty} r^2dr\tilde{R}\mathbf{D}\tilde{R}, \quad \text{(B2)}$$

where the operator $\mathbf{D}$ is taken from the radial Schrödinger equation:

$$\mathbf{D}=\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+k^2-\frac{l(l+1)}{r^2}-U(r)\right], \quad \text{(B3)}$$

so that the exact radial wave function must satisfy $\mathbf{D}R=0$.

Kohn shows that the integral

$$\Lambda_K=J-\int_0^{\infty} jU\tilde{R}r^2dr \quad \text{(B4)}$$

is a variational functional for the quantity

$$\int_0^{\infty} j_l U R_l r^2dr=k^{-1}\sin\delta_l e^{i\delta_l},$$

provided that the trial functions $\tilde{R}$ have the correct asymptotic form. The Green's function formulation in

partial waves for a spherical potential is

$$R(r)=j(kr)-ik\int_0^\infty g(r,r')U(r')R(r')r'^2dr'. \quad \text{(B5)}$$

This guarantees the correct asymptotic form for R.

It is useful to rewrite this equation in an operator notation. If we define

$$\mathbf{G}\equiv ik\int_0^\infty g(r,r')\cdots r'^2dr', \quad \text{(B6)}$$

then we may write (B5) as

$$R=j-\mathbf{G}(UR). \quad \text{(B7)}$$

We will need the expressions $\mathbf{D}j$ and $\mathbf{DG}$. Since j is a spherical Bessel function we have immediately

$$\mathbf{D}j=-Uj. \quad \text{(B8)}$$

It is easy to show that

$$\mathbf{DG}=-\mathbf{I}-U\mathbf{G}. \quad \text{(B9)}$$

As a check, we note that putting (B7) for R we get

$$\mathbf{D}R=\mathbf{D}j-\mathbf{DG}(UR)$$
$$=-Uj+UR+U(j-R)=0. \quad \text{(B10)}$$

In order to ensure that the trial function has correct asymptotic form, we may write

$$\tilde{R}=j-\mathbf{G}(U\tilde{S}), \quad \text{(B11)}$$

where $\tilde{S}$ is a trial function which need not be defined in the region outside the potential. Using (B8) and (B9), we then find

$$\mathbf{D}\tilde{R}=-Uj+U\tilde{S}+U\mathbf{G}(U\tilde{S}). \quad \text{(B12)}$$

Using (B11) and (B12) in the integrand of J, Eq. (B2), we find

$$J=\int_0^\infty r^2dr\ U[j-\mathbf{G}(U\tilde{S})][j-\tilde{S}-\mathbf{G}(U\tilde{S})]. \quad \text{(B13)}$$

Following the procedure of Eqs. (9)–(11) of the text, we define

$$\tilde{v}=rU^{\frac{1}{2}}\tilde{S}, \quad \text{(B14)}$$

$$u=rU^{\frac{1}{2}}j, \quad \text{(B15)}$$

$$\mathbf{L}=\mathbf{I}+[rU^{\frac{1}{2}}\mathbf{G}(U^{\frac{1}{2}}r\cdots)]. \quad \text{(B16)}$$

Using these in (B13) and in the second term of (B4), we find after some manipulation that the Kohn functional is

$$\Lambda_K=-\int_0^\infty dr(\mathbf{L}\tilde{v}-u)^2+\int_0^\infty dr\ \tilde{v}(\mathbf{L}\tilde{v}-2u), \quad \text{(B17)}$$

which has the same form as (B1).

The error functional with identity weighting operator for the complex partial wave equation $\mathbf{L}v-u=0$ is $\Lambda_E=\int_0^\infty dr|\mathbf{L}\tilde{v}-u|^2$. The first term in the Kohn functional (B17) is equivalent to the error functional only for the case of all real quantities.