Variational Approach to the On- and Off-Shell T Matrix*

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A variational procedure for calculating the two-body T matrix $T_l(p,p';s)$ is proposed, and studied numerically for the case of the Reid $^1S_0$ soft-core potential. The method is based on a variational principle of the Schwinger type, in which the trial functions are themselves off-energy-shell T matrices with fixed s and p (or fixed s and p'), which are expressed as linear combinations of a convenient basis set. The variationally calculated T matrix turns out to have the interesting form $T=V+VG'V$, where G' is a finite-rank approximation to the full Green's function, of rank equal to the number of basis functions. It also turns out that for potentials of finite rank the approximation is exact, provided that the space spanned by the basis functions includes the form factors of the potential. Numerical results are given for the Reid potential at energies from −50 to 300 MeV, and show good convergence for both on- and off-shell T matrix elements. The nonvariational estimates obtained directly from the trial functions also converge quite well, but less rapidly than the variational results.

1. INTRODUCTION

In this paper we propose and study a variational approach to the Lippmann-Schwinger equation for the two-body, off-shell, partial-wave T matrix $T_l(p,p';s)$,

$$T_l(p,p';s) = V_l(p,p') + \frac{2}{\pi}\int_0^\infty \frac{V_l(p,p'')T_l(p'',p';s)}{2\mu s - p''^2}p''^2dp'' , \tag{1}$$

where $V_l(p,p')$ is the potential, μ the reduced mass, and s the complex energy parameter; and the normalization is such that the on-shell T matrix and the phase shift δ_l are related by

$$T_l\left(p,p;\frac{p^2}{2\mu}+i\epsilon\right) = -\frac{1}{p}e^{i\delta_l}\sin\delta_l . \tag{2}$$

In the following pages we describe the method, and show by numerical calculations that it does indeed provide a satisfactory way of calculating the T matrix for a realistic soft-core nucleon-nucleon potential. Our fundamental aim, however, is not really to present a new way of solving the Lippmann-Schwinger equation, since there already exist[1-3] a number of perfectly satisfactory numerical methods for solving that equation, and in particular, for dealing with the singularities in the kernel for real positive energies. The two most popular methods of handling the singularities are perhaps the Kowalski-Noyes method[1] of reducing the equation to an integral equation with a nonsingular kernel; and the method of converting Eq. (1) into a principal-value equation for the reactance matrix.[2]

Equations of a similar kind also arise in other contexts, however, with singularities in the kernel that are not at all easy to deal with. In particular, we are interested in the set of coupled integral equations that arise in the *three*-body problem, when finite-rank approximations to the two-body potentials or T matrices are used. In this case the singularities in the kernel depend on both variables, and are therefore not so easy to subtract out. The most popular method of solving these equations has been to deform the integration contour[4] in the complex momentum plane away from the singularities, but the method is unattractively hard to use[5] in calculations involving three-particle final states. The amplitudes needed in this case are analogous to half-off-shell solutions of Eq. (1). Even more difficult to calculate are the fully off-shell three-body amplitudes that will presumably be needed for solving the four-body problem.

Problems of this kind provided the motivation for the present work, since unlike most other methods for solving the Lippmann-Schwinger equation, the method to be developed here generalizes in a straightforward way to these more difficult equations. We have thought it desirable, however, to explore the method first in the more familiar context of two-body scattering, so that it can be tested numerically in an area where other numerical results are available, and so that we can concentrate initially on the essentials of the method itself, rather than on the complexities of the three-body problem.

The variational method to be described here is rather closely related to the method of solving the Lippmann-Schwinger equation by expanding the T

matrix in terms of a suitable set of functions. In the latter method, suppose for example, that our aim is to calculate the particular T matrix element $T_l(p_2, p_1; s)$. Then the solution of Eq. (1) could be expanded in the form

$$T_l(p, p_1; s) = \sum_{n=1}^{N} c_n(p_1) f_n(p), \tag{3}$$

where the functions $f_1(p)$, $f_2(p)$, ... are a conveniently chosen set of functions, presumably complete in some relevant sense, and the coefficients $c_n(p_1)$ are constants to be chosen in some suitable way, so as to make the expansion an approximate solution of Eq. (1).

This expansion procedure is a perfectly sensible, though little explored, way of tackling the Lippmann-Schwinger equation. (We know of no applications for the Lippmann-Schwinger equation itself, but the approach has been used successfully for solving similar three-body equations.[6]) One would expect that only a few terms would be needed in Eq. (3) if the basis functions $f_n(p)$ are well chosen, and a particularly attractive feature of this method is that the solution is available as an analytic function of p, rather than just as a table of numbers.

The essence of the variational method to be described in Sec. 2 is that we use expansions of the form of Eq. (3) as trial functions in a variational expression for $T_l(p_2, p_1; s)$. The variational property then ensures that the final error is of the order of the *square* of the error in Eq. (3). The numerical calculations of Sec. 4 show that even the nonvariational estimates obtained directly from the trial functions converge quite well, but that as expected from the variational property, the variational results converge still faster, even though they are scarcely more difficult to calculate than the nonvariational results.

The variationally calculated T matrix turns out to have the interesting form $T = V + VG'V$ [see Eq. (25)], where G' is a finite-rank approximation to the full Green's function, of rank equal to the number of basis functions in Eq. (3). We also find in Sec. 3 a very encouraging property of the variational calculation, and indeed even of the nonvariational result given by the trial function (3), that the approximate result becomes exact for the case of a finite-rank potential, provided that the space spanned by the basis functions includes the form factors of the potential.

The variational method is based on a variational principle [Eq. (8)] of the kind associated with Schwinger, and can be used to calculate T matrix elements of all types: fully off-shell, half-off-shell, and on-shell. Even in the latter case, however, the method is not equivalent to what is usually referred to as the Schwinger variational method,[7,8] because the variational principles on which the methods are based are not identical. However, there is a formal relationship between these variational principles, and this is discussed in Sec. 3. A slight variant of the Schwinger method proposed by Schwartz[9] is also discussed in Sec. 3.

The variational method described in this paper does not automatically satisfy unitarity, or in other words, does not automatically produce real phase shifts. It would be very easy, however, to modify the method so as to ensure real phase shifts: all that is needed is to apply the same techniques to the principal-value equation for the reactance matrix. We have chosen not to do this, partly because we prefer to have a method that is uniformly straightforward for all T matrix elements at all energies (positive, negative, and complex), and that generalizes easily to more difficult equations; but also because to us it seems an advantage rather than a disadvantage that the phase shifts are not automatically real: The size of the imaginary part of the phase shift then serves as a useful indicator of numerical accuracy.

In Sec. 2 we describe the variational method, and then in Sec. 3 discuss some of its properties. Numerical calculations on the Reid soft-core $^1S_0$ potential are described in Sec. 4.

2. VARIATIONAL METHOD

Let us write the Lippmann-Schwinger equation (1) in operator form as

$$T(s) = V + VG_0(s)T(s), \tag{4}$$

and its transpose as

$$T(s) = V + T(s)G_0(s)V, \tag{5}$$

and let us introduce an alternative Dirac notation for the momentum-space matrix elements,

$$\langle p|T(s)|p'\rangle \equiv T_l(p, p'; s). \tag{6}$$

The starting point for the variational method is the identity (now omitting the label s)

$$\begin{aligned} T = {} & V + VG_0T_1 + T_2G_0V - T_2(G_0 - G_0VG_0)T_1 \\ & + (T_2 - T)(G_0 - G_0VG_0)(T_1 - T). \end{aligned} \tag{7}$$

It is easy to see from Eqs. (4) and (5) that this is valid for arbitrary operators T_1 and T_2. Our interest, however, is in taking T_1 and T_2 to be approximations to T. The last term in Eq. (7) is second order in the differences $T_1 - T$ and $T_2 - T$, so that we get a variational principle for T by omitting this term, thus obtaining

$$[T] = V + VG_0T_1 + T_2G_0V - T_2(G_0 - G_0VG_0)T_1, \tag{8}$$

where T_1 and T_2 are independent approximations to T.

This variational principle is given in Newton's book,[10] but does not appear to have received any significant use in calculations. It is a variational principle of the Schwinger rather than the Kohn-Hulthèn type,[8] but it is not the one usually used in applications of the Schwinger method. We return to this point in Sec. 3.

We suppose, as in Sec. 1, that our specific aim is to calculate the particular T matrix element $\langle p_2|T(s)|p_1\rangle$. From Eq. (8) we immediately obtain a variational principle for this particular T matrix element,

$$[\langle p_2|T|p_1\rangle] = \langle p_2|V|p_1\rangle + \langle p_2|VG_0T_1|p_1\rangle + \langle p_2|T_2G_0V|p_1\rangle - \langle p_2|T_2(G_0 - G_0VG_0)T_1|p_1\rangle , \quad (9)$$

where, for example,

$$\langle p_2|VG_0T_1|p_1\rangle = \frac{2}{\pi}\int_0^\infty \frac{\langle p_2|V|p\rangle\langle p|T_1|p_1\rangle}{2\mu s - p^2}p^2dp . \quad (10)$$

Our procedure is to use trial functions of the form

$$\langle p|T_1|p_1\rangle = \sum_{n=1}^{N} c_n(p_1)f_n(p) , \quad (11)$$

in the variational principle, where the coefficients $c_n(p_1)$ are constants that have yet to be determined. (Remember that for our present purposes p_1 is a fixed parameter.) Similarly, we expand the matrix elements of T_2 in the form

$$\langle p_2|T_2|p\rangle = \sum_{n=1}^{N} d_n(p_2)f_n(p) . \quad (12)$$

[We have chosen to use the same set of functions $f_n(p)$ in Eqs. (11) and (12), but this is clearly not essential.] These equations can be written more concisely if we introduce vectors $|n\rangle$ and $\langle n|$, defined by

$$\langle p|n\rangle = \langle n|p\rangle = f_n(p) . \quad (13)$$

In terms of these, Eqs. (11) and (12) become

$$T_1|p_1\rangle = \sum_{n=1}^{N} c_n(p_1)|n\rangle , \quad (14)$$

$$\langle p_2|T_2 = \sum_{n=1}^{N} d_n(p_2)\langle n| , \quad (15)$$

and the variational expression (9) becomes

$$[\langle p_2|T|p_1\rangle] = \langle p_2|V|p_1\rangle + \sum_{n=1}^{N} c_n(p_1)\langle p_2|VG_0|n\rangle + \sum_{n=1}^{N} d_n(p_2)\langle n|G_0V|p_1\rangle - \sum_{n=1}^{N}\sum_{m=1}^{N} d_m(p_2)c_n(p_1)\langle m|G_0 - G_0VG_0|n\rangle . \quad (16)$$

To fix the values of the constants $c_n(p_1)$ and $d_n(p_2)$, we naturally make use of the variational nature of Eq. (16), and require that the right-hand side be stationary with respect to variations of $c_n(p_1)$ and $d_n(p_2)$. In this way we easily obtain

$$c_n(p_1) = \sum_{m=1}^{N} \Delta_{nm}\langle m|G_0V|p_1\rangle , \quad (17)$$

$$d_m(p_2) = \sum_{n=1}^{N} \langle p_2|VG_0|n\rangle\Delta_{nm} , \quad (18)$$

where Δ is an $N\times N$ matrix defined by

$$(\Delta^{-1})_{mn} = \langle m|G_0 - G_0VG_0|n\rangle . \quad (19)$$

Finally, we substitute Eqs. (17) and (18) into (16) to give us the relatively simple result

$$[\langle p_2|T|p_1\rangle] = \langle p_2|V|p_1\rangle + \sum_{n=1}^{N}\sum_{m=1}^{N} \langle p_2|VG_0|n\rangle\Delta_{nm}\langle m|G_0V|p_1\rangle . \quad (20)$$

This is the expression that we use for the variational calculations in Sec. 4. The required matrix elements can be written explicitly, with the aid of Eqs. (6), (10), (13), and (19), as

$$\langle p_2|VG_0|n\rangle = \frac{2}{\pi}\int_0^\infty \frac{V_l(p_2,p)f_n(p)}{2\mu s - p^2}p^2dp \quad (21)$$

and

$$(\Delta^{-1})_{mn} = \frac{2}{\pi}\int_0^\infty \frac{f_m(p)f_n(p)}{2\mu s - p^2}p^2dp - \left(\frac{2}{\pi}\right)^2\int_0^\infty p'^2dp'\int_0^\infty p^2dp\,\frac{f_m(p')V_l(p',p)f_n(p)}{(2\mu s - p'^2)(2\mu s - p^2)} . \quad (22)$$

As a by-product of the variational calculation, we also obtain two nonvariational approximations, by substituting the values of $c_n(p_1)$ and $d_n(p_2)$ [Eqs. (17) and (18)] into Eqs. (11) and (12), so obtaining

$$\langle p_2|T_1|p_1\rangle = \sum_{n=1}^{N}\sum_{m=1}^{N} f_n(p_2)\Delta_{nm}\langle m|G_0V|p_1\rangle \quad (23)$$

and

$$\langle p_2|T_2|p_1\rangle = \sum_{n=1}^{N}\sum_{m=1}^{N} \langle p_2|VG_0|n\rangle\Delta_{nm}f_m(p_1) . \quad (24)$$

Although these two approximations have been obtained rather indirectly, we emphasize that both of them are perfectly acceptable approximations in their own right, and indeed arise quite naturally if we look for solutions of the Lippmann-Schwinger equation in the form of Eq. (11) or (12), i.e., as sums of functions with unknown coefficients. For example, if we substitute the expansion (11) into the Lippmann-Schwinger equation (4), and determine the values of $c_n(p_1)$ by multiplying on the left by $\langle n|G_0$, with $n=1,\ldots,N$, then we easily find that the resulting values of $c_n(p_1)$ are exactly the same as we found previously by the variational argument. It follows that the corresponding T matrix element is just that given by Eq. (23). A similar argument also applies to Eq. (24).

For some purposes, the nonvariational approximations (23) and (24) have a possible advantage over the variational approximation in being of finite rank. (On the other hand, they are not explicitly symmetric; rather, one is the transpose of the other.) However, the variational property essentially assures us that if the nonvariational approximations are good, then the variational approximation is even better (at least in some average sense), since the error in the variational approximation [the last term in Eq. (7)] is second-order in the errors in T_1 and T_2.

3. DISCUSSION

The variational approximation (20) can be written concisely as an operator equation,

$$[T]=V+\sum_{n=1}^{N}\sum_{m=1}^{N}VG_0|n\rangle\Delta_{nm}\langle m|G_0V, \tag{25}$$

and in a similar way we can also write the two nonvariational approximations (23) and (24),

$$T_1=\sum_{n=1}^{N}\sum_{m=1}^{N}|n\rangle\Delta_{nm}\langle m|G_0V, \tag{26}$$

$$T_2=\sum_{n=1}^{N}\sum_{m=1}^{N}VG_0|n\rangle\Delta_{nm}\langle m|. \tag{27}$$

The variational result is very similar in character to the exact solution of the Lippmann-Schwinger equation in terms of the full Green's function $G(s)=s-H$, namely

$$T=V+VGV, \tag{28}$$

where H is the total Hamiltonian. In fact, Eq. (25) has exactly this form, but with $G(s)$ replaced by a finite-rank approximation $G'(s)$, given by

$$G'=\sum_{n=1}^{N}\sum_{m=1}^{N}G_0|n\rangle\Delta_{nm}\langle m|G_0. \tag{29}$$

As we have already remarked in Sec. 1, the variational method described above is not equivalent to the usual Schwinger method, even in the on-shell case. To help understand the connection, it is convenient to introduce wave operators Ω and Γ, defined by

$$\Omega=1+G_0T, \tag{30}$$

$$\Gamma=1+TG_0. \tag{31}$$

According to (4) and (5), these also satisfy

$$T=V\Omega=\Gamma V. \tag{32}$$

(The significance of Ω and Γ is that Ω produces a scattering wave function by operating to the right on a plane wave of appropriate momentum, and Γ by similarly operating to the left.)

The usual bilinear form of the Schwinger principle[7] is obtained simply by taking the on-shell matrix elements of the variational principle

$$[T]=V\Omega+\Gamma V-\Gamma(V-VG_0V)\Omega. \tag{33}$$

(The stationary property follows easily from the Lippmann-Schwinger equations for Ω and Γ.) There is a formal correspondence between this variational principle and Eq. (8), in that they become equivalent if T_1 is related to Ω by

$$1+G_0T_1=\Omega,$$

and if T_2 is related to Γ by

$$T_2=\Gamma V.$$

In practice, however, the methods are quite different, as is perhaps most clear from the fact that in using Eq. (8) the Born term always appears explicitly in the result, whereas with Eq. (33) it does not.

The variational principle (8) has an important practical advantage over the usual Schwinger principle (33), in that the functions we have to approximate on the right-hand side of Eq. (8) are T matrices, which are perfectly smooth functions, whereas the functions on the right-hand side of Eq. (33) are wave operators or wave functions, which are highly singular functions in momentum space. (The singularities correspond to the asymptotic parts of the wave function in configuration space.) It is therefore reasonable to expect that expansions of the kind used in Sec. 2 will converge much faster in Eq. (8) than they would in Eq. (33).

We are not aware of any systematic studies of the Schwinger principle (33) with a steadily increasing number of basis functions, presumably because of the technical difficulties of evaluating the necessary matrix elements. Such calculations have been carried out,[9] however, with a much more practical variant suggested by Schwartz.[9] This is like the present method in that the trial functions (for the on-shell case) are half-shell T

matrices, but is otherwise entirely different. In the notation of Eq. (33), Schwartz's procedure is simply to construct trial functions for $V\Omega \equiv T_1'$ and $\Gamma V \equiv T_2$, rather than for the wave operators Ω and Γ. In terms of T_1' and T_2 the Schwinger principle (33) becomes

$$[T] = T_1' + T_2 - T_2(V^{-1} - G_0)T_1' . \tag{34}$$

Schwartz[9] has shown in a numerical calculation with a simple potential that the on-shell version of this works satisfactorily in practice, but the rate of convergence is perhaps not impressive. This variational principle becomes equivalent to Eq. (8) if T_1' is related to T_1 by

$$T_1' = V + VG_0T_1 ,$$

but in any practical calculation the two are entirely different.

It is perhaps worth remarking that the variational method of Sec. 2, like other methods of the Schwinger type, is not troubled by the spurious singularities[11] that arise with the Kohn variational method.[12,8] (This difference between the Kohn and Schwinger methods has been noted previously by Schwartz.[9]) The essential difference lies in the matrix which has to be inverted in each case: In the method of Sec. 2 the matrix Δ^{-1} [Eq. (19)] is essentially a representation in the finite basis of $G_0 - G_0VG_0 = G_0(1 - VG_0)$, whereas in the Kohn method the corresponding matrix represents $E - H$. For positive energies, $E - H$ has a continuous spectrum that includes zero, so that it can easily happen that one eigenvalue of the finite matrix is small, especially if the number of basis functions is large. If this happens, the matrix becomes nearly singular, and it is this[11] that causes the difficulties with the Kohn method. With methods of the Schwinger type, on the other hand, the matrix is expected to be singular only when VG_0 has an eigenvalue near 1, which is the condition[13] for a *true* bound-state pole or resonance pole in the T matrix. Therefore there is no reason at all to expect spurious singularities in this case.

A very encouraging feature of the variational method described in Sec. 2 is that the result is exact for potentials of finite rank, provided that the form factors are in the space spanned by the trial functions. This result is in fact even true for the *non*variational approximations (26) and (27), and it is sufficient to prove the result for this case, since the error in the variational result [the final term in Eq. (7)] is then necessarily zero. Specifically, we prove below that Eq. (26) is exact for a rank-one separable potential

$$V = |g\rangle\lambda\langle g| , \tag{35}$$

if $|g\rangle$ is a linear combination of the basis functions. The generalization to potentials of higher rank is straightforward.

For the separable potential case, Eq. (26) becomes

$$T_1 = \sum_{n=1}^{N}\sum_{m=1}^{N} |n\rangle\Delta_{nm}\langle m|G_0|g\rangle\lambda\langle g| , \tag{36}$$

and Eq. (19) becomes

$$(\Delta^{-1})_{mn} = \langle m|G_0|n\rangle - \langle m|G_0|g\rangle\lambda\langle g|G_0|n\rangle . \tag{37}$$

By assumption, $|g\rangle$ is a linear combination of the basis functions, say

$$|g\rangle = \sum_{n=1}^{N} \alpha_n|n\rangle .$$

On multiplying Eq. (37) by α_n and summing over n, we get

$$\sum_{n=1}^{N} (\Delta^{-1})_{mn}\alpha_n = \langle m|G_0|g\rangle - \langle m|G_0|g\rangle\lambda\langle g|G_0|g\rangle ,$$

or

$$\langle m|G_0|g\rangle\lambda = \sum_{n=1}^{N} (\Delta^{-1})_{mn}\alpha_n(\lambda^{-1} - \langle g|G_0|g\rangle)^{-1} .$$

With the aid of this, Eq. (36) easily becomes

$$T_1 = |g\rangle(\lambda^{-1} - \langle g|G_0|g\rangle)^{-1}\langle g| ,$$

which is the exact solution of the Lippmann-Schwinger equation (4) for the separable potential (35). This is the result we set out to prove.

4. NUMERICAL CALCULATIONS

To see how the variational method works in practice, we have carried out numerical calculations with the Reid[14] $^1S_0$ soft-core potential, which is highly repulsive at short distances, and which fits the $^1S_0$ nucleon-nucleon phase shifts quite accurately up to 350 MeV. In momentum space this potential is

$$V_0(p,p') = \frac{1}{4\beta_1 pp'}\sum_{i=1}^{3} v_i \ln\left(\frac{(p+p')^2+\beta_i^2}{(p-p')^2+\beta_i^2}\right) , \tag{38}$$

where $\beta_1 = 0.7$ fm^{-1}, $\beta_2 = 4\beta_1$, $\beta_3 = 7\beta_1$, $v_1 = -10.463$ MeV, $v_2 = -1650.6$ MeV, and $v_3 = 6484.2$ MeV.

The basis functions $f_n(p)$ were chosen to be

$$f_n(p) = \frac{1}{p^2+\beta^2} C_{n-1}^{1}\left(\frac{p^2-\beta^2}{p^2+\beta^2}\right) , \quad n = 1, 2, \ldots, N, \tag{39}$$

where C_{n-1}^{ν} is the Gegenbauer polynomial,[15] a polynomial of degree $n-1$, and where β is a parameter which can be chosen for practical convenience. The functions given by Eq. (39) have the correct p^0 behavior at small p, and at large p have the same p^{-2} behavior as the potential [Eq. (38)]. This set of basis functions is formally equivalent to the set $(p^2+\beta^2)^{-n}$, $n = 1, \ldots, N$, but Eq. (39) has the ad-

vantage numerically that the basis functions so defined are orthogonal on $0 \leq p < \infty$ with a certain weight function [specifically $p^2(p^2+\beta^2)^{-1}$], and this tends to make the matrix Δ^{-1} [Eq. (22)] well conditioned. The functions defined by Eq. (39) are actually Sturmian functions for the Coulomb potential,[16] and the orthogonality property follows from this fact.

Otherwise, however, there is nothing special about our choice of trial functions. Indeed, they have one property that seems quite undesirable, namely, that $f_n(p)$ has poles of order n at $p=\pm i\beta$. The potential itself [Eq. (38)] has branch points at $(p \pm p') = \pm i\beta_t$, so that it seems sensible to require that β be at least as large as 0.7 fm^{-1}. In practice we settled on the value $\beta = 5.0$ fm^{-1} after a small amount of experimentation, our experience being that the convergence was much less satisfactory for values near 0.7 fm^{-1}. We emphasize, however, that we have made no serious attempt to find an optimum set of basis functions.

The singularities in the integrands of Eqs. (21) and (22) were avoided by deforming the integration contour into two straight sections, $[0, -0.525i]$ and $[-0.525i, -0.525i+\infty]$. The latter region was then mapped onto a finite interval, and the integrals along each part of the contour were evaluated by Gaussian quadrature. This proved to be an effective and simple procedure.

The first results (Fig. 1 and Table I) concern the on-shell T matrix at real positive laboratory energies up to 300 MeV. As discussed in Sec. 1, the variational method does not automatically preserve unitarity, though it could easily be adapted to do so, and therefore the phase shift (modulo π) given by Eq. (2) is not automatically real. The imaginary part of the phase shift then serves as a useful indicator of numerical accuracy. In Fig. 1 we show the real part of the phase shift found with the variational method for several values of N, N being the number of basis functions. We also show the values of the phase shifts found by Reid[17] by direct solution of the Schrödinger equation, and our own exact values obtained from the Lippmann-Schwinger equation by numerical matrix inversion. Clearly the convergence of Reδ to the exact values is excellent, since the variational result with $N=6$ is indistinguishable from the exact result at all energies.

The behavior of the variational method at several energies is studied more closely in Table I. It is seen that Reδ does indeed converge rapidly and decisively to the exact result, and that as expected, Imδ converges with equal rapidity to zero. (The convergence is not, however, strictly monotonic. A variational bound of the sort discussed by Kato[18] is not to be expected, since the potential changes sign.)

We also give in Table I the phase shifts obtained with the nonvariational approximation (23) or (24). (Note that these give identical results for the on-shell case, and more generally, for the case $p_1 = p_2$.) Clearly the values again converge steadily to the correct values as N increases, but the convergence is always less rapid than that of the variational method. The advantage of the variational method is perhaps clearest when the nonvariational result is itself reasonably accurate; this is of course expected, from the property that the error in the variational method is of the order of the square of the error in the trial functions.

TABLE I. Phase shifts in degrees with the variational method, and with the nonvariational formula (23) or (24).

E_{lab} (MeV)	N	Reδ		Imδ	
		Var.	Nonvar.	Var.	Nonvar.
40	1	13.5	−10.5	−11.6	0.6
	2	13.1	−8.2	−9.4	6.1
	3	36.5	35.9	−1.1	7.9
	4	42.0	41.7	0.0	−1.2
	5	42.2	42.4	0.0	0.3
	6	42.2	42.2	0.0	0.0
	Exact	42.2			
140	1	2.1	−20.4	−10.0	1.0
	2	−1.6	−22.0	−10.2	11.2
	3	12.8	13.8	−0.3	3.9
	4	15.4	12.7	−0.3	−3.5
	5	15.8	15.2	0.0	−0.2
	6	15.8	15.4	0.0	0.1
	Exact	15.8			
280	1	−14.5	−28.8	−3.7	0.5
	2	−17.0	−35.6	−9.4	13.1
	3	−6.8	−6.4	0.0	0.9
	4	−5.5	−10.8	−0.8	−3.8
	5	−4.7	−5.1	0.0	0.1
	6	−4.7	−4.7	0.0	−0.1
	Exact	−4.7			

TABLE II. Scattering lengths in fm for the variational and nonvariational methods.

N	Var.	Nonvar.
1	−1.1	0.3
2	−1.2	0.1
3	−6.5	−4.8
4	−16.5	−15.5
5	−16.5	−15.5
6	−16.8	−16.2
7	−17.1	−16.7
8	−17.1	−16.7
Exact	−17.1 [a]	

[a] Reid, Ref. 14.

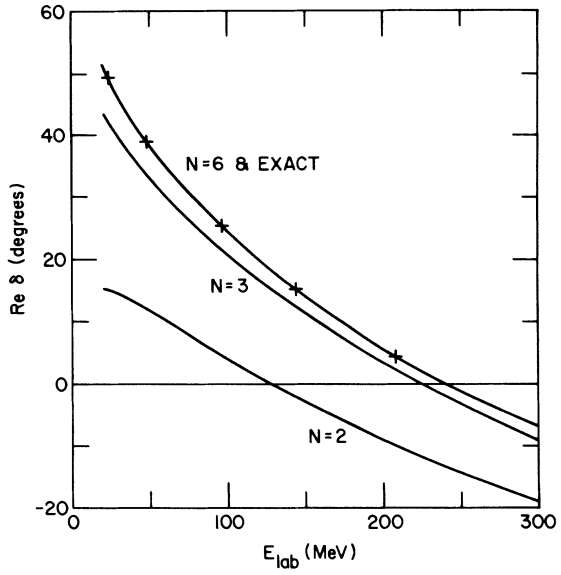

FIG. 1. Variational and exact calculations of the phase shifts for the Reid (Ref.14) $^1S_0$ soft-core potential. The crosses are values found by Reid (Ref. 17).

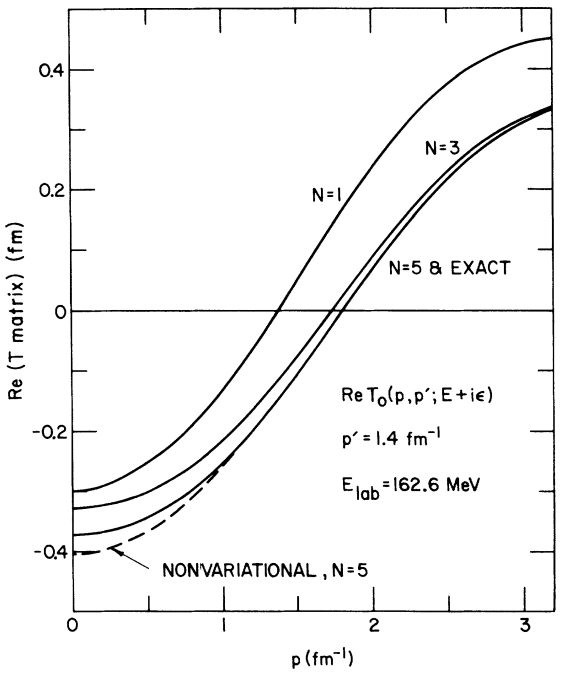

FIG. 3. Half-shell T matrix elements for $E_{lab}=162.6$ MeV obtained by the variational method, and by exact solution. The dashed curve is the nonvariational approximation Eq. (23), with $N=5$.

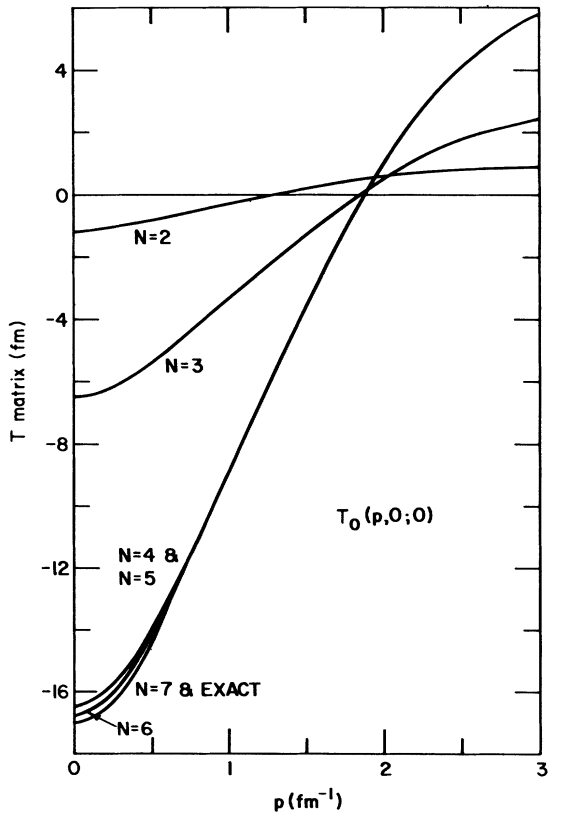

FIG. 2. Half-shell T matrix elements at zero energy obtained by the variational method, and by exact numerical solution.

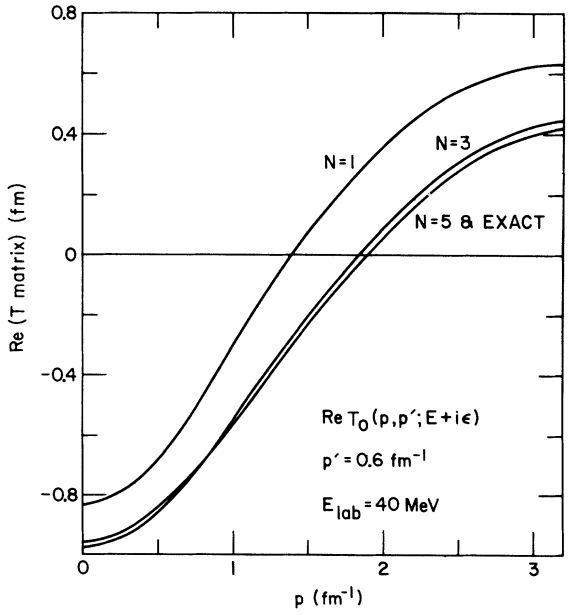

FIG. 4. Off-shell T matrix elements for $E_{lab}=40$ MeV and $p'=0.6$ fm^{-1}, obtained by the variational method, and by exact solution.

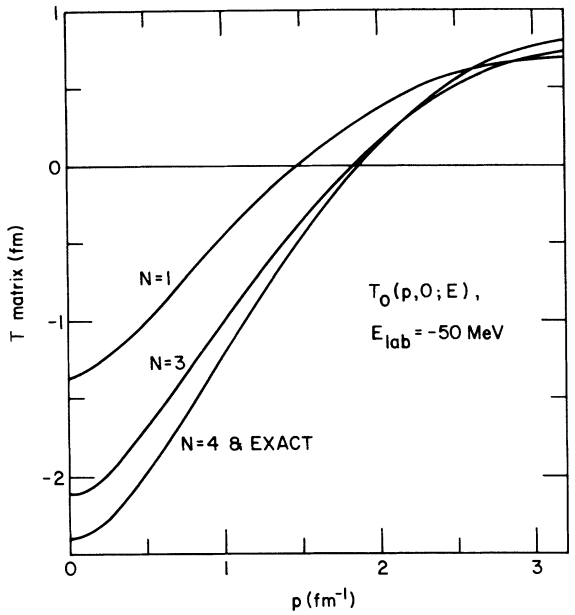

FIG. 5. Off-shell T matrix elements for $E_{lab}=-50$ MeV and $p'=0$, obtained by the variational method, and by exact solution.

Next we consider the case of zero energy. Numerically, this turned out to have the slowest convergence of any that we studied, perhaps because of the nearby pole on the second sheet of the complex energy plane. Nevertheless, the convergence in this case was by no means poor. In Table II we show the scattering lengths obtained with both the variational and nonvariational methods. [With the normalization used in Eq. (2), the scattering length is simply the on-shell T matrix element at zero energy.] Once again, the convergence of the variational method turns out to be much better than the nonvariational: The nonvariational result with $N=8$ is less accurate than the variational result with $N=6$.

The variationally calculated half-off-shell T matrix elements at zero energy are shown in Fig. 2. It is evident that the convergence is slowest for small values of p, and is much faster for larger values of p. The values at $p=0$ are of course the scattering lengths given in Table II. The nonvariational amplitudes have not been shown in Fig. 2, in order to avoid confusing the diagram, but their behavior is qualitatively similar to that of the variational amplitudes in Fig. 2, and a useful indication of their behavior for small p can be obtained from Table II. It is perhaps worth remarking that the nonvariational half-shell amplitudes are the trial functions in the variational calculation of the scattering length, so that the relatively slow convergence in the scattering length calculation is evidently associated with the fact that the trial functions have some difficulty in reproducing the behavior, shown in Fig. 2, of the exact half-shell amplitude at small p.

In Fig. 3 we show the real part of the variationally calculated half-shell T matrix $T_0(p,k,k^2/m+i\epsilon)$, at a laboratory energy of 162.6 MeV (i.e., $k=1.4$ fm^{-1}). Again the convergence is good, and by $N=5$ the variational approximation is exact to within the accuracy of the drawing. [In contrast, the nonvariational approximation (23) at $N=5$, which is also shown, differs considerably from the exact result.] The imaginary part of the variational amplitude is not shown, but converges to the exact result in a similar way. A further check on the calculations follows from the fact[1] that the phase of the half-shell amplitude should be the same as that of the on-shell amplitude $T_0(k,k,k^2/m+i\epsilon)$. We have verified that this is so for the converged half-shell values out to 3 fm^{-1}, and at all energies up to 300 MeV.

Finally, we show in Figs. 4 and 5 the real parts of some fully off-shell T matrix elements, at a positive energy, 40 MeV, and a negative energy, −50 MeV. The behavior of the imaginary parts (not shown) is similar. Clearly the convergence of the variational method is again good. As far as we know, this is true for all energies, and for all off-shell and on-shell momenta.

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Inverse Problem for Heavy-Ion Elastic Scattering and the Connection Between Parametrized Phase-Shift and Optical-Potential Models*

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A method based on the JWKB approximation is presented for constructing a local potential from a complete set of complex phase shifts at a single energy. By introducing the Sabatier transformation the problem is reduced to solving an Abel integral equation, the solution of which is closely connected with the potential. The resulting optical potential is uniquely determined in the noncritical domain, and its range of validity is in keeping with the JWKB approximation. A direct connection between the phase shifts and the optical potential is thereby established. The above procedure is tested for the scattering of medium-energy α particles, and it is found to be quite reliable over an angular range encompassing the diffraction region. Possible applications of the above method to the elastic scattering of medium-energy heavy ions are discussed.

I. INTRODUCTION

The scattering amplitude for elastic scattering of two spinless particles with charge z, z', and relative velocity k/μ is given by

$$f(\theta) = f_c(\theta) + \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)e^{2i\sigma_l}(e^{2i\delta_l}-1)P_l(\cos\theta), \tag{1a}$$

where $f_c(\theta)$ is the point Coulomb scattering amplitude,

$$f_c(\theta) = \frac{-\eta}{2k\sin^2(\frac{1}{2}\theta)}\exp[-2i\eta\ln\sin(\tfrac{1}{2}\theta) + 2i\sigma_0], \tag{1b}$$

$$\sigma_l = \sigma_0 + \sum_{j=1}^{l}\arctan\left(\frac{\eta}{j}\right), \tag{1c}$$

$$\sigma_0 = \arg\Gamma(1+i\eta), \tag{1d}$$

$$\eta = zz'e^2\frac{\mu}{k}, \tag{1e}$$

and Γ is the gamma function. When inelastic channels are open the scattering phase shifts δ_l are complex and $|e^{2i\delta_l}|<1$. In this work we will be interested in the elastic scattering of strongly absorbed projectiles at medium energies. It has become customary to analyze such experiments in terms of two models[1]: (i) the parametrized phase-shift analysis which directly parametrizes the partial-wave amplitudes in (1a)[2]; (ii) the optical-potential analysis which indirectly parametrizes the scattering amplitude in terms of a complex potential. In the above region, either of the above models provides an adequate description of the diffraction scattering in terms of a small number of parameters. Although not identical because of the ambiguity in the significance of the various parameters,[3] the optical-potential and parametrized phase-shift analyses are equivalent insofar as they