Method of Complex Coordinates for Three-Body Calculations above the Breakup Threshold*

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A method is proposed for calculating elastic and inelastic three-particle scattering amplitudes in the breakup region using a coordinate-space variational approach, with each coordinate multiplied by a complex phase factor. The trial wave functions have relatively simple asymptotic forms. The method applies to short-range potentials analytic in coordinate space. A numerical example indicates that the method works well for two-particle scattering.

I. INTRODUCTION

THE three-body problem for short-range potentials is now quite well understood from a mathematical viewpoint, but there is need for improved methods of obtaining numerical solutions to problems of physical interest, particularly at energies where the three-free-particle channel is open ($E>0$). For local potentials, coordinate space methods employing the Kohn variational principle have probably proved to be the most efficient procedure, but so far they have only been used below $E=0$, where the open channels consist of a free particle and a bound pair. The reason for this is that, for every open channel, we must include a term with suitable asymptotic behavior in the trial wave function. For three free particles this term is rather complicated,[1] especially if represented to an accuracy that may well be needed for good convergence fo the Kohn method.

It seems worthwhile, therefore, to investigate alternative methods for solving the three-body problem above $E=0$ which still use coordinate space to take advantage of the locality of the potentials and the near locality of the kinetic energy. One such scheme is related to the contour-distortion method, applicable to potentials including those that are given as a superposition of Yukawa potentials, the case we shall consider from now on. Let us illustrate the idea with a discussion of the two-particle case.

II. TWO-PARTICLE SCATTERING

The contour distortion method[2–5] relates the required scattering amplitude $\langle \mathbf{p}' | T(E) | \mathbf{p}\rangle$ with $\mathbf{p}$, $\mathbf{p}'$ real and $E=p^2=p'^2$ (we choose $\hbar=2m=1$) to the Green's function $\langle \mathbf{k}' | G(E) | \mathbf{k}\rangle$ evaluated for real E but complex $\mathbf{k}$, $\mathbf{k}'$. We have

$$\langle \mathbf{p}' | T(E) | \mathbf{p}\rangle = \langle \mathbf{p}' | V | \mathbf{p}\rangle + \theta^6 \int \langle \mathbf{p}' | V | \mathbf{q}'\theta\rangle \times \langle \mathbf{q}'\theta^* | G(E) | \mathbf{q}\theta\rangle \langle \mathbf{q}\theta^* | V | \mathbf{p}\rangle d\mathbf{q}d\mathbf{q}', \quad (1)$$

where $\theta = e^{-i\alpha}$, $\alpha>0$, and $\mathbf{q}$, $\mathbf{q}'$ are real. By

$$\langle \mathbf{q}'\theta^* | G(E) | \mathbf{q}\theta\rangle$$

we mean

$$\langle \mathbf{q}'\theta^* | G(E) | \mathbf{q}\theta\rangle = \theta^{-3}\delta(\mathbf{q}'-\mathbf{q})[(E-\theta^2 q^2)^{-1}+\cdots].$$

The quantity α must be chosen less than a certain value α_p to ensure that $\langle \mathbf{q}\theta^* | V | \mathbf{p}\rangle$ is analytic for $0 \leq -\arg\theta \leq \alpha$. Thus, if the range of the longest-range component of $V(r)$ is μ^{-1}, we need

$$(\mathbf{p}+\mathbf{q}e^{-i\alpha})^2+\mu^2 \neq 0,$$

which leads to

$$\tan\alpha_p = \mu/p. \quad (2)$$

For real $\mathbf{q}$, $\mathbf{q}'$, the Green's function $\langle \mathbf{q}'\theta^* | G(E) | \mathbf{q}\theta\rangle$ is given by the solution of a Fredholm integral equation[4] with an L^2 kernel, which will have a unique solution unless E is at a bound-state energy. Our suggestion is to solve this equation in coordinate space using a version of the Kohn variational method.

We define $\chi_\theta(\mathbf{r})$ by

$$\chi_\theta(\mathbf{r}) = [\theta^2/(2\pi)^{3/2}] \int d\mathbf{q}' \exp(i\mathbf{q}'\cdot\mathbf{r}) \times \int d\mathbf{q} \langle \mathbf{q}'\theta^* | G(E) | \mathbf{q}\theta\rangle \langle \mathbf{q}\theta^* | V | \mathbf{p}\rangle,$$

so that $\chi_\theta(\mathbf{r})$ falls off exponentially for large $|\mathbf{r}|$ and is given by

$$[E+\theta^2\nabla^2 - V(\mathbf{r}\theta^*)]\chi_0(\mathbf{r}) = V(\mathbf{r}\theta^*)[\exp(i\mathbf{p}\cdot\mathbf{r}\theta^*)/(2\pi)^{3/2}]. \quad (3)$$

Note that the condition (2) limiting the size of the rotation is just that which is required to ensure that the right-hand side of (3) is exponentially decreasing. In terms of $\chi_\theta(\mathbf{r})$ the scattering amplitude is given by

$$\langle \mathbf{p}' | T(E) | \mathbf{p}\rangle = \langle \mathbf{p}' | V | \mathbf{p}\rangle + [\theta^{-3}/(2\pi)^{3/2}] \times \int d\mathbf{r} \exp(-i\mathbf{p}'\cdot\mathbf{r}\theta^*) V(\mathbf{r}\theta^*)\chi_\theta(\mathbf{r}).$$

A variational principle which leads to a second-order accurate estimate of $\langle \mathbf{p}' | T(E) | \mathbf{p}\rangle$ comes from varying χ, χ' in the expression

$$[T] = \langle \mathbf{p}' | V | \mathbf{p}\rangle + \theta^{-3}\langle \mathbf{p}'\theta | V_\theta | \chi\rangle + \theta^{-3}\langle \chi' | V_\theta | \mathbf{p}\theta^*\rangle - \theta^{-3}\langle \chi' | [E+\theta^2\nabla^2 - V_\theta] | \chi\rangle, \quad (4)$$

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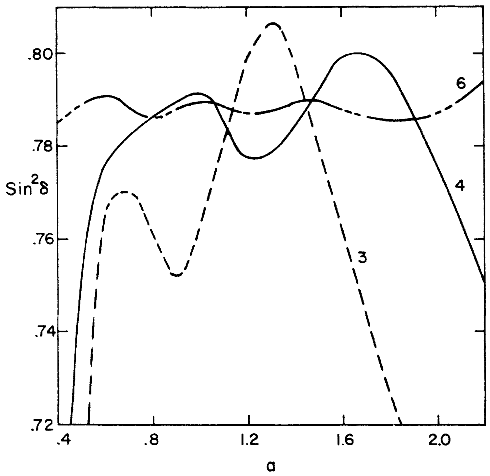

FIG. 1. The imaginary part of the $p=1$ S-wave scattering amplitude plotted against the nonlinear parameter a, for 3, 4, and 6 trial functions.

where we have written V_θ for $V(\mathbf{r}\theta^*)$. If for χ, χ' we take trial functions of the form

$$\chi(\mathbf{r})=\sum_{i=1}^{N} a_i f_i(\mathbf{r}),\qquad \chi'(\mathbf{r})=\sum_{i=1}^{N} b_i f_i(\mathbf{r}),$$

and vary the a_i, b_i, the estimate for $\langle\mathbf{p}'\mid T(E)\mid\mathbf{p}\rangle$ is

$$\langle\mathbf{p}'\mid T(E)\mid\mathbf{p}\rangle=\langle\mathbf{p}'\mid V\mid\mathbf{p}\rangle+\theta^{-3}\langle\mathbf{p}'\theta\mid V_\theta P^N \times[E+P^N(\theta^2\nabla^2-V_\theta)P^N]^{-1}P^N V_\theta\mid\mathbf{p}\theta^*\rangle,\quad(5)$$

where P^N projects onto the space spanned by the functions $f_i(\mathbf{r})$, $i=1,\ldots,N$.

We have tested the proposed method by applying it to an example discussed by Schwartz,[6] S-wave scattering in the potential $-2(e^{-r}/r)$ with $\hbar^2/2m=1$ and $p=1$. We used trial functions of the form $f_i(r)=r^{i-1}e^{-ar}$. In this case, the maximum allowed α is $\alpha_P=45°$, and in Fig. 1 we display the results of the calculation for several different values of N and the nonlinear parameter a, for $\alpha=40°$. There is reasonably rapid convergence of $\mathrm{Im}(e^{i\delta}\sin\delta)$ to its value of 0.78811 with similar results for the real part, though the rate is not equal to that of the ordinary Kohn method. For $\alpha=30°$ the situation changes little but for $\alpha=55°$, no convergence is observed.

III. THREE-PARTICLE SCATTERING

For elastic scattering of particle number 1 from a bound state of particles 2 and 3, the formalism is very similar to the two-body case, and it is sufficient to state the result, which involves a variational principle formally similar to that used by Schlessinger.[7] The elastic amplitude for scattering from an initial state $\mid\mathbf{p},\phi_0\rangle=(2\pi)^{-3/2}\exp(i\mathbf{p}\cdot\mathbf{X})\phi_0(\mathbf{Y})$, consisting of a 23 bound-state wave function $\phi_0(\mathbf{Y})$ and plane wave for particle 1 relative to the 23 c.m. system, is found by varying

$$[T]=\langle\mathbf{p}'\phi_0\mid(V_2+V_3)\mid\mathbf{p},\phi_0\rangle +\theta^{-6}\langle\mathbf{p}'\theta,\phi_0(\theta\mathbf{Y})\mid(V_2+V_3)_\theta\mid\chi\rangle +\theta^{-6}\langle\chi'\mid(V_2+V_3)_\theta\mid\mathbf{p}\theta^*,\phi_0(\theta^*\mathbf{Y})\rangle -\theta^{-6}\langle\chi'\mid[E-\theta^2T-(V_1+V_2+V_3)_\theta]\mid\chi\rangle.\quad(6)$$

A condition on α similar to (2) may be derived from the requirement that $(V_2+V_3)_\theta\mid\mathbf{p}\theta^*,\phi_0(\theta^*\mathbf{Y})\rangle$ decrease at large distances.

The method must be modified if the amplitude for breakup of the 23 bound state into a state of three free particles $\mid\mathbf{p}'\mathbf{q}'\rangle$ is to be calculated. In order to obtain results accurate to second order, we shall need the wave function

$$\mid\chi\rangle=(E-H)^{-1}(V_1+V_2+V_3)\mid\mathbf{p}'\mathbf{q}'\rangle\quad(7)$$

and a straightforward generalization of (4) would involve the function $(V_1+V_2+V_3)\mid\mathbf{p}'\mathbf{q}'\rangle$, which explodes at large distances if $\mathbf{X},\mathbf{Y}\to\mathbf{X}\theta^*,\mathbf{Y}\theta^*$. The remedy is to take out of $\mid\chi'\rangle$ the parts which cause trouble, namely, those in which one of the particles does not interact. Thus, we define a new state $\mid\bar{\chi}'\rangle$ by

$$\mid\bar{\chi}'\rangle=\mid\chi'\rangle-\mid\psi^{(1)}\rangle-\mid\psi^{(2)}\rangle-\mid\psi^{(3)}\rangle,\quad(8)$$

where

$$\mid\psi^{(1)}\rangle=(E-T-V_1)^{-1}V_1\mid\mathbf{p}',\mathbf{q}'\rangle\quad(9)$$

and cyclically so that

$$(E-H)\mid\bar{\chi}'\rangle=\sum_{i=1}^{3}V^{(i)}\mid\psi^{(i)}\rangle,\quad(10)$$

where $V^{(1)}=V_2+V_3$, etc. Now $\mid\bar{\chi}'\rangle$ and the right-hand side of (10) decrease exponentially after a rotation of the coordinates, and a satisfactory variational principle for the break-up amplitude is

$$[T]=\langle\mathbf{p}',\mathbf{q}'\mid V^{(1)}\mid\mathbf{p},\phi_0\rangle+\sum_{i=1}^{3}\langle\psi^{(i)}\mid V^{(1)}\mid\mathbf{p},\phi_0\rangle +\theta^{-6}\langle\chi'\mid V_\theta^{(1)}\mid\mathbf{p}\theta^*,\phi_0(\theta^*\mathbf{Y})\rangle +\theta^{-6}\sum_{i=1}^{3}\langle\psi_\theta^{(i)}\mid V_\theta^{(i)}\mid\chi\rangle -\theta^{-6}\langle\chi'\mid[E-\theta^2T-(V_1+V_2+V_3)_\theta]\mid\chi\rangle.\quad(11)$$

Note that the function $\psi^{(1)}$ is just the χ function of the two-particle 23 system multiplied by a plane wave for the free motion of particle 1.

IV. DISCUSSION

This approach to the problem has several advantages over the standard Kohn method, which in the two-body case involves an additional term with asymptotic form $F(\theta)[\exp(ipr)/r]$ in the trial functions, necessitating very significantly increased computational labor. This difference is magnified in the case of the three-body problem.

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The ordinary Kohn method also suffers from the problem of sporadic singularities[8] in the estimated amplitude, which is related to the fact that one must work at a value of E in the spectrum of the operator $T+V$. In the new method, E is not in the spectrum of $\theta^2 T+V_\theta$, and we expect that no convergence problems will arise. We believe that, for the numerical example discussed above, it is possible to prove the convergence of the method, but the details will not be presented here.

The scheme proposed here may also be superior to the method of analytic continuation from negative E suggested by Schlessinger and Schwartz[9] and recently generalized[10] to include complex E. The effort required to do the computations should be similar in these two approaches, but no continuation with its attendant errors is now needed. In some circumstances it might be advantageous to combine the two methods.

Note added in proof. Dr. Charles Schwartz has kindly pointed out that a coordinate rotation has been previously used in the two-particle problem by T. Regge [Nuovo Cimento **14**, 951 (1959)] and R. Haymaker [University of California Report No. UCRL-17652, Part VIII, 1967 (unpublished)].

ACKNOWLEDGMENT

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Proton-Neutron Final-State Interaction

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The reactions $p(d,2p)n$ and $d(p,2p)n$ were studied at a proton bombarding energy of 16.0 MeV and deuteron bombarding energies of 16.0 and 10.0 MeV. The protons were detected in coincidence with solid-state detectors at angles that allow strong enhancement of the p-n final-state interaction. The coincidence resolving time was sharpened by using time-energy correlation techniques that utilize an on-line SDS-910 computer. The data were analyzed using the "data-simulation technique." A simple theory, which, apart from normalization, contained three adjustable parameters, was found to produce satisfactory fits. In this theory, the final-state interactions are accounted for by assuming additive enhancements for each pair of final-state particles and each spin state. The primary interaction is approximated by the sum of a constant amplitude plus the spectator-effect amplitude. The widths of the final-state interaction peaks are in good agreement with Watson theory using the known singlet p-n scattering length $a_{np}{}^s$ of -23.69 F. The most accurately determined scattering length was extracted from the 16-MeV $p+d$ data and was $a_{np}{}^s=-23.8\pm 0.5$ F. This agreement indicates that interference effects are not important in this reaction at center-of-mass energies above a few MeV if coincidence techniques are employed. With similar methods, a comparative study of the $n+d$ reaction in order to measure the singlet n-n scattering length should be fruitful.

I. INTRODUCTION

A. Three-Body Experiments and Nucleon-Nucleon Interaction

THE nucleon-nucleon interaction plays a fundamental role in our understanding of nuclear physics. Unfortunately, our knowledge of this interaction is incomplete, and there are presently several theoretical potentials that describe the existing two-body scattering data equally well.[1] The study of three-body reactions can, in principle, contribute new information to our knowledge of the nucleon-nucleon interaction in two ways. The first is through investigation of the off-the-energy-shell behavior of the nucleon-nucleon potential, which is, for example, currently being studied in n-p and p-p bremmstrahlung experiments. Quasifree scattering experiments also provide knowledge of the off-the-energy-shell behavior.

The second class of three-body experiments that give nucleon-nucleon potential information consists of those that investigate the neutron-neutron scattering in a final-state interaction, using a reaction such as $n+d\to$

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