Application of the Kohn variational principle to three-particle inelastic scattering*

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We consider the problem of three spinless particles interacting by means of a central potential. The initial state is a free particle labeled number 1 incident on a bound state of particles 2 and 3 and with enough energy to create a three-free-particle final state. We calculate the S-wave elastic scattering amplitude both above and below the inelastic threshold using an extension of the Kohn variational principle suggested by Nuttall. For the asymptotic form, we use the simplest function available. The form used has been shown to be incorrect in certain regions of coordinate space. The trial function we use has up to 32 linear parameters and a range of values for a nonlinear parameter. Below breakup convergence is observed towards a unitary result, but in the inelastic region little evidence of convergence is present.

1. DESCRIPTION OF THE PROBLEM

We consider the problem of three spinless particles interacting by means of a central potential. We are interested in the scattering problem in which particle number 1 is incident on a bound state of particles 2 and 3, but with enough energy to create a three-free-particle final state. The coordinate system used to describe the problem is the same as in the work of Nuttall.[1] We use the vectors $(\vec{X}_i, \vec{Y}_i)$ where for example (we have set $m=\frac{1}{2}$)

$$\vec{X}_1 = \sqrt{\tfrac{2}{3}}\,[\vec{r}_1 - \tfrac{1}{2}(\vec{r}_2+\vec{r}_3)], \qquad \vec{Y}_1 = \sqrt{\tfrac{1}{2}}\,(\vec{r}_2-\vec{r}_3). \tag{1}$$

We shall also have need of the six-vector $\hat{\rho}_i$ defined by

$$\hat{\rho}_i = (\vec{X}_i, \vec{Y}_i). \tag{2}$$

With $\hbar=1$, the Hamiltonian for the three-particle system assumes the form

$$H = -\nabla^2_{\vec{X}_1} - \nabla^2_{\vec{Y}_1} + V_{12} + V_{13} + V_{23}. \tag{3}$$

For this problem Nuttall[1] has shown that the elastic scattering amplitude can be calculated by means of the Kohn principle even in the breakup region provided one takes into account the correct asymptotic wave function. The variational principle has the form

$$\overline{T}_2 = T_2 + \int d\tau\, \psi^+ L \psi^+ \tag{4}$$

In this equation T_2 is a T matrix element describing the elastic scattering process $1+23 \to 1+23$, L is the operator

$$L = -(2\pi)^3(3)^{3/2}(E-H), \tag{5}$$

and ψ^+ is a trial wave function having the asymptotic form

$$\psi^+ \xrightarrow[\rho\to\infty]{} \phi + T_2\psi_2 + T_3\psi_3. \tag{6}$$

In Eq. (6) ϕ is the S-wave part of the incident wave

$$\phi = (2\pi)^{-3}(PX_1)^{-1}\sin(PX_1)\phi_D(Y_1), \tag{7}$$

$\phi_D(Y_1)$ is a bound-state wave function for particles 2 and 3, and ψ_2 is the usual outgoing spherical wave for elastic scattering

$$\psi_2 = -(\tfrac{2}{3})^{3/2}(4\pi X_1)^{-1}e^{iPX_1}(1-e^{-X_1})\phi_D(Y_1). \tag{8}$$

Finally T_3 is a T matrix element describing the inelastic process $1+23 \to 1+2+3$. At the present time there is some controversy about the function ψ_3. If the three particles are well separated, it has the form

$$\psi_3 \sim \rho^{-5/2}e^{iK\rho} \quad (K=\sqrt{E}). \tag{9}$$

However, Nuttall[1] has shown that this function is not correct if two of the particles are close together. Now our criterion for determining the asymptotic region is $\rho \to \infty$ where $\rho^2 = X_1^2 + Y_1^2$, and therefore the asymptotic region includes places with two particles close together. This point has been investigated by Nuttall,[1] and in more detail by Nuttall and Webb.[2] For the present work, we use the form (9) and seek to determine whether or not convergence can be obtained. We assume

$$\psi_3 = \sqrt{i}\,K^{3/2}3^{-3/2}(4\pi)^{-1}\rho^{-5/2}e^{iK\rho}(1-e^{-\rho})^3. \tag{10}$$

The factors of $1-e^{-X_1}$ in Eq. (8) and $1-e^{-\rho}$ in (10) are inserted because of the singularities at $X_1=0$ and $\rho=0$, respectively.

Now for S waves, the elastic scattering ampli-

tude T_2 is a complex constant and may be treated as a single linear parameter in the trial function ψ^+. However, the inelastic scattering amplitude T_3 depends on two angles describing the direction in which the three particles go off (we work in the center-of-mass system) and must be represented by expanding it in terms of a complete set. Thus for the trial wave function we take

$$\psi^+ = \sum_{n=1}^{N} C_n \chi_n + \phi + T_2 \psi_2 + \sum_{m=1}^{M} D_m \theta_m . \tag{11}$$

The expansion functions χ_n are assumed to have the form

$$\chi_n = e^{-(\kappa/2)(Y_1+Y_2)} Y_1^{\,a} Y_2^{\,b} Y_3^{\,c} \tag{12}$$

where κ is a nonlinear parameter, a, b, and c are integers either zero or positive. The expansion functions θ_m have the form

$$\theta_m = \psi_3 Q_1^{\,2a} Q_2^{\,2b} Q_3^{\,2c} , \tag{13}$$

where

$$Q_i = K\rho^{-1} Y_i . \tag{14}$$

In using the variational principle (4), one must evaluate integrals of the form $\int d\tau \psi(E-H)\psi'$ where H is the S-wave part of the full Hamiltonian

$$H = -\frac{1}{X_1^{\,2}} \frac{\alpha}{\alpha X_1}\left(X_1^{\,2} \frac{\alpha}{\alpha X_1}\right) - \frac{1}{Y_1^{\,2}} \frac{\alpha}{\alpha Y_1}\left(Y_1^{\,2} \frac{\alpha}{\alpha Y_1}\right) - \left(\frac{1}{X_1^{\,2}} + \frac{1}{Y_1^{\,2}}\right) \frac{1}{\sin\theta} \frac{\alpha}{\alpha\theta}\left(\sin\theta \frac{\alpha}{\alpha\theta}\right) \tag{15}$$

and

$$d\tau = 8\pi^2 X_1^{\,2} dX_1 Y_1^{\,2} dY_1 \sin\theta d\theta \tag{16}$$

(θ is the angle between $\vec{X}_1$ and $\vec{Y}_1$).
The integrals are three dimensional and for the most part must be evaluated numerically. However the matrix elements involving only the internal functions can be obtained by means of recursion relations developed by Rarita and Present.[3]

All previous variational calculations using the Kohn principle have assumed a fixed form for the asymptotic wave function. Here we see that the number of terms in the asymptotic part is being allowed to vary in much the same way as the number of terms in the internal functions. If one takes an appreciable number of terms in the trial function Ψ^+, the number of matrix elements required will become quite large. This rapid increase is largely due to the fact that the terms coming from the sum over m are not square integrable as are the ones coming from the sum over n. The amount of labor involved in setting up the matrix elements is prodigious if one allows very many terms in the second sum of Eq. (11). Because of this difficulty, we constructed a computer program for the purpose of forming the integrands of the matrix elements. This program will form the quantity $\Psi(E-H)\Psi'$ where Ψ and Ψ' are any of the functions described previously and store the result in algebraic form.

As it turns out, if one transforms the integrands into functions of three coordinates (ρ, α, β) similar to those used by Zickendraht,[4] the integration over ρ can be performed analytically and one is left with functions of two angles to integrate numerically over finite limits. The transformation equations are

$$\begin{aligned} X_1 &= (\rho/\sqrt{2})(1+\sin\alpha\sin\beta)^{1/2} \\ Y_1 &= (\rho/\sqrt{2})(1-\sin\alpha\sin\beta)^{1/2} \\ \cos\theta &= \sin\alpha\cos\beta/(1-\sin^2\alpha\sin^2\beta)^{1/2} \end{aligned} \tag{17}$$

and

$$\int d\tau = \pi^2 \int_0^{\infty} \rho^5 d\rho \int_0^{\pi/2} \sin\alpha\, d\alpha \int_0^{2\pi} d\beta . \tag{18}$$

All the ρ integrations assume the form

$$I(t, B, n) = \int_0^{\infty} d\rho\, \rho^t e^{-B(\alpha,\beta)\rho}(1-e^{-\rho})^n , \tag{19}$$

where t is a positive or negative integer or half integer and n is an integer either zero or positive. We can write down a formula for this integral for any values of t and n. The integration over ρ was performed on the machine along with forming the integrands. Thus the program forms the quantity $\int_0^{\infty}\rho^5 d\rho\, \psi(E-H)\psi'$ and stores the result in algebraic form. For more details see work of Webb.[5]

For the potentials we have made the choice

$$\begin{aligned} V_{23}(r_1) &= V_0 e^{-\mu r_1}, \\ V_{12}(r_3) &= -\tfrac{1}{2} V_0 e^{-\mu r_3}, \quad r_i = \sqrt{2}\, Y_i \\ V_{13}(r_2) &= -\tfrac{1}{2} V_0 e^{-\mu r_2}, \end{aligned} \tag{20}$$

where

$$\begin{aligned} V_0 &= 192.606 \text{ meV}, \\ \mu &= 1.506 \text{ fm}^{-1}. \end{aligned} \tag{21}$$

The potential V_{23} is a nuclear potential which describes the neutron-proton system fairly well at low energy. For example, it binds the deuteron at the right energy and fits the n-p scattering length.[6] The depths of the other two potentials were decreased in order to avoid the additional complexity introduced by the other bound state.

For the potential V_{23} an approximate fit to the deuteron function $\phi_D(Y_1)$ can be constructed after

the manner of Humberston.[7] We obtain

$$\phi_D(Y_1) = 0.175e^{-0.327Y_1}(1-e^{-2.13Y_1}) \times (1-0.60e^{-2.13Y_1}+0.16e^{-4.26Y_1}). \quad (22)$$

The deuteron function is normalized in the following fashion

$$\int |\phi_D(Y_1)|^2 d\vec{Y}_1 = 2^{-3/2}. \quad (23)$$

2. RESULTS AND DISCUSSION

The calculation was carried out at a fixed energy of 5 meV (on our scale breakup occurs at $E=0$), and for a range of values for the nonlinear parameter κ. κ was varied from 0.5 fm^{-1} to 5 fm^{-1} in steps of 0.5 fm^{-1}. We worked with a maximum of 20 internal functions and 10 three-body terms. For this combination of internal and external functions with 10 values for the nonlinear parameter there are 5963 distinct matrix elements involved in the calculation consisting of several hundred thousand individual three-dimensional integrals. On the IBM 360/65 about eight hours of computer time was required to do the calculation at one energy. Of this time, practically all of it was used in evaluating the integrals numerically. The results of the calculation are displayed in Figs. 1 and 2 which show the real and imaginary parts of the elastic scattering amplitude plotted against the nonlinear parameter. In these figures, the symbol (N,M) refers to the number of internal and three-body functions, respectively. In order to interpret these curves, we look for a flat region which tends to persist and which tends to become broader as the number of terms in the trial function increases.

Figures 1 and 2 exhibit some rather strange behavior. There is most likely an unresolved pole in the calculated quantity somewhere in this region. This sort of behavior is common in calculations of this sort[8] and has been discussed rigorously elsewhere.[9]

The plot for $(N,M)=(20,10)$ which represents the maximum number of trial functions used is not shown on the graphs. With the axes scaled as shown, the numbers obtained for $\bar{T}_2$ with 20 internal functions and 10 three-particle terms would not appear. In other words there is evidently no tendency for convergence.

The calculation was also performed below threshold at $E=-1$ meV. For E negative, the asymptotic part of the wave function having to do with three free particles is exponentially damped and therefore need not be included. Exclusion of these terms cuts down tremendously the number of matrix elements involved, especially the ones which must be done numerically. The results of this calculation are shown in Figs. 3 and 4.

An examination of these two figures shows that

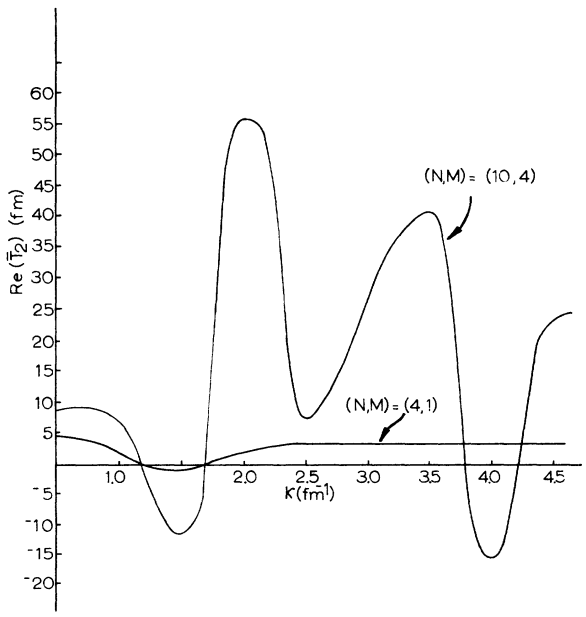

FIG. 1. Real part of the elastic scattering amplitude versus the nonlinear parameter at $E=5$ meV. The symbol (N,M) refers to the number of internal functions and external functions, respectively.

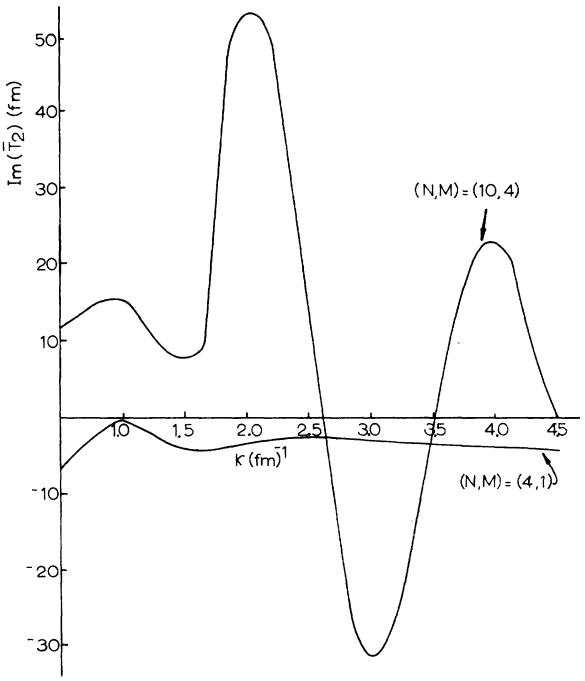

FIG. 2. Imaginary part of the elastic scattering amplitude versus the nonlinear parameter at $E=-1$ meV.

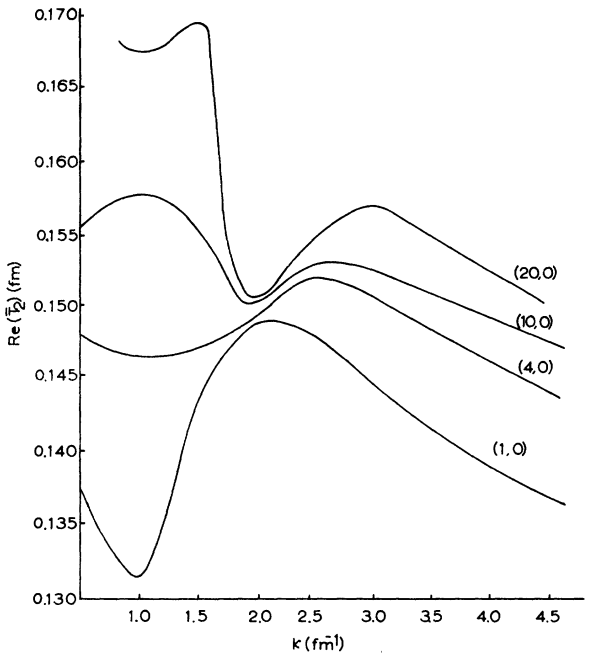

FIG. 3. Real part of the elastic scattering amplitude versus the nonlinear parameter at $E=-1$ meV.

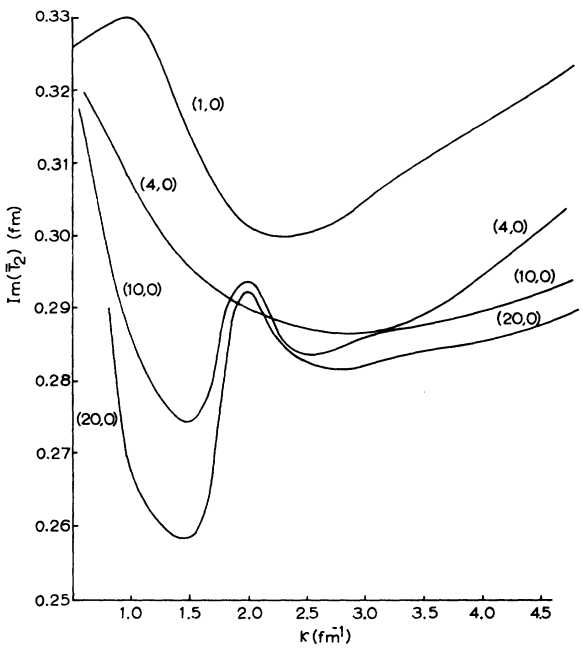

FIG. 4. Imaginary part of the elastic scattering amplitude versus the nonlinear parameter at $E=-1$ meV.

both the real and imaginary parts of the elastic scattering amplitude appear to be converging reasonably well. Again there is some curious behavior for small values of κ, but a flat region shows up even for small values of N and M and appears to become flatter as N and M increase. One can predict with some certainty the value of $\bar{T}_2$ at this energy. The result for the complex number $\bar{T}_2$ below threshold at $E=-1$ meV is

$$\bar{T}_2 = (0.16, -0.28) \text{ fm}. \tag{24}$$

It is worth noting that this result approximately satisfies the unitarity condition which requires that the imaginary part of the scattering amplitude be related to the square of the scattering amplitude. With our normalization T_2 is related to the phase shift by the equation

$$e^{i\delta}\sin\delta = -2P\pi^2\left(\tfrac{2}{3}\right)^{3/2}T_2 \,. \tag{25}$$

The fact that our result below threshold is unitary provides a partial check on the computer program and there is some overlap between the programs used for both calculations.

Since we were unable to obtain convergence above breakup, one of two things is inferred. Either we did not have enough terms in the trial function (which is certainly possible), or the simple asymptotic form will not lead to a converged result. The first of these possibilities cannot be eliminated. The problem we selected is somewhat similar to N-D scattering in the doublet state, and in a 1964 paper,[7] Humberston needed 35 internal functions to produce good convergence in a below breakup calculation. However, the second possibility seems more likely. According to references 1 and 2, the form used is incorrect and therefore we would not expect it to lead to a converged result.

If it is necessary to include all the terms in the asymptotic wave function that are given in Ref. 2, it may not be feasible to calculate neutron-deuteron scattering in this fashion. It is still possible to form the matrix elements on the machine (as a matter of fact, the results presented in Ref. 2 were all checked by a program to form $E-H$ on the functions encountered there), but the sheer number of the integrands and the storage required for them may be too great for present day computers.

Because of these difficulties, it may well be necessary to seek alternative ways of calculating three-body problems in the inelastic region. A recent scheme suggested by Nuttall and Cohen[10] has interesting possibilities. If one puts ρ complex with a positive imaginary part, it is easy to see that the elastic scattering part of the asymptotic wave function as well as the part associated with three particles tends to be damped out. Thus it should be possible to calculate the elastic scattering amplitude in either region without using

either of the functions $T_2\psi_2$ or $T_3\psi_3$ in the asymptotic form. This scheme also renders inconsequential the explicit form of ψ_3. If such a procedure can be made to work, the computational labors involved in the calculation are virtually trivial compared to the problem attacked here. The crucial question is of course, whether or not the convergence rate will be fast enough to make the procedure worthwhile.

More recently McDonald and Nuttall have shown that the method of complex length does work extremely well and provides a systematic method of calculating scattering amplitudes for neutron-deuteron scattering above the inelastic threshold.[11] Also it has been shown that variational principles for the inelastic part of the scattering amplitude exist.[12,13] Thus it may be possible to calculate the entire scattering amplitude without facing the problem of determining explicitly the asymptotic form.

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