

Comparison of Faddeev Method and Resonating Group Method above Breakup Threshold

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The reliability of the resonating group method is studied above the three-body breakup threshold. In particular, the real part of the elastic n - d phase shift is calculated in a model of three spinless bosons interacting by a separable Yamaguchi potential for which exact Faddeev results are available. Spurious singularities which are caused by the distortion part of the resonating group ansatz are eliminated by a least squares method.

1. Introduction

It is well known that spurious singularities can arise in scattering calculations with Kohn's variational principle. These non-physical singularities are due to the fact that part of the scattering solution is expanded into a discrete set of square integrable functions. For energies where only the elastic channel is open various methods have been proposed to avoid such "false resonances"¹. As one of us² has pointed out, another type of singularities is to be expected in calculations of the elastic phase shift above the inelastic threshold, if an open channel is neglected in the trial function. Such an omission may be justified from physical reasons, when the omitted channel is not too strongly coupled to the elastic channel. However, the calculated elastic phase shift will differ strongly from the true one in the vicinity of the above mentioned singularities. In the present work this type of singularities and a method which avoids them² are studied in a numerical example. It will be seen that the resonating group method can yield meaningful results even in an energy region where not all open channels are properly taken into account.

2. The Model and Methods of Calculation

In particular, we have calculated the elastic $l=0$ phase shift of nucleon-deuteron scattering in a three-boson model. The interaction between each pair of particles is a Yamaguchi³ potential,

$$\langle \mathbf{r}' | V | \mathbf{r} \rangle = -V_0 v(\mathbf{r}')v(\mathbf{r}) \quad (1)$$

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with

$$v(r) = \exp \{ -br \} / r, \quad V_0 = 81.3 \text{ MeV}, \quad b = 1.34 \text{ f}^{-1}.$$

The model under consideration is the simplest one to show many-particle features. The separable interaction has the advantage that a (numerical) exact solution can be obtained from the Faddeev equations, even above breakup threshold. We can compare, therefore, the variational result with an exact result. Figure 1 shows the elastic phase shift δ_0 and the inelasticity parameter η_0 as obtained by numerically solving the Faddeev equations⁴; the breakup threshold is at $E=0$, two-particle binding occurs at $E^B = -2.226 \text{ MeV}$.

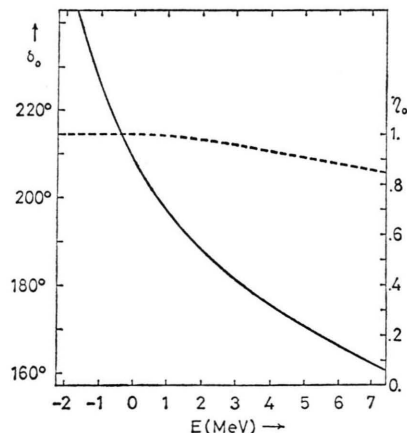


Fig. 1. Exact $l=0$ phase shift δ_0 (full line) and inelasticity parameter η_0 (dashed line) as obtained from the solution of the Faddeev equations; breakup threshold: $E=0$.

As variational approach the resonating group method⁵ has been widely used in single- and multi-channel calculations. Three-particle breakup, however, has not yet been included. An interesting question is, therefore, to what extent resonating



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group results may be reliable above breakup threshold.

In our example an ansatz similar to that of Schwager⁶ has been used for the wave function,

$$\psi = S \{ \Phi_C + \Phi_D \}, \quad (2)$$

where S is a symmetrization operator, Φ_C is a channel function with a flexible relative motion part and Φ_D accounts for distortions of the deuteron. In particular, Φ_C has the form

$$\Phi_C(x_1, y_1) = \varphi_B(x_1) \{ f(y_1) + a_1 g(y_1) + \sum_{n=2}^N a_n \chi_n(a, y_1) \}. \quad (3)$$

Here, $\varphi_B(x_1)$ is the bound state function of the subsystem (2, 3). The relative motion of particle 1 is described by a linear expansion: the function $f(y_1)$ is the regular $l=0$ solution of the free Schrödinger equation, $g(y_1)$ is the irregular solution which is regularized at the origin by a cutoff function and the functions $\chi_n(a, y_1)$ are a truncated set of oscillator functions. The coefficients a_n ($n=1, \dots, N$) are variational parameters, the width parameter a is adjusted to fastest convergence. The distortion part Φ_D has the form

$$\Phi_D(x_1, y_1, \hat{x}_1 \cdot \hat{y}_1) = \sum_{n=N+1}^{N+M} a_n U_n(x_1, y_1, \hat{x}_1 \cdot \hat{y}_1) \quad (4)$$

with variational parameters a_n and two sorts of functions U_n ,

- (i) the ground state ($n=N+1$) and the first excited state ($n=N+2$) of the three-particle system; they are obtained by a separate variational calculation and mainly account for short-ranged correlations⁷,
- (ii) eigenfunctions of the 6-dimensional harmonic oscillator ($n > N+2$).

In a resonating group calculation the Schrödinger equation is usually projected into the test function space,

$$\langle \delta \psi | H - E | \psi \rangle = 0, \quad (5)$$

where $\delta \psi$ denotes all variations of the ansatz (2). When we define functions h_n by writing the expansion (2) as

$$\psi = \sum_{n=0}^{N+M} a_n h_n \quad (6)$$

with $a_0 = 1$ and $h_0 = S \{ \varphi_B(x_1) f(y_1) \}$,

Eq. (5) becomes

$$\langle h_m | H - E | \psi \rangle = 0, \quad m = 1, \dots, N+M. \quad (7)$$

In order to avoid spurious singularities of the first kind ("false Kohn-resonances") we add to the projection space a function ω_1 which is a symmetrized product of the internal motion function $\varphi_B(x_1)$ and a certain relative motion function. Leaving ψ as it is, the variational parameters a_n are now determined by the least squares condition

$$\begin{aligned} \sum_{m=1}^{N+M} |\delta_m|^2 + |\delta_{\omega_1}|^2 &= \min, \\ \delta_m &= \langle h_m | H - E | \psi \rangle, \\ \delta_{\omega_1} &= \langle \omega_1 | H - E | \psi \rangle. \end{aligned} \quad (8)$$

This condition also leads to a set of linear equations for the parameters a_n , but, with an appropriate choice of ω_1 , the new equation does not produce false resonances below the breakup threshold. In our calculation we have chosen ω_1 to be equal to h_0 .

Above the breakup threshold, false resonances of the second type arise from the distortion part Φ_D of the expansion (6). Since the breakup channel has not been included in our ansatz (2) square integrable states will build up in the region of this channel. These states can only decay through the elastic channel where they show up as false resonances. The wrong behaviour of these states which is neither "seen" by the projection principle (5) nor by the least squares principle (8) lies in the fact that they are falling off to zero in a region of space where the true solution would oscillate. Consequently, false resonances of the second type can be suppressed by adding another function ω_2 to the projection space, which is different from zero essentially in this region of coordinate space. The new projection

$$\langle \omega_2 | H - E | \psi \rangle = \delta_{\omega_2}$$

is added to the least squares condition (8),

$$\sum_{m=1}^{N+M} |\delta_m|^2 + |\delta_{\omega_1}|^2 + |\delta_{\omega_2}|^2 = \min. \quad (9)$$

In our calculation the function ω_2 has been chosen to be a long-ranged Gaussian function.

3. Numerical Results and Discussion

Figure 2 shows the results of the variational calculation. Curves a) and b) are obtained with principle (8). In curve a) the trial function consists of Φ_C only (no-distortion approximation). The poor resemblance to the exact solution (Fig. 1) indicates strongly that a deformation of the deuteron has to

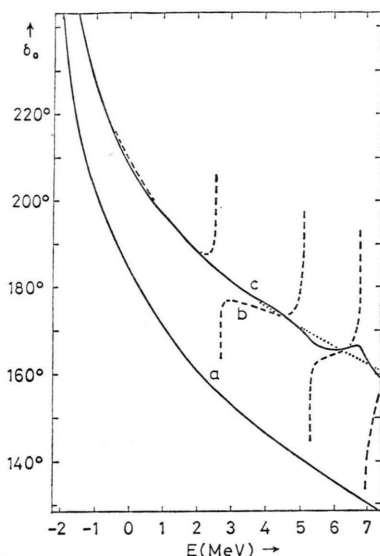


Fig. 2. Resonating group results for the phase shift δ_0 ; a) in no-distortion approximation ($N=12$), b) in distortion approximation ($N=12$, $M=12$), calculated with principle (8) (dashed line), c) in distortion approximation ($N=12$, $M=12$), calculated with principle (9). The exact phase shift from Fig. 1 has been repeated as dotted line where deviations from curve c) are visible.

be taken into account. Curve b) has been calculated including the distortions Φ_D (with $N=12$, $M=12$). Since principle (8) is only able to suppress false channel resonances², singularities appear above the inelastic threshold which are caused by the omission of the inelastic channel. The singularities have been eliminated by the application of principle (9) as shown by curve c). Up to energies of 5 MeV the approximate phase shift c) agrees with the exact one within one degree of angle. At higher energies larger deviations are visible. Two reasons may be responsible for that: Once it is possible that the number of expansion functions does no longer suffice

at these energies; calculations show that the phase shift curve becomes smoother with a higher number of distortion functions. A second reason may be that the breakup channel can no longer be considered as being unimportant at these energies. As can be seen from Fig. 1 the inelasticity parameter η_0 deviates considerably from one at these higher energies. It is clear that the resonating group method with neglected breakup must break down at some energy. The remarkable thing is that it works so well up to several MeV above breakup threshold.

4. Conclusion

From the present example of a simple three-boson calculation the following conclusions can be drawn.

(i) The resonating group method without distortions may give rather poor results. When fragments are more tightly bound than a deuteron and when the particles are fermions the no-distortion approximation may become better but, still, distortions seem to be important.

(ii) With a reasonable number of distortions the resonating group calculation becomes as good as a Faddeev calculation in the elastic energy region.

(iii) The resonating group method with distortions can give reasonable results for the real part of the elastic phase shift up to several MeV above the breakup threshold, even when breakup is neglected in the calculation. This may justify the common practice of performing reaction calculations also above the threshold of an unimportant channel which has to be omitted. Spurious resonances, however, should be suppressed by a least squares technique in this case.

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