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Practical Equations for Three-Particle Scattering Calculations

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A new method is presented for solving the singular integral equations that arise in the Faddeev theory of three-particle scattering. The method is tested by means of an example and found to be practical.

In general, it is more difficult to perform three-particle calculations above the breakup threshold than below. In the Faddeev[1] formalism for nonrelativistic three-particle systems, this difficulty can be attributed to the presence of certain logarithmic singularities in the kernels of the momentum-space integral equations. Three successful techniques for handling these singularities are contour rotation,[2] a method based on the use of Padé approximants to sum a multiple-scattering series,[3] and a modification of the method of moments.[4] The purpose of the present note is to present an alternative approach, which appears to have some advantages over these methods.

The work of Alt, Grassberger, and Sandhas[5] shows that, in general, it is possible to reduce three-particle collision problems to the solution of equations that have the same structure as those which arise when separable two-particle interactions are assumed. Accordingly, here I shall deal with only the equation that arises when each of the pair interactions consists of a single separable term. Furthermore, for the sake of simplicity I shall assume that all of the particles are identical and spinless, and that the two-particle bound state is an s state. This example suffices to illustrate the method; the generalizations to more complicated interactions are not difficult to carry out.

With the assumptions just stated, the two-particle transition operator becomes

$$t(s)=|g\rangle T(s)\langle g|, \tag{1}$$

where s is a complex energy parameter, and $|g\rangle$ is related to the two-particle bound-state wave function $|B\rangle$ with binding energy B by the relation

$$|g\rangle=(-B-H_0)|B\rangle. \tag{2}$$

Here H_0 is the kinetic-energy operator. The propagator T is given by

$$[T(s)]^{-1}=(s+B)\langle B|(s-H_0)^{-1}|g\rangle. \tag{3}$$

Clearly, it has a simple pole at $s=-B$. With this this interaction, it is well known[2,5] that the half-off-shell partial-wave amplitudes for the scattering of one particle from a bound state of the other two can be obtained by solving the equations

$$X_L(q,k;s)=Z_L(q,k;s)+\int_0^\infty Z_L(q,q';s)q'^2\,dq'\,T(s-\tfrac{3}{4}q'^2)X_L(q',k;s),\quad L=0,1,2,\ldots, \tag{4}$$

where

$$Z_L(q,q';s)=\int_{-1}^{1}dx\,P_L(x)g(|\tfrac{1}{2}\vec{q}+\vec{q}'|)g(|\tfrac{1}{2}\vec{q}'+\vec{q}|)/(s-q^2-\vec{q}\cdot\vec{q}'-q'^2),\quad x=\hat{q}\cdot\hat{q}', \tag{5}$$

$$s=-B+\tfrac{3}{4}k^2+i\epsilon=E+i\epsilon.$$

The troublesome logarithmic singularities, referred to above, are associated with the vanishing of the denominator in (5). It is easy to see that this can happen only if

$$q,\ q' < c = (4E/3)^{1/2}. \qquad (6)$$

The singularities can be separated out by using the relation

$$Z_L(q, q'; s) = W_L(q, q'; s) + Y_L(q, q'; s), \qquad (7)$$

where

$$W_L(q, q'; s) = \int_{-1}^{1} \frac{dx\, P_L(x)}{s - q^2 - \vec{q}\cdot\vec{q}' - q'^2} [g(|\tfrac{1}{2}\vec{q} + \vec{q}'|) g(|\tfrac{1}{2}\vec{q}' + \vec{q}|) - \theta(c-q) g((E - \tfrac{3}{4}q^2)^{1/2}) g((E - \tfrac{3}{4}q'^2)^{1/2}) \theta(c - q')], \qquad (8)$$

$$Y_L(q, q'; s) = \theta(c-q) g((E - \tfrac{3}{4}q^2)^{1/2}) (2/qq') Q_L((s - q^2 - q'^2)/qq') g((E - \tfrac{3}{4}q'^2)^{1/2}) \theta(c - q'). \qquad (9)$$

The associated Legendre function Q_L contains the logarithmic singularities. Upon putting (7) into (4), it is not difficult to show that (4) can be replaced with the following two equations:

$$X_L(q, k; s) = R_L(q, k; s) + \int_0^\infty R_L(q, q'; s) q'^2 dq'\, T(s - \tfrac{3}{4}q'^2) X_L(q', k; s), \qquad (10)$$

$$R_L(q, q'; s) = W_L(q, q'; s) + \int_0^c Y_L(q, q''; s) q''^2 dq''\, T(s - \tfrac{3}{4}q''^2) R_L(q'', q'; s). \qquad (11)$$

From (9) and (11), it follows that

$$R_L(q, q'; s) = W_L(q, q'; s), \quad q > c. \qquad (12)$$

The logarithmic singularities in (11) can be treated by simply iterating the equation once to give

$$R_L(q, q'; s) = B_L(q, q'; s) + \int_0^c V_L(q, q''; s) q''^2 dq''\, R_L(q'', q'; s), \qquad (13)$$

where

$$B_L(q, q'; s) = W_L(q, q'; s) + \int_0^c Y_L(q, q''; s) q''^2 dq''\, T(s - \tfrac{3}{4}q''^2) W_L(q'', q'; s), \qquad (14)$$

$$V_L(q, q'; s) = g((E - \tfrac{3}{4}q^2)^{1/2}) T(s - \tfrac{3}{4}q'^2) g((E - \tfrac{3}{4}q'^2)^{1/2}) (4/qq') \times \int_0^c Q_L((s - q^2 - q''^2)/qq'') dq''\, g^2((E - \tfrac{3}{4}q''^2)^{1/2}) T(s - \tfrac{3}{4}q''^2) Q_L((s - q'^2 - q''^2)/q'q''). \qquad (15)$$

It is not hard to see that B_L and V_L are finite and continuous, and therefore (13) can be solved by standard methods. Following Kowalski,[6] it can be shown that the propagator pole [see (3)] in the kernel of (10) can be treated by replacing (10) with the equations

$$\Gamma_L(q, k; s) = R_L(q, k; s) + \int_0^\infty [R_L(q, q'; s) T(s - \tfrac{3}{4}q'^2) - R_L(q, k; s) \gamma_L(k, q)/(\tfrac{3}{4}k^2 + i\epsilon - \tfrac{3}{4}q'^2)] q'^2 dq'\, \Gamma_L(q', k; s), \qquad (16)$$

$$X_L(q, k; s) = \Gamma_L(q, k; s) [1 - \int_0^\infty \gamma_L(k, q') q'^2 dq'\, \Gamma_L(q', k; s)/(\tfrac{3}{4}k^2 + i\epsilon - \tfrac{3}{4}q'^2)]^{-1}. \qquad (17)$$

Here γ_L is any well-behaved function with the property $\gamma_L(k, k) = 1$.

In order to test the practicality of this scheme, a calculation has been carried out for the s-wave, quartet, neutron-deuteron amplitude. Even though the equations presented here are for spinless particles, they can be used for this case by simply taking into account a spin-isospin recoupling coefficient of $-\frac{1}{2}$ in the "potential" Z_L. The two-nucleon interaction was taken to be the same as that used by Sloan.[7] The logarithmic singularities in (14) and (15) were treated by a subtraction technique similar to that of Ref. 3. The range of integration in (16) and (17) was broken up into the intervals $(0, c)$ and (c, ∞), and the points and weights for Gauss-Legendre quadrature were mapped from the interval $(-1, 1)$ onto these intervals by using the transformations

$$q = c(x+1)/2, \quad q = c + (1+x)/(1-x).$$

The same points and weights were used in solving (13). The function γ_0 was taken to be

$$\gamma_0(k, q) = (k^2 + \beta^2)/(q^2 + \beta^2),$$

with $\beta = 1\ \text{fm}^{-1}$. The rate of convergence with respect to the number of quadrature points is illustrated in Table I, where the parameters that

TABLE I. The s-wave, quartet, elastic n-d amplitude at a neutron lab energy of 14.1 MeV, for various sets of quadrature points.

Number of quadrature points $0-c$	$c-\infty$	$\mathrm{Re}(\delta_0)$ (deg)	y_0
6	6	72.80	0.9702
10	6	72.66	0.9719
6	10	72.31	0.9721
10	10	72.14	0.9738
16	10	72.10	0.9758
10	16	72.04	0.9743
16	16	72.00	0.9763

describe the elastic amplitude ($q=k$) at a neutron lab energy of 14.1 MeV are given for various sets of quadrature points. The parameters are the real part of the phase shift δ_0 and the inelasticity y_0.[7] It is seen that the rate of convergence is very good. The last entries in the table agree closely with values of $\mathrm{Re}(\delta_0)=71.9°$ and $y_0=0.978$ found by Sloan.[7,8] The converged off-shell amplitude is shown in Fig. 1, where the known square-root singularity[9] at $q=c$ is clearly revealed. The off-shell elastic amplitude on the interval $0 \le q \le c$ is used in the construction of the breakup amplitude.

In conclusion, it should be noted that in contrast to the contour-rotation technique,[2] the method presented here only requires that the two-particle input be known for real momenta. This is a significant practical advantage, when the two-particle t matrix cannot be obtained analytically. The method of Kloet and Tjon[3] has the same advantage; however, with their technique it is necessary to perform a large number of interpolations. This can lead to a loss of numerical accuracy, as well as necessitating the use of a large amount of computer time. The modified method of moments[4] is also a real-axis technique. An assumption of this approach is that the scattering amplitude can be well approximated by a polynomial on the interval $0 \le q \le c$. Because of the square-root singularity, it is not clear that this assumption is a good one. Finally, there is no reason to believe that the approach presented here will not work just as well for the doublet state of neutron-deuteron scattering. The rate of numerical convergence is determined mainly by the smoothness of the functions B_L and V_L [see Eqs. (14) and (15)], and the same expressions occur in the doublet case.

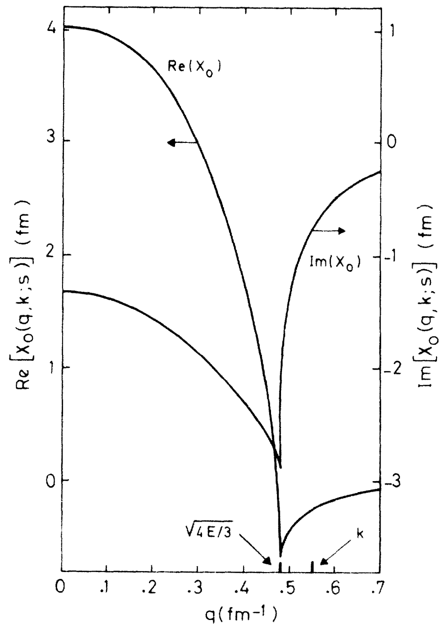

FIG. 1. Amplitude for s-wave, quartet, n-d scattering at a neutron lab energy of 14.1 MeV, as a function of the momentum.

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