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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 Faddeev¹ 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 Sandhas⁵ 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

$$t(s) = |g\rangle T(s) \langle g|, \quad (1)$$

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

$$|g\rangle = (-B - H_0)|B\rangle. \quad (2)$$

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

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

Clearly, it has a simple pole at *s* = −*B*. With 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

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

where

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

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

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

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

The singularities can be separated out by using the relation

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

where

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

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

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:

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

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

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

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

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

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

where

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

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

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

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

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

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		$\text{Re}(\delta_0)$ (deg)	y_0
$0 - c$	$c - \infty$		
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 $\text{Re}(\delta_0) = 71.9^\circ$ 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 singularity⁹ at $q = c$ is clearly revealed. The off-shell elastic amplitude on the interval $0 \leq q \leq c$ 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 Tjon³ 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 moments⁴ 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 $0 \leq q \leq c$. 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

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.

V_L [see Eqs. (14) and (15)], and the same expressions occur in the doublet case.

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