Practical Equations for Three-Particle Scattering Calculations

Michael G. Fuda

Natuurkundig laboratorium der Vrije Universiteit, Amsterdam, The Netherlands

(Received 7 January 1974)

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 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, a method based on the use of Padé approximants to sum a multiple-scattering series, and a modification of the method of moments. 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 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

$$I(s) = |g⟩T(s)⟨g|,$$  \hspace{1cm} (1)

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

$$|g⟩ = (−B − H_0)|B⟩.$$  \hspace{1cm} (2)

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

$$[T(s)]^{-1} = (s + B)(s − H_0)^{-1}|g⟩.$$  \hspace{1cm} (3)

Clearly, it has a simple pole at $s = −B$. With this interaction, it is well known that the 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

$$X_L(q, k; s) = Z_L(q, k; s) + \int_0^m Z_L(q, q'; s)q'^2dq' T(s − \frac{4}{3}q'^2)X_L(q', k; s), \quad L = 0, 1, 2, \ldots,$$  \hspace{1cm} (4)

where

$$Z_L(q, q'; s) = \int_{−1}^{1}dx P_L(x)|\langle \frac{1}{2}q + \frac{1}{2}q' | g(x)|\frac{1}{2}q + \frac{1}{2}q'⟩| / (s − q^2 − \frac{4}{3}q · q' − q'^2), \quad x = \frac{q · q'}{q^2}.$$  \hspace{1cm} (5)

$s = −B + \frac{4}{3}iκ^2 + iκ = E + iκ.$

620
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

\[ q, q' < c = (4E/3)^{1/2}. \]  

(6)

The singularities can be separated out by using the relation

\[ Z_L(q, q'; s) = W_L(q, q'; s) + Y_L(q, q'; s), \]  

(7)

where

\[ W_L(q, q'; s) = \int_1^{\frac{1}{2}} \frac{dx P_L(x)}{s - q^2 - \frac{q^2}{q'}} - \frac{1}{2} \left[ \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \right] \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \]  

\[-\theta(c - q) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \]  

\[ \theta(c - q) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \]  

(8)

\[ Y_L(q, q'; s) = \theta(c - q) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \]  

(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:

\[ X_L(q, k; s) = R_L(q, k; s) + \int_0^{\infty} R_L(q, q'; s) q'^2 dq' T(s - \frac{1}{2} q'^2) X_L(q', k; s), \]  

(10)

\[ R_L(q, q'; s) = W_L(q, q'; s) + \int_0^{\infty} Y_L(q, q''; s) q''^2 dq'' T(s - \frac{1}{2} q''^2) R_L(q'', q'; s). \]  

(11)

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

\[ R_L(q, q'; s) = W_L(q, q'; s), \quad q > c. \]  

(12)

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

\[ R_L(q, q'; s) = B_L(q, q'; s) + \int_0^{\infty} V_L(q, q'', s) q''^2 dq'' R_L(q'', q'; s), \]  

(13)

where

\[ B_L(q, q'; s) = W_L(q, q'; s) + \int_0^{\infty} V_L(q, q'', s) q''^2 dq'' T(s - \frac{1}{2} q''^2) W_L(q'', q'; s), \]  

(14)

\[ V_L(q, q'; s) = \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \]  

\[ \theta(c - q) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \]  

\[ \theta(c - q) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \eta \left( \frac{1}{2} q + \frac{q'}{2} \right) \]  

\[ \times \int_0^{\infty} Q_L(q - q'^2, q'^2, q'^2) T(s - \frac{1}{2} q'^2) Q_L(q, q'^2) / q'^2. \]  

(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, it can be shown that the propagator pole [see (3)] in the kernel of (10) can be treated by replacing (10) with the equations

\[ \Gamma_L(q, k; s) = R_L(q, k; s) + \int_0^{\infty} \left[ R_L(q, q'; s) T(s - \frac{1}{2} q'^2) \right. \]  

\[ - \left. R_L(q, k; s) \gamma_L(q, k, q) / (\frac{3}{2} k^2 + i\epsilon - \frac{1}{2} q'^2) \right] q'^2 dq' \Gamma_L(q', k; s), \]  

(16)

\[ X_L(q, k; s) = \Gamma_L(q, k; s) \left[ 1 - \int_0^{\infty} \gamma_L(q, k, q') q'^2 dq' \Gamma_L(q', k; s) / \left( \frac{3}{2} k^2 + i\epsilon - \frac{1}{2} q'^2 \right) \right]^{-1}. \]  

(17)

Here \( \gamma_L \) 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. 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 \((c, \infty)\), and the points and weights for Gauss-Legendre quadrature were mapped from the interval \((-1, 1)\) on to 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 \( \gamma_0 \) 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.

<table>
<thead>
<tr>
<th>Number of quadrature points</th>
<th>0-c</th>
<th>c-∞</th>
<th>Re(δv) (deg)</th>
<th>y₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-6</td>
<td>6</td>
<td>6</td>
<td>72.80</td>
<td>0.9702</td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>10</td>
<td>72.66</td>
<td>0.9719</td>
</tr>
<tr>
<td>6</td>
<td>10</td>
<td>6</td>
<td>72.31</td>
<td>0.9721</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>10</td>
<td>72.14</td>
<td>0.9738</td>
</tr>
<tr>
<td>16</td>
<td>10</td>
<td>16</td>
<td>72.10</td>
<td>0.9758</td>
</tr>
<tr>
<td>10</td>
<td>16</td>
<td>10</td>
<td>72.04</td>
<td>0.9743</td>
</tr>
<tr>
<td>16</td>
<td>16</td>
<td>16</td>
<td>72.00</td>
<td>0.9763</td>
</tr>
</tbody>
</table>

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 δv and the inelasticity y₀. It is seen that the rate of convergence is very good. The last entries in the table agree closely with values of Re(δv) = 71.9° and y₀ = 0.978 found by Sloan. The converged off-shell amplitude is shown in Fig. 1, where the known square-root singularity at q = c is clearly revealed. The off-shell elastic amplitude on the interval 0 ≤ q ≤ c is used in the construction of the breakup amplitude.

In conclusion, it should be noted that in contrast to the contour-rotation technique, 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 Kloe and Tjon 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 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 ≤ q ≤ 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](image-url)  
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.

The author would like to thank the Dutch Organization for Pure Scientific Research for providing partial support for this work.

8I. H. Sloan, private communication.