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Spline-Galerkin Solution of Integral Equations for Three-Body Scattering above Break-Up

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We investigate a Galerkin method for solving the integral equations for three-body scattering at energies above the break-up threshold. The scattering equations that we consider are one-dimensional integral equations that arise from a separable potential model. Cubic spline approximants with multiple knots are used to construct a non-smooth solution function. Numerical results are obtained both for a system of spin-0 (boson) and spin-$\frac{1}{2}$ (fermion) particles interacting via separable two-body potentials. The results demonstrate that our numerical treatment of this problem is both robust and accurate with a small number of basis functions.

1. INTRODUCTION

The use of separable potentials in the integral equation approach of Faddeev [1] is known to reduce the equations for three-body scattering to a more manageable form [2, 3]. Nevertheless, the numerical treatment of three-body equations, particularly above the break-up threshold, remains a formidable task.

Several practical methods for solving the integral equations for three-body scattering above break-up are known. These include the contour rotation method [4],

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where the integration contour is rotated into the complex momentum plane in order to avoid integrating over singularities; and the Padé method [5], in which a rational expansion approximation is used to sum the multiple scattering series.

An alternative numerical method to those described above, and one that is also advocated as a practical means of solving Faddeev equations, is a projection method [6] in which one seeks to expand the solution of the integral equation in some finite set of basis functions. A difficulty with this approach is that the success of the method often depends on the choice of basis functions for a particular problem. Of particular interest, therefore, is the choice of piecewise local interpolants as basis functions. In this way one may hope to avoid the troublesome problem of selecting an optimum basis set [7]. An additional advantage of this choice of basis functions is that piecewise local interpolation allows considerable flexibility in fitting complicated structure into the solution function.

A collocation method using piecewise Lagrange polynomial functions has been used successfully to solve the integral equations for three-body scattering at energies above the break-up threshold [8]. It is known, however, that the Lagrange polynomial does not yield the best interpolation, and that a better choice is provided by the spline [9]. The advantage of using spline functions as a basis for solving Faddeev equations has been recognized by several authors [10, 11]. Recently, cubic B-splines have been shown [11] to provide an excellent basis for solving the equations of [3] in a Galerkin method approach.

The present paper is devoted to an investigation of the numerical treatment of three-body integral equations at energies above the break-up threshold in which use is made of a Galerkin method approach with cubic B-spline approximants. The numerical procedure is an extension of the method employed in [11] for solving three-body scattering below break-up. Novel features of the present problem are a logarithmic singularity structure in the kernel, and a non-smooth (C_1 discontinuity) in the solutions of the integral equations.

Section 2 gives a mathematical formulation of the method for integral equations of the second kind. Section 3 gives a brief review of the integral equations for three-body scattering. Section 4 describes the numerical procedure, and Section 5 gives our numerical results. An appendix describes the origin of the cusp in the three-body transition amplitude above break-up.

2. Theory

The problem, from which our physical problem is taken, is the solution to the operator equation

$$(\mathscr{I} - \mathscr{K}) f = y, \tag{2.1}$$

where f, $y \in C[a, b]$, the space of continuous functions defined on the closed inter-

val $[a, b]$, $\mathscr{I}$ is the identity operator, and $\mathscr{K}$ is a linear operator defined on a subset of $C[a, b]$.

In the scattering problems we consider here, $\mathscr{K}$ is the integral operator given by

$$\mathscr{K}f = \int_a^b K(\cdot, t) f(t)\, dt, \tag{2.2}$$

where the kernel K has a Cauchy principal value type singularity. That is, K has the form

$$K(\cdot, t) = \tilde{K}(\cdot, t)/(t-u) \tag{2.3}$$

for some $u \in [a, b]$. Also, at some known value $\eta \in [a, b]$ the function $f(\eta)$ has a discontinuous derivative.

To solve this problem numerically we seek to find an approximation to f which satisfies some interpolation property or variational principle. We thus look for an approximation that satisfies the properties of f. For such a purpose the linear space of cubic splines forms an ideal setting. To be precise, let π_N be a partition of the interval $[a, b]$, defined by the knots $\{t_i\}$, such that $a = t_1 \leqslant \cdots \leqslant t_N = b$. On this partition, together with the extended knots $t_{-2} \leqslant t_{-1} \leqslant t_0 \leqslant t_1$, and $t_N \leqslant t_{N+1} \leqslant t_{N+2} \leqslant t_{N+3}$, we can construct the cubic B-splines. For a partition π_N we can construct $N+2$ B-splines denoted by $\{B_i;\ i = 0,..., N+1\}$, where B_i is non-zero over the interval $(t_{i-2},\ t_{i+2})$ and is a cubic polynomial over each subinterval $(t_{i+j},\ t_{i+j+1})$, $j = -2,..., 1$, with the added restriction that we get C_2 continuity everywhere. Such continuity is obtained if the knots are simple, that is, if $t_{i+j} < t_{i+j+1}$, $j = -2,..., 1$. If, however, multiple knots are introduced, then loss of continuity ensues. To be precise, if for some j, $t_j = t_{j+1}$, then at that point C_1 continuity is obtained, while for $t_{j-1} = t_j = t_{j+1}$, C_0 continuity is obtained. Hence, to ensure that the approximation emulates the C_0 continuity of f at η, we place a triple knot at η and keep the other knots simple. In all such cases $\{B_i;\ i = 0,..., N+1\}$ is a basis for the linear space S_N of cubic splines with partition π_N. For numerically stable methods of evaluating B-splines under all conditions see [12].

Using this linear space, we approximate f by the linear combination given by

$$\sum_{i=0}^{N+1} \alpha_i B_i, \tag{2.4}$$

and seek an appropriate set of coefficients $\{\alpha_i\}$.

To aid us in this search for appropriate coefficients, we define a residual function r by the relation

$$r = \sum_{i=0}^{N+1} \alpha_i (\mathscr{I} - \mathscr{K})\, B_i - y; \tag{2.5}$$

then $\{\alpha_i\}$ are chosen to minimize r in some fashion.

One such method is to choose $N+2$ abscissae values s_j, $j=0,\ldots, N+1$, and then to solve the linear system of equations given by

$$r(s_j)=0, \qquad j=0,\ldots, N+1. \tag{2.6}$$

This is the method of collocation. The choice of collocation points $\{s_j\}$ is only restricted by the Schoenberg–Whitney theorem [13], which requires that $t_{i-2}<s_i<t_{i+2}$, $i=0,\ldots, N+1$. For a more elementary proof of this theorem see [9].

As can be expected, a bad choice of collocation points will result in a poor approximation. Hence, we choose to calculate our coefficients α_i, $i=0,\ldots, N+1$ by solving the system of linear equations given by

$$(r, B_i)=0, \qquad i=0,\ldots, N+1. \tag{2.7}$$

where $(\cdot,\cdot)$ defines the inner product on $C[a, b]$, namely

$$(\psi, \phi)=\int_a^b \psi(x)\,\phi(x)\,dx. \tag{2.8}$$

This is the classical Galerkin technique.

To analyze this method, let G_N be the mapping of $C[a, b]$ onto S_N, such that, for $\psi \in C[a, b]$, $G_N\psi$ is the best approximation of ψ by S_N in the norm defined by the inner product. That is,

$$G_N\psi=\sum_{i=0}^{N+1} \lambda_i B_i, \tag{2.9}$$

where λ_i are the solutions to the linear system

$$\sum_{i=0}^{N+1} \lambda_i(B_i, B_j)=(\psi, B_j), \qquad j=0,\ldots, N+1. \tag{2.10}$$

See [6] for the theoretical development of this result. The operator G_N is a projection operator, which is easily deduced from the properties of cubic splines.

For our problem we consider

$$G_N r=\sum_{i=0}^{N+1} \lambda_i B_i. \tag{2.11}$$

Then to find the λ_i's we have to solve

$$\sum_{i=0}^{N+1} \lambda_i(B_i, B_j)=(r, B_j), \qquad j=0,\ldots, N+1. \tag{2.12}$$

Due to the linear independence of our B-spline basis, the solution to this system is

$\lambda_i = 0$ for all i, that is, $G_N r = 0$ (the zero function), if and only if $(r, B_j) = 0$, $j = 0,..., N+1$. Hence, the Galerkin procedure gives us a solution $g \in S_N$ such that

$$G_N(\mathscr{I} - \mathscr{K})\, g = G_N\, y. \tag{2.13}$$

The G_N here defined is a continuous least squares approximation operator, and one property of least squares approximation by cubic splines is that there exists a strictly increasing set of abscissae τ_i, $i = 0,..., N+1$, such that $t_{i-2} < \tau_i \leqslant t_{i+2}$, where the error of approximation is zero; see [9]. Thus

$$r(\tau_i) = 0, \qquad i = 0,..., N+1, \tag{2.14}$$

and, hence, the Galerkin procedure is a collocation procedure with $\{\tau_i\}$ the set of collocation points.

To solve the system of equations $(r, B_i) = 0$, we need to perform two integrations numerically. To this end we choose a standard numerical quadrature, namely,

$$\int_a^b F(x)\, dx \approx \sum_{j=1}^{p} \omega_j F(x_j), \tag{2.15}$$

for some suitably chosen x_j, $j = 1,..., p$. Then, for any $k = 0,..., N+1$, we write

$$\begin{aligned}(r, B_k) &= \int_a^b r(x)\, B_k(x)\, dx \\ &\approx \sum_{j=1}^{p} \omega_j r(x_j)\, B_k(x_j),\end{aligned} \tag{2.16}$$

while

$$r(x_j) = \sum_{i=0}^{N+1} \alpha_i \left[B_i(x_j) - \int_a^b \frac{\tilde{K}(x_j, s)}{(s-u)} B_i(s)\, ds \right] - y(x_j). \tag{2.17}$$

The integral in this equation needs careful attention due to the presence of the singularity. We write

$$\int_a^b \frac{\tilde{K}(x_j, s)}{s-u} B_i(s)\, ds = \sum_{k=i-2}^{i+1} \int_{t_k}^{t_{k+1}} \frac{\tilde{K}(x_j, s)}{s-u} B_i(s)\, ds. \tag{2.18}$$

For all k such that $u \notin (t_k, t_{k+1})$ we have

$$\int_{t_k}^{t_{k+1}} \frac{\tilde{K}(x_j, s)}{s-u} B_i(s)\, ds \approx \sum_{q=1}^{p} \omega_q \frac{\tilde{K}(x_j, s_q)}{q_q - u} B_i(s_q), \tag{2.19}$$

for suitable s_q in the interval (t_k, t_{k+1}).

If $u \in (t_k, t_{k+1})$ then we subtract out the singularity [14] as follows:

$$\int_{t_k}^{t_{k+1}} \frac{\tilde{K}(x_j, s)}{s-u} B_i(s)\, ds$$

$$= \int_{t_k}^{t_{k+1}} \left\{ \frac{\tilde{K}(x_j, s)\, B_i(s) - \tilde{K}(x_j, u)\, B_i(u)}{s-u} \right\} ds + \tilde{K}(x_j, u)\, B_i(u) \ln \left| \frac{t_{k+1}-u}{t_k-u} \right|$$

$$\approx \sum_{q=1}^{p} \omega_q \frac{\tilde{K}(x_j, s_q)}{s_q-u} B_i(s_q)$$

$$- \sum_{q=1}^{p} \omega_q \frac{\tilde{K}(x_j, u)}{s_q-u} B_i(u) + \tilde{K}(x_j, u)\, B_i(u) \ln \left| \frac{t_{k+1}-u}{t_k-u} \right|, \tag{2.20}$$

for appropriate s_q in the interval (t_k, t_{k+1}). The first term in this expression is the usual quadrature formula, while the second and third terms are adjustments to account for the singularity.

Using these equations we obtain a spline approximation $g_N \in S_N$ to our unknown function f. The numerical results we obtain lead us to believe that the method outlined here does converge with a fourth order rate of convergence. That is, the theory developed for a continuous kernel holds for the type of singularity treated here. Thus, using the uniform norm, we assume that for some β,

$$\| f - g_N \| \leqslant \beta \| f - G_N f \|, \tag{2.21}$$

analogous to theorem 2 in [6, p. 51]. Using the Peano kernel theorem [15], we have

$$\| f - G_N f \| \leqslant \frac{5}{384} \| f^{(4)} \| h_N^4, \tag{2.22}$$

with h_n the maximum knot spacing over the knots $(t_0, \ldots, t_{v-1}, t_{v+1}, \ldots, t_{N+1})$. Hence if our assumption is correct, fourth order convergence is attained.

3. Three-Body Integral Equations

In this section we briefly describe the three-body integral equations. In order to test the numerical method described in the previous section, we consider three simple cases. The first is a model boson problem, so called because the three particles are identical with no spin or isospin. For the second, we choose a system of three spin-$\frac{1}{2}$ and isospin-$\frac{1}{2}$ particles in a spin-quartet and isospin-doublet configuration. The third is a spin-doublet and isospin-doublet configuration. These last two configurations are found in the scattering of neutrons from deuterons.

For each of the above three cases, we shall consider a system of equal mass par-

ticles and set the particle mass $M=1$. We denote by $(\mathbf{p}, \mathbf{q})$ the two independent Jacobi momentum variables in the three-body center-of-mass frame. Here $\mathbf{q}$ is the relative momentum between two particles and $\mathbf{p}$ is the momentum of the third particle relative to the center-of-mass of the other two. The pairwise interactions are chosen to be s-wave separable potentials of the Yamaguchi [16] form

$$V_m(\mathbf{q}, \mathbf{q}') = \lambda_m (q^2 + \beta_m^2)^{-1} (q'^2 + \beta_m^2)^{-1}, \tag{3.1}$$

where λ_m and β_m are strength and range parameters, and m is used to denote internal quantum numbers of the interacting pair. In the case of spin-$\frac{1}{2}$ particles we use different parameters λ_m, β_m for the spin-triplet ($m=t$) and spin-singlet ($m=s$) configurations. For the boson model we use the $m=t$ interaction.

For the interactions given in Eq. (3.1) it is known that the Faddeev equations reduce [2, 3] to a set of coupled integral equations in one continuous momentum variable. We now describe the integral equations for the three cases discussed above.

Consider the scattering of a particle from a bound state of the other two, described by quantum number $m=t$. For a particle with incident momentum k and a target with binding energy $-\varepsilon$, the scattering energy in the three-body center-of-mass frame is

$$E = \tfrac{3}{4} k^2 - \varepsilon. \tag{3.2}$$

The $L=0$ partial wave half-shell transition amplitudes $\{T_{mt}(p; E+i0);\ m=t, s\}$ satisfy a set of coupled integral equations

$$T_{mt}(p; E+i0) = Z_{mt}(p, k; E+i0) - \sum_n \int Y_{mn}(p, p'; E+i0)\, T_{nt}(p'; E+i0)\, p'^2 dp', \tag{3.3}$$

where the kernels Y_{mn} are given by

$$Y_{mn}(p, p'; E+i0) = Z_{mn}(p, p'; E+i0)\, \tau_n(E+i0-\tfrac{3}{4}p'^2). \tag{3.4}$$

The effective three-body potentials Z_{mn} are defined by the integrals

$$Z_{mn}(p, p'; E+i0) = -\chi_{mn} \frac{4}{3\pi} \int_{-1}^{1} \frac{\phi_m(q_1)\, \phi_n(q_2)\, dy}{p^2 + p'^2 + pp'y - E - i0}, \tag{3.5}$$

where

$$\begin{aligned} q_1 &= (\tfrac{1}{4}p^2 + p'^2 + pp'y)^{1/2}, \\ q_2 &= (p^2 + \tfrac{1}{4}p'^2 + pp'y)^{1/2}, \end{aligned} \tag{3.6}$$

and

$$\phi_m(q) = \frac{C_m}{(q^2 + \beta_m^2)} \tag{3.7}$$

is a two-body vertex function. We take $C_s = 1$ and choose the constant C_t so that the bound state wavefunction is normalized to unity. The constant C_t is given by

$$C_t = [2\alpha\beta_t(\alpha + \beta_t)^3]^{1/2}, \tag{3.8}$$

where $\alpha = \sqrt{\varepsilon}$.

The constant χ_{mn} in Eq. (3.5) is a spin–isospin recoupling coefficient [2]. For the boson model $\chi = 2$ and the effective potential is purely attractive. For the spin-quartet system there is no $m = s$ subsystem and $\chi_{tt} = -1$, which means that the effective potential is purely repulsive. For the spin-doublet system χ_{mn} is given by the matrix

$$\chi_{mn} = \begin{pmatrix} -\frac{1}{2} & \frac{3}{2} \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix}. \tag{3.9}$$

In this case the effective potential has both an attractive and repulsive piece.

The effective propagator $\tau_m(z)$ in Eq. (3.3) has its origin in the two-particle transition matrix t_m. We write

$$t_m(q, q'; z) = \phi_m(q)\, \tau_m(z)\, \phi_m(q'), \tag{3.10}$$

where

$$\tau_m(z) = C_m^{-2} \left[\frac{1}{\lambda_m} + \frac{2}{\pi} \int_0^\infty \frac{q^2\, dq}{(q^2 + \beta_m^2)^2 (q^2 - z)} \right]^{-1}. \tag{3.11}$$

In the spin-triplet ($m = t$) configuration $\tau_t(z)$ has a bound state pole at $z = -\varepsilon$. This gives $\lambda_t = -2\beta_t(\beta_t + \alpha)^2$. For z along the real axis, $z = -\xi^2 + i0$, $\xi > 0$, the pole structure of this function can be written

$$\tau_t(-\xi^2) = -\frac{3}{4} \frac{S(\xi)}{\xi^2 - \varepsilon - i0}, \tag{3.12}$$

where

$$S(\xi) = \frac{(\xi + \beta_t)^2}{\alpha(\alpha + \beta_t)[1 + 2\beta_t/(\alpha + \xi)]}. \tag{3.13}$$

The denominator in Eq. (3.12) leads to a Cauchy-type singularity $(p'^2 - k^2 - i0)^{+1}$ in the kernel of Eq. (3.3).

An additional logarithmic singularity structure in the kernel of Eq. (3.3) leads to a C_1 discontinuity in the three-body transition amplitude. A discussion of this non-smooth behaviour is given by Larson and Hetherington in [8]. For completeness,

we describe in the appendix an alternative derivation of the cusp singularity, based on an analysis of the logarithmic integrands in the kernel of Eq. (3.3). This completes our description of the three-body integral equations.

4. Numerical Procedure

This section describes our numerical procedure for solving the integral equation in Eq. (3.3).

In order to construct the spline basis, we first map the momentum variable $p \in [0, \infty)$ onto a finite interval $[-1, +1]$, using

$$p(x) = \left(\frac{1+x}{1-x}\right), \qquad x \in [-1, +1]. \tag{4.1}$$

We partition this interval $[-1, +1]$ by N knots $-1 = x_1 \leqslant x_2 \leqslant x_3 \cdots x_N = +1$, with mesh spacing $h_N = \max\{(x_{i+1} - x_i);\ 1 \leqslant i < N\}$. Three of the knots are placed in coincidence at $p_c(x) = \sqrt{\frac{4}{3}E}$. This will ensure that the spline approximate solution to Eq. (3.3) has C_1 discontinuity at p_c. On this partition, together with the extended knots $x_{-2} \leqslant x_{-1} \leqslant x_0 \leqslant x_1$ and $x_N \leqslant x_{N+1} \leqslant x_{N+2} \leqslant x_{N+3}$, we construct a basis of $N+2$ cubic B-splines $\{B_i;\ i = 0,..., N+1\}$, using the method of Cox and de Boor [12].

The approximate transition amplitude $T_{mt}^{(N)}$ is given by the cubic spline

$$T_{mt}^{(N)}(p(x); E + i0) = \sum_{i=0}^{N+1} a_{mi}(E + i0)\, B_i(x), \tag{4.2}$$

where $\{a_{mi}(E + i0);\ i = 0,..., n+1;\ m = t, s\}$ are complex spline coefficients. These coefficients are obtained from a solution of the linear system of equations

$$\sum_{m=s,t} \sum_{i=0}^{N+1} a_{mi}(E + i0)[(B_i, B_j)\, \delta_{mn} + A_{mi,nj}(E + i0)] = C_{nj}(E + i0), \qquad j = 0,..., N+1, \qquad n = s, t. \tag{4.3}$$

Here, $A_{mi,nj}$ is a moment integral of the kernel Y_{mn} in Eq. (3.3)

$$A_{mi,nj}(E + i0) = 2 \int_{-1}^{1} \int_{-1}^{1} Y_{mn}(p(x), p'(x'); E + i0) \times \frac{B_i(x)\, B_j(x')\, dx\, dx'}{(1-x')^2}, \tag{4.4}$$

and

$$C_{nj}(E + i0) = \int_{-1}^{1} Z_{nt}(p(x), k; E + i0)\, B_j(x)\, dx. \tag{4.5}$$

In practice, the numerical evaluation of the integral in Eq. (4.4) is difficult, because the integrand contains both logarithmic and Cauchy-type singularities. For integration over the logarithmic singularities, we break up the region of integration and use a standard Gauss–Legendre quadrature formula. A method of subtraction [14] is used to integrate over the Cauchy singularities.

An iterative improvement $\bar{T}_{mt}^{(N)}$ to the spline approximation $T_{mt}^{(N)}$ is obtained from the spline expansion coefficients $\{a_{mi};\ i=0,\ldots,N+1;\ m=s,t\}$ by the formula [17]

$$\bar{T}_{mt}^{(N)}(p; E+i0) = Z_{mt}(p, k; E+i0) - \sum_{n} \sum_{i=0}^{N+1} a_{ni}(E+i0)\, D_{m,ni}(p; E+i0), \quad (4.6)$$

where

$$D_{m,ni}(p; E+i0) = 2\int_{-1}^{1} Y_{mn}(p, p'(x'); E+i0)\, \frac{B_i(x')}{(1-x')^2}\, dx'. \quad (4.7)$$

The integral in Eq. (4.7) is one-dimensional and therefore easier to evaluate than the integral of Eq. (4.4).

5. Numerical Results and Discussion

We obtain numerical results for both the three-boson and three-fermion systems described in Section 3 using the numerical procedure described in Section 4. These numerical results are compared with a reference solution obtained by solving the three-body integral equations with a Padé method [5].

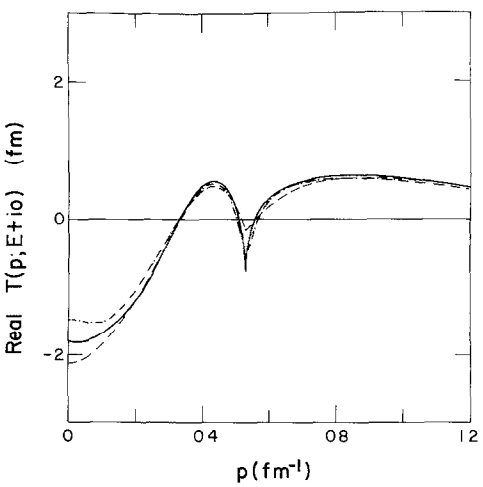

FIG. 1. Real part of the half-shell transition amplitude for a three-boson system. The solid curve is the reference solution, the broken curve is for $N=9$, and the dotted curve is for $N=19$. The knots are uniformly spaced.

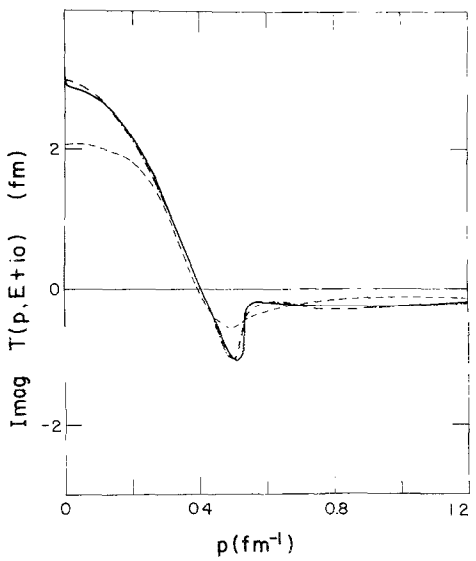

FIG. 2. Imaginary part of the half-shell transition amplitude. Curves as labelled in Fig. 1.

For our numerical example we have chosen parameters for the two-particle potential given by Eq. (3.1) to be $\beta_t = 1.4498\ \text{fm}^{-1}$, $\lambda_t = -8.1978\ \text{fm}^{-3}$, $\beta_s = 1.1648\ \text{fm}^{-1}$ and $\lambda_s = -2.9471\ \text{fm}^{-3}$. These parameters are chosen so that the Yamaguchi potential will approximately describe low energy neutron–proton scattering in the s-wave spin-1 (t) and spin-0 (s) channels.

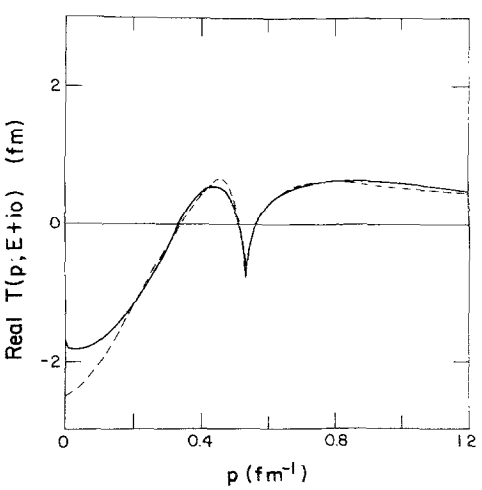

FIG. 3. Real part of the half-shell transition amplitude for a three-boson system. The solid curve is the reference solution. The broken curve is for $N = 9$. The knots are non-uniformly spaced.

Our first results are for the three-boson system. In order to get an impression of the robustness of the algorithm we have tried several different distributions of the knots. In each case three knots are placed in coincidence at the position of the C_1 discontinuity. We are, however, free to choose the position of the interior knots in each of the two sections between the C_1 discontinuity and the end points of the interval $x \in [-1, 1]$.

We first consider uniformly spaced knots. Figures 1 and 2 illustrate the real and imaginary parts of the $L=0$ half-shell transition amplitude at a scattering energy $E=4\varepsilon$. Only a finite interval along the p-variable from 0 to 1.2fm^{-1} is shown. This interval includes the on-shell value of the momentum $k=0.5981$ fm^{-1} and the C_1 discontinuity at $p_c=0.5349$fm^{-1}. The approximate spline solutions with $N=9$ and $N=19$ are indicated by broken and dotted lines respectively. For $N=9$ we have only two interior knots in each section. It is observed that, even with such a small number of uniformly spaced knots, it is possible to determine the structure of the solution to the integral equation. When the number of knots is increased, the solution shows a better agreement with our reference solution.

In the case of functions with singularities it is known that good interpolation cannot be obtained with uniformly spaced knots. On the other hand, as shown in the Appendix, the solution has a square root term, $\sqrt{p-p_c}$, at the C_1 discontinuity. A recommendation [18] for the optimal approximation of a square-root function by cubic splines on the interval [0, 1] is to use the following formula for the knots;

$$t_j = j/(P+1)^8, \qquad j=0,\ldots, P+1, \tag{5.1}$$

where P denotes the number of free knots counting multiplicities.

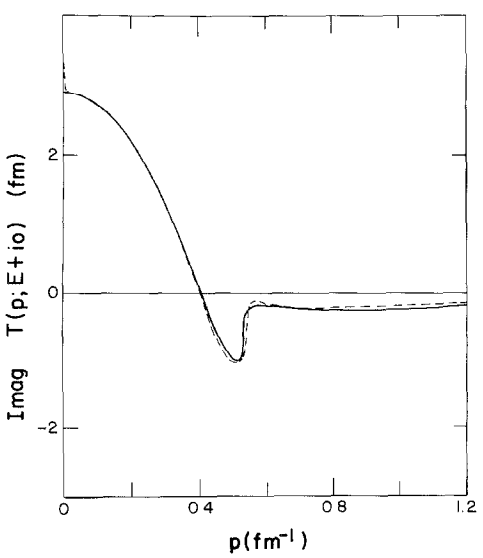

FIG. 4. Imaginary part of the half-shell transition amplitude. Curves as labelled in Fig. 3.

TABLE I

Approximate Solution for a System of Three Identical Bosons

	Uniform		Non-uniform	
N	$\|T_N - T\|_2$	$\|\bar{T}_N - T\|_2$	$\|T_N - T\|_2$	$\|\bar{T}_N - T\|_2$
9	0.865	0.339	0.230(1)	0.185
11	0.500	0.277	0.155(1)	0.994(−1)
13	p.297	0.202	0.938	0.384(−1)
15	0.193	0.150	0.498	0.446(−1)
17	0.152	0.128	0.201	0.333(−1)
19	0.140	0.126	0.299(−1)	0.244(−1)
21	0.137	0.126	0.120	0.186(−1)

Note. The L_2 error norm for several choices of knots with both uniform and non-uniform spacing is shown. The Galerkin solution T_N and iterative improvement $\bar{T}_N$ are compared with a reference solution T.

Figures 3 and 4 illustrate the real and imaginary parts of the half-shell transition amplitude with non-uniformly spaced knots (5.1). The approximate solution with $N=9$ is indicated by the broken line. The result with $N=19$ is indistinguishable from the reference solution on these figures. It is seen that when the simple knots, i.e., those not in multiplicities, are chosen in accordance with the formula in Eq. (5.1), then the C_1 discontinuity is reproduced accurately, even with a small number of knots.

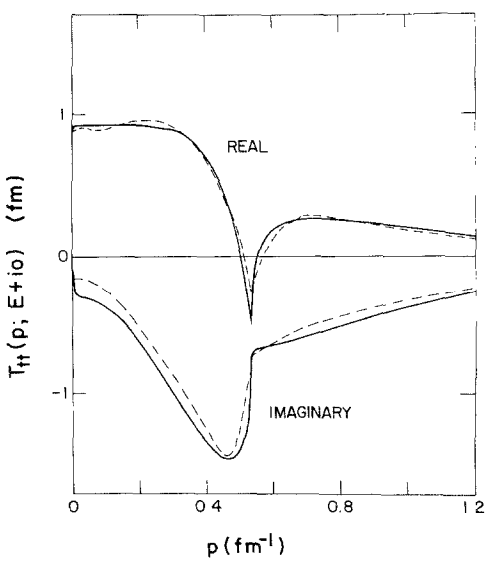

FIG. 5. Half-shell transition amplitude for three spin-$\frac{1}{2}$ particles in a quartet spin configuration. The solid curve is the reference solution. The broken curve is for $N=9$ with non-uniformly spaced knots.

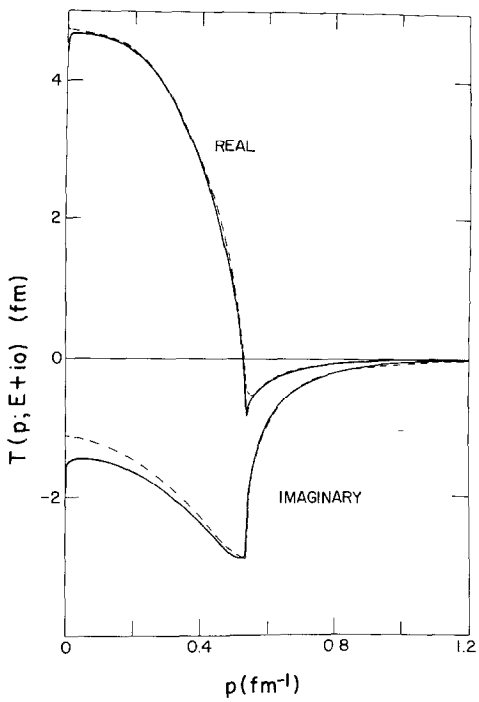

FIG. 6. Half-shell transition amplitude T_{tt} for three spin-$\frac{1}{2}$ particles in a doublet spin configuration. Curves as labelled in Fig. 5.

Table I shows the convergence behaviour of the three-boson transition amplitude using both the uniform and non-uniform meshes. The L_2 norm is used to describe the convergence as the number of knots N is increased. Both the Galerkin solution, T_N, and the iterative improvement, $\bar{T}_N$, given by Eq. (4.6), are compared with our reference solution. For a given number of knots the iterative improvement performs better, and in the case of non-uniform spacing much better, than the Galerkin solution. The greater accuracy of the iterative improvement in the case of non-uniform spacing can be attributed to the fact that this mesh reproduces the C_1 discontinuity more accurately than the uniform mesh.

We next turn our attention to the three-fermion case. Figure 5 illustrates the $L=0$ half-shell transition amplitude for the quartet spin configuration, again at the scattering energy $E=4\varepsilon$. Also shown is the Galerkin solution with $N=9$ on a non-uniform mesh. The solution with $N=11$ is indistinguishable from the reference solution on this figure. The corresponding result for the doublet spin configuration is illustrated in Fig. 6. In the doublet case we solve a set of coupled integral equations for the transition amplitude T_{tt} and T_{st}.

Our numerical results demonstrate that accurate results can be obtained with only a small number of basis functions. Moreover, the algorithm is invariant to the

mesh structure, and it performs well with an arbitrary distribution of simple knots. Given a square-root behaviour in the solution function, we introduce properly spaced knots for the interpolating spline. This is shown to reproduce the non-smooth behaviour accurately. It must be noted that our numerical technique allows for the positioning of simple knots, as well as triple knots, with no special effort. Hence, the generality and versatility of the algorithm makes it worthwhile as an alternative accurate method for solving integral equations that describe three-body scattering above break-up.

APPENDIX: C_1 DISCONTINUITY IN THE HALF-SHELL AMPLITUDE

The three-body half-shell amplitude $T_{mi}(p; E+i0)$ has a C_1 discontinuity at momentum $p_c = \sqrt{\frac{4}{3}E}$. This C_1 discontinuity results from the integration of logarithmic singularities in the effective potential $Z_{mn}(p, p': E+i0)$ defined by Eq. (3.5). In this appendix we describe the origin of the C_1 discontinuity and its singular behaviour.

We first perform the integration in Eq. (3.5). We denote by Z^p the principal value part of this integral and write

$$Z^p_{mn}(p, p'; E) = -\frac{C_m C_n}{(R_m - E)}[S(R_n, R_m) - S(R_n, E)], \tag{A1}$$

where

$$\begin{aligned} R_m &\equiv R_m(p) = \tfrac{3}{4}p^2 - \beta_m^2, \\ R_n &\equiv R_n(p') = \tfrac{3}{4}p'^2 - \beta_n^2. \end{aligned} \tag{A2}$$

Here,

$$\begin{aligned} S(s, t) &= -\frac{1}{2pp'}\frac{1}{s-t}\ln\left|\frac{(A_+ - s)(A_- - t)}{(A_- - s)(A_+ - t)}\right|, \qquad s \neq t \\ &= -\frac{1}{(A_+ - t)(A_- - t)}, \qquad s = t \end{aligned} \tag{A3}$$

and

$$A_\pm \equiv A_\pm(p, p') = p^2 + p'^2 \pm pp', \tag{A4}$$

where $A_\pm > 0$.

At positive energies, $E > 0$, logarithmic singularities are contained in the terms

$$F_+(p, p'; E) = \ln|A_+ - E|, \tag{A5}$$

$$F_-(p, p'; E) = \ln|A_- - E|, \tag{A6}$$

where, for simplicity, we have suppressed a multiplicative factor involving the parameters β_m and β_n. Integration of the logarithmic singularity in Eq. (A5) does not result in any C_1 discontinuity, and we concentrate on the logarithmic term in Eq. (A6). The singularities in Eq. (A6) occur on the real axis of the p'-integration only when $p \leqslant p_c$ and $p' \leqslant p_c$. Thus, to study the origin of the C_1 discontinuity, the integral over p' need be taken only to the upper limit p_c.

We are thus led to examine the integral

$$I(u) = \int_0^1 \ln(u^2 + v^2 - uv - \tfrac{3}{4})\, \Psi(u, v)\, dv, \tag{A7}$$

where we have introduced dimensionless variables $u = p/p_c$ and $v = p'/p_c$ and Ψ is a smooth function of u, v obtained from the remaining factors.

We first consider the special case $\Psi(u, v) = 1$, and write

$$\begin{aligned} I(u) &= \int_0^1 \ln[(v - \tfrac{1}{2}u)^2 - \tfrac{3}{4}(1 - u^2)]\, dv, \qquad u < 1, \\ &= \int_0^1 \ln[v - \tfrac{1}{2}u)^2 + \tfrac{3}{4}(u^2 - 1)]\, dv, \qquad u > 1. \end{aligned} \tag{A8}$$

Then, from standard tables of integrals [19], we obtain the result

$$I(u) = 2\ln(u - \tfrac{1}{2}) - \tfrac{1}{2}u \ln \left| \frac{(u - \frac{1}{2})^2}{u^2 - \frac{3}{4}} \right| - 2 + \bar{I}(u) \tag{A9}$$

where

$$\begin{aligned} \bar{I}(u) &= a \ln \left| \frac{(1 - \frac{1}{2}u + a)(\frac{1}{2}u + a)}{(1 - \frac{1}{2}u - a)(\frac{1}{2}u - a)} \right|, \qquad u < 1 \\ &= 2b \left[\tan^{-1} \left(\frac{1 - \frac{1}{2}u}{b} \right) + \tan^{-1} \left(\frac{\frac{1}{2}u}{b} \right) \right], \qquad u > 1 \end{aligned} \tag{A10}$$

and

$$a = \sqrt{\tfrac{3}{4}(1 - u^2)}, \qquad b = \sqrt{\tfrac{3}{4}(u^2 - 1)}. \tag{A11}$$

Although $I(u)$ is continuous with the value $-2(\ln 2 + 1)$ at $u = 1$, its derivative is discontinuous. It is a simple exercise to show that

$$\frac{dI}{du} \propto \frac{1}{\sqrt{u - 1}}, \qquad \text{for } u > 1. \tag{A12}$$

Hence, we find the result that the derivative of $I(u)$ is infinite at the point $u = 1 + \varepsilon$ as $\varepsilon \to 0$.

More generally, if $\Psi(u, v)$ is a smooth function of v, we expand Ψ in the form

$$\Psi(u, v) = \sum_{n=0}^{\infty} a_n(u)(v - \tfrac{1}{2}u)^{2n} + \sum_{n=0}^{\infty} b_n(u)(v - \tfrac{1}{2}u)^{2n+1}. \tag{A13}$$

The even terms in this expansion, i.e., those under the first summation, lead to an integral in Eq. (A7) (see [19]) with a similar discontinuity in the derivative as was found in the case $\Psi(u, v) = 1$. Thus, in general, the integral in Eq. (A7) has a square root singularity $(p - p_c)^{1/2}$ at $p = p_c$.

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