The Solution of Faddeev Integral Equations
for Three-Body Scattering by Means of B-Splines

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A method for the solution of Fredholm integral equations of the second kind with sigularities both in the kernel and in the solution is developed, based on the approximation of the solution by B-splines. The main problem of this method, the distribution of knots, is extensively investigated. The Faddeev equations describing the physical problem of pion deuteron elastic scattering are solved as an application of this method. © 1990 Academic Press, Inc.

1. INTRODUCTION

The numerical treatment of the integral equations for three-body scattering, the Faddeev [1] or AGS equations [2]—Fredholm integral equations of the second kind—is a complicated affair due to the singularities both in the kernel and in the solution.

Different methods have been developed in the past to solve these equations of which the contour rotation method [3–5] and the Padé-approximant approach [6] are the most widely used today. The contour rotation method consists of solving the integral equation along the line obtained by rotation of the positive real axis into the complex plane. It requires the analytical continuation of the kernel for complex values of its arguments. The solution for real arguments is obtained from the solution for complex arguments in a second step involving an integration. For higher energies the maximum angle of rotation becomes smaller and hence the integration contour comes closer to the real axis where the singularities in the kernel occur. This necessitates the use of more integration points [7]. The analytical continuation of the kernel is not required if the integral equation is solved along the real axis as is done in the Padé-approximant approach. Successive iterations of the integral equation are required to determine the coefficients in this rational approximation of the solution. The calculation of these iterations is time consuming due to the singular integrands involved.

A conceptually much simpler method to solve the integral equations of three-body scattering along the real axis is the spline method we describe here. The usefulness of this method for the solution of singular integral equations was studied by Atkinson [8] for the case of weakly singular kernels, but only for solutions

belonging to the space $C^4[a, b]$. Later on, Schneider [9] and Graham [10] investigated the convergence of this method for the case where the solution has isolated singular points as well. The latter two authors make the remark that non-uniform meshes have better convergence properties than equidistant distributions. Eyre *et al.* [11, 12] applied the spline method to the AGS equations, first employing equidistant knot-distributions only, but later on also using non-uniform meshes. Below we describe the spline method in more detail, but here we want to point out one additional advantage of this approach over the contour rotation method and the Padé-approximant method. Product integration makes use of the expansion of the solution in terms of suitably chosen basis functions. Then the original integral equation is turned into a set of linear equations for the expansion coefficients. (Using splines as a basis, singularities of the solutions of the type x^α can be accurately approximated.) Once these coefficients are known, an approximation of the solution exists for any positive real value of its argument. The extra inter-polation procedure to obtain an approximation of the solution for arbitrary positive real arguments, as is needed in the contour rotation method as well as in the Padé approach, is in the spline method not required. This is of importance in the calculation of breakup amplitudes in the three-body scheme [13].

In the spline method the singularities of the kernel can be treated in a straightforward way using subtraction. The singularity in the solution, however, requires special attention. This is due to the fact that the basic ingredient of the spline method consists of the approximation of the solution by a set of basis func-tions. Obviously the accuracy of such a method for solving integral equations is closely connected to the extent to which the solution can be approximated by these basis functions at all. Therefore the approximation problem should be looked at first, particularly since the solution of the three-body scattering equations has a square root behaviour at a certain point [14, 15]. For that reason the elementary problem of the approximation of a square root function by a finite set of basis functions will be discussed in detail.

Then as a test of the method an integral equation is constructed which has a singularity structure which is the same as that of the three-body scattering equa-tions in all relevant aspects. However, in this example an analytical solution is known and therefore not only the convergence, but also the accuracy, of the numerical solution can be tested. Using the outcome of this example as a guideline, we applied the method to the three-body approach to pion–deuteron scattering and results for the pion–deuteron scattering amplitude will be shown.

The organisation of this paper is as follows. In Section 2 the spline method to solve integral equations is explained in detail. In Section 3 the elementary problem of how to approximate a square root function in an optimal way is investigated. Section 4 is devoted to the solution by the spline method of the aforementioned specially constructed example. The questions of knot distribution and convergence are addressed. The solution by the spline method of the three-body integral equa-tions describing the physical problem of pion-deuteron elastic scattering is discussed in Section 5.

2. The Solution of Fredholm Integral Equations by Means of Splines

The spline method for solving integral equations consists of the following. Consider the integral equation

$$f(x) = g(x) + \int_a^b K(x, y) f(y) \, dy \qquad (2.1)$$

with $f \in C[a, b]$. Choose a finite dimensional subspace $S^n \subset C[a, b]$ and choose a set $\{B_i(x)\}$ of basisfunctions for S^n. Approximate the unknown function f by an element of S^n. The problem of solving the integral equation is then reduced to the determination of the expansion coefficients c_i in such a way that the residual function $r(x)$:

$$r(x) = \sum_i c_i \left[B_i(x) - \int_a^b K(x, y) B_i(y) \, dy \right] - g(x) \qquad (2.2)$$

is minimal in some sense. When it is required that r vanishes in certain points x_j,

$$r(x_j) = 0, \qquad (2.3)$$

this method is called collocation. The points x_j are called collocation points. The coefficients c_i can be found by solving the corresponding set of linear equations:

$$\sum_i M_{ji} c_i = g_j \qquad (2.4)$$

with

$$M_{ji} = B_i(x_j) - \int_a^b K(x_j, y) B_i(y) \, dy, \qquad (2.5a)$$

$$g_j = g(x_j). \qquad (2.5b)$$

The procedure described above is valid for any finite dimensional subspace S^n. Knowledge of the singularity structure of the solution can serve as a guiding principle for the choice of a suitable subspace; when it is known, e.g., that the solution has a discontinuous derivative at some point it is advantageous to use an S^n whose elements also have a discontinuous derivative at that point.

A suitable subspace that is capable to exhibit this feature is the subspace spanned by cubic B-splines. A cubic B-spline ("hill" or "hump" function) is a positive definite function defined by a set of points called knots; between neighbouring knots it is a cubic polynomial and at the knots these polynomials are glued together smoothly. To define n cubic B-splines, $n + 4$ knots are needed; these knots are allowed to coincide. The B-splines lose some smoothness at a point where knots coalesce (a multiple knot). They can be evaluated in a numerically stable manner using the method of Cox [16, 17] and de Boor [18].

To be specific, consider n knots t_i,

$$a = t_1 \leqslant t_2 \leqslant \cdots \leqslant t_n = b, \qquad (2.6)$$

together with the extended knots $t_{-2} \leqslant t_{-1} \leqslant t_0 \leqslant a$ and $b \leqslant t_{n+1} \leqslant t_{n+2} \leqslant t_{n+3}$. These knots determine $n+2$ B-splines B_i, $i = 0, ..., n+1$, where B_i is non-zero only in the interval $[t_{i-2}, t_{i+2}]$ and is a cubic polynomial in each subinterval $[t_{i+j}, t_{i+j+1}]$, $j = -2, ..., +1$. If only simple knots are used, i.e., $t_i < t_{i+1}$, then the B_i have continuous second derivatives over the whole interval $[a, b]$; if a triple knot is used ($t_j = t_{j+1} = t_{j+2}$ for some j) the B_i ($i = j-2, ..., j+4$) are continuous at that knot, but do not have continuous derivatives there. In this way a finite dimensional subspace S^n of $C[a, b]$ can be constructed whose elements have a discontinuous derivative at the triple knots. The above results can be easily generalised for higher order B-splines.

A topic that has to be discussed when collocation is used to solve integral equations together with B-splines as a basis, is that of the distribution of the knots over the interval $[a, b]$. Is there an optimal distribution of knots such that for a fixed number of basis functions the difference between the numerical and the exact solution measured in some norm is minimal? To answer this question the factors that determine this difference should be known. These factors have been investigated in a mathematically thorough study of collocation as a means of solving integral equations by Philips [19]. The main and intuitively obvious factor is the extent to which the solution can be approximated by elements of S^n at all. This implies the somewhat simpler problem: is there an optimal distribution of knots such that for a fixed number of basisfunctions the difference between approximated and exact function measured insome norm is minimal? Note that the solution of the integral equations for three-body scattering is a smooth function apart from the square root singularity. Splines are well suited to approximate smooth functions; therefore the main errors in the approximation of the solution by splines are expected to occur in the region of non-smooth behaviour, i.e., in the neighbourhood of the square root singularity. Furthermore, for the description of elastic scattering the solution is required at a point very near the square root singularity. The basic problem of how to distribute knots to approximate the square root function in the neighbourhood of its singular point in an optimal way should hence be examined first.

3. The Approximation of x^α by Means of Splines

Rice [20] presents rigorous results on the distribution of knots to approximate functions of the form x^α on the interval $[0, 1]$ in an optimal way. Consider a function $f(x)$ defined on $[0, 1]$ with L_p norm:

$$\|f\|_p = \left[\int_0^1 |f(x)|^p \, dx \right]^{1/p}, \qquad 1 \leqslant p < \infty \tag{3.1a}$$

$$\|f\|_\infty = \max_{x \in [0, 1]} |f(x)|. \tag{3.1b}$$

The function f is to be approximated by spline functions $S_\pi^k(x)$ defined by the set π of n knots $\{t_i\}$ with $t_i \leqslant t_{i+1}$. $S_\pi^k(x)$ is a polynomial of degree $k-1$ or less in $[t_i, t_{i+1}]$. The distance in the p norm of f from the set S_π^k of all functions $S_\pi^k(x)$ is defined as

$$\operatorname{dist}_p(f, S_\pi^k) = \inf_{s \in S_\pi^k} \|f - s\|_p. \tag{3.2}$$

Let $f(x) = x^\alpha$, $\alpha > 0$ and consider the following partition π_q of $[0, 1]$:

$$t_j = \left(\frac{j-1}{n-1}\right)^q, \qquad j = 1, ..., n. \tag{3.3}$$

Extend this partition such that each knot is a $(k-1)$-tuple knot. Then, according to Rice [20],

$$\operatorname{dist}_\infty(x^\alpha, S_{\pi_q}^k) = O(n^{-r}), \tag{3.4}$$

with

$$r = \begin{cases} \alpha q & q < k/\alpha \\ k & q \geqslant k/\alpha. \end{cases} \tag{3.5}$$

In particular, the smallest optimal knot distribution exponent to approximate the square root function ($\alpha = \frac{1}{2}$) with cubic splines ($k = 4$) is $q = 8$. These results hold for a large number n of basis functions. More generally, when the distance is measured in the p norm,

$$\operatorname{dist}_p(x^\alpha, S_{\pi_q}^k) = O(n^{-r}), \tag{3.6}$$

with

$$r = \begin{cases} (1 + \alpha p)q & q < (1 + kp)/(1 + \alpha p) \\ k & q \geqslant (1 + kp)/(1 + \alpha p). \end{cases} \tag{3.7}$$

In practice it is important to know for what value of n the above results hold. Therefore we performed calculations to approximate $x^{1/2}$ by means of cubic splines using the following knot distribution:

$$t_j = \left(\frac{j-1}{n-1}\right)^q, \qquad j = 1, ..., n,$$

$$t_{-2} = t_{-1} = t_0 = t_1 = 0; \qquad t_{n+3} = t_{n+2} = t_{n+1} = t_n = 1. \tag{3.8}$$

Simple knots were used in the calculations, except for the endpoints. The triple knots were considered only in connection with the theoretical investigation of the rate of convergence. We used simple knots in the expectation that for them an even

better or at least the same accuracy and rate of convergence would be attained. With the aid of these knots a basis of $S_{\pi_q}^{k=4}$ was constructed consisting of $n+2$ B-splines $\{B_i \mid i=0, ..., n+1\}$. To project an element f from $C[0, 1]$ on $S_{\pi_q}^{k=4}$, $n+2$ collocation points x_j are needed, which were taken as

$$x_0 = t_1, \qquad x_1 = (t_1 + t_2)/2, \qquad x_2 = t_2, ...,$$

$$x_{n-1} = t_{n-1}, \qquad x_n = (t_{n-1} + t_n)/2, \qquad x_{n+1} = t_n. \tag{3.9}$$

A projector $P: C[0, 1] \to S_{\pi_q}^{k=4}$ is defined by

$$Pf = \sum_{i=0}^{n+1} c_i B_i, \tag{3.10}$$

with c_i determined by the solution of the system of linear equations:

$$\sum_{i=0}^{n+1} B_i(x_j) c_i = f(x_j), \qquad j = 0, ..., n+1. \tag{3.11}$$

In this way we approximated $x^{1/2}$ on $[0, 1]$ by means of splines and calculated the differences

$$E_\infty := \max_{x \in [0,1]} \left| x^{1/2} - \sum_i c_i B_i(x) \right| \tag{3.12}$$

and

$$E_1 := \int_0^1 \left| x^{1/2} - \sum_i c_i B_i(x) \right| dx. \tag{3.13}$$

This was done employing 10 Gauss–Legendre integration points over each subinterval $[x_j, x_{j+1}]$ $(j = 0, ..., n)$ obtaining $10(n+1)$ integration points u_k to calculate E_1; for E_∞ we calculated the lower bound

$$\max_{k \in \{1, ..., 10(n+1)\}} \left| u_k^{1/2} - \sum_i c_i B_i(u_k) \right| \tag{3.14}$$

The results for E_1 and E_∞ obtained in this way are shown in Figs. 1 and 2, where the error is plotted as a function of the number of collocation points for different values of the knot distribution exponent q. The theoretical predictions about the rate of convergence as a function of the knot distribution exponent were indeed observed for $n \geqslant 30$, both in the L_∞ and in the L_1 norm. Note that for large values of the number of knots n, the best approximation to $x^{1/2}$ in het L_∞ norm is indeed obtained when the knot distribution exponent is equal to 8. For smaller numbers of basis functions (e.g., between 15 and 30, a typical number used in the solution of the AGS-type [2] integral equations) the error in the L_∞ norm was smallest for
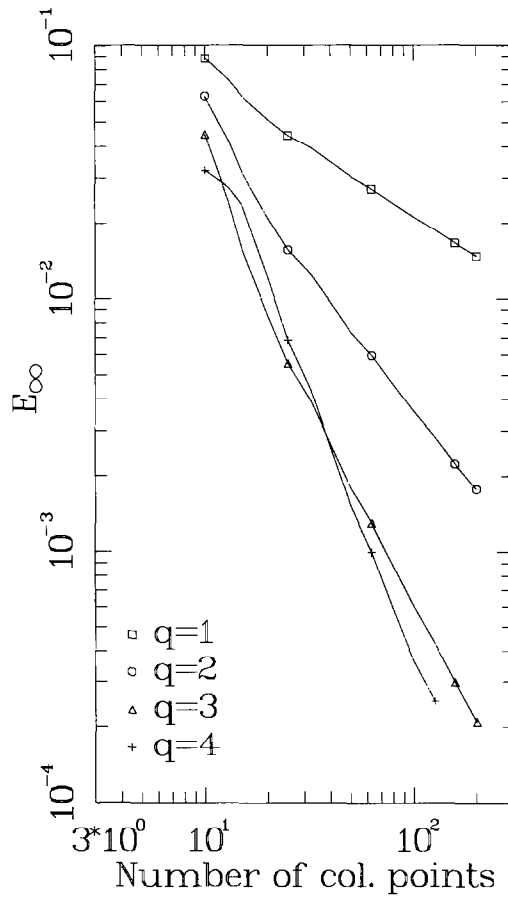
FIG. 1. Difference in L_∞ norm between $\sqrt{x}$ and the spline approximation as a function of the number of collocation points for different values of the distribution exponent q.

a distribution exponent equal to 3 or 4; an exponent equal to 8 was actually the worst of all distributions we tried. This fact has been overlooked so far in the literature [12]. Concerning the error in the L_1 norm, a distribution exponent of 3 is favourable in this range of numbers of collocation points.

We also tried to approximate the square root function by the set spanned by spline functions defined by [21, 22]

$$S_i(t_j) = \delta_{ij}, \tag{3.15}$$

instead of by the set of functions spanned by B-splines. This basis has been used in the literature [21, 23]. Our numerical results with this basis however showed much larger errors due to oscillations.
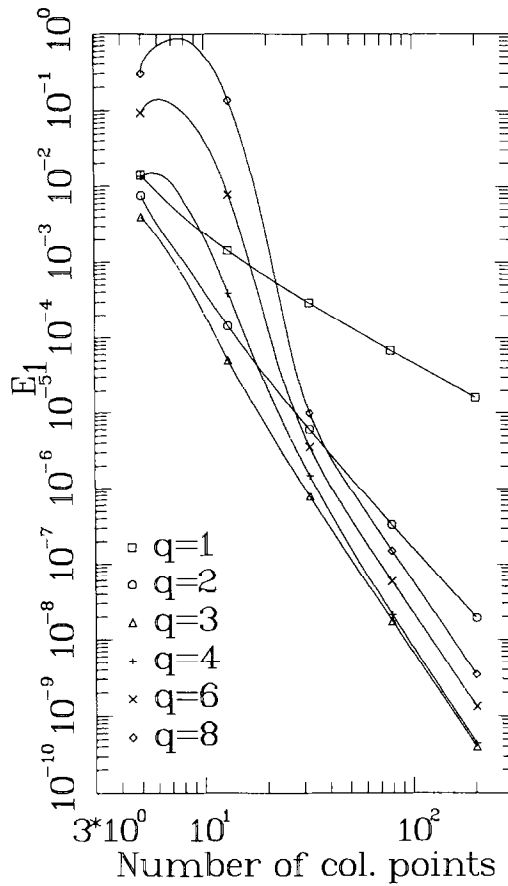
FIG. 2.   Same as Fig. 1, but now the difference is measured in L_1 norm.

From this we conclude that in order to approximate $x^{1/2}$ by a rather limited (<30) number of splines it is advantageous to use a distribution exponent of 3 together with B-splines as a basis.

4. THE ANALYTICALLY SOLVABLE EXAMPLE

To test the accuracy and convergence of the spline method an example was constructed, such that the kernel and the solution have similar singularity structures—as far as they are important to test the spline method—as the AGS-type integral equations. In the latter the kernel $K(x, y)$ is logarithmically singular for points (x, y) on curves $F(x, y) = 0$ which are ellipses in the (x, y) plane (the

so-called Amado ellipses [24]) and the solution $f(x)$ has a square root behaviour at the point where $\partial F(x, y)/\partial y = 0$. In the example

$$f(x) = g(x) + \int_a^b K(x, y) f(y) \, dy, \tag{4.1}$$

the following kernel, solution, and inhomogeneous term have been chosen:

$$K(x, y) = C \ln |x^2 + y^2 - R^2| \tag{4.2a}$$

$$f(x) = \begin{cases} R - x & x \leqslant R \\ R - x + (x - R)^{1/2} & x > R \end{cases} \tag{4.2b}$$

$$g(x) = f(x) - \int_a^b K(x, y) f(y) \, dy \tag{4.2c}$$

$$C = [(2R)^{3/2} \pi]^{-1}. \tag{4.2d}$$

The full expression for the inhomogeneous term is not given here because of its length but it can be obtained from straightforward calculation of the integral involved, using standard tables [25]. The equation was solved on the interval $[-0.75, 2.0]$ with a singularity at $R = 1$. For a plot of the inhomogeneous term see Fig. 3. For different knot-distributions and for different numbers of basis functions the numerical solution was compared with the analytical one and their difference in the L_∞ and L_1 norm was determined in the same way as described in the previous section. The knots were distributed as follows. First, knots were distributed over $[0, 1]$ using a distribution exponent q as

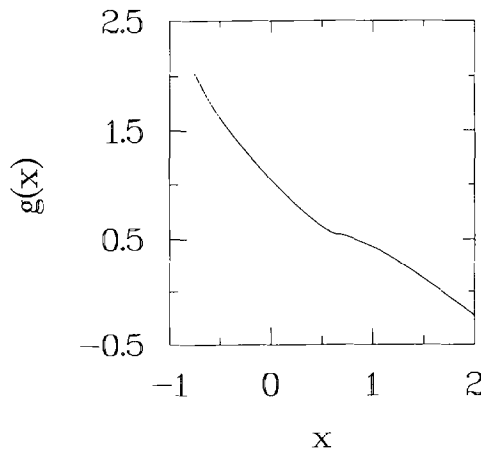$$t_j = \left(\frac{j-1}{n-1}\right)^q, \qquad j = 1, ..., n; \tag{4.3}$$

FIG. 3. The inhomogeneous term $g(x)$. Note that it is a smooth function everywhere, in particular at $x = 1$ where the solution of the integral equation has a square root behaviour.

then these knots were mapped linearly from $[0, 1]$ to $[R, b]$. Again using Eq. (4.3), but now for a fixed exponent $q = 3$ only, knots were generated on $[0, 1]$. Next these were mapped into $[a, R]$ using a linear mapping such that $0 \to R, 1 \to a$. The calculation of

$$\int_a^b K(x_j, y) B_i(y) \, dy = \sum_k \int_{t_k}^{t_{k+1}} K(x_j, y) B_i(y) \, dy \qquad (4.4)$$

was done in the following way. In the case that the kernel was not singular in the interval $[t_k, t_{k+1}]$, six Gauss–Legendre points were used to calculate the integral over this interval; in case the kernel was singular in some point $s \in [t_k, t_{k+1}]$ this interval was divided into subintervals $[t_k, s]$ and $[s, t_{k+1}]$. The kernel was split into a regular part and an irregular part,

$$\ln |x^2 + y^2 - R^2| = \ln |y - s| + \ln |y + s|, \qquad (4.5)$$

where the regular part was integrated using six Gauss–Legendre points and the irregular part was integrated via

$$\int_s^{t_{k+1}} \ln \left| \frac{y - s}{d} \right| f(y) \, dy = d \int_0^1 f(du + s) \ln(u) \, du \approx \sum_l f(du_l + s) \, w_l \qquad (4.6)$$

with $u = (y - s)/d$, $d = t_{k+1} - s$ and using six points $\{u_l\}$ and weights $\{w_l\}$ corresponding to $\ln(u)$ as a weightfunction. Coinciding singularities were handled via $\ln |(y - s)^2| = 2 \ln |y - s|$.

For a larger number of collocation points and for a larger distribution exponent q, some knots can come very close to the singularity R. For an x_j just larger than R, no singularities occur in the integrand in Eq. (4.4) and hence no subtraction is performed. However, the nearby singularity strongly influences the behaviour of the integrand and causes inaccuracies if the integration is carried out numerically. Atkinson [8] has shown how one can remove this difficulty: perform the subtraction also in intervals sufficiently close to, but not containing, the singularity. (We actually followed that procedure in the case of pion–deuteron scattering, Section 5.) The main purpose of the example studied in the present section is not the determination of the integrals in Eq. (4.4), but the study of the accuracy and convergence of the solution as a function of the distribution of the knots. Therefore we did not use the sophisticated subtraction techniques or its refinements [8] for larger numbers of collocation points. Instead we used the fact that the basis functions $B_i(x)$ are cubic polynomials

$$B_i(x) = \sum_{l=0}^3 a_l x^l \qquad (4.7)$$

in each interval $[t_j, t_{j+1}]$. The coefficients a_l are known when the knots are determined. Note that:

$$\int_{t_k}^{t_{k+1}} K(x_j, y) B_i(y) dy = \sum_{l=0}^{3} a_l \int_{t_k}^{t_{k+1}} \ln |x_j^2 + y^2 - R^2| \, y^l \, dy. \tag{4.8}$$

The integrals at the right-hand side can be performed analytically, so the calculation reduces to a summation and function evaluations. We used double precision to determine the coefficients a_l, the integrals in Eq. (4.8), and their sum. This procedure improved the accuracy with which the integrals in Eq. (4.4) could be determined.

The results are shown in Fig. 4. Note that the accuracy of the numerical solution of the integral equation in the L_∞ norm in this example is indeed determined to a
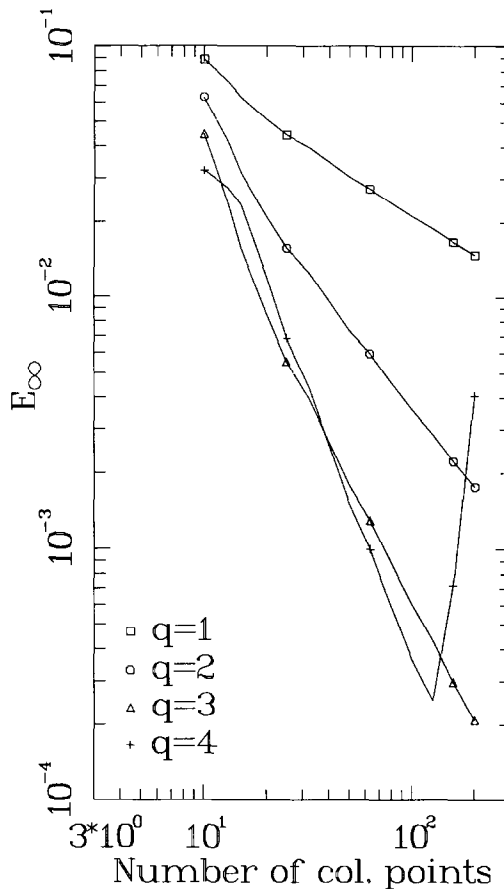

FIG. 4.   The difference in L_∞ norm between the actual solution and the numerical result as a function of the number of collocation points for different values of the distribution exponent q.

large extent by the accuracy of the approximation of the square-root part; the rate of convergence in both cases is about the same. The fact that the accuracy of the solution becomes worse for $q = 4$ and more than 150 collocation points is due to numerical inaccuracies of some of the integrals of Eq. (4.4). This merely illustrates the fact that one should be very careful in applying a large distribution exponent in combination with a large number of collocation points. For a required level of accuracy of the solution and for a limited amount of computational effort, one may either employ more knots, following a power law distribution with a lower exponent, or less knots with a higher distribution exponent. In the latter case it turns out that eventually additional effort is needed to calculate the integrals (4.4) to the accuracy required.

This example was also studied with the other set of basis functions discussed in the previous section. As expected from the results of the approximation problem, also in the solution of this integral equation large oscillations show up. Furthermore, it should be noted that the elements from the set spanned by those basis functions do have a continuous second derivative everywhere, since knots are not allowed to coincide in that case. Such functions are therefore less suited to approximate a function with a discontinuous derivative at some point. This basis should therefore not be used to solve integral equations when the solution is known to have discontinuous derivatives at some points.

5. PION–DEUTERON SCATTERING

We applied the spline method to the physical problem of pion deuteron elastic scattering as described by an AGS-type equation which has been widely used for the πNN system [7, 26–38]

$$X_{\beta\alpha}(q, k) = Z_{\beta\alpha}(q, k) + \sum_{\gamma} \int_0^\infty Z_{\beta\gamma}(q, q')\, G_\gamma(q')\, X_{\gamma\alpha}(q', k)\, q'^2\, dq', \qquad (5.1)$$

where the subscripts α, β, and γ number different coupled channels.

The one-particle exchange driving term is denoted by $Z_{\beta\alpha}$, $X_{\beta\alpha}$ is the transition amplitude, and G_γ is the propagator of the interacting pair. The arguments q and k are the relative momentum between a spectator particle and an interacting pair and the initial pion on-shell momentum, respectively.

Different stages of refinement of this three-body approach to the πNN system have led to different forms of the terms Z and G; here we use expressions and the two-body input from Thomas [38]. It is the standard non-relativistic three-body AGS equation for two identical fermions and one different particle, supplemented by the use of relativistic kinematics for the pion ("RPK"). Since amplitudes are known from the literature in this case [38], both the accuracy of the spline method and the correctness of the computer code can be tested.

As input, the $^3S_1 - {}^3D_1\, NN$ and all S and P πN partial waves are used, with form

factor parametrisations and parameters from Thomas [38] resulting in at most 18 coupled integral equations.

These were solved by the spline method using the following knots. First the knots were distributed homogeneously over $(-1, 0)$ and $(0, 1)$. These knots, together with the points -1 and 0, were redistributed over $[-1, +1]$ by the mapping

$$\xi(x) = \begin{cases} x^d, & 0 \leqslant x \leqslant 1 \\ -|x|^d, & -1 \leqslant x < 0, \end{cases} \tag{5.2}$$

using a distribution exponent d. Call these points ξ_j, $j = 1, ..., 2m$, with $\xi_1 = -1$ and $\xi_{m+1} = 0$. Finally, these knots were mapped onto $[0, \infty)$ by

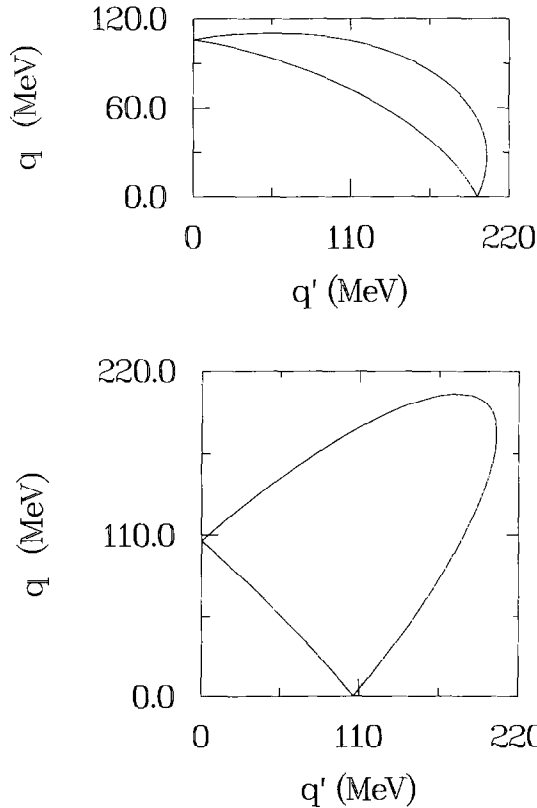$$t(\xi) = c \frac{1 + \xi}{1 - \xi}, \tag{5.3}$$

FIG. 5. The curves in (q, q') plane on which the singularities in the kernel $Z_{\beta\gamma}(q, q')$ are located. The upper picture corresponds to β resp. γ indicating a NN resp. πN pair; the lower picture corresponds to β and γ both indicating a πN pair.

TABLE I

Convergence of the Amplitudes $X_{dd}(k, k)$ as a Function of the Number of Collocation Points N_{COL}

N_{COL}	0^+	1^-	1^+	2^-	2^+
9	$-31.828 + 2.8112\,i$	$-60.756 + 11.689\,i$	$31.362 + 8.8693\,i$	$11.807 + 1.3170\,i$	$175.47 + 32.280\,i$
17	$-31.363 + 2.3270\,i$	$-61.872 + 12.967\,i$	$30.929 + 8.5220\,i$	$11.448 + 1.2529\,i$	$171.19 + 26.445\,i$
25	$-31.310 + 2.3537\,i$	$-61.645 + 12.885\,i$	$30.837 + 8.5142\,i$	$11.473 + 1.2490\,i$	$172.65 + 26.463\,i$
33	$-31.239 + 2.3426\,i$	$-61.525 + 12.806\,i$	$30.852 + 8.5384\,i$	$11.482 + 1.2495\,i$	$174.73 + 27.041\,i$
9	$-31.765 + 2.4205\,i$	$-58.516 + 11.630\,i$	$29.687 + 8.7279\,i$	$11.669 + 1.2760\,i$	$174.71 + 30.345\,i$
17	$-31.522 + 2.3882\,i$	$-61.505 + 13.039\,i$	$31.511 + 8.6896\,i$	$11.699 + 1.2914\,i$	$175.81 + 27.142\,i$
25	$-31.278 + 2.3458\,i$	$-61.656 + 12.838\,i$	$31.003 + 8.5460\,i$	$11.485 + 1.2499\,i$	$173.63 + 26.642\,i$
33	$-31.235 + 2.3390\,i$	$-61.532 + 12.785\,i$	$30.910 + 8.5496\,i$	$11.484 + 1.2493\,i$	$174.72 + 27.003\,i$

Note. Other parameters have the following values: $N_x = 16$, $N_{REG} = 4$, $N_{LEG} = 4$, $N_{LOG} = 4$. For the meaning of these parameters see the text. The upper part of the table corresponds to $d = 2$, the lower part to $d = 3$. Although coupling between different L-values to form a total angular momentum J was taken into account in the calculation of the $J^\pi = 1^-$ and 2^+ amplitudes only the results for the lowest L-values are shown in this and the following tables. The amplitudes are given in units of 10^{-3} fm.

c being the point where the square root singularity occurs. (The point c is known in advance [14, 15].) We call these knots t_j, $j = 1, ..., 2m$, with $t_1 = 0$ and $t_{m+1} = c$. Three extra knots were placed at t_1 and t_{2m} and two extra ones at c, making t_1 and t_{2m} fourfold knots and c a triple knot. As collocation points we used

$$s_1 = 0, \qquad s_2 = (t_1 + t_2)/2, \qquad s_3 = t_2, ...,$$

$$s_{m+1} = t_m, \qquad s_{m+2} = (t_m + t_{m+1})/2, \qquad s_{m+3} = t_{m+1} = c,$$

$$s_{m+4} = (t_{m+1} + t_{m+2})/2, \qquad s_{m+5} = t_{m+2}, ..., \tag{5.4}$$

$$s_{2m+2} = t_{2m-1}, \qquad s_{2m+3} = (t_{2m-1} + t_{2m})/2, \qquad s_{2m+4} = t_{2m}.$$

TABLE II

Convergence of the Amplitudes as a Function of N_x

N_x	0^+	1^-	1^+	2^-	2^+
8	$-31.234 + 2.3388\,i$	$-61.510 + 12.781\,i$	$30.905 + 8.5494\,i$	$11.484 + 1.2493\,i$	$174.71 + 27.003\,i$
12	$-31.235 + 2.3390\,i$	$-61.528 + 12.784\,i$	$30.909 + 8.5496\,i$	$11.484 + 1.2493\,i$	$174.72 + 27.003\,i$
16	$-31.235 + 2.3390\,i$	$-61.532 + 12.785\,i$	$30.910 + 8.5496\,i$	$11.484 + 1.2493\,i$	$174.72 + 27.003\,i$
20	$-31.235 + 2.3390\,i$	$-61.534 + 12.785\,i$	$30.910 + 8.5497\,i$	$11.484 + 1.2493\,i$	$174.72 + 27.004\,i$

Note. Other parameters have the following values: $N_{COL} = 33$, $N_{REG} = 4$, $N_{LEG} = 4$, $N_{LOG} = 4$, $d = 3$.

TABLE III

Convergence of the Amplitudes as a Function of N_{REG}

N_{REG}	0^+	1^-	1^+	2^-	2^+
2	$-31.236 + 2.3388\,i$	$-61.542 + 12.789\,i$	$30.904 + 8.5499\,i$	$11.484 + 1.2495\,i$	$174.73 + 27.010\,i$
4	$-31.235 + 2.3390\,i$	$-61.532 + 12.785\,i$	$30.910 + 8.5496\,i$	$11.484 + 1.2493\,i$	$174.72 + 27.003\,i$
8	$-31.235 + 2.3390\,i$	$-61.532 + 12.785\,i$	$30.910 + 8.5496\,i$	$11.484 + 1.2493\,i$	$174.72 + 27.003\,i$

Note. Other parameters have the following values: $N_{COL} = 33$, $N_x = 16$, $N_{LEG} = 4$, $N_{LOG} = 4$, $d = 3$.

Since the position of the singularity c in the solution $X_{\beta\alpha}(q, k)$ is different for different channels β (an NN or πN pair), two sets of knots were used. In the case of a deuteron final state the on-shell momentum k was used as an additional knot.

Once the B-splines and collocation points are defined, the integrals

$$\int_0^\infty Z_{\beta\gamma}(q_j, q')\, G_\gamma(q')\, B_i(q')\, q'^2\, dq' \tag{5.5}$$

need to be calculated. This was done in the following way. The calculation of the function $Z_{\beta\gamma}(q, q')$ requires the evaluation of an integral; the Cauchy-type singularity which occurs in its integrand for some values of q and q' was handled using subtraction [39, 40]. The integral over the regularised integrand was determined by $N_x = 16$ Gauss–Legendre points. The calculation of the function $G_\gamma(q')$ also requires the evaluation of an integral which was done using 20 Gauss–Legendre points.

In the q' integration two types of singularities occur. Logarithmic singularities occur in $Z_{\beta\gamma}(q, q')$ for certain values of q and q' and a Cauchy-type singularity occurs in $G_\gamma(q')$, if γ denotes a channel containing a deuteron. The latter was handled by subtraction. The logarithmic singularities in $Z_{\beta\gamma}(q, q')$, which are located on a curve in the (q, q') plane (see Fig. 5), were treated by subtraction in a small region around these singularity curves. A function which contains $\ln(|q' - s_i|)$ explicitly and regularises the singularity was subtracted and the

TABLE IV

Convergence of the Amplitudes as a Function of N_{LEG}

N_{LEG}	0^+	1^-	1^+	2^-	2^+
2	$-31.236 + 2.3390\,i$	$-61.542 + 12.780\,i$	$30.909 + 8.5496\,i$	$11.464 + 1.2266\,i$	$174.72 + 27.014\,i$
4	$-31.235 + 2.3390\,i$	$-61.532 + 12.785\,i$	$30.910 + 8.5496\,i$	$11.484 + 1.2493\,i$	$174.72 + 27.003\,i$
8	$-31.235 + 2.3390\,i$	$-61.532 + 12.785\,i$	$30.910 + 8.5497\,i$	$11.484 + 1.2494\,i$	$174.72 + 27.004\,i$

Note. Other parameters have the following values: $N_{COL} = 33$, $N_x = 16$, $N_{REG} = 4$, $N_{LOG} = 4$, $d = 3$.

TABLE V

Convergence of the Amplitudes as a Function of N_{LOG}

N_{LOG}	0^+	1^-	1^+	2^-	2^-
2	$-31.235 + 2.3389\,i$	$-61.532 + 12.785\,i$	$30.910 + 8.5496\,i$	$11.483 + 1.2495\,i$	$174.72 + 27.006\,i$
4	$-31.235 + 2.3390\,i$	$-61.532 + 12.785\,i$	$30.910 + 8.5496\,i$	$11.484 + 1.2493\,i$	$174.72 + 27.003\,i$
8	$-31.235 + 2.3390\,i$	$-61.532 + 12.785\,i$	$30.910 + 8.5496\,i$	$11.484 + 1.2493\,i$	$174.72 + 27.003\,i$

Note. Other parameters have the following values: $N_{COL} = 33$, $N_x = 16$, $N_{REG} = 4$, $N_{LEG} = 4$, $d = 3$.

regularised kernel was integrated over this small region using $N_{LEG} = 4$ Gauss–Legendre points; the added singular function was integrated using $N_{LOG} = 4$ points and weights corresponding with the log function as a weight function. In regions were the integrand is regular, $N_{REG} = 4$ Gauss–Legendre points were used to integrate over each subinterval defined by two adjacent collocation points.

We tested the numerical accuracy of the method by varying the total number of knots (and so the total number of collocation points) and the distribution of the knots around the square root singularity. The numbers of integration points, N_x, N_{REG}, N_{LEG}, and N_{LOG} were also varied to test convergence as a function of these numbers. The results for the amplitudes $X_{dd}(k, k)$, corresponding to a deuteron in the initial and final state, are tabulated in Tables I–V for several values of the total angular momentum J and parity π. The amplitudes are normalised such that $X_{dd}(k, k) = (1/k) \exp(i\delta) \sin \delta (fm)$ and are obtained for a pion laboratory energy of

TABLE VI

Comparison with the Results of Thomas [38]

J^π	This work	Thomas
0^+	$-31.2 + 2.3i$	$-31 + 2i$
1^-	$-61.6 + 12.78i$	$-58 + 12i$
1^+	$30.9 + 8.5i$	$31 + 8i$
2^+	$179.3 + 28.0i$	$179 + 28i$

Note. Our results were obtained with 33 collocation points. In Thomas' work not all possible channels were included and the coupling between amplitudes with different *L*-values was ignored; only in the 2^+ case were the included channels specified. We also used these specified channels in the 2^+ case and turned off the coupling in the 1^- and 2^+ case; in other cases all possible channels were included. The difference in the 1^- amplitude is attributed to the fact that probably in our calculation not the same channels were used as in Thomas' calculation.
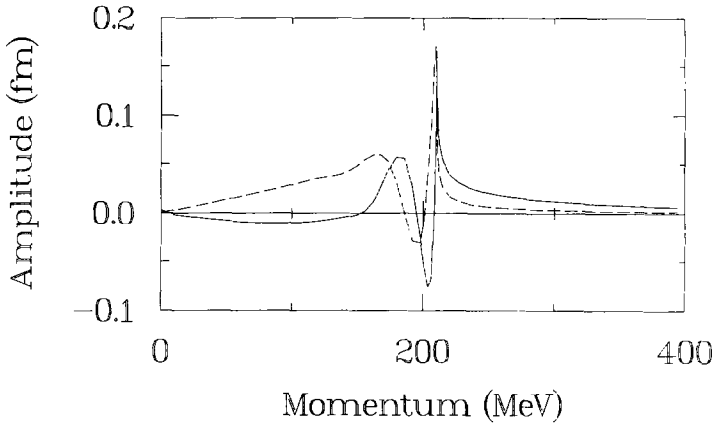
FIG. 6. Amplitude $X_{dd}(q, k)$ for $J^\pi = 0^+$ as a function of pion final momentum for a pion kinetic lab energy of 140 MeV. The solid curve corresponds to the real part of the amplitude, the dashed curve to the imaginary part.

47.7 MeV. A comparison with results from the literature is made in Table VI. Results for the amplitude $X_{dd}(q, k)$ as a function of q for $J^\pi = 0^+$, 1^-, and 2^+ for a pion kinetic lab energy of 140 MeV are shown in Figs. 6–8. These results can be compared in a qualitative sense with the results obtained by Matsuyama [23]. He solved a slightly different set of equations by a similar method but used a different set of splines and did not address the question of the knot distribution.

Some brief remarks about the computer code are appropriate here. The time-consuming parts of the program were written in completely vectorisable form. For the calculation of the 0^+, 1^-, 1^+, 2^-, and 2^+ amplitudes using the following number of collocation and integration points $N_{COL} = 33$, $N_x = 16$, and $N_{REG} = N_{LEG} = N_{LOG} = 4$, 20% of the time was spent to determine the kernel Z and the rest
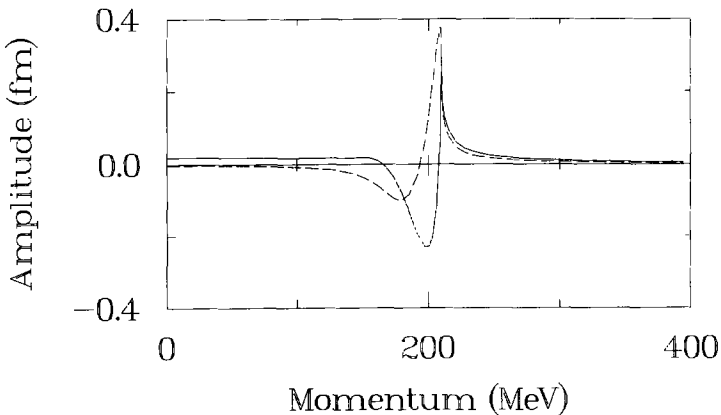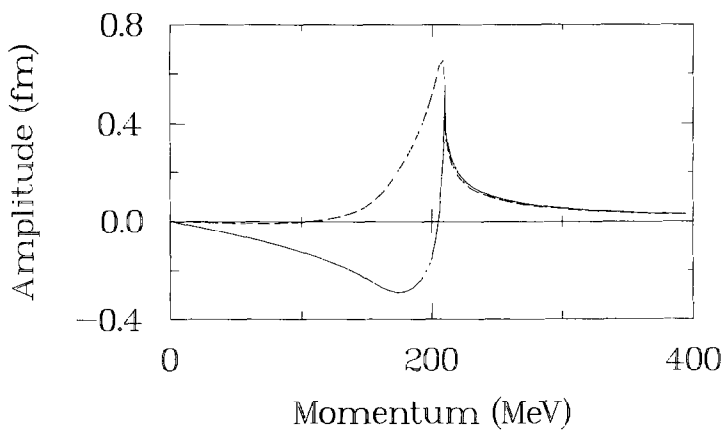

FIG. 7. Same as Fig. 6, now for $J^\pi = 1^-$.

FIG. 8. Same as Fig. 6, now for $J^\pi = 2^+$.

of the time was needed to solve the systems of linear equations. In fact, the number of integration points could have been reduced to $N_{REG} = N_{LOG} = 2$ (see Tables III and V), but since the calculation of Z requires only a small part of the total time it was not necessary to do so.

As is seen from the numerical results, the spline method is a quickly converging method for the solution of the πd three body integral equations along the real axis. The accuracy of the spline method with 33 collocation points is somewhat better than that of the contour rotation method with 32 points, when the convergence of the absolute value of the amplitude is considered [7]. Furthermore, the convergence of the contour rotation method deteriorates with increasing energy [7].

Therefore we conclude that the spline method is an attractive alternative for the solution of the integral equations for three-body scattering.

REFERENCES

1. L. D. FADDEEV, *Sov. Phys. JETP* 12, 1014 (1961).
2. E. O. ALT, P. GRASSBERGER, AND W. SANDHAS, *Nucl. Phys. B* 2, 167 (1967).
3. J. M. HETHERINGTON AND L. H. SCHICK, *Phys. Rev. B* 137, B935 (1965).
4. R. AARON AND R. D. AMADO, *Phys. Rev.* 150, 857 (1966).

5. R. T. Cahill and I. H. Sloan, *Nucl. Phys. A* **165**, 161 (1971).
6. W. M. Kloet and J. A. Tjon, *Ann. Phys. (NY)* **79**, 407 (1973).
7. A. S. Rinat and A. W. Thomas, *Nucl. Phys. A* **282**, 365 (1977).
8. K. Atkinson, *Numer. Math.* **19**, 248 (1972).
9. C. Schneider, *Math. Comput.* **153**, 207 (1981).
10. I. G. Graham, *Math. Comput.* **160**, 519 (1982).
11. M. Brannigan and D. Eyre, *J. Math. Phys.* **24**, 1548 (1983).
12. A. Alaylioglu, D. Eyre, M. Brannigan, and J. P. Svenne, *J. Comput. Phys.* **62**, 383 (1986).
13. I. R. Afnan and A. W. Thomas, in *Modern Three-Hadron Physics*, edited by A. W. Thomas (Springer-Verlag, Berlin, 1977).
14. D. D. Brayshaw, *Phys. Rev.* **176**, 1855 (1968).
15. N. M. Larson and J. H. Hetherington, *Phys. Rev. C* **9**, 699 (1974).
16. M. G. Cox, *J. Inst. Math. Appl.* **10**, 134 (1972).
17. M. G. Cox, *J. Insti. Math. Appl.* **15**, 95 (1975).
18. C. de Boor, *J. Approx. Theory* **6**, 50 (1972).
19. J. L. Phillips, *SIAM J. Numer. Anal.* **9**, 14 (1972).
20. J. R. Rice, in *Symposium on Approximation with Special Emphasis on Spline Functions*, edited by I. G. Schoenberg (Academic Press, New York, 1969), p. 349.
21. W. Glöckle, G. Hasberg, and A. R. Naghabian, *Z. Phys. A* **305**, 217 (1982).
22. J. Stoer and R. Bulirsch, *Introduction to Numerical Analysis* (Springer-Verlag, New York, 1980).
23. A. Matsuyama, *Phys. Lett.* **152**, 42 (1985).
24. E. W. Schmid and H. Ziegelmann, *The Quantum Mechanical Three-Body Problem* (Vieweg, Braunschweig, 1974).
25. I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic Press, New York, 1980).
26. I. R. Afnan and A. W. Thomas, *Phys. Rev. C* **10**, 109 (1974).
27. I. R. Afnan and B. Blankleider, *Phys. Rev. C* **22**, 1638 (1980).
28. M. Araki, Y. Koike, and T. Ueda, *Nucl. Phys. A* **389**, 605 (1982).
29. M. Araki and T. Ueda, *Nucl. Phys. A* **379**, 449 (1982).
30. Y. Avishai and T. Mitzutani, *Nucl. Phys. A* **326**, 352 (1979).
31. Y. Avishai and T. Mitzutani, *Nucl. Phys. A* **338**, 377 (1980).
32. Y. Avishai and T. Mitzutani, *Nucl. Phys. A* **352**, 399 (1981).
33. Y. Avishai and T. Mitzutani, *Phys. Rev. C* **27**, 312 (1983).
34. B. Blankleider and I. R. Afnan, *Phys. Rev. C* **24**, 1572 (1981).
35. H. Garcilazo, *Nucl. Phys. A* **360**, 411 (1981).
36. H. Garcilazo, *Phys. Rev. C* **35**, 1804 (1987).
37. A. S. Rinat, Y. Starkand, and E. Hammel, *Nucl. Phys. A* **364**, 486 (1981).
38. A. W. Thomas, *Nucl. Phys. A* **258**, 417 (1976).
39. L. Pretorius and D. Eyre, *J. Comput. Appl. Math.* **18**, 235 (1987).
40. M. I. Haftel and F. Tabakin, *Nucl. Phys. A* **158**, 1 (1970).