Solving Three-Body Integral Equations with Blending Functions

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This paper investigates a numerical method for solving three-body integral equations. The method is a finite element approach similar to that of Hammerlin *et al.* which utilizes an approximating surface in three-dimensional space, commonly referred to as "Coons' patches" or "blending functions." However, unlike Hammerlin *et al.* who use smoothest splines the present paper uses a basis of C^0 piecewise polynomial functions. Numerical accuracy of the approximation is tested in a single-variable three-boson model at bound energies and scattering threshold. It is shown that the method converges to exact three-body solutions, and that the rate of convergence is much faster than a usual tensor product of C^0 piecewise polynomial functions. The blending function approximation can be used to construct finite-rank separable approximations of the three-body amplitude, which should be of use in four-body calculations. \bigcirc 1987 Academic Press. Inc.

1. INTRODUCTION

System of three or more particles can be described by solving integral equations [1-3]. Although several numerical methods are available for solving such equations [4], these methods are difficult to apply to problems that have more than one continuous variable [5]. A remarkably successful approach has been to reduce the dimension (number of continuous variables) of the multiparticle equation by introducing a finite-rank separable approximation in the subsystem amplitudes [6]. In this way one can reduce the problem of solving a complicated multidimensional integral equations.

Even with the considerable simplification introduced by the separable approximation, it has not been possible to continue calculations further than the four-body problem [7]. Several methods for constructing separable approximations of the three-body amplitude have been investigated [8–12]. Often these methods require a contour rotation technique [13] in order to avoid singularities at positive three-body energies. Nevertheless, separable approximations have proved a

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valuable aid for solving four-body integral equations that desribe both nuclear [14-15] and atomic [16] systems.

Thus far, useful finite-rank approximations of the three-body amplitude are based on the use of global elements. Finite elements, such as splines [17], can, however, be used to solve integral equations [18]. Indeed, the finite element method has been used successfully for the numerical treatment of integral equations that arise in few-body problems [19–24]. It is of interest, therefore, to investigate the utility of separable expansions based on the use of finite elements.

The present method is based on a surface approximation devised by Coons [25-27], sometimes called Coons' patches, and applied in later work to the numerical treatment of integral equations [28-29]. (Throughout this paper we shall adopt the term "blending function" rather than "Coons' patches.") Reference [28] uses smoothest splines as a basis for constructing blending functions. Our approach is based on the use of piecewise Lagrange polynomials. The basis functions in this case are C^0 functions.

The purpose of the present paper is to investigate the utility of the blending function method for solving integral equations that describe quantum few-body systems. The order of convergence is one criterion which determines the utility of the method. Another is the accuracy of the solution for a given mesh spacing. In practice one seeks an accurate solution to the integral equation using a small number of basis functions.

We shall consider a model problem of three identical spin-zero bosons interacting via rank-one separable potentials. Using this model, the three-body Faddeev integral equations reduce to a Lippmann–Schwinger-type integral equation, which we shall refer to as the Amado–Lovelace [30] equation. Our numerical method for solving the Amado–Lovelace equation is first to approximate the effective potential by a blending function. The Amado–Lovelace equation then reduces to algebraic equations, which we solve. The result is a matrix of coefficients for a finite-rank separable approximation of the three-body amplitude.

Our main reason for choosing C^0 basis functions to solve the Amado-Lovelace equation is that the approximating surface can be determined from function values that lie entirely within the domain of the kernel of the integral equations. This is not the case, for example, with the smoothest splines used in Ref. [28]. To construct the approximating surface for smoothest splines of order m > 2 requires additional information such as derivative information on the boundary of the domain, or function values on an extended domain (see Ref. [28]). Since this additional information is difficult to obtain it makes sense to use the C^0 basis functions. It should also be remarked that C^0 functions are simpler than smoothest splines and are therefore easier to work with.

Section 2 describes the blending function. A general procedure is given for solving integral equations of the second kind. Section 3 describes the application of the blending function method to the Amado-Lovelace integral equation. Our numerical results are given in Section 4, and a summary is given in Section 5.

2. PROCEDURE FOR INTEGRAL EQUATIONS

This section describes the blending function and also the kernel approximation method for solving integral equation of the second kind. For simplicity, and to illustrate the method, we consider the homogeneous integral equation

$$\lambda f(s) = -\int_{x}^{\beta} K(s, t) f(t) dt, \qquad (2.1)$$

where the continuous kernel K(s, t) is defined on the square $[\alpha, \beta] \times [\alpha, \beta]$. In general, there are an infinite sequence of numbers $\{\lambda_i\}$ and corresponding eigenfunctions $\{f_i\}$ that solve Eq. (2.1).

To begin, we partition the interval $[\alpha, \beta]$ by n+1 nodal points $\{t_i\}_{i=1}^{n+1}$, where $\alpha = t_1 < t_2 < \cdots < t_{n+1} = \beta$. The only restriction is that the number of subintervals n = (m-1)l, where l is the number of elements. On this partition we define a set of n+1 linearly independent functions $\{\phi_i\}_{i=1}^{n+1}$ satisfying the condition $\phi_i(t_j) = \delta_{ij}$. Each function $\phi_i(s)$ is a piecewise polynomial of order m (degree m-1). We restrict our discussion to a uniform mesh with spacing h. For polynomials of degree m-1 we consider an interval [0, (m-1)h] which contains m nodal points 0, h, ..., (m-1)h. The interval is spanned by m basis functions $\{\phi_i\}_{i=1}^m$. We give as an example the functions for m = 2,

$$\phi_1(s) = 1 - s/h,$$

$$\phi_2(s) = s/h.$$
(2.2)

The functions for m = 3 and 4 are given in Ref. [24]. Basis functions for m = 2, 3, and 4 are illustrated in Fig. 1. Notice that each nodal point has one (and ony one) non-zero basis function. Since the mesh is uniform we can use the *m* functions $\{\phi_i\}_{i=1}^m$ to construct the entire set $\{\phi_i\}_{i=1}^{n+1}$.

We seek a finite dimensional approximation of the bivariate function K(s, t). An operator Q_n will map K onto the usual tensor product space

$$Q_n K(s, t) = \sum_{i=1}^{n+1} \sum_{j=1}^{n+1} \alpha_{ij} \phi_i(s) \phi_j(t), \qquad (2.3)$$

where

$$\alpha_{ii} = K(t_i, t_i). \tag{2.4}$$

An alternative approximation, and one that we shall be concerned with in this paper, is defined by the operator R_n , which maps the kernel K onto a blending function

$$R_n K(s, t) = \sum_{i=1}^{n+1} \phi_i(s) \ K(t_i, t) + \sum_{j=1}^{n+1} K(s, t_j) \ \phi_j(t) - Q_n K(s, t).$$
(2.5)



FIG. 1. Basis functions $\{\phi_i\}_{i=1}^m$ for (a) linear, (b) quadratic, and (c) cubic polynomials.

The blending function (Eq. (2.5)) can achieve a better approximation of the function K(s, t) than the tensor product (Eq. (2.3)). This is because the blending function uses more information from the functions K(s, t) than does the tensor product. While the tensor product interpolates from a set of points (s_i, t_j) , the blending function interpolates from a network of lines in the (s, t)-plane.

For the purpose of solving integral equations it is convenient to rewrite Eq. (2.5) in a more compact form. As in [28] we define extended basis functions

$$\zeta_{i}(s) = \begin{cases} \phi_{i}(s) & i = 1, ..., n + 1, \\ K(s, t_{i-(n+1)}) & i = n + 2, ..., 2n + 2, \end{cases}$$

$$\eta_{j}(s) = \begin{cases} \phi_{j}(s) & j = 1, ..., n + 1, \\ K(t_{j-(n+1)}, s) & j = n + 2, ..., 2n + 2, \end{cases}$$
(2.6)

and introduce a matrix $B = (\beta'_{ij})$, i, j = 1, ..., 2n + 2, defined by

$$B = \left(\frac{-A}{I} + \frac{I}{0}\right). \tag{2.7}$$

Here $A = (\alpha_{ij})$, $I = (\delta_{ij})$, and 0 is the zero matrix, where i, j = 1, ..., n + 1. With this notation Eq. (2.5) becomes

$$R_n K(s, t) = \sum_{i=1}^{2n+2} \sum_{j=1}^{2n+2} \beta'_{ij} \zeta_i(s) \eta_j(t).$$
(2.8)

We remark that if the kernel is symmetric, that is, K(s, t) = K(t, s), then $\zeta_i = \eta_i$.

Next we turn to the integral equation (2.1). The approximation is to replace the kernel K in Eq. (2.1) by the projection $R_n K$ defined by Eq. (2.8). Following the procedure of Ref. [28] we obtain

$$\lambda f(s) = -\sum_{i=1}^{2n+2} \sum_{j=1}^{2n+2} \beta'_{ij} \zeta_i(s) v_j, \qquad (2.9)$$

where

$$v_{j} = \int_{\alpha}^{\beta} \eta_{j}(t) f(t) dt.$$
 (2.10)

Equations (2.9) and (2.10) can be rewritten in the form of an eigenvalue problem, namely

$$\lambda v = M v. \tag{2.11}$$

Here v is the column vector $v = (v_1, v_2, ..., v_{2n+2})^T$ and M is a $(2n+2) \times (2n+2)$ matrix given by

$$M = -PB, \tag{2.12}$$

where $P = (P_{ij})$, i, j = 1, ..., 2n + 2 is the inner product

$$P_{ij} = \int_{\alpha}^{\beta} \eta_i(s) \zeta_j(s) \, ds. \tag{2.13}$$

Let $\{v_i\}_{i=1}^{2n+2}$ be the 2n+2 eigenvalues of the matrix M. Since the eigenvalue problem (2.11) represents a discretization of the integral equation (2.1), the eigenvalues of the matrix M may be regarded as approximations to 2n+2 of the eigenvalues $\{\lambda_i\}$ of Eq. (2.1). The eigenvector $d_i = (d_{i,1}, d_{i,2}, ..., d_{i,2n+2})^T$, corresponding to the eigenvalue v_i , yields the function

$$g_i(s) = \sum_{j=1}^{2n+2} d_{i,j} \eta_j(s), \qquad (2.14)$$

which may be regarded as an approximation to the eigenfunction f_i of Eq. (2.1) corresponding to the eigenvalue v_i .

To evaluate the inner product (2.13) we must integrate the kernel K of Eq. (2.1). These integrals are performed using a standard Gauss-Legendre quadrature formula. Although a quadrature can destroy the order of convergence of the method, it has been pointed out in Ref. [28] that the order of convergence should be maintained if the quadrature rule has at least the same order of convergence as the blending function method. Some of the inner products involve only the basis functions $\{\phi_i\}_{i=1}^{n-1}$. We provide an exact expression for the matrix elements

$$P_{ij} = \int_{\alpha}^{\beta} \phi_i(s) \phi_j(s) \, ds, \qquad (2.15)$$

where i, j = 1, ..., n + 1. These elements are defined by $m \times m$ matrices. For m = 2

$$\frac{h}{6} \begin{bmatrix} 2 & 1\\ 1 & 2 \end{bmatrix}. \tag{2.16}$$

The matrices for m = 3 and 4 are given in Ref. [24]. Further details can be found for example in Strang and Fix [31].

Finally, we can say something about the rate of convergence of the above method. We assume that the kernel has continuous derivatives of order at least 2m. Although the numerical method described above is different from that of Hammerlin *et al.* [28–29] we may expect the blending function approximation to yield roughly the same numerical results. The expected numerical errors in the eigenvalue using the blending function method are $O(h^{2m})$ [28–29]. This contrasts favorably with the tensor approximation, which has a rate of convergence $O(h^m)$ [32].

3. Aplications to the Three-Body System

In this section we use blending functions to construct finite-rank approximations of the three-body amplitude. In order to test the utility of the method for solving integral equations that arise in few-body problems we consider a simple model problem of three identical spin-zero bosons interacting via a separable pairwise potential. It will be assumed that this potential can support a single two-body bound state. We shall restrict our discussion to the angular momentum l=0 case. Also, the energy is restricted to scattering threshold and the three-body bound state region.

We use the variable q to denote the relative two-particle momentum, and use p to denote the relative momentum of one particle with respect to the center-of-mass of the remaining pair. For the case of a rank-one separable two-body potential, and after partial wave decomposition, the Amado-Lovelace integral equation takes the single-channel form

$$X(p, p'; E) = U(p, p'; E) - \frac{2}{\pi} \int_0^\infty U(p, p''; E) X(p'', p'; E) D(p''; E) p''^2 dp'', \quad (3.1)$$

where E is the total three-body energy. The solution X(p, p'; E) of Eq. (3.1) is proportional to the three-body amplitude. Our normalizations are chosen so that the s-wave phase shift, $\delta(k)$, for elastic scattering at incident momentum k is given by

$$X(k, k; E) = -\frac{3}{4}e^{-i\delta(k)}\frac{\sin\delta(k)}{k}.$$
(3.2)

Here the scattering energy is

$$E = \frac{3}{4}k^2 - b, \tag{3.3}$$

and b is the (positive) two-body binding energy.

The scattering length a is defined by

$$a = \frac{4}{3}X(0, 0; -b). \tag{3.4}$$

Three-body bound states lie in the energy region E < -b. These bound states satisfy the homogeneous form of Eq. (3.1). Let $\Phi_r(p)$ be the three-body vertex function. This function satisfies the homogeneous integral equation

$$\Phi_r(p) = -\frac{2}{\pi} \int_0^\infty U(p, p'; -B_r) D(p'; -B_r) \,\Phi_r(p') \,p'^2 dp', \qquad (3.5)$$

where B_r is the (positive) three-body binding energy, and r labels the bound state.

The function U(p, p'; E) is an energy-dependent effective three-body potential defined by the integral

$$U(p, p'; E) = -\int_{-1}^{1} \frac{Q(q_1) Q(q_2) dy}{p^2 + p'^2 + pp' y - E},$$
(3.6)

where

$$q_1 = (\frac{1}{4}p^2 + p'^2 + pp'y)^{1/2}, \qquad (3.7)$$

$$q_2 = (p^2 + \frac{1}{4}p'^2 + pp'y)^{1/2}, \qquad (3.8)$$

and Q(q) is a two-body vertex function.

For our simple model problem we choose a Yamaguchi [33] potential. This simple potential does not adequately describe the nucleon-nucleon interaction [6]. For this purpose more refined finite-rank potentials have been developed [34]. In our case we employ the Yamaguchi potential in order to simplify the three-body equations for the purpose of numerical calculations.

The two-body vertex function is

$$Q(q) = \frac{C}{q^2 + v^2},$$
 (3.8)

where v is a range parameter and

$$C = [2\gamma v(\gamma + v)^3]^{1/2}, \qquad (3.9)$$

where $\gamma = \sqrt{b}$.

The function D(p; E) is

$$D(p; E) = S[(\frac{3}{4}p^2 - E)^{1/2}](\frac{3}{4}p^2 - b - E)^{-1}, \qquad (3.10)$$

where, for the Yamaguchi potential,

$$S(\xi) = \frac{(\xi + v)^2}{\gamma(\gamma + v)[1 + 2v/(v + \xi)]}.$$
(3.11)

Before we apply the blending function, it is convenient first to map the momentum variable p onto a finite interval. We use the mapping

$$p = \left(\frac{1+x}{1-x}\right),\tag{3.12}$$

where $x \in [-1, 1]$. Next, we symmetrize Eq. (3.1). We define

$$\widetilde{X}(x, x'; E) = \omega(p) X(p, p'; E) \omega(p'), \qquad (3.13)$$

$$\widetilde{U}(x, x'; E) = \omega(p) \ U(p, p'; E) \ \omega(p'), \tag{3.14}$$

where

$$\omega(p(x)) = \frac{p(x)}{(1-x)} \left[D(p(x); E) \right]^{1/2}.$$
(3.15)

In this notation Eq. (3.1) becomes

$$\tilde{X}(x, x'; E) = \tilde{U}(x, x'; E) - \frac{4}{\pi} \int_{-1}^{1} \tilde{U}(x, x''; E) \,\tilde{X}(x'', x'; E) \, dx''.$$
(3.16)

To conclude this section we briefly describe the blending function method for solving Eq. (3.16). Following the procedure described in Section 2, we approximate the function \tilde{U} by the blending function $R_n \tilde{U}$ where

$$R_n \tilde{U}(x, x'; E) = \sum_{i=1}^{2n+2} \sum_{j=1}^{2n+2} \beta'_{ij}(E) \zeta_i(x) \eta_j(x').$$
(3.17)

The solution functions \tilde{X} can be approximated by

$$R_n \tilde{X}(x, x'; E) = \sum_{i=1}^{2n+2} \sum_{j=1}^{2n+2} X_{ij}(E) \zeta_i(x) \eta_j(x'), \qquad (3.18)$$

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where the matrix $X = (X_{ii})$ is a solution of the algebraic equations

$$\left[I + \frac{4}{\pi}BP\right]X = B. \tag{3.19}$$

Notice that expression (3.18) is a finite-rank approximation of the three-body amplitude. Three-body bound states are found by solving Eq. (3.16) when the first term on the right-hand side is set to zero. Our method for solving the homogeneous equation exactly follows the procedure described in Section 2.

4. NUMERICAL RESULTS

This section gives our numerical results for the blending function method. Results for an approximation method using tensor product are also shown for the purpose of comparison. All calculations are performed on a CDC Cyber 750 computer in single precision.

In order to check our algorithm for solving integral equations we have solved a simple test problem [18, 28]. This test problem is the homogeneous integral equation (2.1) defined on the interval [0, 1] with

$$K(s, t) = -\sin\left[\frac{\pi}{2}(s+t)\right].$$
(4.1)

The largest eigenvalue for this problem is given by $0.5 + \pi^{-1} = 0.81830989$. The eigenvalue equation (2.11) is solved using IMSL subroutine EIGRF. Tables I-III show the error in the eigenvalue using both tensor product and blending function approximations. Results for this simple test problem are close to those obtained by Hammerlin *et al.* [18, 28] but are not exactly the same because the basis functions are different from those used by Hammerlin.

We calculate the rate of convergence as follows: Suppose e(h) is the error when h is the mesh spacing. Then

$$e(h) \approx ch^{\beta},\tag{4.2}$$

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Errors in the First Eigenvalue for the test Problem Using m = 2

n	3	б	12
Tensor	3.7(-2)	9.3(-3)	2.3(-3)
Blending	4.3(-4)	2.7(-5)	1.7(-6)

n	4	8	16	32
Tensor Blending	-6.6(-5) 1.3(-9)	-2.2(-6) 1.5(-12)	-1.0(-7)	-6.1(-9)

Errors in the First Eigenvalue for the Test Problem Using m = 3

where c is an unknown constant and β is the rate of convergence. By halving the mesh size and taking the ratio of errors, e(h)/e(h/2), we can eliminate c. We obtain

$$\beta \approx \left[\log(2)\right]^{-1} \log\left[\frac{e(h)}{e(h/2)}\right]. \tag{4.3}$$

Table IV shows the calculated rates of convergence β obtained from errors corresponding to the smallest values of h (largest n) shown in Tables I-III, respectively. These values agree with theoretical estimates in the case of linear and cubic polynomials. The quadratics do better than expected from theoretical estimates. In fact, for smoothest splines, the quadratics are known [18, 29] to exhibit superconvergence. However, the anomalously large convergence rate of 9.8 for blending functions is probably due to the fact that the error reaches machine accuracy for n > 8, as indicated in Table II.

Next, we turn to the Amado-Lovelace integral equation and finite-rank separable approximations of the three-body amplitude. The exact solution of this problem is not known. The integral equation can be solved only by approximate numerical methods. For our numerical example we have chosen nuclear scales. We set $h^2/m = 41.468 \text{ MeV} \cdot \text{fm}^2$. The two-body parameters are chosen to be $v = 1.4498 \text{ fm}^{-1}$ and b = 2.225 MeV. With this choice of parameters, the three-boson system has two bound states: a ground state and a first excited state lying close to the scattering threshold.

Tables V-X show the approximate three-body binding energies and scattering lengths. Results using the tensor product approximation (Eqs. (2.2)-(2.3)) are shown in Tables V, VII, and IX. We remark that the difference between these results and those of Ref. [24] is due to the symmetric structure of the integral equation (3.16). In addition, for the scattering length we now approximate the inhomogenous term of the integral equation (3.16). These differences have only a

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Errors in the First Eigenvalue for the Test Problem Using m = 4

n	3	6	12
Tensor	-1.4(-3)	-9.4(-5)	-6.0(-6)
Blending	6.2(-7)	2.7(-9)	1.1(-11)

	Rates of convergence			
т	2	3	4	-
Tensor	2.0	4.0	4.0	
Blending	4.0	9.8	7.9	

TABLE	IV
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Ground State Energy (MeV) Using Tensor Approximation

n			
m	12	24	48
2	24.566787	25.269222	25.451416
3	25.454757	25.509093	25.512526
4	25.551912	25.515364	25.512933

TABLE VI

Ground State Energy (MeV) Using Blending Function Approximation

п			
m	6	12	24
2	25.447224	25.507869	25.512453
3	25.403113	25.512827	25.512750
4	25.269358	25.511528	25.512763

TABLE VII

First Excited State Energy (MeV) Using Tensor Approximation

п			
m	12	24	48
2	2.266521	2.351936	2.371661
3	2.386100	2.378640	2.378364
4	2.381812	2.379723	2.378640

TABLE VIII

	Blending Funct	6 12 24 229549 2.372894 2.378184 322340 2.378298 2.378507	
n -			
т	6	12	24
2	2.229549	2.372894	2.378184
3	2.322340	2.378298	2.378507
4	2.350965	2.378441	2.378507

First Excited State Energy (MeV) Using

small effect on calculated values. Results using the blending function approximation (Eq. (2.8)) are shown in Tables VI, VIII, and X.

For a given number of mesh intervals n the blending function approach leads to twice as many algebraic equations as the method based on tensor product approximation. In order to make a useful comparison between the two methods one should compare results that are obtained by solving roughly the same number of algebraic equations. We may take agreement in results from polynomials of different order m as an indication of the accuracy of the approximation.

Since exact results are not available, we estimate the rates of convergence as follows: Suppose f(h) is the approximate solution when h is the grid size. Then

$$f(h) \approx f + ch^{\beta},\tag{4.4}$$

where f is the unknown value, c is a constant, and β is the rate of convergence. By halving the mesh size twice we can eliminate the constants f and c. We obtain

$$\beta \approx [\log(2)]^{-1} \log \left[\frac{f(h) - f(h/2)}{f(h/2) - f(h/4)} \right].$$
(4.5)

Equation (4.5) gives an indication of the rate of convergence, provided that h is sufficiently small and f(h), f(h/2), and f(h/4) are monotone.

Table XI shows the estimated rates of convergence β for each of the examples

TABLE IX

Scattering Length	(fm)	Using Ten	sor Approximation
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n			
т	12	24	48
2	24.833632	21.377110	20.651261
3	20.501988	20.430349	20.420145
4	20.121943	20.403308	20.418411

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n			
m	6	12	24
2	21.689002	20.491116	20.423928
3	21.694881	20.425429	20.419455
4	22.281788	20.427806	20.419459

TABLE	Х
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Scattering Length (fm) Using Blending Function Approximation

tabulated in Tables V–X. These results are in general agreement with results obtained from our simple test problem (see Table IV). Our results show that the blending function method has a higher rate of convergence than the method based on tensor product approximation.

5. SUMMARY

We have solved the three-body problem using a finite element approach. Blending functions yield accurate numerical solutions and, in addition, may be used to construct finite-rank separable approximations of the three-body amplitude. We have shown in these examples that the rates of convergence for the blending function method are superior to a tensor product of piecewise Lagrange polynomials.

One disadvantage of the blending function method is that a numerical quadrature must be used to evaluate some of the inner products (2.13). For a coarse mesh (n=6) the accuracy of the blending function method is not significantly better than the tensor product of piecewise Lagrange polynomials. On the other hand, for a fine mesh (n=24) the additional cost in CPU time of using blending functions rather than Lagrange functions is offset by the higher accuracy solutions.

We now discuss the application of the present method to few-body problems. In the Faddeev-Yakubovskii approach the four-body problem is described by an integral equation that has a kernel which is constructed by first solving the three-

Estimated Rates of Convergence						
m	v	VI	VII	VIII	IX	X
2	1.95	3.73	2.12	4.76	5.18	4.16
3	3.98	Not monotone	4.76	8.07	2.81	7.73
4	3.91	7.61	0.95	8.70	4.22	7.80

TABLE XI

body problem. The blending function approximation of the three-body amplitude (3.18) is a surface interpolant that can be used to compute the four-body kernel in an accurate and efficient manner. The success of the blending function approximation of the three-body amplitude reported in this paper strongly suggests that the method will be useful in finite element solutions of the four-body integral equation.

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