Configuration-space Faddeev calculations: Supercomputer accuracy on a personal computer

N. W. Schellingerhout* and L. P. Kok
Institute for Theoretical Physics, University of Groningen, P.O. Box 800, 9700 AV Groningen, The Netherlands

G. D. Bosveld
Kernfysisch Versneller Instituut, Groningen, The Netherlands
(Received 24 March 1989)

The bound-state three-body problem is solved using the Faddeev-Noyes equations. The infinite domain of these equations is dealt with using a transformation of the hyperradius instead of the usual cutoff. The Faddeev-Noyes equations are reduced to a matrix equation by spline approximation and orthogonal collocation. This matrix equation is solved using a method that is based on the tensor structure of the matrices and reduces storage requirements by at least two orders of magnitude, thus allowing personal computers to produce results that previously could only be obtained with very large computers. Some of the results obtained with these methods are presented.

I. INTRODUCTION

The quantum-mechanical three-body problem has been an area of active research during the last three decades. Urged by the desire to gain insight in the nucleon-nucleon interaction, many workers have calculated three-nucleon bound states. The scattering problem for neutral particles has also successfully been tackled. Among the most commonly used methods are variational,[1,2] hyperspherical,[3,4] Green's function Monte Carlo,[5,6] and Faddeev calculations.[7–12] Most workers now consider these problems solved and devote their attention to the scattering problem of three charged particles, or the problem of more than three particles.

Indeed, for most applications the accuracy of three-particle bound states that can be calculated by the various numerical methods is better than that of experiment. The research on muon-catalyzed fusion, however, requires the determination of three-particle bound states of (muonic) atoms to a very high accuracy, which currently can only be obtained by variational[13–18] and hyperspherical[19,20] calculations. Although variational calculations are very successful for atomic systems, these methods rely heavily on the amount of work which can be done analytically, limiting the potentials that can be treated to a small set. Also, the accuracy of the wave function remains a problem. In this paper we present a method for solving the three-particle bound-state problem based on the configuration-space Faddeev equations. It can be used on small computers to obtain results with an accuracy that is comparable to that of conventional supercomputer calculations, or on very large computers in order to obtain highly accurate results. We believe that this method makes configuration-space Faddeev calculations competitive with variational calculations.

We will state the three-body problem by the Faddeev-Noyes equations, which are solved using a method similar to that used by Payne and co-workers.[11,21] It reduces the differential equations into a matrix eigenvalue equation which is usually of very large order and therefore difficult to solve on present-day computers. We have derived an alternative representation for the matrices that appear in this equation, based on the tensor structure that is inherent to the solution method mentioned above. Also, we have shown that it is possible to maintain this structure during the process of solving the matrix equation.

In the next section we describe the Faddeev-Noyes equations for the bound-state case.[22] We then describe the solution technique used by us. Although it is largely based on the techniques used by Payne and co-workers, finite-difference techniques can also be used,[9,23] without altering the validity of the remaining sections. In Sec. IV we concentrate on the solution of the resulting matrix problem, and introduce a solution technique that uses the tensor structure of the matrices. In Sec. V we show and discuss some of the results that were obtained with our method. In the Appendix we have included the content of the matrices that occur throughout this paper.

II. FADDEEV-NOYES EQUATIONS

The Faddeev equations in configuration space were first used by Noyes,[22] to study the three-body scattering problem. We derive these equations for three nonidentical particles, after which we review the effect of the (anti)symmetrization condition on the Faddeev-Noyes equations, when two or three particles are identical.

We will follow Noyes and use *mass-weighted* Jacobi coordinates to remove the particle masses from the equations:

$$\mathbf{R}=\frac{m_1\mathbf{r}_1+m_2\mathbf{r}_2+m_3\mathbf{r}_3}{m_1+m_2+m_3}\,,$$
$$\mathbf{x}_1=\frac{1}{\hbar}\left[\frac{2m_2m_3}{m_2+m_3}\right]^{1/2}(\mathbf{r}_2-\mathbf{r}_3)\,, \tag{1}$$
$$\mathbf{y}_1=\frac{1}{\hbar}\left[\frac{2m_1(m_2+m_3)}{m_1+m_2+m_3}\right]^{1/2}\left[\mathbf{r}_1-\frac{m_2\mathbf{r}_2+m_3\mathbf{r}_3}{m_2+m_3}\right].$$

 ©1989 The American Physical Society

The subscripts 1,2,3 can be replaced by cyclic permutations, giving the definitions for $(\mathbf{x}_2,\mathbf{y}_2)$ and $(\mathbf{x}_3,\mathbf{y}_3)$. We write an eigenstate of the operators $\mathbf{x}_i$, $\mathbf{y}_i$, and $\mathbf{R}_{(i)}$ with eigenvalues $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{R}$ as $|\mathbf{xyR}\rangle_i$. These states are related to the eigenstate $|\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\rangle$ of the set of position operators of the three particles by

$$|\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\rangle=\frac{2}{\hbar^2}\left[\frac{m_1m_2m_3}{m_1+m_2+m_3}\right]^{1/2}|\mathbf{x}_i\mathbf{y}_i\mathbf{R}\rangle_i \ . \tag{2}$$

The three-particle Schrödinger equation

$$(H-E)|\Psi\rangle=0 \ , \tag{3}$$

can—after separating out the center-of-mass motion—be expressed as

$$(H_0+\kappa^2+V_1+V_2+V_3)|\Psi\rangle=0 \ , \tag{4}$$

where we use V_i to denote the interaction between particles j and k, and H_0, which can be written (using the Jacobi coordinates) as

$$H_0=-\nabla^2_{\mathbf{x}_i}-\nabla^2_{\mathbf{y}_i} \ . \tag{5}$$

Furthermore, we have written $\kappa^2=-E'$, where E' is the energy of the system in its rest frame.

The Faddeev decomposition[24] consists of replacing Eq. (4) by three coupled equations for the so-called *Faddeev components* $|\psi_i\rangle\equiv G_0V_i|\Psi\rangle$:

$$\begin{aligned}|\psi_1\rangle&=G_1V_1(|\psi_2\rangle+|\psi_3\rangle) \ ,\\ |\psi_2\rangle&=G_2V_2(|\psi_3\rangle+|\psi_1\rangle) \ ,\\ |\psi_3\rangle&=G_3V_3(|\psi_1\rangle+|\psi_2\rangle) \ .\end{aligned} \tag{6}$$

Addition of these three equations gives the Schrödinger equation for the total state $|\Psi\rangle=|\psi_1\rangle+|\psi_2\rangle+|\psi_3\rangle$. In these equations we have used the Green's functions G_i:

$$G_i(z)=(z-H_0-V_i)^{-1}=(\nabla^2_{\mathbf{x}_i}+\nabla^2_{\mathbf{y}_i}-\kappa^2-V_i)^{-1} \ , \tag{7}$$

with $z=-\kappa^2$. Equation (6) can be used for the bound-state problem, and also for the scattering case, by adding a driving term which describes the initial condition.[25] In the bound-state case, the Faddeev equations lead to a unique solution even for systems containing charged particles.[26]

When two of the particles in the system are identical, we must symmetrize (for bosons) or antisymmetrize (for fermions) the wave function with respect to the exchange of these particles. We can label the two identical particles as particles 2 and 3. If we assume that the potentials satisfy the condition $P_{23}V_2P_{23}=V_3$, then we find that the second and third Faddeev equations are equivalent, and that the Faddeev components must satisfy the following symmetry conditions:

$$\begin{aligned}P_{23}|\psi_1\rangle&=p|\psi_1\rangle \ ,\\ P_{23}|\psi_2\rangle&=p|\psi_3\rangle \ ,\end{aligned} \tag{8}$$

where $p=+1$ if particles 2 and 3 are identical bosons, and $p=-1$ if they are identical fermions.

When all three particles are identical, we find that the three Faddeev equations are equivalent. Furthermore, we have $\psi_1=\psi_2=\psi_3=\psi$ and

$$P_{23}|\psi\rangle=p|\psi\rangle \ . \tag{9}$$

As an example we write the explicit form of the symmetry requirements for a system in which particles 2 and 3 are electrons in the singlet state. In that case, we can easily write down the conditions for the spatial part of the Faddeev amplitudes. (The Faddeev amplitudes are defined by $\psi_i(\mathbf{x},\mathbf{y})={}_i\langle\mathbf{xy}|\psi_i\rangle$, where ${}_i\langle\mathbf{xy}|$ is a simultaneous eigenstate of the operators $\mathbf{x}_i$ and $\mathbf{y}_i$.) These conditions are

$$\begin{aligned}\psi_1(-\mathbf{x},\mathbf{y})&=\psi_1(\mathbf{x},\mathbf{y}) \ ,\\ \psi_2(-\mathbf{x},\mathbf{y})&=\psi_3(\mathbf{x},\mathbf{y}) \ .\end{aligned} \tag{10}$$

The antisymmetry of the wave function is entirely contained in the spin function, and the spatial part must therefore be symmetric.

The configuration-space Faddeev-equations can be reduced to coupled partial differential equations by expanding the Faddeev amplitudes onto a bipolar harmonic basis:

$$|\psi_i\rangle=\sum_\alpha(x_iy_i)^{-1}|\phi^i_\alpha\rangle_i|\alpha\rangle_i \ , \tag{11}$$

where we have chosen the decomposition so that

$${}_i\langle\mathbf{xy}|\phi^i_\alpha\rangle_i={}_i\langle\hat{\mathbf{x}}\hat{\mathbf{y}}|\phi^i_\alpha(x,y) \ , \tag{12}$$

$${}_i\langle\mathbf{xy}|\alpha\rangle_i={}_i\langle xy|\alpha(\hat{\mathbf{x}},\hat{\mathbf{y}}) \ , \tag{13}$$

and $\alpha(\hat{\mathbf{x}},\hat{\mathbf{y}})$ is the following *bipolar harmonic*:

$$\begin{aligned}\alpha(\hat{\mathbf{x}},\hat{\mathbf{y}})&=[Y_{l_\alpha}(\hat{\mathbf{x}})\otimes Y_{L_\alpha}(\hat{\mathbf{y}})]_{LM}\\ &=\sum_{m_\alpha}\sum_{M_\alpha}(l_\alpha m_\alpha L_\alpha M_\alpha|LM)Y_{l_\alpha m_\alpha}(\hat{\mathbf{x}})Y_{L_\alpha M_\alpha}(\hat{\mathbf{y}}) \ .\end{aligned} \tag{14}$$

When dealing with particles with (iso)spin, the basis functions are tensor products of the bipolar harmonics and the spin-isospin basis functions. We will not go into this, since the extension is straightforward.[9] The symmetry requirements of Eqs. (8) and (9) can be met by restricting the set of basis functions to functions that satisfy these conditions.

The terms in the expansion (11) are usually called *channels*. (These must not be confused with the four channels of three-particle scattering theory.[25])

The Faddeev equations can be written in configuration space by multiplying each equation from the left with ${}_i\langle\alpha|{}_i\langle x_iy_i|x_iy_iG_i^{-1}$, and inserting unit operators of the form

$$\int\int dx\,dy\sum|xy\rangle_i|\beta\rangle_{i\,i}\langle\beta|_i\langle xy| \ .$$

Using the orthonormality of the channel basis, and explicitly writing the remaining matrix elements we arrive at

$$(\Delta^0_{i,\alpha}-\kappa^2)\phi^i_\alpha(x_i,y_i)-\sum_\beta v^i_{\alpha\beta}(x_i,y_i)\phi^i_\beta(x_i,y_i)=\sum_{\beta,\gamma} v^i_{\alpha\gamma}(x_i,y_i)\sum_{j\,(\neq i)}\int\int d\hat{\mathbf{x}}_i d\hat{\mathbf{y}}_i \frac{x_i y_i}{x_j y_j}\gamma^*(\hat{\mathbf{x}}_i,\hat{\mathbf{y}}_i)\phi^j_\beta(x_j,y_j)\beta(\hat{\mathbf{x}}_j,\hat{\mathbf{y}}_j)\ , \tag{15}$$

with

$$\Delta^0_{i\alpha}=\frac{\partial^2}{\partial x_i^2}+\frac{\partial^2}{\partial y_i^2}-\frac{l_\alpha(l_\alpha+1)}{x_i^2}-\frac{L_\alpha(L_\alpha+1)}{y_i^2}\ , \tag{16}$$

and

$$v^i_{\alpha\beta}(x,y)=\int\int dx'dy'_i\langle xy|_i\langle\alpha|V_i|\beta\rangle_i|x'y'\rangle_i\ . \tag{17}$$

Note that the Faddeev equations can only be written in the form (15) if the matrix elements ${}_i\langle\alpha|V_i|\beta\rangle_i$ are *local*.

It is convenient to use polar coordinates

$$x_i=\rho\cos\theta_i\ ,\qquad y_i=\rho\sin\theta_i\ , \tag{18}$$

and to average over M, so that we can rewrite Eq. (15) into

$$(\Delta^1_{i,\alpha}-\kappa^2)\phi^i_\alpha(\rho,\theta_i)-\sum_\beta v^i_{\alpha\beta}(\rho\cos\theta_i)\phi^i_\beta(\rho,\theta_i)=\sum_{\beta,\gamma} v^i_{\alpha\gamma}(\rho\cos\theta_i)\sum_{j\,(\neq i)}\int_{\Omega_{ji}} d\theta_j\left[\sum_M \frac{\gamma^*(\hat{\mathbf{x}}_i,\hat{\mathbf{y}}_i)\beta(\hat{\mathbf{x}}_j,\hat{\mathbf{y}}_j)}{(2L+1)\sin 2|\mu_{ji}|}\right]\phi^j_\beta(\rho,\theta_j)\ , \tag{19}$$

where $\Delta^1_{i,\alpha}$ is $\Delta^0_{i,\alpha}$ expressed in polar coordinates, Ω_{ji} denotes the interval $[\theta_-,\theta_+]$, where $\theta_-=|\theta_i-|\mu_{ji}||$ and

$$\theta_+=\frac{\pi}{2}-\left|\frac{\pi}{2}-\theta_i-|\mu_{ji}|\right|$$

(cf. Fig. 1), and the numbers $|\mu_{ij}|$ are defined by

$$\cos\mu_{ij}=\left[\frac{m_i m_j}{(m_i+m_k)(m_j+m_k)}\right]^{1/2}\ , \tag{20}$$

where $\{i,j,k\}$ is a permutation of $\{1,2,3\}$.

Equation (19) is an elliptic partial (integro-)differential eigenvalue equation, having unique solutions when boundary conditions are specified on a closed surface.

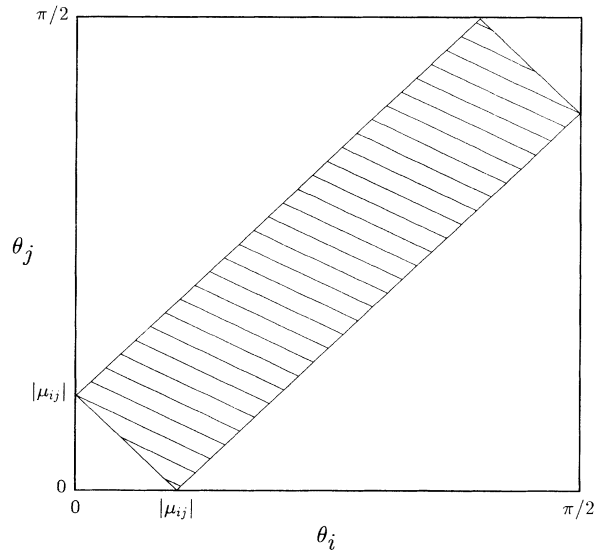

FIG. 1. Domain of integration for matrix elements.

For the bound-state case the boundary conditions are

$$\phi^i_\alpha(\rho,0)=\phi^i_\alpha(\rho,\pi/2)=\phi^i_\alpha(0,\theta)=\phi^i_\alpha(\infty,\theta)=0\ , \tag{21}$$

for all i and α.

In the next section we will describe the numerical solution of Eq. (19) using the spline method.

III. SOLUTION OF THE DIFFERENTIAL EQUATION

The Faddeev-Noyes equations are defined on an infinite interval, which must in some way be reduced to a finite interval to make them suitable for numerical solution techniques. Usually, this is done by factoring out the (known) asymptotic behavior of the Faddeev amplitudes, and demanding that the *reduced* amplitudes F are constant outside a finite interval.[21] This gives $\partial F/\partial\rho=0$ as the approximate boundary condition. We use another approach, which makes sure that the boundary conditions are exact. This method consists of a transformation of the variable ρ to a variable r (not to be confused with the particle coordinates $\mathbf{r}_i$):

$$r=1-e^{-\lambda\rho}\ . \tag{22}$$

This transformation maps the interval $[0,\infty)$ onto $[0,1)$. It is not the only transformation that can be used, but it has proven to work well. The parameter λ can be used to optimize the accuracy of the numerical solution. (Note that when a cutoff method is used, there is also a parameter: the cutoff radius.) It plays an important role in the asymptotic behavior of the transformed amplitudes. As a function of ρ, the asymptotic behavior (for short-range potentials) is

$$\phi^i_\alpha(\rho,\theta_i)\sim A(\theta)\rho^{-1/2}e^{-\kappa\rho}\ , \tag{23}$$

so that transformed wave functions have the following asymptotic behavior:

$$\phi^i_\alpha(r,\theta_i)\sim A(\theta)\ln(1-r)(1-r)^{\kappa/\lambda}\ . \tag{24}$$

Thus the number κ/λ is the exponent of the lowest-order term of the asymptotic behavior (24).

Apart from the absence of approximations on the boundary, the transformation method has the advantage of not destroying self-adjointness of the differential operator. (In the cutoff method, a function depending on κ is factored out.)

Now we expand the channel amplitudes ϕ^i_α on a *bicubic spline basis:*[21,27]

$$\phi^i_\alpha(r,\theta)=\sum_{m=0}^{M+1}\sum_{n=0}^{N+1} a^i_{\alpha mn} s_m(r) s_n(\theta) , \tag{25}$$

where M is the number of intervals in which we subdivide the interval $[0,1)$, and N the number of intervals in which we subdivide the interval $[0,\pi/2]$. The cubic Hermite spline functions s_i are piecewise cubic polynomials, nonzero on two adjoining intervals, and have a continuous first derivative.

An even-numbered spline function equals 1 in the center of its domain, whereas an odd-numbered spline equals 0 and has unit derivative there. The boundary conditions (21) can therefore be met by dropping the first and one-but-last basis function:

$$\phi^i_\alpha(r,\theta)=\sum_{m=1}^{M}\sum_{n=1}^{N} a^i_{\alpha mn} s_m(r) s_n(\theta) , \tag{26}$$

where we have relabeled s_{M+1} to s_M and s_{N+1} to s_N.

A numerical approximation of the solution to the Faddeev-Noyes equations can be obtained by substituting Eq. (26) into (19) and requiring that the differential equation is satisfied in the four two-point Gauss-quadrature points of each interval. This method is known as *orthogonal collocation,* and provides fourth-order convergence.[28,29] Orthogonal collocation reduces the Faddeev-Noyes equations to a matrix equation:

$$(A-\kappa^2 B-C)\mathbf{a}=D\mathbf{a} , \tag{27}$$

where the matrix A contains the differential terms, B the unit term associated with the eigenvalue, C the terms containing the potential on the left-hand side, and D the right-hand side of the Faddeev-Noyes equations. The vector $\mathbf{a}$ contains the expansion coefficients $a^i_{\alpha mn}$. (Note that the matrices carry eight indices: $A_{\alpha_i pq,\beta_j mn}$.) In the Appendix we show the contents of these matrices explicitly.

The solution of Eq. (27) is far from trivial, since the order of the matrices is usually very large. Close examination of the matrices reveals that except for D they are very sparse. Therefore we must look for a solution method that does not require inversion of this matrix. The method introduced by Payne[21] is to substitute an estimate κ_0 for κ and to introduce a parameter Λ:

$$(A-\kappa_0^2 B-C)\mathbf{a}=\Lambda D\mathbf{a} . \tag{28}$$

By regarding this equation as an eigenvalue problem in Λ the original problem can be solved: When 1 is an element of the spectrum, we have substituted a correct value for κ_0. It is important to note that (according to Payne) the eigenvalue we look for ($\Lambda=1$) is the smallest in the spectrum. This means that an iterative method for the "inverted" problem [$A\mathbf{x}=\lambda B\mathbf{x}\rightarrow B\mathbf{x}=(1/\lambda)A\mathbf{x}$] can be expected to converge very rapidly. As a consequence, we can avoid (implicit) inversion of the matrix D. Payne has proposed to use the unsymmetric *Lanczos* algorithm and found it a very powerful method for solving the eigenvalue problem.[21,30]

In the following section we will discuss an alternative method, based on an observation concerning the special structure of the matrices, caused by the numerical solution technique.

IV. AN ALTERNATIVE SOLUTION TECHNIQUE

The solution of matrix problem (27) requires a very large computer, when the number of intervals in the mesh and the number of channels become large. One part of the problem consists of the number of flops that is required to solve the problem. This, however, is usually not prohibitive (although the inversion of the left-hand side can be very expensive for fine grids). The second, and most important part, is the amount of memory required to store the matrices. In practice, it is impossible to store the matrices in central memory, and a very large background memory is required. On small computers, background memory often has low storage capacity and low access speed, making the solution of the matrix problem prohibitively expensive.

It is possible to reduce the amount of storage required, by recognizing that the matrices can be constructed from tensor products. This is an immediate consequence of the solution method that was used: the Faddeev-amplitude ψ_i is expanded on a basis which is decomposed; every basis function can be written as the product of functions depending on only one variable. As an example, we show that the matrix B can be written explicitly as a tensor product. Its elements can be described by

$$B_{\alpha_i pq,\beta_j mn}=\delta_{\alpha\beta}\delta_{ij} s_m(r_p) s_n(\vartheta_q) . \tag{29}$$

Note that we write (r_p,ϑ_q) to denote the value taken by the coordinates (r,θ) in the collocation point which is labeled (p,q). The above expression is equivalent to

$$B=1\otimes 1\otimes S\otimes S , \tag{30}$$

where the first matrix is defined in the space of amplitude numbers, the second in the space of channel numbers, and so on. The matrices S are defined by

$$S_{pm}=s_m(r_p) . \tag{31}$$

Clearly, the tensor representation requires much less storage than a representation where the tensor products are explicitly calculated. Furthermore, the inverse of a tensor product is the tensor product of the inverses of the components, so it is also expected that the number of flops required to solve the matrix equation can be reduced. We now introduce a notation, to make the remainder of this paper more clear. Using this notation, we can write (30) as

$${}^{*}_{*}B^{*}_{*}={}^{*}1\otimes_{*}1\otimes S_{*}\otimes S^{*} , \tag{32}$$

where the presence of an asterisk on a corner of a matrix means that this matrix works in the space associated with that corner. From the top-left corner to the top-right corner we have the amplitude numbers, channel numbers, spline and collocation point numbers in the r direction, and the spline and collocation point numbers in the θ direction.

Unfortunately, it is not possible to decompose all the matrices fully into tensor products, but by transferring the term containing the matrix C to the right-hand side and again introducing a parameter Λ, it is possible to write the resulting equation in the following form:

$$(M_*\otimes^*_*\mathbb{1}\otimes S^*+N_*\otimes^*_*Q^*)\mathbf{a} = \Lambda\,{}^*_*P^*_*(S_*\otimes^*_*\mathbb{1}\otimes S^*+S_*\otimes^*_*J^*)\mathbf{a}\ . \quad (33)$$

This form does not seem to be much of an improvement when compared to the original equation (27), because there is still a matrix P which acts in all four spaces. However, it should be noted that this matrix (containing the matrix elements $v^i_{\alpha\beta}$) is diagonal in three of these spaces. When the potential is central it is also diagonal in the fourth—i.e., the channel-number—space.

The contents of the remaining matrices in Eq. (33) are described below.

- M describes the terms in the differential operator that contain only operators in r space. (This is the only matrix that depends on κ.)
- N describes the r-space part of the remaining terms of the differential operator.
- Q contains the θ-, channel-, and amplitude-space part of these terms.
- J contains the θ-, channel-, and amplitude-space part of the integrals that occur in the right-hand side of the Faddeev-Noyes equations.

It should be noted that Q is diagonal in both the amplitude and the channel space, so that J is the matrix requiring by far the most storage. For the explicit form of the elements of these matrices, see the Appendix.

Note that in the language of operators, Payne and coworkers iterate

$$\psi_1=\Lambda G_1 V_1(\psi_2+\psi_3)\ , \quad (34)$$

whereas we solve

$$\psi_1=\Lambda G_0 V_1(\psi_1+\psi_2+\psi_3)\ . \quad (35)$$

In other words, in our method the entire potential is scaled by Λ, whereas in Eq. (34) only a part of the potential is scaled.

Since the parameter Λ can be regarded as the coupling constant of the potential, the solutions to Eq. (33) represent the set of potential strengths for which there is a bound state at a given energy. This means that when we substitute for $-\kappa^2$ the exact ground-state energy, 1 will be the smallest eigenvalue in the spectrum, unless the set of "inverted" potentials ($V_i\rightarrow -V_i$) supports bound states at even smaller strengths. But even then, 1 is among the smallest elements of the spectrum. It is therefore possible to apply the Lanczos algorithm on

$$M_*\otimes^*_*\mathbb{1}\otimes S^*+N_*\otimes^*_*Q^*)^{-1}\,{}^*_*P^*_*(S_*\otimes^*_*\mathbb{1}\otimes S^*+S_*\otimes^*_*J^*)\mathbf{a}=\frac{1}{\Lambda}\mathbf{a}\ . \quad (36)$$

In general, it will not be necessary to invert $M\otimes\mathbb{1}\otimes S+N\otimes Q$ explicitly since the Lanczos algorithm is soley based on multiplications of basis vectors by the matrix in Eq. (36), but the special structure of this matrix makes it relatively easy to perform the inversion explicitly. We show an example method here, based on the simultaneous diagonalization of matrices in both terms. We write

$$(M_*)^{-1}N_*=C_*\Pi_*(C_*)^{-1}\ , \quad (37)$$

$$({}^*_*\mathbb{1}\otimes S^*)^{-1}\,{}^*_*Q^*={}^*_*D^*\,{}^*_*\Xi^*({}^*_*D^*)^{-1}\ , \quad (38)$$

where Π and Ξ are diagonal. These diagonalizations can be obtained by the QZ algorithm,[31] at relatively low cost—the matrices that must be diagonalized usually have order 100 or smaller. Using Eqs. (37) and (38), we can write

$$(M_*\otimes^*_*\mathbb{1}\otimes S^*+N_*\otimes^*_*Q^*)^{-1}=(C_*\otimes^*_*D^*)({}^*_*\mathbb{1}^*_*+\Pi_*\otimes^*_*\Xi^*)^{-1}(C_*\otimes^*_*D^*)^{-1}(M_*\otimes^*_*\mathbb{1}\otimes S^*)^{-1}\ . \quad (39)$$

This is an expression for the explicit inverse, which can be stored in a relatively small amount of memory.

We solve Eq. (36) by application of the Lanczos algorithm.[30] This algorithm generates a biorthogonal basis set by repeated multiplication of a pair of estimate vectors with the matrix on the left-hand side of (36). This basis is then used to approximate the matrix by an $n\times n$ tridiagonal matrix. In general, the number of iterative steps n that is needed to obtain an accurate approximation is very small.

In the next section we present some of the numerical results that were obtained using the tensor method.

V. SOME RESULTS

In this section we discuss some of the results obtained with a program that solves the Faddeev-Noyes equations by methods described in the preceding sections. All calculations were performed on a VAX 8600 computer, using 64 bit floating point real numbers (VAX double precision).

We find the transformation method to be a very general method of dealing with the infinite interval. The cutoff method fails in some cases, such as for very strongly bound states (factoring out the asymptotic behavior

gives rise to very large variations in magnitude of the reduced wave function). Furthermore, the transformation method has a parameter λ which can be used to scale the interval to obtain optimal results. In the cutoff method it is necessary to use a nonuniform grid in order to obtain a reasonable accuracy. The amount of nonuniformity can be expressed by the ratio between the sizes of neighboring intervals. The optimal value for this ratio, however, is grid-size dependent. We have found that $(S_\rho)^I$ must be approximately a constant to obtain the best results for every number of intervals, where S_ρ is the ratio of the lengths of neighboring intervals in the ρ direction, and I the number of intervals. The grid dependency complicates investigation of the convergence properties of the method. In the transformation method we can afford to keep the grid uniform, because the transformation has an effect similar to the use of a nonuniform grid.

The parameter λ must be chosen so that κ/λ is a number larger than 1, but otherwise there is no strict limitation to this number. Figure 2 is an illustration of this fact. (Here we have used the Malfliet-Tjon-V (MT-V) potential[32] with parameters from Ref. 33: $V_A=570.3316$ MeV fm and $V_R=1438.4812$ MeV fm; for the nucleon mass we used $\hbar^2/M=41.47$ MeV fm^2.) From this figure we see that any value of κ/λ between 1 and 3 will do. The large error that appears when κ/λ is chosen smaller than 1 is probably caused by the singularity at infinity, which must be compensated by a wave function that goes to zero at least as fast as $1-x$ does, for $x\to 1$. For high values of κ/λ the error is caused by the lack of grid points near the origin. (This situation is comparable to that of choosing the grid too uniform when using the cutoff method.) Thus we have a method that is stable, and that requires only one parameter instead of three.

The first results we show are ground-state energies of a three-nucleon system described by the MT-V potential. This potential is defined as an s-wave potential, acting between three identical bosons. It has been used as a test case by many groups, so that the result is rather well established. The variational upper bounds are $-8.22(2)$ (MeV),[34] -8.244,[35] and -8.26.[36] Further results are -8.251, $-8.26(1)$, and -8.251, corresponding to a hyperspherical (a result by Fabre de la Ripelle, quoted in Ref. 37), a Green's function Monte Carlo[38] (GFMC), and a configuration-space Faddeev calculation,[33] respectively. In Table I we show the results of our calculations, using parameters inferred from Ref. 32 ($V_A=578.089$ MeV fm and $V_R=1458.047$ MeV fm), and $\hbar^2/M=41.47$ MeV fm^2. The longest calculation (using five channels and a grid of 31×34 intervals) took the VAX less than an hour of CPU time, and less than six megabytes of storage (including storage for program code, run-time unit, and all other data). These requirements are quite modest, so that a personal computer equipped with a large RAM disk and floating-point coprocessor can obtain similar results in a few hours of CPU time.

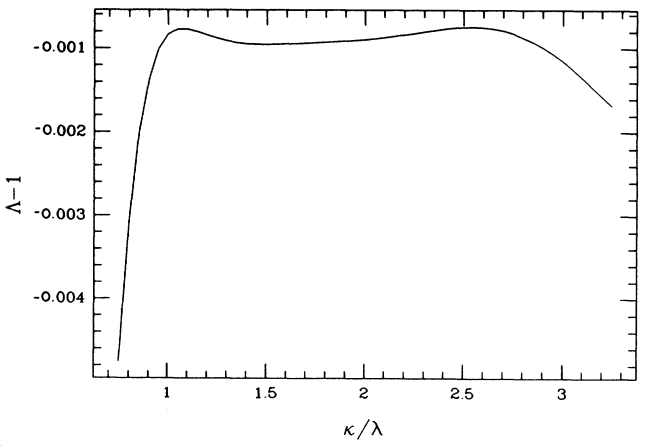

FIG. 2. The number $\Lambda-1$ as a function of κ/λ for the MT-V potential, using $E_0=-7.53976$ MeV, one channel, and a 10×12 grid.

The last column in this table contains extrapolations to infinite grid size, whereas the last row contains an extrapolation to an infinite number of channels (the errors are estimates, and probably smaller than given here). The first of these extrapolations is not just a cosmetic improvement of the accuracy of the calculations, but it is based on the observation that the error in the eigenvalue (and the wave function) behaves as

$$\kappa-\hat{\kappa}=ah^4+bh^6+ch^8+\cdots, \tag{40}$$

where a, b, and c are constants. This means that we can reduce the error by taking a suitable linear combination of the results for different grid sizes h, and thereby canceling the lowest-order terms in the series.

The extrapolation to an infinite number of channels is a more complicated matter. Also it will be more difficult to find an improved wave function than it is to find an improved energy. However, extrapolation does give an indication of the energy that can be expected for an infinite number of channels. Our best result for the binding energy is 8.2526 MeV, which we estimate to be approximately 0.2 keV below the actual value. This result is in excellent agreement with those mentioned above, and an improvement in the accuracy of approximately one order of magnitude. The accuracy reached here gives an indication of the power of the tensor method: in combination with a very large computer, it is possible to obtain results with a very high degree of precision.

We also used our program to calculate binding energies of two-electron atoms and similar systems. Variational methods have been very successful in this area and very accurate results have been obtained, so that we can use these cases to test the correctness and the performance of

TABLE I. Convergence of the partial-wave series and the spline approximation for the MT-V potential, using $\kappa/\lambda=2$.

N_{ch}	15×17	21×24	31×34	∞
1	8.044 53	8.041 50	8.042 22	8.0427±0.0001
2	8.231 14	8.228 44	8.229 18	8.2297±0.0001
3	8.251 25	8.248 60	8.249 33	8.2499±0.0001
4	8.253 63	8.250 98	8.251 72	8.2522±0.0001
5	8.253 99	8.251 35	8.252 09	8.2526±0.0001
∞	8.2542	8.2515	8.2523	8.2528±0.0002

our programs. We show results for the helium atom, and the $e^-e^+e^-$ system in Tables II and III, respectively. The helium atom was modeled using an infinitely massive nucleus. (This calls for special measures concerning the evaluation of the elements in the integral matrix D.) The most accurate calculation (11 channels on a 28×32 grid) is comparable in size to the 34-channel calculations performed by Payne and co-workers,[12] since the matrices for a system containing only two identical particles are four times as large as those for a system containing three identical particles. This calculation required less than 12 hours of CPU time and less than 30 megabytes of storage.

Our results compare well to the Faddeev results of Cravo and Fonseca,[39] who use a Sturmian expansion for the potential. The results for the highest number of terms used by them are 2.905 16 a.u. for the helium atom and 0.263 029 a.u. for the $e^-e^+e^-$ system. This expansion leads to binding energies that converge to a wrong value, whereas the partial-wave series does converge to the correct value (within the estimate error limits). The accuracy is not nearly as high as that of variational calculations performed by Yeremin, Frolov, and Kutukova[15] (which result in $2.903\,724\,377\,05\pm5\times10^{-11}$ a.u. for the helium atom, and $0.262\,005\,070\,232\,5\pm5\times10^{-13}$ a.u. for the $e^-e^+e^-$ system), but our results were obtained on a relatively small computer, and in contrast to variational results, we expect the wave function to be approximately as accurate as the energy eigenvalue. Also, we expect that the accuracy can be greatly enhanced by using extrapolation techniques such as the ones mentioned above on finer grids. Note that extrapolation techniques work best for fine grids, where a large number of terms can be canceled, and the error of the remaining terms is small. The tensor method allows much finer grids to be used than classical methods, making extrapolation very effective.

VI. DISCUSSION AND CONCLUSION

The tensor representation of the matrices that occur in the numerical solution of the Faddeev-Noyes equations reduces the amount of storage required by two or more orders of a magnitude (typically eight times the number of intervals used in the r direction). As we have shown in Sec. V this makes it possible to obtain results of considerable accuracy on small computers.

The tensor method also has the advantage that it is very simple to update the matrix system when one of the parameters changes. For example, we can change the estimate energy κ by changing just one (very small) matrix. Also, the dependence on the potential is confined to just one matrix, the other matrices are more or less universal to the three-body problem.

Another aspect of the method described here is the transformation of the infinite interval to a finite interval. This procedure reduces the error due to inaccuracies in the boundary conditions to zero, and keeps the differential operator self-adjoint. This can be of importance since it enables the use of algorithms for symmetrical matrices when we use a finite-difference method instead of the spline method. This makes the solution to the matrix problem easier to obtain and more accurate. (The spline method, on the other hand, has the advantage of giving quite accurate results on relatively coarse grids, due to the smoothness of the basis functions.) Furthermore, the transformation method is stable and requires only one parameter, whereas the cutoff method has three parameters, of which two are grid-size dependent (the ratio of the sizes of neighboring intervals must be chosen closer to 1 as the number of intervals increases.)

Finally, we transfer all the terms containing the potentials to the right-hand side, and introduce a new parameter which acts as a simultaneous strength parameter of the potentials, instead of introducing a parameter in the right-hand side of the original equations. Our method has the advantage over the method suggested by Payne of keeping the spectrum real (cf. discussion above), giving physically significant data for every calculation, and obtaining more than one state at once (excited states show up in the spectrum as eigenvalues smaller than 1). The method suggested by Payne does not render physically significant data when an incorrect energy eigenvalue is substituted, since in that case $\Lambda\neq1$ and therefore, we have solved a problem that is related to the original problem in a peculiar, nonphysical way.

A disadvantage of ordering the terms so that all the terms containing the potential are on the right-hand side is that the Lanczos algorithm does not converge as fast as it does when using Payne's method, but this is largely compensated for by the fact that the Lanczos steps themselves are somewhat cheaper due to the tensor structure.

The storage requirements have until now restricted

TABLE II. Convergence of the partial-wave series and the spline approximation for the helium atom, using $\kappa/\lambda=3$.

N_{ch}	14×16	20×23	28×32	∞
1	2.937 439	2.937 089	2.937 001	2.936 963±0.000 008
2	2.946 335	2.945 991	2.945 906	2.945 869±0.000 008
3	2.908 036	2.907 769	2.907 700	2.907 671±0.000 002
4	2.908 122	2.907 855	2.907 787	2.907 757±0.000 002
5	2.904 812	2.904 559	2.904 493	2.904 465±0.000 002
7	2.904 266	2.904 018	2.903 953	2.903 924±0.000 002
9	2.904 132	2.903 885	2.903 820	2.903 791±0.000 002
11	2.904 090	2.903 843	2.903 778	2.903 749±0.000 002
∞	2.904 06	2.903 81	2.903 75	2.903 72±0.000 02

TABLE III. Convergence of the partial-wave series and the spline approximation for the $e^-e^+e^-$ system, using $\kappa/\lambda=3$.

N_{ch}	9×10	12×14	17×19	∞
1	0.256 88	0.249 45	0.246 61	0.245 36±0.000 11
2	0.274 58	0.270 28	0.269 11	0.268 60±0.000 05
3	0.263 69	0.260 69	0.259 96	0.259 64±0.000 03
4	0.269 25	0.264 84	0.263 65	0.263 13±0.000 05
5	0.266 01	0.262 76	0.261 96	0.261 60±0.000 04
6	0.267 65	0.263 74	0.262 73	0.262 29±0.000 05
7	0.266 65	0.263 17	0.262 31	0.261 93±0.000 03
∞	0.266 97	0.263 36	0.262 43	0.262 02±0.000 04

configuration-space Faddeev calculations to relatively coarse grids, and it was therefore not possible to obtain high-accuracy results. The tensor representation enables the use of much finer grids, which—in combination with higher-order methods—makes these calculations competitive in problems where high accuracy is needed, such as muon-catalyzed fusion. We are presently engaged in the implementation of our programs on a Cyber 205 vector computer, and investigating the effectiveness of different higher-order methods. Extrapolation techniques seem especially promising.

The programs that we used are written in VAX FORTRAN and can be easily implemented on personal computers. The source code can be obtained from one of the authors (N.W.S.) A full description of the methods used is given in the report of Bosveld and Schellingerhout.[40]

ACKNOWLEDGMENTS

We are indebted to the Werkgroep Gebruik Supercomputers for granting the funds to experiment with configuration-space Faddeev calculations on the Cyber 205 of the University of Amsterdam.

APPENDIX

When we express $\Delta^1_{i,\alpha}$ in r instead of ρ, we find

$$\Delta^2_{i,\alpha}=\lambda^2(1-r)^2\frac{\partial^2}{\partial r^2}-\lambda(1-r)\left[\lambda-\frac{1}{\rho(r)}\right]\frac{\partial}{\partial r}+\frac{1}{\rho^2(r)}\frac{\partial^2}{\partial\theta_i^2}-\frac{l_\alpha(l_\alpha+1)}{\rho^2(r)\cos^2\theta_i}-\frac{L_\alpha(L_\alpha+1)}{\rho^2(r)\sin^2\theta_i}\ , \tag{A1}$$

where $\rho(r)=-\lambda^{-1}\ln(1-r)$.

The Faddeev-Noyes equations (19) expressed in the variables θ_i and r, reduce after collocation in the points $(r,\theta_i)=(r_p,\vartheta_q)$ to the following matrix equation [cf. Eq. (27)]:

$$(A-\kappa^2B-C)\mathbf{a}=D\mathbf{a}\ , \tag{A2}$$

where the matrices A through D are defined as

$$A_{i\alpha pq,j\beta mn}=\delta_{ij}\delta_{\alpha\beta}\left[\lambda^2(1-r_p)^2s_m''(r_p)s_n(\vartheta_q)-\lambda^2(1-r_p)s_m'(r_p)s_n(\vartheta_q)+\frac{\lambda(1-r_p)}{\rho(r_p)}s_m'(r_p)s_n(\vartheta_q)+\frac{1}{\rho^2(r_p)}s_m(r_p)s_n''(\vartheta_q)-\left[\frac{l_\alpha(l_\alpha+1)}{\rho^2(r_p)\cos^2\vartheta_q}+\frac{L_\alpha(L_\alpha+1)}{\rho^2(r_p)\sin^2\vartheta_q}\right]s_m(r_p)s_n(\vartheta_q)\right]\ , \tag{A3}$$

$$B_{i\alpha pq,j\beta mn}=\delta_{ij}\delta_{\alpha\beta}s_m(r_p)s_n(\vartheta_q)\ , \tag{A4}$$

$$C_{i\alpha pq,j\beta mn}=\delta_{ij}v^i_{\alpha\beta}(\rho(r_p)\cos\vartheta_q)s_m(r_p)s_n(\vartheta_q)\ , \tag{A5}$$

$$D_{i\alpha pq,j\beta mn}=\frac{16\pi^2}{2L+1}(1-\delta_{ij})\sum_M\sum_\gamma v^i_{\alpha\gamma}(\rho(r_p)\cos\vartheta_q)s_m(r_p)\times\int_{\Omega_{ij}}\frac{d\theta_j}{\sin2|\mu_{ji}|}\gamma^*(\nu_{ji}(\theta_j,\vartheta_q))s_n(\theta_j)\beta(\nu_{ij}(\vartheta_q,\theta_j))\ . \tag{A6}$$

Here we have used the definition

$$\nu_{ij}(\theta,\theta')=\frac{\cos^2\mu_{ij}\cos^2\theta'+\sin^2\mu_{ij}\sin^2\theta'-\cos^2\theta}{2\cos\mu_{ij}\sin\mu_{ij}\cos\theta'\sin\theta'}\ . \tag{A7}$$

This function has the property $\nu_{ji}(\theta_j,\theta_i)=\hat{\mathbf{x}}_i\cdot\hat{\mathbf{y}}_i$. (The channel basis functions can be chosen to depend only upon this value.)

As mentioned in Sec. IV, the tensor representation of (A2) reads

$$(M_*\otimes^*_*\mathbf{1}\otimes S^*+N_*\otimes^*_*Q^*)\mathbf{a}=\ {}^*_*P^*_*\circ(S_*\otimes^*_*\mathbf{1}\otimes S^*+S_*\otimes^*_*J^*)\mathbf{a}\ . \tag{A8}$$

The matrices used in this equation read

$$M_{pm}=\lambda^2(1-r_p)^2 s_m''(r_p)-\lambda^2(1-r_p)s_m'(r_p)+\frac{\lambda(1-r_p)}{\rho(r_p)}s_m'(r_p)-\kappa^2 s_m(r_p)\ , \tag{A9}$$

$$S^{qn}=s_n(\vartheta_q)\ , \tag{A10}$$

$$N_{pm}=\frac{1}{\rho^2(r_p)}s_m(r_p)\ , \tag{A11}$$

$$\overset{ij}{\alpha\beta}Q^{qn}=\overset{ij}{\alpha\beta}\delta\,\overset{i}{\alpha}O^{qn}\ , \tag{A12}$$

with

$$\overset{i}{\alpha}O^{qn}=s_n''(\vartheta_q)-\left[\frac{l_{\alpha_i}(l_{\alpha_i}+1)}{\cos^2\vartheta_q}+\frac{L_{\alpha_i}(L_{\alpha_i}+1)}{\sin^2\vartheta_q}\right]s_n(\vartheta_q)\ . \tag{A13}$$

For $\overset{*}{*}P\overset{*}{*}$ we have

$$\overset{ik}{\alpha\gamma}P_{pr}^{qs}=\overset{ik}{}\delta_{pr}^{qs}\,\overset{ik}{\alpha\gamma}U_p^q\ , \tag{A14}$$

with

$$\overset{ik}{\alpha\gamma}U_p^q=v_{\alpha_i\gamma_k}(\rho(r_p)\cos\vartheta_q)\ . \tag{A15}$$

Finally, we have for S_* and $\overset{*}{*}J^*$:

$$S_{pm}=s_m(r_p)\ , \tag{A16}$$

$$\overset{kj}{\gamma\beta}J^{sn}=\overset{kj}{}R\,\overset{kj}{\gamma\beta}I^{sn}\ , \tag{A17}$$

with

$$\overset{ij}{}R=1-\delta_{ij}\ , \tag{A18}$$

$$\overset{kj}{\gamma\beta}I^{qn}=\frac{16\pi^2}{2L+1}\sum_M\int_{\Omega_{ji}}d\theta_j\frac{1}{\sin 2|\mu_{ji}|}\gamma^*(\nu_{ji}(\theta_j,\vartheta_q))\times s_n(\theta_j)\beta(\nu_{ij}(\vartheta_q,\theta_j))\ . \tag{A19}$$

*Electronic address: SCHELLIN@HGRRUG5.

[1] L. M. Delves, Adv. Nucl. Phys. **5**, 1 (1972), and sources quoted therein.

[2] J. Carlson, V. R. Pandharipande, and R. B. Wiringa, Nucl. Phys. **A401**, 59 (1983).

[3] J. L. Ballot and M. Fabre de la Ripelle, Ann. Phys. (N.Y.) **127**, 62 (1980).

[4] C. D. Lin and X. H. Liu, Phys. Rev. A **37**, 2749 (1988).

[5] J. G. Zabolitzky and M. H. Kalos, Nucl. Phys. **A356**, 114 (1981).

[6] K. E. Schmidt, in *Models and Methods in Few-Body Physics, Proceedings, Lisboa, Portugal, 1986,* Vol. 273 of *Lecture Notes in Physics,* edited by L. S. Ferreira, A. C. Fonseca, and L. Streit (Springer-Verlag, Berlin, 1987), pp. 363–407.

[7] A. N. Mitra, Nucl. Phys. **32**, 529 (1962).

[8] I. R. Afnan and N. D. Birell, Phys. Rev. C **16**, 823 (1977).

[9] C. Gignoux and A. Laverne, Phys. Rev. Lett. **29**, 436 (1972).

[10] S. P. Merkuriev, C. Gignoux, and A. Laverne, Ann. Phys. (N.Y.) **99**, 30 (1976).

[11] G. L. Payne, J. L. Friar, B. F. Gibson, and I. R. Afnan, Phys. Rev. C **22**, 823 (1980).

[12] C. R. Chen, G. L. Payne, J. L. Friar, and B. F. Gibson, Phys. Rev. C **31**, 2266 (1985).

[13] C. L. Pekeris, Phys. Rev. **112**, 1649 (1958).

[14] K. Frankowsky and C. L. Pekeris, Phys. Rev. **146**, 46 (1966); **150**, 366 (1966).

[15] A. Yeremin, A. M. Frolov, and E. B. Kutukova, Few-Body Systems **4**, 111 (1988).

[16] K. Szalewicz, H. J. Monkhorst, W. Kolos, and A. Scrinzi, Phys. Rev. A **36**, 5494 (1987).

[17] S. E. Haywood, H. J. Monkhorst, and K. Szalewicz, Phys. Rev. A **37**, 3393 (1988).

[18] S. A. Alexander and H. J. Monkhorst, Phys. Rev. A **38**, 26 (1988).

[19] M. I. Haftel and V. B. Mandelzweig, Phys. Lett. A **120**, 232 (1987).

[20] M. I. Haftel and V. B. Mandelzweig, Ann. Phys. (N.Y.) **150**, 48 (1983).

[21] G. L. Payne, in Ref. 6, pp. 64–99.

[22] H. P. Noyes and H. Fiedeldey, in *Three-Particle Scattering in Quantum Mechanics. Proceedings of the Texas A&M Conference,* edited by J. Gillespie and J. Nuttall (Benjamin, New York, 1968), pp. 195–294.

[23] D. M. Young and R. T. Gregory, *A Survey of Numerical Mathematics* (Addison-Wesley, Reading, MA, 1973).

[24] L. D. Faddeev, Zh. Eksp. Teor. Fiz. **39**, 1459 (1961) [Sov. Phys.—JETP **12**, 1014 (1961)].

[25] W. Glöckle, *The Quantum Mechanical Few-Body Problem* (Springer-Verlag, Heidelberg, 1983).

[26] Y. E. Kim and A. Tubis, Annu. Rev. Nucl. Sci. **24**, 69 (1974).

[27] C. de Boor, *A Practical Guide to Splines* (Springer-Verlag, Berlin, 1978).

[28] C. de Boor and B. Swartz, SIAM (Soc. Ind. Appl. Math.) J. Num. Anal. **10**, 582 (1973).

[29] P. M. Prenter, *Splines and Variational Methods* (Wiley, New York, 1975).

[30] Y. Saad, SIAM (Soc. Ind. Appl. Math.) J. Num. Anal. **19**, 485 (1982).

[31] G. H. Golub and C. F. Van Loan, *Matrix Computations* (Johns Hopkins University Press, Baltimore, 1983).

[32] R. A. Malfliet and J. A. Tjon, Nucl. Phys. **A127**, 161 (1969).

[33] J. L. Friar, B. F. Gibson, and G. L. Payne, Phys. Rev. C **24**, 2279 (1981).

[34] J. Carlson and V. R. Pandharipande, Nucl. Phys. **A371**, 301 (1981).

[35] C. Ciofi degli Atti and S. Simula, Nuovo Cimento Lett. **41**, 101 (1984).

[36] Y. Akaishi, in Ref. 6, pp. 324–362.

[37] J. L. Friar, in *Few-Body Problems in Particle, Atomic, Nuclear, and Molecular Physics,* Proceedings of the XIth European Conference on Few-Body Physics, Fontevraud, 1987, edited by J.-L. Ballot and M. Fabre de la Ripelle (Springer-Verlag, Wien, 1987), pp. 51–63.

[38] J. G. Zabolitzky, K. E. Schmidt, and M. H. Kalos, Phys. Rev. C **25**, 1111 (1982).

[39] E. Cravo and A. C. Fonseca, Few-Body Systems **5**, 117 (1988).

[40] G. D. Bosveld and N. W. Schellingerhout, Institute for Theoretical Physics, University of Groningen, Groningen, The Netherlands, Report No. 231, 1989 (unpublished).