Solution of three-body Coulomb problems for $J=0$

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The Schrödinger equation for the S state of the three-body system with arbitrary charge and mass has been solved directly using finite-element analysis. In this analysis, the wave function is approximated piecewise using polynomial interpolation functions. The energy and wave function converge to their exact values as the number of elements is increased. In contrast to standard variational calculations, the error in the expectation value of physical observables is comparable to the error in the energy. Results are reported here for the helium atom and the muonic molecular ion $dd\mu^+$.

I. INTRODUCTION

The standard approach to solving few-body problems in atomic and molecular physics is the variational method. Trial wave functions are constructed from parametrized Hylleraas- and Slater-type functions and the energy is minimized. This method is undeniably the most efficient means for obtaining highly accurate energies.

However, the variational method does not solve the Schrödinger equation; it minimizes the energy. Thus, while the variational wave function is optimized in the region of the continuum where the contribution to the Hamiltonian is large, there is no reason to expect this wave function to be equally well determined in other regions of space. Indeed, if the error in the energy is one part in 10^6, the average error in the wave function is one part in 10^3 in the region where the probability density is large; the wave function may exhibit much larger localized error elsewhere. Consequently, if one uses a variational wave function to calculate the expectation value of an operator, the accuracy of the result can be much less than that for the energy, particularly if the integral receives a large contribution from a region of space where the probability density is low. For example, variational values for the δ function of the interparticle distance are notoriously poor unless the correct cusp behavior is explicitly built into the trial wave function.

Unlike the variational approach, the finite-element (FE) method offers a direct means for solving the Schrödinger equation for few-body problems. By approximating the wave function piecewise via locally defined interpolation functions, it is possible to obtain a wave function that is accurate over the entire continuum. Hence the FE wave functions are well suited for calculating physical observables and other matrix elements. Note that the success of this method does not rely on the nature of the potential and that additional interactions can be incorporated directly into Hamiltonian.

In this paper we report results in which the FE method is used to solve the Schrödinger equation for three-body Coulomb systems. The FE wave functions are found to be uniformly accurate over the continuum, as evidenced by the fact that the error in non-Hamiltonian expectation values is equal to the error in the energy.

In the next section, we provide a brief summary of the finite-element method; more complete details are given in Refs. 1 and 2. In Sec. III, we compare FE results for the helium atom and the muonic molecular ion $dd\mu^+$ with those obtained using the variational method[4–6] and the correlation function hyperspherical harmonic (CFHH) method.[7,8]

II. FINITE-ELEMENT SOLUTION FOR THE THREE-BODY SYSTEM

The Schrödinger wave function for a three-body system with total angular momentum J and z component m may be written as[3]

$$\Psi^J_m=\sum_{s=1}^{2J+1}[D^J(R)]^*_{ms}\chi^J_s(\rho,\xi,\cos\varphi)\ , \tag{1}$$

where $[D^J(R)]^*_{ms}$ are the coefficients of the irreducible representation of the three-dimensional rotation group and χ^J_s are functions of the three coordinates ρ, ξ, and $\cos\varphi$ which specify the relative configuration of the three masses. ξ is the distance between particles 2 and 3, ρ is the distance between particle 1 and the center of mass of particles 2 and 3, and $\cos\varphi=\hat{\rho}\cdot\hat{\xi}$.

The functions $\chi^J_s(\rho,\xi\cos\varphi)$ can be obtained by solving a set of $2J+1$ coupled equations. For the special case $J=0$, we have (dropping the indices on χ)

$$\int\int\int\left[\frac{1}{\mu}\frac{\partial\chi}{\partial\rho}\frac{\partial\chi}{\partial\rho}+\frac{1}{M}\frac{\partial\chi}{\partial\xi}\frac{\partial\chi}{\partial\xi}+\left[\frac{1}{\mu\rho^2}+\frac{1}{M\xi^2}\right](1-\cos^2\varphi)\frac{\partial\chi}{\partial\cos\varphi}\frac{\partial\chi}{\partial\cos\varphi}+2\chi(V-E)\chi\right]\rho^2d\rho\,\xi^2d\xi\,d\cos\varphi \tag{2}$$

where M and μ are given by

$$M=\frac{m_2m_3}{m_2+m_3}\ , \tag{3a}$$

$$\mu=\frac{m_1(m_2+m_3)}{m_1+m_2+m_3}\ . \tag{3b}$$

Atomic units are used throughout, with $e=\hbar=m_1=1$,

and $m_1 \leq m_2 \leq m_3$.

In order to solve Eq. (2) using the FE method, the three-dimensional space spanned by ρ, ξ, and $\cos\varphi$ is truncated and discretized into small regions called elements. The cutoff values ρ_c and ξ_c are chosen large enough that the wave function is essentially zero for $\rho \geq \rho_c$ or $\xi \geq \xi_c$. For the special case $m_2 = m_3$, the wave function is symmetric or antisymmetric about the plane $\varphi = 0$ and the equation can be solved on the domain $\cos\varphi \in [0,1]$ with the appropriate boundary condition.

In each element N, we approximate the solution to Eq. (2) with a locally defined basis which is a product of fourth degree Lagrange polynomials in the ρ, ξ, and $\cos\varphi$,

$$\chi^N(\rho,\xi,\cos\varphi) = \sum_{i,j,k=1}^{5} \chi^N_{ijk}\phi_i(\rho)\phi_j(\xi)\phi_k(\cos\varphi) \ . \tag{4}$$

The Lagrange polynomials have the unique property that the expansion coefficients χ^N_{ijk} are the value of the wave function at 125 nodes in the element. The nodes are arranged symmetrically in a $5\times5\times5$ array.

Substituting Eq. (4) into Eq. (2) we obtain a generalized eigenvalue problem for element N,

TABLE I. Finite-element parameters for helium. The number of elements is 196. The order of FE matrices is 12 448.

ρ	0.0	0.25	0.5	1.0	2.0	4.0	6.0	8.0
ξ	0.0	0.25	0.5	1.0	2.0	4.0	6.0	8.0
$\cos\varphi$		−1.0	−0.5	0.0	0.5	1.0		

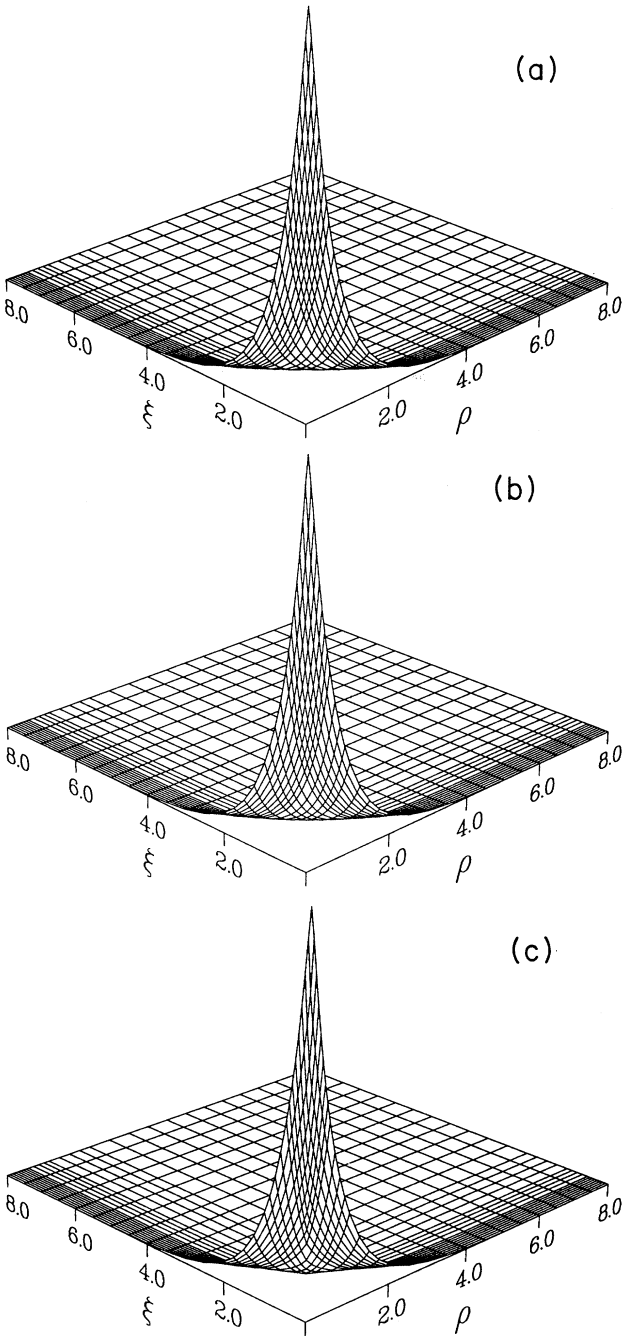

FIG. 1. Ground-state helium wave function at (a) $\cos\varphi = -1$, (b) $\cos\varphi = 0$, and (c) $\cos\varphi = 1$.

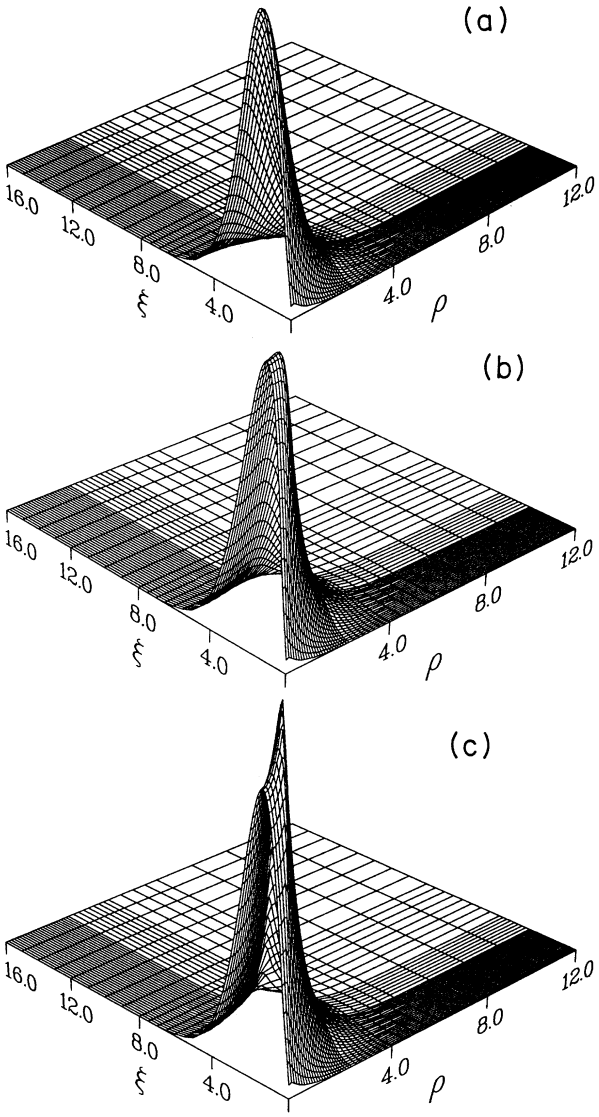

FIG. 2. $dd\mu^+(J=0,\nu=0)$ wave function at (a) $\cos\varphi = 0$, (b) $\cos\varphi = 0.9$, and (c) $\cos\varphi = 1$.

TABLE II. Expectation values for helium with mass polarization included in the Hamiltonian. Both variational and CFHH calculations incorporate explicit electron-nuclear cusps into the wave functions.

	Variational (Ref. 4)	CFHH (Ref. 7)	Finite element
$\|E\|$	2.903 30	2.903 30	2.903 26
$\langle r_{12} \rangle$	1.422 25	1.422 25	1.422 28
$\langle r_{13} \rangle$	0.929 61	0.929 61	0.929 63
$\langle r_{23} \rangle$	0.929 61	0.929 61	0.929 63
$\langle r_{12}^2 \rangle$	2.517 06	2.517 06	2.517 14
$\langle r_{13}^2 \rangle$	1.193 83	1.193 84	1.193 86
$\langle r_{23}^2 \rangle$	1.193 83	1.193 84	1.193 86
$\langle 1/r_{12} \rangle$	0.945 70	0.945 70	0.945 66
$\langle 1/r_{13} \rangle$	1.688 08	1.688 08	1.688 05
$\langle 1/r_{23} \rangle$	1.688 08	1.688 08	1.688 05
$\langle \delta(r_{23}) \rangle$	1.809 67	1.809 67	1.809 66

$$\bar{H}^N \chi^N = E \bar{U}^N \chi^N . \tag{5}$$

$\bar{H}^N$ and $\bar{U}^N$ are symmetric matrices of order 125 and the vector χ^N contains the unknown expansion coefficients. All of the matrix elements can be integrated exactly using six-point Gauss quadrature with the exception of the Coulomb interaction of particle 1 with particles 2 and 3. These matrix elements were integrated using 24-point Gauss quadrature unless the element included a point where the interparticle distance r_{12} or r_{13} was zero; in this case, the quadrature was increased to 48 point.

In order to guarantee continuity of the wave function across the element boundaries, all of the local matrices $\bar{H}^N$ and $\bar{U}^N$ are mapped onto two global matrices $\bar{H}$ and $\bar{U}$. Global matrix elements that correspond to nodes that are on a boundary between two elements receive contributions from both local matrices. The unknown global vector χ, which contains the value of the wave function at every node in the grid, must satisfy the boundary conditions of the problem. Every component of the vector $\bar{\chi}$ that corresponds to a node where $\rho=\rho_c$ or $\xi=\xi_c$ is set to zero. The remaining components are found by solving the generalized eigenvalue problem,

$$\mathbf{H}\chi = E\bar{U}\chi \tag{6}$$

using subspace iteration.[1]

III. RESULTS

In order to show the flexibility of the FE approach to the three-body problem, we solved the Schrödinger equation for an atomic system and a muonic molecular ion. For the helium atom, we used the finite mass of the α particle, thereby incorporating mass polarization directly. The ground-state wave function (Fig. 1) was obtained using only 196 elements (Table I). Using the convention $m_1 \leq m_2 \leq m_3$, ξ is the distance from the α particle to the first electron and ρ is the distance from the second electron to the center of mass of the α particle and the first electron. No attempt was made to optimize the grid and the results were stable with respect to minor variation in the discretization. FE values for the energy and powers of particle distances are compared with those obtained using the variational method[4] and the CFHH method[7] in Table II. The accuracy of the FE expectation values is comparable to that of the FE energy. The error in the

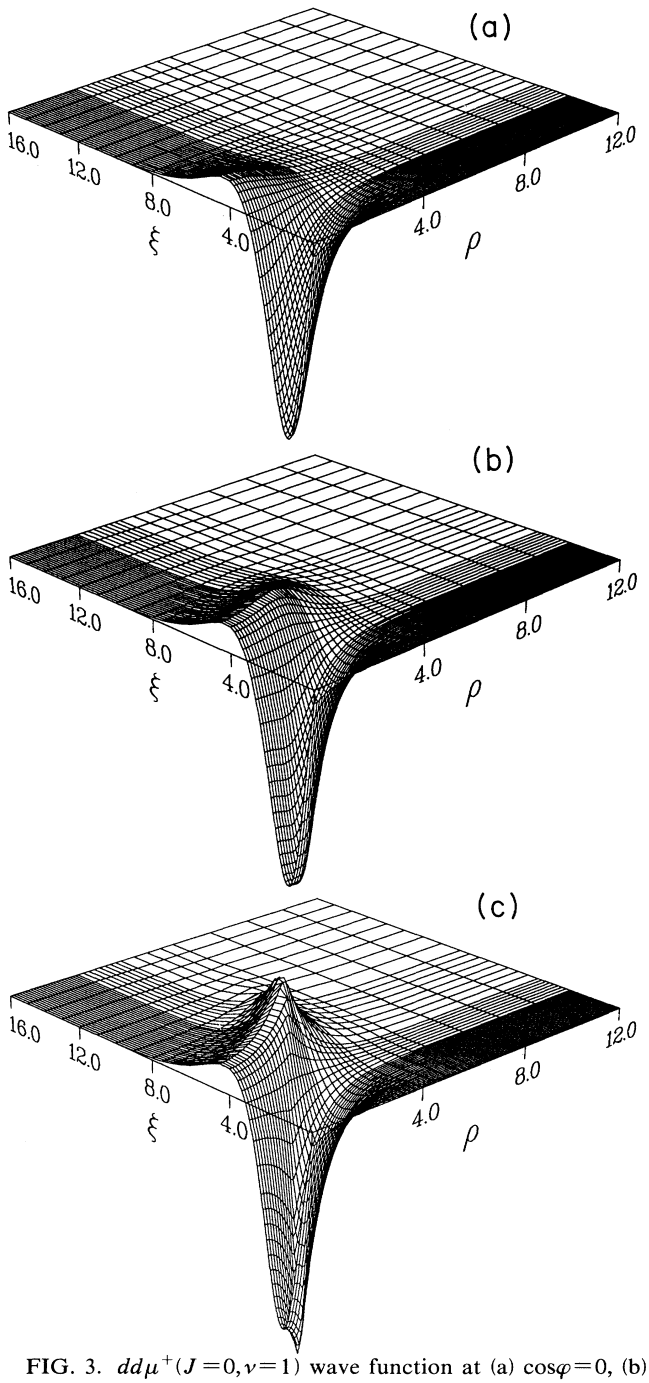

FIG. 3. $dd\mu^+(J=0,\nu=1)$ wave function at (a) $\cos\varphi=0$, (b) $\cos\varphi=0.9$, and (c) $\cos\varphi=1$.

TABLE III. Finite-element parameters for $dd\mu^+$. The number of elements is 480. The order of FE matrices is 31 248.

ρ	0.0	0.4	0.8	1.2	1.6	2.0	2.4	3.2	4.0	6.0	12		
ξ	0.0	0.4	0.8	1.2	1.6	2.0	2.4	3.2	4.0	6.0	8.0	12.0	16.0
$\cos\varphi$		0.0	0.5	0.9	0.99	1.0							

TABLE IV. Expectation values for $dd\mu^+(0,0)$ ($m_\mu=\hbar=e=1$). The binding energy ε is given in eV. For the CFHH method, the eigenvalue of the effective Schrödinger equation (0.5312) differs from $\langle H\rangle$ (0.5311); the latter,which is generally more accurate, was used in calculating the binding energy given below.

	Variational (Ref. 5)	Variational (Ref. 6)	CFHH (Ref. 8)	Finite element
$\lvert E\rvert$	0.5311	0.5311	0.5311	0.5310
ε	325.07	325.07	325.05	324.51
$\langle r_{12}\rangle$	2.120	2.120	2.121	2.119
$\langle r_{13}\rangle$	2.120	2.120	2.121	2.119
$\langle r_{23}\rangle$	2.834	2.834	2.836	2.832
$\langle 1/r_{12}\rangle$	0.7285		0.7284	0.7284
$\langle 1/r_{13}\rangle$	0.7285		0.7284	0.7284
$\langle 1/r_{23}\rangle$	0.3948		0.3945	0.3949

FE energy can be used to estimate the error in other physical observables. Excited S-state energies were not accurate because the grid was truncated at $8a_0$. However, additional FE calculations with larger values of ξ_c and ρ_c and more elements improved the accuracy of the excited states (and the ground state as well).

For the calculation on $dd\mu^+$ we used the mass values $m_\mu=206.7686m_e$ and $m_d=3670.481m_e$. The $dd\mu^+(J=0,\nu=0,1)$ wave functions (Figs. 2 and 3) were obtained with 480 elements (Table III). Smaller elements were needed near $\varphi=0$ in order to allow an accurate approximation of the cusp in the wave function when the muon-deuteron distance goes to zero. Otherwise the results were extremely stable with respect to variations in the grid. Values for the energy and geometry for $dd\mu^+$ ($J=0,\nu=0$) are given in Table IV and compared to the most accurate variational results[5,6] and the CFHH results.[8] As expected, the results for $\nu=1$ were less accurate since the excited-state wave function is much more extended in space.

One of the attractive features of FE analysis is the ability to construct the grid in such a way that more basis functions can be used where the wave function has a more complex structure, as in a region of the continuum where an interparticle distance approaches zero. Note that this is not the same thing as building in explicit cusp behavior, a procedure that is necessary to obtain accuracy in the variational method. Furthermore, the accuracy of the FE wave function can be improved locally without affecting its value elsewhere. This is generally not the case if one is using global basis functions in a variational calculation.

The advantages of FE analysis are clear. One can obtain accurate solutions to the Schrödinger equation for simple systems without constructing trial wave functions specific to the problem at hand. Expectation values obtained with FE wave functions are in general as accurate as the energy. In one- and two-dimensional FE calculations on simple systems, extremely high accuracy has been obtained for ground and excited states.[2] The main disadvantage of this method is that the FE matrices for three-dimensional calculations are extremely large. In order to improve the current results (larger values for ξ_c and ρ_c, finer discretization) and to extend the analysis to excited states ($J\neq 0$), it is necessary to develop new out-of-core routines to handle extremely large generalized eigenvalue problems. We are also investigating the advantages of choosing different coordinates to represent the three-body system. Finite-element analysis of few-body systems is undeniably computer intensive; however, it is the most direct method for solving the Schrödinger equation.

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