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Multibox strategy for constructing highly accurate bound-state wave functions for three-body systems

Alexei M. Frolov
Department of Physics, University of Windsor, Windsor, Ontario, Canada N9B 3P4

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Variational, multibox approach is proposed to construct extremely accurate, bound-state wave functions for arbitrary three-body systems. The high efficiency of our present approach is based on an optimal choice of nonlinear parameters in the exponential basis functions. The proposed method is very flexible, since the final wave function can also include a large number of separately optimized cluster fragments. The wave functions obtained are very compact and highly accurate. Such wave functions can be used to compute various bound state properties for different three-body systems. The proposed approach has been successfully tested on a large number of actual systems. It is shown that the present approach can be used to solve various three-body problems with, in principle, arbitrary precision. In particular, the long-standing problem of highly accurate determination of the weakly bound (1,1) states in the $dd\mu$ and $dt\mu$ muonic molecular ions has finally been solved. The determined binding energies are $-1.974\,988\,088\,0 \pm 5 \times 10^{-10}$ eV and $-0.660\,338\,74 \pm 1 \times 10^{-8}$ eV, respectively.

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In this study an advanced and variational approach is proposed and discussed. This approach can be used to determine to high accuracy, the bound-state spectra for various three-body systems. In fact, the proposed approach is found to be very effective and quite simple in solving a large number of bound-state, three-body problems. The accuracy of the bound-state determination in this approach is usually higher than in other competing methods, and more important, the accuracy can easily be increased. It should be mentioned, however, that highly accurate calculations are of great importance for many Coulomb three-body systems. For instance, to compute the hyperfine splitting in the helium-muonic atoms one needs to determine the electron-nucleus and electron-muonic delta functions with a maximal absolute error less than 1×10^{-8} a.u. [1]. The total bound-state energies for such systems are ≈ 400 a.u. It can be estimated from this that the required wave function must reproduce the ground state energy with an absolute error less than $\approx 1 \times 10^{-18}$ a.u. Only for such highly accurate wave functions, eight significant figures as required for the two mentioned delta functions, are stable. Also, the electron-positron and nucleus-nucleus delta functions are very important for predicting the corresponding annihilation rates in the Ps^- ion and fusion rates in the muonic molecular ions, respectively (see, e.g. [2–4]). Moreover, highly accurate nonrelativistic wave functions can be used to compute relativistic and Q.E.D. corrections for some actual atoms and ions. In fact, this is the only way to compute these corrections, since the alternative approach based on the Dirac equations cannot be used directly for three-body systems (see, e.g., [5]).

The nonrelativistic Hamiltonian for an arbitrary Coulomb three-body system can be written in the form

$$H = -\frac{1}{2m_1}\nabla_1^2 - \frac{1}{2m_2}\nabla_2^2 - \frac{1}{2m_3}\nabla_3^2 + \frac{q_3 q_2}{r_{32}} + \frac{q_3 q_1}{r_{31}} + \frac{q_2 q_1}{r_{21}},$$

where the so-called quasiatomic units $[\hbar = 1, e = 1, m_{min} = 1,$ and $m_{min} = \min(m_1, m_2, m_3)]$ are used. In this equation q_1, q_2, q_3 are the particle charges, while m_1, m_2, m_3 are their masses. The main goal of the present study is to determine (with high accuracy) the bound states of the corresponding Schrödinger equation $(H-E)\Psi = 0$, where H is the Hamiltonian and $E < 0$. Another goal is to perform highly accurate computations of various bound-state properties. To determine the bound-state energies and corresponding wave functions we apply an improved version of the exponential variational expansion in relative coordinates r_{32}, r_{31}, and r_{21} (where $r_{ij} = r_{ji} = |\vec{r}_i - \vec{r}_j|$, for more details see, e.g., [6]). Note, however, that the three relative coordinates r_{32}, r_{31}, and r_{21} are not really independent, since e.g., $|r_{ik} - r_{jk}| \leq r_{ij} \leq r_{ik} + r_{jk}$, where $(i,j,k) = (1,2,3)$. In general, this produces a few additional restrictions on possible values of nonlinear parameters that can be used in actual variational wave functions [1]. In fact, such relations between the nonlinear parameters are needed to guarantee convergence of the corresponding integrals in all matrix elements [6]. Obviously, in this case the optimization of these nonlinear parameters in the exponential variational expansion cannot be very effective.

To avoid this problem and increase the total efficiency of the exponential variational expansion in this study, the so-called mixed form of the basis functions is used [1]. In such a form the three perimetric coordinates u_1, u_2, and u_3 are used to represent the exponential part of each basis function. The angular, and other parts, of each basis function can be written either in the relative coordinates or in perimetric coordinates. The perimetric coordinates are simply related to the three relative coordinates: $u_i = \frac{1}{2}(r_{ik} + r_{ij} - r_{jk})$, and therefore, $r_{ij} = u_i + u_j$, where $(i,j,k) = (1,2,3)$. The perimetric coordinates are truly independent, and each of them varies from 0 to $+\infty$.

Thus, in the general case, the trial wave function for the (L,M) bound state in an arbitrary three-body system is represented in the form

$$\Psi_{LM}=\frac{1}{2}(1+\kappa\hat{P}_{21})\times\sum_{i=1}^{N}\sum_{\ell_1=\epsilon}^{L}C_i\mathcal{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\phi_i(r_{32},r_{31},r_{21})\times\exp(-\alpha_i u_1-\beta_i u_2-\gamma_i u_3)\times\exp(\imath\delta_i u_1+\imath e_i u_2+\imath f_i u_3), \quad (1)$$

where C_i are the linear (or variational) parameters, α_i, β_i, γ_i, δ_i, e_i, and f_i are the nonlinear parameters, and i is the imaginary unit. The functions $\mathcal{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})$ are the so-called Schwartz [7] or bipolar harmonics, L is the total angular momentum, and M is the eigenvalue of the $\hat{L}_z$ operator. An additional family of polynomial-type functions $\phi_i(r_{32},r_{31},r_{21})$ can also be used in calculations to represent some interparticle correlations. The operator $\hat{P}_{21}$ is the permutation of the identical particles in symmetric three-body systems, where $\kappa=\pm 1$, otherwise $\kappa=0$. In the present study $\kappa=-1$ for the triplet state of the helium atom, $\kappa=(-1)^L$ for the $pp\mu$ and $dd\mu$ symmetric systems, and $\kappa=0$ for the $dt\mu$ ion. Furthermore, in all present calculations it is assumed that $\phi_i(r_{32},r_{31},r_{21})=1$ for $i=1,\ldots,N$.

In general, by using the variational expansion Eq. (1) one can determine energy levels and variational wave functions for such systems with very high accuracy. Obviously, the main problem is the optimal choice of the nonlinear parameters in Eq. (1). To perform such an optimization in a very effective manner, presently we have developed a variational, multibox approach. This approach is essentially based on an optimal (or smart) choice of the nonlinear parameters in the exponential part basis functions Eq. (1) [8]. Note that, the use of perimetric coordinates in the exponents of Eq. (1), instead of the relative coordinates, significantly simplifies the partial (or complete) optimization of the nonlinear parameters. Indeed, the parameters α_i,β_i, and γ_i $(i=1,\ldots,N)$ in Eq. (1) can be arbitrary positive numbers, while the parameters δ_i,e_i, and $f_i(i=1,\ldots,N)$ can be arbitrary real numbers. The simple conditions $\alpha_i>0$, $\beta_i>0$, and $\gamma_i>0$ $(i=1,\ldots,N)$ must be obeyed to guarantee convergence of all integrals needed in computations. In fact, such a choice of nonlinear parameters, i.e., without any restriction, means that one can now use very effective optimization procedures, and therefore significantly better optimize these parameters than was possible in our previous works (see, e.g., [6]). If the exponential variational expansion is written in relative coordinates, then some of the nonlinear parameters can be negative. In earlier works (see, e.g., [6]), however, we could not use negative values for some of the nonlinear parameters since their optimization can generate infinite expressions for matrix elements. The negative nonlinear parameters are critically important in some cases for representing interparticle correlations. In particular, negative nonlinear parameters are really needed in highly accurate calculations of weakly bound, excited and cluster states. Complex values for some of the nonlinear parameters in Eq. (1) are used to provide high accuracy for adiabatic systems, where $\min(m_1,m_2)\gg m_3$ and $q_1q_2>0$ (for more details see, e.g., [6]). Note that, for such systems our method, based on Eq. (1), does not make use of the Born-Oppenheimer approximation [9].

In general, the expansion Eq. (1) can be obtained by a discretization of the Fourier (or Laplace-Fourier [10]) integral transform for the unknown wave function. Then, the unknown values of the exact wave function at some quadrature points (or lattice points) are replaced by the linear variational coefficients C_i, which do not depend upon the nonlinear parameters in Eq. (1). The general approach for generating variational expansions by using discretization of the different integral transformations can be found in [11–13] (see also references therein). In general, the optimization of the linear parameters C_i in Eq. (1) cannot produce highly accurate wave functions unless the nonlinear parameters are varied. In fact, only methods based on the optimization of the nonlinear parameters in Eq. (1) can produce extremely accurate wave functions. In particular, our present consideration deals with such an optimization.

It should be mentioned that initially the so-called regular [14] and quasirandom choices [12] of the nonlinear parameters in the exponential variational expansion were proposed and used. Later, the quasirandom choice was applied to compute the bound-state spectra in muonic molecular ions [15]. This simple approach allows one to compute various bound states relatively quickly, but the final accuracy is not sufficient for solving many actual problems. For our present purposes, it is important to note that if the regular or quasirandom choices of nonlinear parameters are used, then the nonlinear parameters in Eq. (1) are not real parameters in the method. They are usually called either the lattice points, or quadrature points. In fact, in these cases a few nonlinear parameters can be introduced for improving the overall efficiency of the method. For instance, if the nonlinear parameters are chosen quasirandomly from one $\alpha-\beta-\gamma$ box in three-dimensional space [or six-dimensional space for Eq. (1)], then by using some effective algorithms for optimization of the box parameters, one can accelerate the convergence of the results. However, the final accuracy of this improved method is still not sufficient for some Coulomb three-body problems.

To improve the final accuracy of Eq. (1) significantly in our earlier work [6] another approach was proposed. To choose the nonlinear parameters in Eq. (1) we used a two-stage procedure [6]. In fact, the first $6N_0$ (or $3N_0$) such parameters have been optimized carefully by using some very effective algorithms. Here and below, N_0 is the total number of terms in the short-term or booster function, which is significantly less than the total number N of basis functions used in calculations. In general, the first stage of our method [6] generates very compact and accurate booster wave functions. However, later it was found that the approach in [6] has the two following disadvantages: (1) the second stage of the method is not effective; and (2) the construction of the highly accurate booster functions requires extensive computational resources. Inefficiency of the second stage devaluates, in fact, the whole method. Indeed, it was observed that a better booster function does not always mean higher final accuracy. The reason is obvious, since the second stage function essentially repeats the corresponding booster function. In other words, the quasirandom choice of the lattice points $\alpha_i,\beta_i,\gamma_i,\delta_i,e_i$, and $f_i(i=1,\ldots,N)$ used in the second stage of the procedure is far from an optimal choice. An optimal choice must produce, in the general case, the lowest final (variational) energy for a given booster function. The second disadvantage means that it takes a quite long time for some systems to produce sufficiently accurate booster wave functions, but main point is that without such an accurate booster function the whole two-stage method cannot work successfully.

Initially, our goal was to improve the second stage of the method [6]. Also, we wanted to develop an independent procedure, which could be used independently and effectively even in those cases when the highly accurate booster wave function is unknown. The initial improvement has been achieved by using the computerized version of the box optimization, and by applying the perimetric coordinates in the exponents of Eq. (1) [1]. Then it became clear that the use of two, three, five, etc. different boxes, for choosing the lattice points α_i, β_i, γ_i, δ_i, e_i, and f_i in Eq. (1), produces significantly better variational energies. Finally, the approach has been developed to perform high precision, variational, bound-state calculations for arbitrary three-body systems. Briefly, in our present approach nonlinear parameters α_i, β_i, γ_i, δ_i, e_i, and f_i in Eq. (1) are chosen quasirandomly as in the older procedure (see, e.g., [15,16]), but now we are using a few (up to 10) different boxes. In fact, this means that we propose to use a multibound integration domain for the original Fourier integral transform wave function (see, e.g., [12]). The geometrical sizes and positions of these boxes are optimized, i.e., they are the actual nonlinear parameters of the method. Furthermore, there are also some scaling parameters, which are optimized for each step (or each pass) of the procedure. These parameters are used to find a proper balance between different parts of the trial function. Briefly, our present approach is a synthesis of the quasirandom choice of the nonlinear parameters from one box (see, e.g., [16]) and multiscaling optimization of such parameters [6].

Let us present the following simplified version of the procedure. The simplification means the use of the three-box version and restriction to a few scaling parameters. Furthermore, we shall assume that all exponents in Eq. (1) are real. In other words, all parameters δ_i, e_i, and f_i in Eq. (1) equal zero identically for $i=1,\ldots,N$. In fact, these parameters are really needed only for highly accurate calculations of the adiabatic (or close to them) three-body systems. Finally, the total number of nonlinear parameters in this version equals 28. This version of the procedure has been used extensively in our present calculations (see below). The choice of the nonlinear parameters in Eq. (1) proceeds as follows. Let i be the number (or index) of the basis function in Eq. (1) $(1\leqslant i\leqslant N)$ and $k=\mathrm{mod}(i,3)+1$, where $\mathrm{mod}(i,3)$ designates the modular division (i.e., an integer remainder after division of i by 3). Now, the parameters α_i, β_i, and γ_i are chosen from the three positive intervals $[A_1^{(k)},A_2^{(k)}]$, $[B_1^{(k)},B_2^{(k)}]$, and $[G_1^{(k)},G_2^{(k)}]$:

$$\alpha_i=\langle\langle\tfrac{1}{2}i(i+1)\sqrt{2}\rangle\rangle(A_2^{(k)}-A_1^{(k)})+A_1^{(k)}, \tag{2}$$

$$\beta_i=\langle\langle\tfrac{1}{2}i(i+1)\sqrt{3}\rangle\rangle(B_2^{(k)}-B_1^{(k)})+B_1^{(k)}, \tag{3}$$

$$\gamma_i=\langle\langle\tfrac{1}{2}i(i+1)\sqrt{5}\rangle\rangle(G_2^{(k)}-G_1^{(k)})+G_1^{(k)}. \tag{4}$$

Here the symbol $\langle\langle\cdots\rangle\rangle$ designates the fractional part of a real number. Such a choice of the α_i, β_i, and γ_i parameters is the first (main) stage of the procedure. The total number of actual nonlinear parameters used in this stage equals 18 $(2\times3\times3$ for the considered three-box version). In fact, for many Coulomb three-body systems the first stage already produces very accurate results and the second stage is not needed.

The second stage is essentially a scaling of the lattice points chosen in the first step. The scaling itself is performed as follows. The families of the parameters α_i, β_i, and γ_i (which correspond to the same k) are multiplied by the positive factors $\lambda_{k,1}$, $\lambda_{k,2}$, and $\lambda_{k,3}$, respectively. Then, these three parameters $\lambda_{k,1}$, $\lambda_{k,2}$, and $\lambda_{k,3}$ are also varied. The total number of such additional parameters equals nine (3×3). Also, one additional variational parameter is used to perform a scaling for all lattice points in Eq. (1). Finally, this method produces a properly balanced wave function that represents the considered bound state very accurately.

Note that, the high efficiency of our present strategy for choosing of the lattice points in Eq. (1) is based on the fact that in Eqs. (2)–(4) any additional condition for the $A_1^{(k)},A_2^{(k)},\ldots,G_2^{(k)}$ points is not used. In particular, either $A_1^{(k)}\leqslant A_2^{(k)}$, or $A_1^{(k)}\geqslant A_2^{(k)}$. The same is true for the $B_1^{(k)},B_2^{(k)},G_1^{(k)},G_2^{(k)}$ points. Furthermore, for any k the relative position of the interval $[A_1^{(k)},A_2^{(k)}]$ with respect to the intervals $[A_1^{(k-1)},A_2^{(k-1)}]$ and $[A_1^{(k+1)},A_2^{(k+1)}]$ can be arbitrary. This is also true for the $[B_1^{(k)},B_2^{(k)}]$ and $[G_1^{(k)},G_2^{(k)}]$ intervals. The results of calculations for different systems indicate clearly that such a freedom in choosing the lattice points is one of the main advantages of our present approach. In fact, this allows the generation of extremely accurate variational wave functions for different systems (see results below).

Our present procedure can be modified easily to the case when the short term (or booster) wave function is known. In this case the index i in Eqs. (2)–(4) changes from N_0+1 to N. Here N_0 is the number of basis functions in the booster function, while N is the total number of basis functions used. The cases when three-, four- and many-cluster functions are included in calculations can be considered in analogous manner. In any case, our presently developed multibox approach produces a variationally optimal, orthogonal complement to the original cluster wave function. In other words, by using our present procedure one can obtain the best (in the variational sense) correction to the wave function known from separate computations. This is an obvious advantage of our present approach in comparison with the original method used in [6]. Indeed, now the use of a more accurate booster wave function does mean better final accuracy for the total wave function.

TABLE I. The total energies (E) of the ${}^{\infty}$He atom $[2^3S(L=0)$-state$]$ in atomic units $(m_e=1,\hbar=1,e=1)$ and for some (L,ν) states in the $pp\mu$, $dd\mu$, and $dt\mu$ muonic molecular ions in muon-atomic units $(m_\mu=1,\hbar=1,e=1)$.

N	$E[{}^{\infty}\text{He};2^3S(L=0)\ \text{state}]$	$E[pp\mu;(0,0)\ \text{state}]$	$E[dd\mu;(0,0)\ \text{state}]$
600	−2.175 229 378 236 791 301 785 2	−0.494 368 202 488 828 302 7	−0.531 111 135 402 281 544 0
800	−2.175 229 378 236 791 305 644 1	−0.494 368 202 489 242 294 2	−0.531 111 135 402 375 706 6
1000	−2.175 229 378 236 791 305 712 5	−0.494 368 202 489 311 905 9	−0.531 111 135 402 384 135 5
2000	−2.175 229 378 236 791 305 737 7	−0.494 368 202 489 343 263 3	−0.531 111 135 402 386 302 8
2250	−2.175 229 378 236 791 305 738 1	−0.494 368 202 489 344 591 5	−0.531 111 135 402 386 345 1
2500	−2.175 229 378 236 791 305 738 4	−0.494 368 202 489 345 469 4	−0.531 111 135 402 386 374 5
	−2.175 229 378 236 791 301 794[a]	−0.494 386 820 248 931 69[a]	−0.531 111 135 402 385 75[a]
N	$E[dt\mu;(1,0)\ \text{state}]$	$E[dd\mu;(1,1)\ \text{state}]$	$E[dt\mu;(1,1)\ \text{state}]$
600	−0.523 191 455 489 821 946	−0.473 686 733 349 049 0	−0.48 199 152 778 643 2
1000	−0.523 191 456 282 037 570	−0.473 686 733 827 595 5	−0.48 199 152 962 856 7
1700	−0.523 191 456 315 607 405	−0.473 686 733 842 229 5	−0.48 199 152 995 582 9
1900	−0.523 191 456 315 772 556	−0.473 686 733 842 447 5	−0.48 199 152 996 358 7
2100	−0.523 191 456 315 858 429	−0.473 686 733 842 550 7	−0.48 199 152 996 694 7
2300	−0.523 191 456 315 906 521	−0.473 686 733 842 606 2	−0.48 199 152 996 960 1
2500	−0.523 191 456 315 927 175	−0.473 686 733 842 637 1	−0.48 199 152 997 083 4
2700	−0.523 191 456 315 937 144	−0.473 686 733 842 653 5	−0.48 199 152 997 171 3
	−0.5231914563027[a]	−0.4736867338415[a]	−0.481991528744[a]

[a] The best variational results known from earlier calculations.

In the present study, the proposed method is applied to the helium atom with infinitely heavy nucleus (or the ${}^{\infty}$He atom, for short) in its 2^3S state and to the $pp\mu$, $dd\mu$, and $dt\mu$ muonic molecular ions. To designate the bound states in muonic molecular ions, it is very convenient to use rotational (L) and vibrational (v) quantum numbers. Such a (L,v) classification scheme is based on the adiabatic (or molecular) picture for muonic molecular ions. However, all three particle masses in muonic molecular ions $pp\mu$, $pd\mu$, $pt\mu$, $dd\mu$, $dt\mu$, and $tt\mu$ are quite comparable with each other, and therefore, the so-called adiabatic approximation [9] cannot be applied successfully to these systems. Nevertheless, the approximate (L,v) classification scheme is very convenient for muonic molecular ions. In the present study, we consider the symmetric muonic molecular ions $pp\mu$ and $dd\mu$ in their ground (0,0) states and the nonsymmetric ion $dt\mu$ in its (1,0) and (1,1) states, respectively. For the $dd\mu$ ion we also discuss the (1,1) state. Note that the (1,1) states are weakly bound states in both $dd\mu$ and $dt\mu$ ions (see, e.g., [16]). Highly accurate determination of such states is very complicated, since it includes a large number of principal difficulties (see, e.g., [15]). In fact, the known energies of the (1,1) states for both $dd\mu$ and $dt\mu$ ions are significantly less accurate than appropriate values obtained for other bound states in muonic molecular ions [17]. However, such weakly bound states are of interest in some applications (see, e.g., [18]).

For the ground states in the $pp\mu$ and $dd\mu$ ions, highly accurate calculations have been recently performed [1]. Comparison of our present results with analogous results from [1] seems to be very interesting. Note that the method used in [1] is essentially a version of the two-stage strategy developed in [6]. For the symmetric muonic ions $pp\mu$ and $dd\mu$ our presently used booster functions coincide exactly with those functions used in [1]. To illustrate the advantages of our present approach we decided not to use any booster function for all other considered systems, i.e., for the 2^3S state of the ${}^{\infty}$He atom, for the $dd\mu$ ion in its excited (1,1) state and for $dt\mu$ ion in its both (1,0) and (1,1) states.

The results of our present calculations are presented in Tables I and II. Table I contains highly accurate energies for the 2^3S state of the ${}^{\infty}$He atom. The total number of basis functions used in calculations varies from 600 up to 2700. In general, the total energies presented in Table I are significantly more accurate than analogous results known from previous calculations. A large number of other bound-state properties for the 2^3S state of the ${}^{\infty}$He atom have been computed earlier [1]. For most of these properties our present values coincide almost exactly with the values determined in [1]. Note only that our computed value for the electron-nucleus cusp [19,20] (−1.999 999 999 996 81 a.u., for $N=2500$) coincides with the exact value (−2.0 a.u.) in 12 significant figures. The corresponding value for the electron-nucleus delta functions is 1.320 355 082 930 3 a.u.

Variational energies for the muonic molecular ions $pp\mu$, $dt\mu$, and $dd\mu$ can also be found in Table I. All energies for these systems are presented in muon-atomic units $(\hbar=1,e=1,m_\mu=1)$. The particle masses used in our present calculations are $m_p=1836.152\,701 m_e$, $m_d=3670.483\,014 m_e$, $m_t=5496.921\,58 m_e$, and $m_\mu=206.768\,262 m_e$ [21]. In all cases optimization of the nonlinear parameters has been performed for $N=600$ basis functions. Note that the results obtained with $N=600$ basis func-

TABLE II. The expectation values $\langle X_{ij} \rangle$ in muon atomic units ($m_\mu = 1, \hbar = 1, e = 1$) of some properties for the ground (0,0) states in the $pp\mu$ and $dd\mu$ muonic molecular ions. The notations 1 and 2 designate the hydrogen nuclei, while 3 stands for the muon (μ^-).

$\langle X_{ij} \rangle$	$pp\mu$	$dd\mu$
$\langle \delta_{31} \rangle$	0.131 500 862	0.158 738 97
$\langle \delta_{21} \rangle$	$0.393\,700\,5 \times 10^{-4}$	$0.243\,871 \times 10^{-5}$
$\langle \delta_{321} \rangle$	$0.554\,30 \times 10^{-4}$	0.4274×10^{-5}
ν_{31}	−0.898 787 919 95	−0.946 671 449 2
$\overline{\nu}_{31}^{\mathrm{a}}$	−0.898 787 928 781 951 609 94	−0.946 671 431 052 228 77
ν_{21}	4.440 106 25	8.875 716
$\overline{\nu}_{21}^{\mathrm{a}}$	4.440 122 200 669 269 058 32	8.875 837 564 471 088 95
ε^{b} (eV)	−253.150 192 338 596 952 1	−325.070 689 006 603 665

[a] The exact values from Eq. (6).

[b] The binding energy. The conversion factor is $27.211\,396\,1 (m_\mu / m_e)$.

tions for such systems have comparable and even better accuracy than our previous results from [16,22] computed with $N = 1000$ and 1200 basis functions. However, it may be more important to note that in contrast with the original two-stage approach [6], the presently performed optimization significantly improves the overall accuracy of the wave functions with total number of basis functions $N \geqslant 600$.

Table I also includes the best variational results known for the corresponding systems from earlier calculations (see [1,16]). In fact, the results of our present calculations (energies and bound-state properties) for all considered muonic molecular systems have significantly better accuracy than results known from earlier calculations [23]. In general, the accuracy of our present variational calculations for muonic molecular ions is quite comparable to the accuracy of the best atomic computations. In particular, by using our presently developed approach we can finally solve the long-standing problem of highly accurate determination of the weakly bound (1,1) states in the $dd\mu$ and $dt\mu$ muonic molecular ions. Indeed, by using the results presented in Table I one can easily evaluate the binding energies for the weakly bound (1,1) states in the $dd\mu$ and $dt\mu$ muonic molecular ions as follows:

$$\varepsilon(dd\mu) = -1.974\,988\,088\,0 \pm 5 \times 10^{-10} \ \text{eV},$$

$$\varepsilon(dt\mu) = -0.660\,338\,74 \pm 1 \times 10^{-8} \ \text{eV},$$

where the conversion factor $27.211\,396\,1 (m_\mu / m_e)$ has been used. In other words, these weakly bound states are now known with the absolute error less than 6×10^{-6} K and 3.7×10^{-5} K, respectively. Here, the conversion factor is $11\,604.448 \ \mathrm{K} \cdot (\mathrm{eV})^{-1}$. Finally, these energy levels have been determined with accuracy that is obviously sufficient for future experiments. The comparison of energies from Table I with the results obtained in [15] shows amazing progress relative to the 1985 level of computational technology.

The highly accurate wave functions can be used to determine the expectation values of many bound-state properties, e.g., the nuclear-nuclear and three-particle delta functions and two-particle cusps [19]. The results for some of these expectation values for the $pp\mu$ and $dd\mu$ ions [ground (0,0) states] are presented in Table II. They include expectation values for the delta functions (δ_{31}, δ_{21}, and δ_{321}) and cusps (ν_{31} and ν_{21}). Here and in Table II the notations 1 and 2 designate the hydrogen nuclei (p or d), while 3 means the negatively charged muon (μ^-). A large number of other expectation values for these systems can be found in [22]. The two-body cusp is determined in a traditional manner [19]:

$$\nu_{ij} = \frac{\left\langle \delta(\mathbf{r}_{ij}) \cdot \frac{\partial}{\partial r_{ij}} \right\rangle}{\langle \delta(\mathbf{r}_{ij}) \rangle}, \tag{5}$$

where $\delta_{ij} = \delta(\mathbf{r}_{ij})$ is the appropriate Dirac δ function and $(ij) = (32)$, (31), and (21). The exact (or predicted) value of the two-body cusp $\overline{\nu}_{ij}$ equals [20]

$$\overline{\nu}_{ij} = q_i q_j \frac{m_i m_j}{m_i + m_j}, \tag{6}$$

where q_i and q_j are the charges and m_i and m_j are the masses of the i and j particles ($i \neq j = 1,2,3$). Obviously, for the considered symmetric systems $\langle \delta(\mathbf{r}_{31}) \rangle = \langle \delta(\mathbf{r}_{32}) \rangle, \nu_{31} = \nu_{32}$, and $\overline{\nu}_{31} = \overline{\nu}_{32}$. In general, the coincidence between the predicted and computed two-particle cusp values indicates the quality of the wave functions. For the systems presented in Table II such a coincidence is very good.

Thus, in the present study, the advanced, multibox variational approach has been proposed to perform highly-accurate, variational, bound-state calculations for three-body systems. The proposed approach is found to be very flexible, since the final variational wave function can also include a large number of separately optimized cluster fragments. This version of the method can be called the improved two-stage strategy [6]. The very high efficiency of our present approach is based on an optimal and simple choice of nonlinear parameters in the trial wave functions. The nonlinear parameters are chosen quasirandomly from three (also from five, seven, ten, etc.) different and optimized boxes. The approach has been tested for a large number of quite complicated three-body systems. It was found that this approach works very effectively and surprisingly well for all such systems. In fact, we can say briefly that this method for highly accurate three-body calculations has been developed and successfully tested for a large number of three-body systems. Note also that our present universal approach can be used to solve various three-body problems with, in principle, arbitrary precision.

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