

## High-precision, variational, bound-state calculations in Coulomb three-body systems

Alexei M. Frolov

*Department of Physics, University of Windsor, Windsor, Ontario, Canada N9B 3P4*

(Received 25 April 2000)

The present study contains high-precision variational results for a number of bound states in various Coulomb three-body systems. In particular, we discuss the bound-state properties for the  $2^3S$  state of the  ${}^\infty\text{He}$  atom, the bound  $S(L=0)$  and  $P(L=1)$  states in symmetric muonic molecular ions, and ground states in the  ${}^3\text{He}^{2+}\mu^-e^-$  and  ${}^4\text{He}^{2+}\mu^-e^-$  atoms. The accuracy achieved for the total energies in these systems is significantly higher than known from the previous works. These results have been obtained by using a package of FORTRAN programs and a pretranslator written by D.H. Bailey from NASA [D.H. Bailey, ACM Trans. Math. Softw. **21**, 379 (1995)]. This multiprecision FORTRAN package can completely eliminate all problems related to numerical instabilities at large dimensions, which are crucial for high-precision, bound-state calculations in few-body systems. In fact, the multiprecision FORTRAN programs open another avenue in the study of bound states in few-body systems.

PACS number(s): 02.70.-c, 36.10.Dr

In this paper we present the advanced, high-precision results of bound-state, variational calculations for some Coulomb three-body systems. In particular, we consider the bound-state properties for the  $2^3S$  state of the  ${}^\infty\text{He}$  atom, the bound  $S(L=0)$  and  $P(L=1)$  states in the symmetric muonic molecular ions  $pp\mu, dd\mu, tt\mu$ , and the ground states in the  ${}^3\text{He}^{2+}\mu^-e^-$  and  ${}^4\text{He}^{2+}\mu^-e^-$  atoms. The accuracy achieved for the total energies in these systems is significantly higher than known from previous works. Our present results have been obtained by applying a recently developed FORTRAN translator with extended numerical accuracy. This powerful, multiprecision FORTRAN translator was written by Bailey from NASA [1]. This translator (called NASA-FORTRAN, for short) allows one to perform calculations, in principle, with arbitrary accuracy (for more details, see [1]). Moreover, any program written in FORTRAN-90 can automatically be transformed to an arbitrary precision version by using a pretranslator, which was also written by Bailey [1]. In our present study we have used the numerical accuracy which corresponds to the 48 and 64 exact decimal figures per computer word. It should be mentioned here that the packages developed by Bailey open another avenue in the study of bound states in few-body systems.

In fact, for the physics of few-body systems the invention of such a translator means a revolutionary turn. Indeed, by using this translator one can eliminate all problems related with numerical instabilities for the finite-dimension eigenvalue problems (at large dimensions). This means that now we can use practically nonlimited sets of basis functions in few-body, bound-state calculations. As a result, one can obtain the energies and other properties for such systems with an arbitrary number of correct (or stable) decimal figures. To illustrate this in the present study we consider the helium atom ( ${}^\infty\text{He}$ ) in its  $2^3S$  (triplet) state, the symmetric muonic molecular ions  $pp\mu, dd\mu$ , and  $tt\mu$  in their  $S(L=0)$ – and  $P(L=1)$  states, and the helium-muonic atoms  ${}^3\text{He}^{2+}\mu^-e^-$  and  ${}^4\text{He}^{2+}\mu^-e^-$  in their ground  $S(L=0)$  states. The bound-state properties of the triplet states of  ${}^\infty\text{He}$  atoms have never been determined to high accuracy. In contrast with this, the energies and a number of other bound

state properties for the  $S(L=0)$  states in muonic molecular ions have been computed recently with very high accuracy [2]. The comparison between the results from [2] and those calculated presently using NASA-Fortran is of great interest. This is also the case for the helium-muonic atoms ( ${}^3\text{He}^{2+}\mu^-e^-$  and  ${}^4\text{He}^{2+}\mu^-e^-$ ) in their ground  $S(L=0)$  states. For such systems, it is very interesting to recalculate the corresponding hyperfine splitting (see, e.g. [3–5]) for both atoms and compare results with [6]. Note that the multiprecision FORTRAN has already been used in calculations of the bound  $S(L=0)$  states for the nonsymmetric muonic molecular ions  $pd\mu, pt\mu$ , and  $dt\mu$  [7].

Note that the methods discussed below can be used for arbitrary three-body systems, but presently, we restrict ourselves to a consideration of the Coulomb three-body systems. To determine the bound states in such systems the exponential variational expansion in relative coordinates is used (for more details see, e.g., [2] and references therein). In the general case, the trial wave function for the  $(L, M)$  bound state is represented in the form

$$\begin{aligned} \Psi_{LM} = & \frac{1}{2} (1 + \kappa \hat{P}_{21}) \sum_{i=1}^N \sum_{\ell=1}^L C_i \mathcal{Y}_{LM}^{\ell, \ell/2}(\mathbf{r}_{31}, \mathbf{r}_{32}) \\ & \times \exp(-\alpha_i u_1 - \beta_i u_2 - \gamma_i u_3) \\ & \times \exp(i\delta_i u_1 + i e_i u_2 + i f_i u_3) \end{aligned} \quad (1)$$

where  $C_i$  are the linear (or variational) parameters,  $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i$ , and  $f_i$  are the nonlinear parameters. The functions  $\mathcal{Y}_{LM}^{\ell, \ell/2}(\mathbf{r}_{31}, \mathbf{r}_{32})$  are the so-called Schwartz [8] or bipolar harmonics,  $L$  is the total angular momentum, and  $M$  is the eigenvalue of the  $\hat{L}_z$  operator. The three perimetric coordinates  $u_1, u_2$ , and  $u_3$  are simply related with the three relative coordinates:  $u_i = \frac{1}{2}(r_{ik} + r_{ij} - r_{jk})$  and  $r_{ij} = r_{ji} = u_i + u_j$ , where  $(i, j, k) = (1, 2, 3)$ . The operator  $\hat{P}_{21}$  is the permutation of the identical particles in symmetric systems, where  $\kappa = \pm 1$ , otherwise  $\kappa = 0$ . In fact, in the present study all three possible values of  $\kappa$  are used:  $\kappa = -1$  for the triplet

state of the helium atom and for the  $P(L=1)$  states in the muonic molecular ions;  $\kappa=0$  for the ground states in the muonic-helium atoms; and  $\kappa=1$  for the  $S(L=0)$  states in the muonic molecular ions.

The use of perimetric coordinates in the exponents of Eq. (1) instead of the relative coordinates (see, e.g., [2]) significantly simplifies partial (or complete) optimization of the nonlinear parameters in Eq. (1) (see, e.g., [6]). Indeed, the parameters  $\alpha_i$ ,  $\beta_i$ , and  $\gamma_i$  ( $i=1, \dots, N$ ) in Eq. (1) can be arbitrary positive numbers, while the parameters  $\delta_i$ ,  $e_i$ , and  $f_i$  ( $i=1, \dots, N$ ) can be arbitrary real numbers. The simple conditions  $\alpha_i > 0$ ,  $\beta_i > 0$ , and  $\gamma_i > 0$  ( $i=1, \dots, N$ ) must be obeyed to guarantee convergence of all integrals needed in the computations. In fact, such a choice for the nonlinear parameters means that one can now use very effective optimization procedures, and therefore, perform significantly better optimization of these parameters than was possible in our previous work [9]. In the last case, we could not use the negative values for some of these parameters, since the three relative coordinates  $r_{32}$ ,  $r_{31}$ , and  $r_{21}$  are not completely independent. Negative values of the nonlinear parameters are critically important in many cases to represent accurately some interparticle correlations. In particular, the 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 needed to provide high accuracy also for the adiabatic systems, where, e.g.,  $\min(m_1, m_2) \gg m_3$  and  $q_1 q_2 > 0$  (for more detail see, e.g., [2]). Note that our method does not make use of the Born-Oppenheimer approximation [10].

In fact, in our present study only the  $L=0$  and  $L=1$  cases are considered. Furthermore, all nonlinear parameters  $\delta_i$ ,  $e_i$ , and  $f_i$  in the basis functions have been chosen to be equal to zero for  $i=1, \dots, N$ . This means that all basis functions are real functions, and therefore, all matrix elements of the Hamiltonian and overlap matrices are also real. This can be done, since all considered systems are certainly not adiabatic. Indeed, even for the  $tt\mu$  ion the numerical value of the so-called adiabatic parameter [10]  $\tau = (m_\mu/m_t)^{1/4} \approx 0.44039$ , i.e.,  $\tau \gg 0$ . The use of the complex exponents in Eq. (1) does not accelerate convergence significantly even for the  $tt\mu$  ion, but instead it makes all calculations much more complicated. Moreover, in our present calculations we have used the two following methods to construct basis functions in Eq. (1). First, we used the two-stage procedure which is based on the optimization of the nonlinear parameters in the first  $N_0$  trial wave functions ( $N_0 < N$ ), while the nonlinear parameters in the rest  $N - N_0$  basis functions are chosen quasirandomly. The second method is the quasirandom choice for all  $(3N)$  nonlinear parameters in Eq. (1). Presently, the first approach has been used for the helium and helium-muonic atoms and also for the  $S(L=0)$  states of the muonic molecular ions (for more details, see [2] and [6]). In all these cases, a partial optimization has been performed for the boost wave function consisting of  $N_0=200$  basis functions. The second (quasi-random) choice is applied only for the  $P(L=1)$  states in the muonic molecular ions. It was found that both choices of nonlinear parameters in Eq. (1) provide a very comparable accuracy in computations with  $N_{max}=2500$  basis functions. This is obvious, since even a very detailed optimization of the nonlinear parameters in the

relatively short, booster function cannot significantly improve results for the total wave function which includes a very large number of basis functions. This means that even a careful optimization of the very compact, booster wave functions cannot improve drastically the final accuracy if the total number of basis functions used (i.e.,  $N$ ) is significantly larger than the number of terms in the booster function (i.e.,  $N_0$ ). In other words, the final result is determined primarily by the  $N$  (for very large  $N$ ), rather than by a combination of  $N$  and  $N_0$  (when  $N_0 \ll N$ , e.g.,  $N \approx 10N_0$ ).

Now, let us briefly discuss the advantages which are provided by the invention of the MPFUN package of FORTRAN programs and the pretranslator written by Bailey. It is known that the central problem of all few-body, variational, highly accurate computations is the stability of matrix diagonalization routines (partial or complete diagonalization) at large dimensions (see, e.g., [2]). For instance, in the case of Eq. (1), the solution of the original Schrödinger equation  $H\Psi = E\Psi$  is reduced to the following matrix form:  $(\hat{H} - E\hat{S})\vec{C} = \vec{0}$ , where  $\hat{H}$  and  $\hat{S}$  are the matrices of the Hamiltonian and overlap.  $\vec{C}$  is the vector of the variational (linear) coefficients from Eq. (1). In fact, at large dimensions all three matrices  $\hat{S}$ ,  $\hat{H}$ , and  $\hat{H} - E\hat{S}$  are ill-conditioned. Formally, a matrix  $\hat{A}$  is ill-conditioned if its corresponding condition number  $N(\hat{A}) = \log_{10}(|\lambda_{max}|/|\lambda_{min}|)$  is very large (see, e.g., [11,12]). Here,  $|\lambda_{max}|$  and  $|\lambda_{min}|$  designate the maximal and minimal eigenvalues (absolute values) of the  $\hat{A}$  matrix. In actual computations any of the  $\hat{S}$ ,  $\hat{H}$ , and  $\hat{H} - E\hat{S}$  matrices can be ill-conditioned. But the most serious problems are related, as a rule, with the ill-conditioned overlap matrix  $\hat{S}$ . In this case, the basis vectors [i.e., the basis functions in Eq. (1)] are almost linearly dependent [13]. In this case, for the two close unit-norm vectors  $\vec{C}$  and  $\vec{C} + \delta\vec{C}$  (where  $\|\delta\vec{C}\| \ll \|\vec{C}\|$ ), the difference between the corresponding scalar products  $\langle \vec{C}, \hat{S}\vec{C} \rangle$  and  $\langle \vec{C} + \delta\vec{C}, \hat{S}(\vec{C} + \delta\vec{C}) \rangle$  can be  $\approx 10^{N(\hat{S})} (\gg 1)$ . This implies numerical instability in the diagonalization process. In fact, the accuracy of the  $E$  determination decreases rapidly when the condition number  $N(\hat{S})$  grows. By using the new NASA-FORTRAN with extended numerical precision, one can avoid all problems related with the presence of ill-conditioned matrices. Indeed, the new NASA-Fortran allows us to keep as many significant figures as needed to stabilize the diagonalization process. Finally, we can now concentrate on the physics of few-body systems, rather than apply very specific tricks to solve the mentioned problem of numerical instability.

To illustrate how the new NASA-FORTRAN works for real systems, we consider the bound  $2^3S$  state of the  ${}^{\infty}\text{He}$  atom, the bound  $S(L=0)$  and  $P(L=1)$  states in the symmetric muonic molecular ions, and the ground states in the  ${}^3\text{He}^{2+}\mu^-e^-$  and  ${}^4\text{He}^{2+}\mu^-e^-$  atoms. All constants, conversion factors, and particle masses used in our present calculations have been taken from [14]. In particular, the particle masses are

$$m_p = 1836.152701m_e, \quad m_d = 3670.483014m_e,$$

$$m_t = 5496.92158m_e, \quad m_\mu = 206.768262m_e,$$

TABLE I. The expectation values  $\langle X_{ij} \rangle$  in atomic units ( $m_e = 1, \hbar = 1, e = 1$ ) of some properties for the  $2^3S$  state of the helium atom with infinitely heavy nucleus.  $N$  designates the number of basis functions used. The notations 1 and 2 designate the two electrons, while 3 stands for the nucleus.

$\langle X_{ij} \rangle$	$N = 1800$	$N = 2200$	$N = 2500$
$E$	-2.175229378236791291621	-2.175229378236791299265	-2.175229378236791301794
$\langle r_{21}^{-1} \rangle$	0.268197855414848	0.268197855414848	0.268197855414848
$\langle r_{31}^{-1} \rangle$	1.15466415297211	1.15466415297211	1.15466415297211
$\langle r_{21} \rangle$	4.44753521696268	4.44753521696268	4.44753521696268
$\langle r_{31} \rangle$	2.55046267687692	2.55046267687692	2.55046267687692
$\langle r_{21}^2 \rangle$	23.04619747997229	23.04619747997229	23.04619747997229
$\langle r_{31}^2 \rangle$	11.46432162228457	11.46432162228457	11.46432162228457
$\langle r_{21}^3 \rangle$	136.742510330358	136.742510330358	136.742510330358
$\langle r_{31}^3 \rangle$	65.2150926304579	65.2150926304579	65.2150926304579
$\langle r_{21}^4 \rangle$	916.389433776757	916.389433776757	916.389433776757
$\langle r_{31}^4 \rangle$	428.402273125949	428.402273125949	428.402273125949
$\langle (r_{31}r_{32})^{-1} \rangle$	0.560729635682927	0.560729635682927	0.560729635682927
$\langle (r_{31}r_{21})^{-1} \rangle$	0.322696221719855	0.322696221719855	0.322696221719855
$\langle (r_{31}r_{21}r_{32})^{-1} \rangle$	0.186586074203096	0.186586074203094	0.186586074203093
$\tau_{31}$	0.562788947402921	0.562788947402921	0.562788947402921
$\tau_{21}$	$-1.58392170882503 \times 10^{-2}$	$-1.58392170882503 \times 10^{-2}$	$-1.58392170882503 \times 10^{-2}$
$\langle f \rangle$	$2.74346694293978 \times 10^{-2}$	$2.74346694293978 \times 10^{-2}$	$2.74346694293978 \times 10^{-2}$
$\langle \mathbf{r}_{31} \cdot \mathbf{r}_{32} \rangle$	$-5.87771177015738 \times 10^{-2}$	$-5.87771177015738 \times 10^{-2}$	$-5.87771177015738 \times 10^{-2}$
$\langle \mathbf{r}_{31} \cdot \mathbf{r}_{21} \rangle$	17.314036668301	17.314036668301	17.314036668301
$\langle -\frac{1}{2} \nabla_1^2 \rangle$	1.08761468911840	1.08761468911840	1.08761468911840
$\langle -\frac{1}{2} \nabla_3^2 \rangle$	2.18267150894282	0.218267150894282	2.18267150894282
$\langle \nabla_1 \nabla_2 \rangle$	$7.44213070602412 \times 10^{-3}$	$7.44213070602413 \times 10^{-3}$	$7.44213070602414 \times 10^{-3}$
$\langle \nabla_1 \nabla_3 \rangle$	-2.18267150894282	-2.18267150894282	-2.18267150894282
$\langle \delta_{31} \rangle$	1.32035508284857	1.32035508305351	1.3203550829745
$\langle \delta_{21} \rangle$	0.0	0.0	0.0
$\langle \delta_{321} \rangle$	0.0	0.0	0.0
$\nu_{31}$	-1.9999999894905	-2.00000000452699	-2.00000000167468
$\nu_{31}^a$	-2.0	-2.0	-2.0
$\eta$	$3.86992 \times 10^{-17}$	$1.77976 \times 10^{-17}$	$1.08525 \times 10^{-17}$
$\varepsilon$	-4.768236019558047429	-4.768236019558047637	-4.768236019558046682

<sup>a</sup>The exact two-particle cusp value [Eq. (3)].

$$m_{3\text{He}} = 5495.885 2m_e, \quad m_{3\text{He}} = 7294.299 6m_e.$$

For the helium atom and helium-muonic atoms ( $^3\text{He}^{2+}\mu^-e^-$  and  $^4\text{He}^{2+}\mu^-e^-$ ) only atomic units ( $\hbar = 1$ ,  $e = 1$ , and  $m_e = 1$ ) are used. For the muonic molecular ions all results are given in muon-atomic units ( $\hbar = 1$ ,  $e = 1$ , and  $m_\mu = 1$ ).

The numerical values for some of the properties (i.e., expectation values) for the  $2^3S$  state of the  $^\infty\text{He}$  atom can be found in Table I. In this table all such values are presented in atomic units. The physical meaning for all of the expectation values in Table I is quite clear from the notations used. So, here we wish to make only the few following remarks. In Table I the notations 1 and 2 mean negatively charged electrons, while the notation 3 designates the infinitely heavy nucleus. The notations  $\delta_{31}$ ,  $\delta_{21}$ , and  $\delta_{321}$  stand for the two- and three-particle Dirac  $\delta$  functions, respectively. In fact, the expected values for  $\langle \delta_{21} \rangle$  and  $\langle \delta_{321} \rangle$  for the  $2^3S$  state of the  $^\infty\text{He}$  atom equal zero identically. This is the so-called Fermi hole effect (see, e.g., [15]).

The two-body cusp ratios are determined in a traditional manner [16,17],

$$\nu_{ij} = \frac{\left\langle \frac{\delta(\mathbf{r}_{ij}) \cdot \frac{\partial}{\partial \mathbf{r}_{ij}}}{\delta(\mathbf{r}_{ij})} \right\rangle}{\langle \delta(\mathbf{r}_{ij}) \rangle}, \quad (2)$$

where  $\delta_{ij} = \delta(\mathbf{r}_{ij})$  is the appropriate Dirac  $\delta$  function and  $(ij) = (21)$  and  $(31)$ . The exact value of  $\nu_{ij}$  equals

$$\bar{\nu}_{ij} = q_i q_j \frac{m_i m_j}{m_j + m_j}, \quad (3)$$

where  $q_i$  and  $q_j$  are the charges and  $m_i$  and  $m_j$  the masses of the particles. However, the expected value of the electron-electron cusp (or  $\nu_{21}$  cusp) is not determined uniformly, since  $\langle \delta_{21} \rangle = 0$ . It is also assumed that  $\bar{\nu}_{21} = 0$  identically. This formally follows from the Fermi hole effect [15].

The expectation values of the two interparticle cosine functions are determined traditionally,

$$\tau_{ij} = \langle \cos(\mathbf{r}_{ik} \wedge \mathbf{r}_{jk}) \rangle = \left\langle \frac{\mathbf{r}_{ik} \cdot \mathbf{r}_{jk}}{r_{ik} \cdot r_{jk}} \right\rangle, \quad (4)$$

TABLE II. The total energies ( $E$ ) in muon-atomic units ( $m_\mu = 1, \hbar = 1, e = 1$ ) for the ground  $S(L=0)$  states of symmetric muonic molecular ions.  $N$  designates the number of basis functions used.

$N$	$E(pp\mu)$	$E(dd\mu)$	$E(tt\mu)$
1400	-0.49438682024891802	-0.53111113540238425	-0.54637422561381507
1600	-0.49438682024892353	-0.53111113540238336	-0.54637422561381615
1800	-0.49438682024892639	-0.53111113540238425	-0.54637422561381655
2000	-0.49438682024892849	-0.53111113540238486	-0.54637422561381664
2200	-0.49438682024893003	-0.53111113540238539	-0.54637422561381668
2500	-0.49438682024893169	-0.5311111540238575	-0.5467422561381371

where  $(i,j,k)=(1,2,3)$ . The quantity  $\langle f \rangle$  is expressed in terms of the relative coordinates  $(r_{31}, r_{32}, r_{21})$  or perimetric coordinates  $(u_1, u_2, u_3)$  [where  $u_i = \frac{1}{2}(r_{ij} + r_{ik} - r_{jk})$  and  $(i,j,k)=(1,2,3)$ ] as follows:

$$\begin{aligned} \langle f \rangle &= \langle \psi | \frac{u_1}{r_{32}} \frac{u_2}{r_{31}} \frac{u_3}{r_{21}} | \psi \rangle \\ &= \int \int \int |\psi(u_1, u_2, u_3)|^2 u_1 u_2 u_3 du_1 du_2 du_3. \end{aligned} \quad (5)$$

The value  $\langle f \rangle$  can be calculated directly or by applying  $\tau_{ij}$ . Their coincidence indicates that  $\tau_{21}, \tau_{32}, \tau_{31}$  and  $\langle f \rangle$  have been computed correctly. The equalities

$$\tau_{21} + \tau_{32} + \tau_{31} = 1 + 4\langle f \rangle \quad (6)$$

hold for an arbitrary three-body system. For symmetric systems we have  $\tau_{32} = \tau_{31}$ .

The virial factor  $\eta$  is determined as follows:

$$\eta = \left| 1 + \frac{\langle V \rangle}{2\langle T \rangle} \right|, \quad (7)$$

where  $\langle T \rangle$  and  $\langle V \rangle$  are the expectation values of the kinetic and potential energy, respectively. The deviation of the factor  $\eta$  from zero indicates, in principle, the quality of the wave function used. The appropriate binding energies  $\varepsilon$  are given in eV (the conversion factor is 1 a.u. = 27.211 396 1 eV). Note, however, that even an exact coincidence of the factor  $\eta$  with 0 does not indicate a high quality of the wave function. In fact, such a coincidence can be significantly improved artificially, as well as the corresponding coincidence for two-particle cusp values, by varying some of the linear and nonlinear parameters in the wave function. However, in our present study such an ‘‘advanced, scientific method’’ of improving wave functions has not been used.

TABLE III. The total energies ( $E$ ) in muon atomic units ( $m_\mu = 1, \hbar = 1, e = 1$ ) for the ground  $P(L=1)$  – states of symmetric muonic molecular ions.  $N$  designates the number of basis functions used.

$N$	$E(pp\mu)$	$E(dd\mu)$	$E(tt\mu)$
1400	-0.46845843630337135	-0.51362395679262942	-0.53326344981910582
1600	-0.46845843630337626	-0.513623956792666100	-0.53326344982010159
1800	-0.46845843630338003	-0.51362395679267359	-0.53326344982023228
2000	-0.46845843630338143	-0.51362395679267741	-0.53326344982031475
2200	-0.46845843630338226	-0.51362395679267890	-0.53326344982035642
2500	-0.46845843630338344	-0.51362395679268025	-0.53326344982037656

Note that some expectation values in Table I can be expressed as linear combinations of other properties. For instance, for the three relative vectors  $\vec{r}_{32}$ ,  $\vec{r}_{31}$ , and  $\vec{r}_{21}$  we have

$$\vec{r}_{32} - \vec{r}_{31} + \vec{r}_{21} = 0. \quad (8)$$

Therefore, the three following equalities  $[(i,j,k)=(1,2,3)]$ :

$$\vec{r}_{ik} \cdot \vec{r}_{jk} = \frac{1}{2}(r_{ik}^2 + r_{jk}^2 - r_{ij}^2) \quad (9)$$

hold in any case. For the appropriate expectation values one finds (see Table II)

$$\langle \vec{r}_{ik} \cdot \vec{r}_{jk} \rangle = \frac{1}{2}(\langle r_{ik}^2 \rangle + \langle r_{jk}^2 \rangle - \langle r_{ij}^2 \rangle). \quad (10)$$

Analogously, since  $\vec{p}_1 + \vec{p}_2 + \vec{p}_3 = 0$ , we write

$$\langle \vec{p}_i \cdot \vec{p}_j \rangle = \frac{1}{2}(p_k^2 - p_i^2 - p_j^2) \quad (11)$$

and

$$\langle \vec{p}_i \cdot \vec{p}_j \rangle = \frac{1}{2}(\langle p_k^2 \rangle - \langle p_i^2 \rangle - \langle p_j^2 \rangle) \quad (12)$$

$[(i,j,k)=(1,2,3)]$ . Moreover, if the three  $\vec{p}_i$  are determined by the relations  $\vec{p}_i = (-\iota)\vec{\nabla}_i$  in Cartesian coordinates, then one finds

$$\langle \vec{\nabla}_i | \vec{\nabla}_j \rangle = \langle -\vec{\nabla}_i \cdot \vec{\nabla}_j \rangle = \left\langle -\frac{1}{2}\nabla_k^2 \right\rangle - \left\langle -\frac{1}{2}\nabla_i^2 \right\rangle - \left\langle -\frac{1}{2}\nabla_j^2 \right\rangle, \quad (13)$$

TABLE IV. The expectation values  $\langle X_{ij} \rangle$  in atomic units ( $m_e = 1, \hbar = 1, e = 1$ ) of some properties for the ground states of the  ${}^3\text{He}^{2+}\mu^-e^-$  and  ${}^4\text{He}^{2+}\mu^-e^-$  helium-muonic atoms, respectively.  $N$  designates the number of basis functions used. The notations 1 and 2 designate the electron and muon, respectively, while 3 stands for the nucleus.

$\langle X_{ij} \rangle$	$N=2000$	$N=2200$	$N=2500$
$E$	-399.04233683286251593	-399.04233683286251960	-399.04233683286252384
$\langle \delta_{21} \rangle$	0.3136819444	0.3136819823	0.3136820042
$\langle \delta_{31} \rangle$	0.3206115479	0.3206115304	0.3206115091
$\langle \delta_{32} \rangle$	$2.01499388439 \times 10^7$	$2.01499388438 \times 10^7$	$2.01499388440 \times 10^7$
$\eta$	$1.803651 \times 10^{-16}$	$1.452855 \times 10^{-16}$	$1.291539 \times 10^{-16}$
$E$	-402.63726303513543127	-402.63726303513543620	-402.63726303513544403
$\langle \delta_{21} \rangle$	0.3137604521	0.3137604246	0.3137604273
$\langle \delta_{31} \rangle$	0.3206314979	0.3206315214	0.3206315471
$\langle \delta_{32} \rangle$	$2.07001373520 \times 10^7$	$2.07001373510 \times 10^7$	$2.07001373521 \times 10^7$
$\eta$	$2.148075 \times 10^{-16}$	$1.68369 \times 10^{-16}$	$1.04044 \times 10^{-16}$

where  $(i, j, k) = (1, 2, 3)$ . The expectation values from both sides of this equality can be found in Table I. Note, however, that the last three equalities are obeyed only in Cartesian coordinates and only if  $\vec{p}_i = (-i)\vec{\nabla}_i$ . In the present study such a choice is used, and therefore,  $\langle -\vec{\nabla}_i \cdot \vec{\nabla}_j \rangle$  can be expressed through  $\langle -\frac{1}{2}\nabla_i^2 \rangle$  and vice versa. Moreover, in the symmetric systems we have  $\langle p_1^2 \rangle = \langle p_2^2 \rangle$  and  $\langle \vec{r}_{31} \cdot \vec{r}_{21} \rangle = \langle \vec{r}_{32} \cdot \vec{r}_{21} \rangle$ . This simplifies some of the equations presented above. Moreover, for the symmetric systems ( $1=2$ ) one easily finds that  $-\langle \vec{\nabla}_1 \cdot \vec{\nabla}_2 \rangle$  is always negative, since  $\langle \vec{\nabla}_1 | \vec{\nabla}_2 \rangle = -\langle \vec{\nabla}_1 \cdot \vec{\nabla}_2 \rangle = -\langle -\frac{1}{2}\nabla_3^2 \rangle < 0$ .

The variational energies for the  $S(L=0)$  and  $P(L=1)$  bound states in the symmetric muonic molecules  $pp\mu$ ,  $dd\mu$ , and  $tt\mu$  are presented in Tables II and III. All energies in Tables II and III are given in muon-atomic units ( $m_\mu = 1, e = 1, \hbar = 1$ ). The variational energies and  $\langle \delta_{ij} \rangle$  expectation values [ $(ij) = (21)$ , (31), and (32)] for the ground  $S(L=0)$  states in the  ${}^3\text{He}^{2+}\mu^-e^-$  and  ${}^4\text{He}^{2+}\mu^-e^-$  helium-muonic atoms can be found in Table IV.

A convergence of the computed properties for the  $2^3S$  state of the helium atom (see Table I) indicates clearly that our present method can produce extremely accurate wave functions. Briefly, the accuracy of the obtained wave functions is far beyond the accuracy of the wave functions previously known for the considered systems. Moreover, by using such high-precision wave functions one can make significant progress in the study of bound states in various few-body systems. In particular, a number of bound-state properties for the  $2^3S$  state in the  ${}^\infty\text{He}$  atom have presently been determined with extremely high accuracy. Furthermore, such a very high accuracy is observed not only for the regular properties (e.g., for  $\langle r_{ij}^n \rangle$ ,  $\langle \mathbf{r}_{ij} \cdot \mathbf{r}_{ik} \rangle$ , etc), but also for the  $\delta_{31}$  delta-function expectation value and for the  $\nu_{31}$  two-particle cusp.

The variational energies and some other properties for the symmetric muonic molecular ions  $pp\mu$ ,  $dd\mu$ , and  $tt\mu$  have recently been computed to high accuracy [2]. In fact, bound-state computations for such systems have been performed for years (see, e.g., [18–20] and references therein), and now many of the bound-state properties of muonic molecular ions

are quite well known. Presently, by using the new NASA-Fortran we have determined the bound-state energies for the symmetric muonic molecular ions  $pp\mu$ ,  $dd\mu$ , and  $tt\mu$  with at least two more correct decimal figures (in comparison to [2]). Furthermore, the other bound-state properties (i.e., geometrical and dynamical properties) for these ions have also been computed presently more accurately than their values given in [2] (they are not presented in Tables II and III). In fact, by using the new NASA-FORTRAN it is straightforward to determine as many decimal figures as needed. In other words, now the accuracy of few-body bound state computations can be arbitrarily high.

Based on the results given in Table IV, one can evaluate the ground-state energies of the helium-muonic atoms with maximal error less than  $\pm 2 \times 10^{-15}$  a.u. This means that our present energies are  $\approx 50$  times more accurate than those computed only one year ago [6]. Note also that for the helium-muonic atoms the hyperfine splittings are of significant interest, since it can be easily measured experimentally. The theoretical expressions for the hyperfine splittings takes the form (see, e.g., [6])

$$\Delta \nu({}^4\text{He}) = 14\,229.180\,061\,055 \langle \delta(\mathbf{r}_{e\mu}) \rangle \text{ MHz},$$

$$\Delta \nu({}^3\text{He}) = 10\,671.885\,079\,542 \langle \delta(\mathbf{r}_{e\mu}) \rangle \quad (14)$$

$$+ 2553.907\,751\,447\,6 \langle \delta(\mathbf{r}_{eN}) \rangle \text{ MHz},$$

where  $\Delta \nu({}^3\text{He})$  and  $\Delta \nu({}^4\text{He})$  are the hyperfine splittings for the  ${}^3\text{He}^{2+}\mu^-e^-$  and  ${}^4\text{He}^{2+}\mu^-e^-$  helium-muonic atoms, respectively. In these equations  $\langle \delta(\mathbf{r}_{e\mu}) \rangle$  and  $\langle \delta(\mathbf{r}_{eN}) \rangle$  are the expectation values for the electron-muonic (21) and electron-nucleus (31)  $\delta$  functions, respectively. From these formulas and our expectation values in Table IV we find  $\Delta \nu({}^4\text{He}) \approx 4464.554$  MHz and  $\Delta \nu({}^3\text{He}) \approx 4166.390$  MHz. They are very close to the values computed previously [6] and to the experimentally known values:  $\Delta \nu({}^4\text{He}) \approx 4464.95$  MHz and  $\Delta \nu({}^3\text{He}) \approx 4166.41$  MHz [6]. Thus, based on the results from [6] and the results of the present study (see Table IV) one can say that the total relativistic and QED corrections are  $\approx 20$  kHz for the  ${}^3\text{He}^{2+}\mu^-e^-$  atom, and  $\approx 400$  kHz for the  ${}^4\text{He}^{2+}\mu^-e^-$  atom. It is still not quite

clear why the hyperfine splitting for the  ${}^3\text{He}^{2+}\mu^-e^-$  atom agrees with the known experimental value in  $\approx 20$  times better than in the case of the  ${}^4\text{He}^{2+}\mu^-e^-$  atom. Also, it should be mentioned that despite a significant progress made in bound-state computations for the considered Coulomb three-body systems some problems still remain. For instance, the observed (almost perfect) convergence for the variational bound-state energies does not mean a similar improvement in coincidence of the computed and predicted two-particle cusp values. In fact, the determined internuclei cusp values (i.e. the  $\nu_{21}$  cusps) for all symmetric muonic molecular ions have almost the same quality as in [2]. Such a problem has also been detected for some other bound-state properties. Obviously, this problem requires a separate investigation.

In conclusion, it should be mentioned that the invention of the powerful multiprecision FORTRAN (i.e., NASA-FORTRAN, developed by D.H. Bailey) has created a completely new situation for the whole of few-body physics. In fact, one can now use extremely large basis sets in bound-state, variational

computations. All bound-state properties for the three-, four-, and more-body systems can now be determined, in principle, to arbitrarily high accuracy. This is a very important step for future progress in few-body physics. However, it is easy to predict some possible complications. One of them is related with an extensive use of *a priori* nonoptimal, few-body basis sets with very slow convergence. However, such a slow convergence can be compensated for by using very large numbers of basis functions in computations. In general, an improvement of relatively short variational wave functions will be replaced by the use of very large basis sets. Obviously, this will require significantly more powerful computers, but in principle, such calculations can be performed already. In fact, this means a fundamental change for the whole of few-body physics.

It is a pleasure to thank Mark M. Cassar for his valuable help and the Natural Sciences and Engineering Research Council of Canada for financial support.

- 
- [1] David H. Bailey, ACM Trans. Math. Softw. **21**, 379 (1995), and references therein. The name of the package is MPFUN.
- [2] A. M. Frolov, Phys. Rev. A **59**, 4270 (1999).
- [3] S. D. Lakdawala and P. J. Mohr, Phys. Rev. A **22**, 1572 (1980); **24**, 2224 (1981).
- [4] K. N. Huang and V. W. Hughes, Phys. Rev. A **20**, 706 (1979); **21**, 1071E (1980); **26**, 2330 (1982).
- [5] R. J. Drachman, J. Phys. B **14**, 2733 (1981); **16**, L749 (1983).
- [6] A. M. Frolov, Phys. Rev. A **61**, 022509 (2000).
- [7] A. M. Frolov, Phys. Rev. A (to be published).
- [8] C. L. Schwartz, Phys. Rev. **123**, 1700 (1961).
- [9] A. M. Frolov, Phys. Rev. A **57**, 2436 (1998).
- [10] M. Born and J. R. Oppenheimer, Ann. Phys. (Paris) (Paris) **84**, 457 (1927).
- [11] G. E. Forsythe, M. A. Malcom, and C. B. Moller, *Computer Methods for Mathematical Computations* (Prentice-Hall, Englewood Cliffs, NJ, 1977); see also R. A. Horn and C. R. Johnson, *Matrix Analysis* (Cambridge University Press, Cambridge, England, 1985).
- [12] J. J. Dongara, J. R. Bunch, C. B. Moler, and G. W. Steart, *LINPACK User's Guide* (SIAM, Philadelphia, 1979), and references therein.
- [13] P. R. Halmos, *Finite-Dimensional Vector Spaces* (D. Van Nostrand Company, Princeton, NJ, 1958).
- [14] E. R. Cohen and B. N. Taylor, Phys. Today **52(8)**, 9 (1999).
- [15] N. H. March, W. H. Young, and S. Sampanthar, *The Many-Body Problem In Quantum Mechanics* (Dover Publications, New York, 1995), pp. 36–42.
- [16] T. Kato, Commun. Pure Appl. Math. **10**, 151 (1957).
- [17] R. T. Pack and W. Byers-Brown, J. Chem. Phys. **45**, 556 (1966).
- [18] A. K. Bhatia and R. J. Drachman, Phys. Rev. A **30**, 2138 (1984).
- [19] A. M. Frolov and V. D. Efros, Pis'ma Zh. Éksp. Teor. Fiz. **39**, 544 (1984) [JETP Lett. **39**, 449 (1984)].
- [20] A. K. Bhatia and R. J. Drachman, Comments At. Mol. Phys. **22**, 281 (1989).