Advanced variational approach for high-precision bound-state calculations in three-body systems.

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(July 19, 2002)

Abstract

The results of high precision variational calculations are reported for a number of bound states in various Coulomb three-body systems, including helium and helium-muonic atoms, some adiabatic systems (H_2^+, D_2^+ and DT^+ ions) and muonic molecular ions $pp\mu, dd\mu, tt\mu$ and $dt\mu$. The hyperfine splittings for the double electron-excited states in the helium-muonic $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms have also been determined. The results of our present study are significantly more accurate than results known from earlier calculations for all considered systems and states. Our present approach can be used to determine the bound state spectra in various three-body systems to arbitrary high accuracy. We also discuss a number of complications which are usually detected in high precision bound state calculations of few-body systems.

PACS: 31.25.Eb, 31.25.Nj and 36.10.Dr

In this communication we report the results of high precision, bound states calculations for a number of Coulomb three-body systems. Presently, our main goal was to perform highly accurate computations of various three-body systems with different particle masses, charges and permutation symmetries. Note that recently a significant progress has been achieved in theoretical and computational studies of the bound state spectra in various three-body systems [1]. In particular, now by using our approach developed in [1] one can determine the bound state energies and corresponding wave functions for an arbitrary three-body system to a very high accuracy. In this study we want to improve previously computed energies and wave functions to the limits which are significantly exceed any present and future experimental needs. In other words, the maximal computational uncertainties for all computed energies and other bound state properties must be negligibly small.

Presently, for high precision computations we also apply the variational approach developed in [1]. This approach was found to be very effective and sufficiently flexible in applications to various three-body systems [1]. To illustrate the efficiency of this approach [1] below we consider a large number of Coulomb three-body systems (and different states in such systems). This includes a few systems which are traditionally known as complicated cases for highly accurate variational methods based on the use of the relative coordinates r_{32}, r_{31} and r_{21} (see below). In particular, highly accurate variational results are presented for the adiabatic ions H_2^+, D_2^+ and DT^+. The heavy, non-symmetric adiabatic ion DT^+ is one of the most complicated systems for our present approach [1]. We are also consider the weakly-bound (1,1)-states in the $dd\mu$ and $dt\mu$ muonic molecular ions. Highly accurate determination of these weakly-bound states was a long-standing (since 1959, see [2]) unsolved and very complicated problem for various computational methods. The helium-muonic $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms in their electron-excited states can also be considered as examples of quite complicated Coulomb three-body systems with the two-shell, cluster structure.

In addition to such complicated (and extremely complicated) systems and states we also discuss some Coulomb three-body systems which are 'traditionally convenient' for highly accurate variational expansions written in the relative coordinates r_{32}, r_{31} and r_{21}. These are

the helium atom $^\infty He$ ($2^3S(L = 0)$−state) and $pp\mu$ muonic molecular ion ($S(L = 0)$−state). Highly accurate results for analogous 'convenient' systems such as Ps^-, $^\infty H^-$ ions and $^\infty He$ atom ($1^1S(L = 0)$−state) will be presented elsewhere.

It should be mentioned that our present approach [1] is based on a few fundamental ideas. First, we apply the so-called fast convergent and universal variational expansions written in the relative coordinates r_{32}, r_{31} and r_{21}. Here and below $r_{ij} = | \vec{r}_i - \vec{r}_j | = r_{ji}$ and $i \neq j = (1, 2, 3)$ and $\vec{r}_1, \vec{r}_2$ and $\vec{r}_3$ are the position vectors of the first, second and third particle, respectively. Note that all these position vectors are determined to the same center, i.e. the relative coordinates are translationally and rotationally invariant. In fact, all our present trial wave functions are written in the perimetric coordinates u_1, u_2, u_3 (see below) which are closely related with the relative coordinates, but always positive and truly independent. The use of perimetric coordinates simplifies significantly the optimization of non-linear parameters in the trial wave functions. Finally, the overall efficiency of our approach increases drastically.

The fast convergent variational expansion means that: (1) the use of a very few basis functions allows one to obtain a quite accurate energy for an arbitrary Coulomb three-body (symmetric) system [3], and (2) the variational energies $E(N)$ computed with the use of N basis functions rapidly (exponentially) converge when the number of basis functions N grows. Note also that by the universal variational expansion we mean the expansion which can successfully be applied to various three-body systems, including the one-center systems (e.g., the H^- ion or He atom), systems with three comparable masses (e.g., the Ps^- and $pp\mu$ ions), the semi-adiabatic systems (e.g., the $dt\mu$ and $tt\mu$ ions) and adiabatic systems (e.g., the DT^+ and T_2^+ ions). It should be mentioned that our present approach does not use any of the Born-Oppenheimer (or adiabatic) approximations [4] for the adiabatic and similar systems.

Second, the flexibility and efficiency of our variational approach [1] is based on the optimization of non-linear parameters in the trial (variational) wave functions. Presently, the multi-box strategy [1] is applied for optimization of such non-linear parameters. In fact, we

are using the three-box version of our procedure [1] which includes 28 non-linear parameters (18 principal parameters and 10 scaling parameters). For the adiabatic systems the analogous procedure contains 40 non-linear parameters [5]. Note, however, that our approach [1] was developed in such a way that the total number of actual non-linear parameters can be different for different systems, states, permutation symmetries and number of basis functions N. In general, the total number of such parameters can now be varied between 2 and $6N$, where N is the total number of basis functions used.

Third, our present calculations are performed using high-precision arithmetic – arithmetic accurate to the equivalent of 72 to 116 decimal digits. These calculations were performed using MPFUN, a multiple-precision, Fortran-90 computation package developed by one of the authors (DHB) [6]. This software includes a multiple-precision computation library, plus translation modules that permit one to utilize the library from standard Fortran-90 code, with only minor changes to the user's source code. In particular, one identifies multiple precision variables and constants with special datatypes, and then during program execution the appropriate library routines are automatically called. We believe this to be the first instance of the usage of high-precision numerical software in Coulomb three- and many-body systems. Previous applications of the MPFUN software have mostly been in the realm of "experimental mathematics." These include the discovery of several new mathematical identities (including a new formula for π that permits one to calculate arbitrary individual binary or hexadecimal digits), and the identification of certain constants that arise in quantum field theory [7].

As mentioned above in this study we consider the bound state spectra in various Coulomb three-body systems, including atoms, quasi-atoms, ions and muonic molecular ions. The high precision numerical results of such a study are discussed below. In general, the Coulomb three-body system contains three point particles with charges q_1, q_2, q_3 and masses m_1, m_2, m_3. Below, we shall use only atomic units in which $\hbar = 1, e = 1, m_e = 1$, where m_e is the mass of an electron and e is the charge on a proton. These units, however, are not very convenient for the muonic molecular ions $pp\mu, dd\mu, tt\mu$ and $dt\mu$ considered below. For these

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systems, the so-called muon-atomic (or quasi-atomic) units ($\hbar = 1, e = 1, m_{min} = m_\mu = 1$, where $m_{min} = \min(m_1, m_2, m_3)$) are more appropriate. As is well known in these units the non-relativistic Hamiltonian for an arbitrary Coulomb three-body system can be written in the following form

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

where all charges and masses must be expressed in terms of e and m_{min}, respectively. In the general case, the operator H has the discrete and continuous spectra. Our present main goal is to determine (with maximal possible accuracy) the energies and wave functions of the considered bound states. Such energies and wave functions are determined by solving the corresponding Schrödinger equation $(H - E)\Psi = 0$, where H is the Hamiltonian from Eq.(1) and $E < 0$.

In order to determine the bound state energies and corresponding wave functions we apply an improved version [1] of the exponential variational expansion in perimetric coordinates u_1, u_2 and u_3. 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 $+\infty$. 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 [1]:

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

where C_i are the linear (or variational) parameters, $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i$ and f_i are the non-linear parameters and $\imath$ is the imaginary unit. The functions $\mathcal{Y}_{LM}^{\ell_1, \ell_2}(\mathbf{r}_{31}, \mathbf{r}_{32})$ are the so-called Schwartz [8] or bipolar harmonics, L is the total angular momentum, M is the eigenvalue of the $\hat{L}_z$ operator. In actual calculations one can use only those Schwartz harmonics for which $\ell_1 + \ell_2 = L + \epsilon$, where $\epsilon = 0$ or 1. The first choice of ϵ corresponds to the natural space parity $\pi = (-1)^L$, while the second choice represents states with the unnatural space

parity $\pi = (-1)^{L+1}$. An additional family of polynomial-type functions $\phi_i(r_{32}, r_{31}, r_{21})$ can also be used in calculations to represent some inter-particle 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 $pp\mu, dd\mu$ and $tt\mu$ symmetric systems and $\kappa = 0$ for the $dt\mu$ ion. Also, $\kappa = 1$ for the H_2^+ and D_2^+ ions, and $\kappa = 0$ for the DT^+ ion and both helium-muonic atoms. Furthermore, in all present calculations it is assumed that $\phi_i(r_{32}, r_{31}, r_{21}) = 1$ for $i = 1, \ldots, N$.

Note that the variational expansion Eq.(2) can also be written in the following (short) form

$$\Psi = \sum_{i=1}^{N} C_i K_{LM}^i(\mathbf{r}_{31}, \mathbf{r}_{32}) \psi_i(u_1, u_2, u_3; \vec{\omega}_i) \quad , \tag{3}$$

where $i = 1, 2, \ldots, N$ and N is the total number of basis functions ψ_i used. C_i are the linear (or variational) coefficients, u_1, u_2, u_3 are the perimetric coordinates and $\vec{\omega}_i = (\alpha_i, \beta_i, \gamma_i, d_i, e_i, f_i)$ is the six-dimensional, $i-$dependent vector of the non-linear parameters associated with the given basis function ψ_i. Also, in the last formula $K_{LM}^i(\mathbf{r}_{31}, \mathbf{r}_{32}) = \mathcal{Y}_{LM}^{\ell_1(i), \ell_2(i)}(\mathbf{r}_{31}, \mathbf{r}_{32})$ is the corresponding angular factor. Note that the variational expansion Eq.(2) (or Eq.(3)) can be obtained by discretization of the Fourier integral transformation [9] for the wave function written in the perimetric coordinates. The general approach for generating variational expansion by using discretization of the different integral transformations can be found in [10]. Note also that this variational expansion (Eq.(2)) is assumed to be a fast convergent expansion. As we mentioned above, this means that already a very few basis functions $\psi_i(u_1, u_2, u_3; \vec{\omega}_i)$ can approximate quite accurately the bound state energy and corresponding wave function [3]. For instance, the first 100 basis functions in Eq.(2) used for the considered $S(L = 0)-$state of the $pp\mu$ ion allow one to obtain 99.99999 % of the total energy (and even more, if the optimization of non-linear parameters is applied). This means that the total contribution to the $pp\mu$ energy for the rest of 3500 basis wave functions (see Table I) is less than $1 \cdot 10^{-5}$ %. However, such a small contribution is ex-

tremely important to obtain highly accurate results for this system (see results Table I). This means that all basis functions with $101 \leq N \leq 3500$ form almost linearly dependent combination, or in other words almost zero vector. Analogous situation can be found for all other systems and states considered in this study. In general, at large dimensions (N) the additional basis functions do not contribute significantly to the energy, but complicate solution of the corresponding eigenvalue problem due to increasing linear dependence. This indicates clearly that high precision bound state calculations are essentially based on the use of almost linearly dependent vectors [11] and almost degenerated (or ill-conditioned) matrices [12]. In general, the absolute norms of such almost linearly dependent vectors are very close to zero [11].

To illustrate the general situation let us consider the matrix representation of the original Shrödinger equation. In fact, by using the variational expansion Eq.(3) for the trial wave function Ψ one can reduce the original bound state problem to the following matrix eigenvalue form

$$(\hat{H} - E \cdot \hat{S})\vec{C} = 0 \quad , \quad or \quad (\hat{\Lambda}^{-\frac{1}{2}}\hat{U}^{-1}\hat{H}\hat{U}\hat{\Lambda}^{-\frac{1}{2}} - E)\vec{\mathcal{C}} = 0 \quad , \tag{4}$$

where $\hat{H}$ is the Hamiltonian matrix $H_{n,n'} = \langle \psi_n \mid \hat{H} \mid \psi_{n'} \rangle$ and $\hat{S} = \hat{U}^{-1}\hat{\Lambda}\hat{U}$ is the positive overlap matrix $S_{n,n'} = \langle \psi_n \mid \psi_{n'} \rangle$. In general, for truly independent basis sets all eigenvalues of $\hat{S}$ are positive. In actual bound state calculations, most of the eigenvalues of $\hat{H}$ are also positive, but some of them can be negative. In fact, only such negative eigenvalues of $\hat{H}$ are of interest for our present study, since they represent the case of discrete spectrum. The main problem of high precision bound state calculations for few-body systems is related to the fact that all matrices in Eq.(4) (i.e. the $\hat{S}, \hat{H}$ and $(\hat{H} - E \cdot \hat{S})$ matrices) are extremely ill-conditioned. Briefly, this means that all these (symmetric) matrices contain very large and very small matrix elements [13]. In the general case, for an arbitrary finite-dimensional matrix $\hat{A}$ one can determine the condition number $\kappa(\hat{A})$ [13] as the ratio of maximal and minimal of all matrix elements (by absolute value). The matrix elements equal zero identically must be ignored during this procedure. In fact, in the case of Eq.(3) all mentioned

$\hat{S}, \hat{H}$ and $(\hat{H} - E \cdot \hat{S})$ matrices do not have matrix elements which are equal zero identically. In general, the condition number $\kappa(\hat{A})$ is a characteristics of solvability of system of linear equations $\hat{A}\mathbf{x} = \mathbf{y}$ [12]. Note that all operations with ill-conditioned matrices are very complicated, but their inversion, decomposition and diagonalization become extremely complicated.

These serious troubles have a very simply explanation, since, in general, the numerical accuracy can easily be lost even in usual arithmetic operations with ill-conditioned matrices [12]. The solution of a linear system and eigenvalue problem with ill-conditioned matrices produces a significant loss of numerical accuracy. This known fact can be formulated as the following general rule [14]: if $\kappa(\hat{A})$ is 10^k, the solution of a linear system (or eigenvalue problem) computed in $t-$digit (decimal) arithmetic will have no more than $t - k$ accurate figures. In our present study the condition numbers for the $\hat{S}, \hat{H}$ and $(\hat{H} - E \cdot \hat{S})$ matrices in Eq.(5) were $\approx 10^{60} - 10^{72}$. Therefore, in order to produce the result which is accurate in 30 decimal figures, one has to use arithmetic with 84 - 100 digits. For some systems the actual situation is even worse, but in these cases all matrices can be scaled and this can have a beneficial effect on the overall numerical stability. However, in general, even a perfect scaling strategy cannot remove all troubles related with ill-conditioned matrices, since the main source of such troubles is related with the original physical problem, rather than with the chosen computational strategy.

However, the presence of ill-conditioned matrices in Eq.(4) is only one of numerous problems related with this eigenvalue equation. A separate problem is related with the condensation of positive eigenvalues E to the threshold energy E_{tr}. This problem can be detected already for relatively small N, but at large dimensions ($N \geq 3000$) this can produce a significant loss of numerical accuracy. To illustrate the problem let us consider the muonic molecular ion $pp\mu$ which has only one bound state with $L = 0$. In this case, already one exponential basis function in Eq.(2) with optimized non-linear parameters reproduces quite accurately the corresponding bound state energy [3]. According to the "separation theorem"

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[15], [16] (see, also [17]) the second, third and higher eigenvalues of the Hamiltonian for $pp\mu$ ion converge to the threshold energy which represents the two-particle dissociation channel (i.e. $pp\mu = p\mu + p$, $E_{tr} = E_{p\mu} = -0.5/(1 + m_\mu/m_p) \approx$ -0.449393964390975805 $m.a.u.$). Finally, in actual calculations a large number of higher eigenvalues of Eq.(4) can be found to be very close to the threshold energy E_{tr} (condensation of eigenvalues). This means that our original eigenvalue problem is essentially replaced by eigenvalue problem for degenerated matrices. In fact, at very large dimensions ($N \geq 3000$) the matrix $(\hat{H} - E \cdot \hat{S})$ (for the $pp\mu$) ion is almost degenerated. The reduction of this matrix to the $\Lambda^+\Lambda$, L^+DL and other forms [12] complicates significantly. In the general case, this is another source of numerical errors. An effective way to avoid all troubles related with the use of ill-conditioned and almost degenerated matrices in Eq.(4) is to perform all arithmetic operations with the extended numerical precision [6].

The results of our present calculations can be found in Tables I - IV. The particle masses used in our present calculations are $m_p = 1836.152701$ m_e, $m_d = 3670.483014$ m_e, $m_t = 5496.92158$ m_e and $m_\mu = 206.768262$ m_e [18]. For the helium nuclei in the helium-muonic atoms we used the following masses (in atomic units) [18], [19] $M_{^3He^{2+}} = 5495.8852$ and $M_{^4He^{2+}} = 7294.2996$. The nucleus in the $^\infty He$ atom is assumed to be infinitely heavy. The results for the $2^3S(L = 0)-$state in the helium atom with infinitely heavy nucleus $^\infty He$ are presented in Table I. This state is a relatively low-lying state in the bound state spectrum of helium atom. In fact, this state can be computed with incredible high numerical accuracy, since the presence of Fermi hole (see, e.g. [20]) in the electron density distribution simplifies significantly the consideration of the electron-electron correlations at short distances. Briefly, this means that the electron-electron delta-function equals zero identically for all triplet states in two-electron systems. This explains why the computed energies for triplet states in any two-electron system are more accurate, in general, than corresponding results for the singlet states. In fact, the triplet $2^3S(L = 0)-$state in the helium atom with infinitely heavy nucleus $^\infty He$ is an ideal test for any computational method.

Tables I and II contain highly accurate variational results for a number of muonic

molecular ions $pp\mu, dd\mu, dt\mu$ and $tt\mu$. Presently, to designate the bound states in muonic molecular ions we shall apply the $(L, \nu)-$classification scheme, where L and ν are the corresponding rotational and vibrational quantum numbers. For the $pp\mu$ ion we consider the ground bound $S(L = 0)-$state (or (0,0)-state) and rotationally excited $P(L = 1)-$state (or (1,0)-state). For the $tt\mu$ ion only the $P(L = 1)-$state (or (1,0)-state) is discussed. The best variational energies obtained in earlier calculations for all 22 bound states in six muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$ can be found in [1]. Our present results (see Tables I and II) for all considered states are more accurate than energies presented in [1]. Note that, all muonic molecular ions can easily be created and observed experimentally.

Obviously, the most interesting bound states in muonic molecular ions are the two weakly-bound (1,1)-states in the $dd\mu$ and $dt\mu$ muonic molecular ions. It was assumed that such 'resonance' states can play a central role in the muon-catalyzed nuclear $(d, t)-$ and $(d, d)-$fusion (see, e.g. [21], [22]). To predict the efficiency of muon-catalyzed fusion in the equimolar deuterium-tritium mixture one has to know the (1,1)-energy level in the $dt\mu$ ion with the accuracy $\approx 0.01\ K$ (or $\approx 10^{-6}\ eV$). On the other hand, the amplitude of attractive muon-nuclear potential in the $dt\mu$ ion is $\approx 1\ keV = 1000\ eV$. Finally, the maximal computational uncertainty for the energies of these weakly-bound (1,1)-states can be estimated as $\approx 1 \cdot 10^{-9}$. Such an accuracy can easily be produced for the helium atom or for the Ps^- ion. However, the considered (1,1)-states in the $dd\mu$ and $dt\mu$ ions are extremely weakly-bound systems consisting of the three particle with comparable masses (m_μ, m_d and m_t). In general, the wave functions of weakly-bound systems vanish effectively only at very large distances. The actual computations situation for the (1,1)-states in the $dd\mu$ and $dt\mu$ is even worse than for the DT^+ ion (almost unbound systems). Our long-time experience in three-body bound state calculations, indicates that the (1,1)-state in the $dt\mu$ ion is one of most complicated cases for high precision calculations. The complexity of this system is related with the overall structure of the weakly-bound state, rather than with particle masses or charges. Note that highly accurate results for the (1,1)-state in the $dt\mu$ ion were produced only recently [1].

The total energies (in muon-atomic units) for the (1,1)-states in the $dd\mu$ and $dt\mu$ ions can be found in Table II. In general, the energies from Table II for these ions are more accurate than results obtained for these states in [1]. In fact, by using these results and relatively simple asymptotic formulas one can easily evaluate the total energies for the weakly bound (1,1)-states in the $dd\mu$ and $dt\mu$ muonic molecular ions as follows

$$E(dd\mu; L = 1, \nu = 1) = -0.473686733842725 \pm 4 \cdot 10^{-15} \quad m.a.u. \quad ,$$

$$E(dt\mu; L = 1, \nu = 1) = -0.4819915299739 \pm 4 \cdot 10^{-13} \quad m.a.u. \quad ,$$

where the muon-atomic units ($m_\mu = 1, \hbar = 1$ and $e = 1$) are used. The binding energies for these states can now be evaluated with uncertainties less than $2.3 \cdot 10^{-11}$ eV and $2.3 \cdot 10^{-9}$ eV, respectively. The corresponding binding energies are

$$\varepsilon(dd\mu; L = 1, \nu = 1) = -1.974988087995 \pm 23 \cdot 10^{-12} \quad eV \quad ,$$

$$\varepsilon(dt\mu; L = 1, \nu = 1) = -0.6603386864 \pm 23 \cdot 10^{-10} \quad eV \quad ,$$

Here, the conversion factor $27.2113961(m_\mu/m_e)$ was used. This means that our present results are significantly more accurate than the energies determined in [1].

Highly accurate results for the ground states in the adiabatic ions H_2^+, D_2^+ and DT^+ are presented in Table III. These ions are of increasing interest in various applications mainly related with astrophysics, plasma physics and nuclear $(d, t)-$ and $(d, d)-$fusion. The properties of these ions are discussed in our earlier studies [5]. The bound state properties for the H_2^+ and D_2^+ ions determined in [5] coincide very well with the results obtained in [23] and [24] (for the energies, see also [25]). Note that the current accuracy for the energies presented in Table III is quite comparable to the accuracy of the best atomic calculations. The energies of the considered adiabatic ions H_2^+ and D_2^+ (other similar ions HD^+, HT^+ and T_2^+ are considered in [5]) can now be predicted with uncertainties less that $1 \cdot 10^{-20}$ $a.u.$ For the DT^+ ions such an minimal uncertainty is $\approx 1 \cdot 10^{-16}$ $a.u.$ A large number of other bound state properties were also determined quite accurately (see [5]).

However, our progress in computations of the nuclear-nuclear contact properties in such systems is quite modest [5]. In general, the contact property X can be written in the form

$$\langle X \rangle = \langle \delta(\mathbf{r}_{ij}) \hat{F}(\mathbf{x}_i, \mathbf{p}_j) \rangle \quad , \tag{5}$$

where $\hat{F}$ is an arbitrary, in principle, operator which depends on the dynamical variables ($\mathbf{x}_i$ and $\mathbf{p}_j$) of the considered system. The delta-functions and cusps [26], [27] are the two examples of quite simple contact operators. However, these expectation values of the nuclear-nuclear delta-function (as well as the triple delta-function) are of great importance in numerous applications. This follows e.g. from the fact that these values determine the nuclear fusion probabilities in the corresponding system. Unfortunately, the best current deviation obtained with our bound state wave functions for the nuclear delta-functions varies between $\approx 10^{18}$ (for the H_2^+ ion) and $\approx 10^{28}$ (for the DT^+ and T_2^+ ions). On the other hand, note that the same wave functions are almost perfect for the energy and many other properties. Obviously, the problem of contact nuclear-nuclear properties for adiabatic systems needs a further investigation, but it was shown in [5] that the agreement between the computed and predicted values for nuclear-nuclear delta-functions is improving when more accurate wave functions are used.

Presently, we also consider the double electron excited $1s_\mu 3s_e-$states in the ${}^3He^{2+}\mu^- e^-$ and ${}^4He^{2+}\mu^- e^-$ helium-muonic atoms which have never been computed earlier. Our present goal is to evaluate the hyperfine splitting in these systems to the accuracy $\pm 1\ kHz$. The numerical computations of helium-muonic atoms contain a number of difficulties, since these systems have the two-shell (cluster) structure. In fact, by using the hydrogen-like two-shell model one can easily obtain some approximate results for the energies and properties in such systems. However, an accurate description of the helium-muonic atoms requires an extensive use of numerical methods and significant computational resources. The main problem here is related with the electron-muonic correlations. In our present calculations of the helium-muonic atoms we applied the same approach [1] which was successfully used for other three-body systems. The results of numerical calculations for the second $1s_\mu 3s_e-$electron excited

$S(L = 0)-$states of the helium-muonic atoms are presented in Table IV. This Table include the total energies (in atomic units) and hyperfine splittings (in MHz). The formulas for the hyperfine splitting $\Delta\nu$ in the $S(L = 0)-$states of the helium-muonic atoms take the form (for more details see, e.g. [28], [29] and also [30])

$$\Delta\nu(^3He^{2+}\mu^-e^-) = 10671.885079542 \cdot \langle\delta(\mathbf{r}_{e^-\mu^-})\rangle \ + \ 2553.9077514476 \cdot \langle\delta(\mathbf{r}_{e^-He})\rangle \ \ MHz \ ,$$

$$\Delta\nu(^4He^{2+}\mu^-e^-) = 14229.180061055 \cdot \langle\delta(\mathbf{r}_{e^-\mu^-})\rangle \ \ MHz$$

where $\langle\delta(\mathbf{r}_{e^-\mu^-})\rangle$ and $\langle\delta(\mathbf{r}_{e^-He})\rangle$ are the expectation values for the electron-muonic and electron-nucleus delta functions, respectively. The expectation values of all delta-functions in these formulas must be expressed in atomic units. Finally, by using the results from Table IV one can evaluate the corresponding hyperfine splittings for the second electron excited $1s_\mu 3s_e-$states in the helium-muonic atoms as $\approx 154.3058 \pm 3 \cdot 10^{-4} \ MHz$ ($^3He^{2+}\mu^-e^-$) and $\approx 165.3482 \pm 3 \cdot 10^{-4} \ MHz$ ($^4He^{2+}\mu^-e^-$). Note that these states have never been discussed in earlier studies.

The results from Table IV indicate the efficiency of our present approach for advanced theoretical research in various few-body systems. Indeed, by considering these states for the first time we have solved the problem completely, since now the hyperfine splittings in both helium-muonic atoms are known with uncertainties which are less than $0.3 \ kHz$. In fact, such an accuracy is significantly higher than maximal experimental accuracy known for these systems ($\approx 10 \ kHz$, see discussion in [1]). Furthermore, the improved theoretical results for the helium-muonic atoms must also include the relativistic and quantum-electrodynamics (radiative) corrections [31], [32]. However, such corrections are relatively small (≈ 0.02 - 0.5 MHz). To emphasize the efficiency of our present approach we want to note that it took almost 30 years to produce a comparable numerical accuracy ($\approx 1 \ kHz$) for the ground $1s_\mu 1s_e-$states in the helium-muonic atoms (see, e.g. [28], [33] - [35]).

In the present study, we discuss an advanced variational approach for high-precision bound-state calculations in three-body systems [1]. The proposed approach is found to be very flexible and effective for solving three-body bound state problems. Its flexibility is based

on the use of fast convergent variational expansion written in the perimetric coordinates and a large number of separately optimized non-linear parameters. In fact, the total number of non-linear parameters can also be varied for different systems, considered bound states, number of basis functions N and required computational accuracy. The efficiency of our present approach is based on the use of high-precision numerical software (MPFUN) specifically developed to perform calculations with extended numerical precision. Our present approach has been successfully tested for a large number of Coulomb three-body systems, with different particle masses, nuclear (or particle) charges and permutation symmetries. All our presently computed results are significantly more accurate than results known from previous calculations for the considered systems and states.

In conclusion, we want to note that our present approach is the most appropriate method for high precision variational calculations of the bound state spectra in the non-relativistic three-body systems. For an arbitrary Coulomb three-body system this approach allows one to obtain extremely accurate (i.e. essentially exact) numerical solutions. It is important to note that numerical accuracy of such solutions can be made arbitrarily high. Briefly, one can say that now the Coulomb three-body systems can effectively be studied numerically [36], rather than experimentally. This means that from now on the non-relativistic Coulomb three-body problem can be considered as a technical or computational problem, rather than a scientific problem. For the non-Coulomb three-body systems our present approach allows one to concentrate on the physics of the problem (e.g. on the potential reconstruction).

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[36] The remaining unsolved problem is related with the accurate evaluation of the nuclear-nuclear contact properties in the adiabatic systems, e.g. in the DT^+ ion [5].

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 $(L,\nu)-$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 is the total number of basis functions used in Eq.(2).

N	$E(^{\infty}He; 2^3S(L = 0)-$state)	N	$E(pp\mu; (0,0)-$state)
2500	-2.175229378236791305738 9644	2900	-0.494368202489347718
2750	-2.175229378236791305738 9677	3100	-0.494368202489347776
3000	-2.175229378236791305738 9710	3300	-0.494368202489347839
3250	-2.175229378236791305738 9731	3500	-0.494368202489347872
3500	-2.175229378236791305738 9742	3700	-0.494368202489347899
3750	-2.175229378236791305738 9753	3800	-0.494368202489347909
	-2.1752293782367913057 3891[a]		-0.4943682024893455[a]

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

TABLE II. The total energies (E) of some (L, ν)−states in the $pp\mu, tt\mu, dd\mu$ and $dt\mu$ muonic molecular ions in muon-atomic units $(m_\mu = 1, \hbar = 1, e = 1)$. N designates the number of basis functions used in Eq.(2).

N	$E(pp\mu; (1,0)$−state)	$E(tt\mu; (1,0)$−state)
2750	-0.468 458 436 303 383 938	-0.533 263 449 820 381 89
3000	-0.468 458 436 303 384 288	-0.533 263 449 820 382 30
3250	-0.468 458 436 303 384 504	-0.533 263 449 820 382 69
3500	-0.468 458 436 303 384 684	-0.533 263 449 820 382 89
3750	-0.468 458 436 303 384 803	-0.533 263 449 820 383 02
	-0.468 458 436 303 383 44[a]	-0.533 263 449 820 376 56[a]
N	$E(dd\mu; (1,1)$−state)	$E(dt\mu; (1,1)$−state)
2900	-0.473 686 733 842 675 6	-0.481 991 529 972 380
3100	-0.473 686 733 842 694 8	-0.481 991 529 972 721
3300	-0.473 686 733 842 707 2	-0.481 991 529 973 090
3500	-0.473 686 733 842 716 7	-0.481 991 529 973 278
3700	-0.473 686 733 842 719 7	-0.481 991 529 973 412
3800	-0.473 686 733 842 720 3	———
	-0.473 686 733 842 653[a]	-0.481 991 529 971 713[a]

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

TABLE III. The total energies E (in atomic units $m_e = 1, \hbar = 1, e = 1$) and binding energies ε (in eV) for the ground states of some adiabatic H_2^+−like ions. N designates the number of basis functions used in Eq.(2).

N	H_2^+	D_2^+	DT^+
2000	-0.59713906312340507364	-0.59878878433068346368	-0.59913066285505615
2200	-0.59713906312340507438	-0.59878878433068346419	-0.59913066285505942
2400	-0.59713906312340507463	-0.59878878433068346439	-0.59913066285506088
2600	-0.59713906312340507474	-0.59878878433068346447	-0.59913066285506164
3000	-0.59713906312340507481	-0.59878878433068346453	-0.59913066285506218
3500	-0.59713906312340507483	-0.59878878433068346455	-0.59913066285506275
$E_p^{(a)}$	-0.59713906312340507 [5]	0.598787843306835 [5]	-0.599130662855023

$^{(a)}$The best variational energies (in $a.u.$) known from earlier calculations.

TABLE IV. The convergence of the total energies E in atomic units and hyperfine splittings ΔH (in MHz) for the second electron excited $1s_\mu 3s_e$−states for the $^3He^{2+}\mu^- e^-$ (3) and $^4He^{2+}\mu^- e^-$ (4) helium-muonic atoms.

N^a	$E(3)$	$\Delta H(3)$	$E(4)$	$\Delta H(4)$
1000	-398.597957663903039272	154.3056	-402.261928652266220979	165.3481
1500	-398.597957663903043734	154.3057	-402.261928652266220992	165.3482
2000	-398.597957663903044910	154.3058	-402.261928652266220996	165.3482
2500	-398.597957663903045392	154.3058	-402.261928652266220998	165.3482
3000	-398.597957663903045630	154.3058	-402.261928652266220998	165.3482

^{a}The number of basis functions used in calculations.