Highly accurate calculations of the rotationally excited bound states in three-body systems

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(Dated: August 3, 2010)

Abstract

An effective optimization strategy has been developed to construct highly accurate bound state wave functions in various three-body systems. Our procedure appears to be very effective for computations of weakly bound states and various excited states, including rotationally excited states, i.e. states with \( L \geq 1 \). The efficiency of our procedure is illustrated by computations of the excited \( P^+(L = 1) \)–states in the \( dd\mu, dt\mu \) and \( tt\mu \) muonic molecular ions, \( P(L = 1) \)–states in the non-symmetric \( pd\mu, pt\mu \) and \( dt\mu \) ions and \( ^2\!P(L = 1) \)– and \( ^2\!P(L = 1) \)–states in He atom(s).

PACS: 31.15.ac, 31.15.vj and 36.10.Ee

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In this study we develop a new optimization strategy which is used to construct extremely accurate variational wave functions in arbitrary three-body systems. As follows from the results of numerical computations this procedure is a very effective method to determine highly accurate, bound state wave functions in various three-body atoms, ions, muonic ions, etc. It can be applied not only to ground states, but, in principle, to arbitrary excited states in three-body systems, including very weakly bound states, rotationally and vibrationally excited states, Rydberg states in atoms, etc. Our computational goal in this work is to determine the highly accurate solutions of the corresponding Schrödinger equation for the bound state spectra $H\Psi = E\Psi$, where $E < 0$, and $H$ is the non-relativistic Hamiltonian of an arbitrary three-body system. In particular, for Coulomb three-body systems the Hamiltonian $H$ takes the form

$$H = -\frac{\hbar^2}{2m_a} \left( \frac{m_a}{m_1} \nabla_1^2 + \frac{m_a}{m_2} \nabla_2^2 + \frac{m_a}{m_3} \nabla_3^2 \right) + \frac{q_3q_2e^2}{r_{32}} + \frac{q_3q_1e^2}{r_{31}} + \frac{q_2q_1e^2}{r_{21}}$$

(1)

where $m_1, m_2, m_3$ and $q_1, q_2, q_3$ are the particle masses and charges, respectively. Also, in this equation $\hbar = \frac{h}{2\pi}$ is the reduced Planck constant, $e$ is the electron’s electric charge and $m_a$ is the mass of some elementary particle. Below, we shall use the following units: $\hbar = 1$, $e = -1$ and $m_a = \min(m_1, m_2, m_3) = 1$. Such a choice of units corresponds to the atomic units in the case of atoms/ions, where $m_a = m_e$, and to the muon-atomic units in the case of muonic atoms/ions and muon-molecular ions, where $m_a = m_\mu$. We shall not assume a priori that some particle masses are infinite.

In this work, all solutions of the Schrödinger equation are approximated with the use of a finite set of exponents which explicitly depend upon three relative coordinates $r_{32}, r_{31}$ and $r_{21}$. In the case of bound states with angular momentum $L$ ($L \geq 1$) this exponential ansatz is written in the form

$$\Psi = \frac{1}{2} (1 + \kappa \hat{P}_{21}) \sum_{i=1}^{N} \sum_{\ell_1=0}^{L} C_i(\ell_1) \gamma_{L0}^{(\ell_1,\ell_2)}(n_{32}, n_{31}) \exp(-\alpha_1 r_{32} - \beta_1 r_{31} - \gamma_1 r_{21})$$

(2)

where $r_{ij} = r_{ji}$ are the three relative coordinates, $n_{3i} = \frac{r_{3i}}{r_{3j}} = -n_{3j}$ and $\ell_1 + \ell_2 = L$ (or in some cases $\ell_1 + \ell_2 = L + 1$, see below). The operator $\hat{P}_{21}$ in this equation is the permutation of the two identical (1 and 2) particles, e.g., electrons, muons, nuclei. The parameter $\kappa$ equals zero for non-symmetric three-body systems, while for symmetric three-body systems we have $\kappa = (-1)^L$. The coefficients $C_i$ in Eq.(2) are the linear variational parameters of the method, which are determined by solving the corresponding Schrödinger equation. The
parameters $\alpha_i, \beta_i, \gamma_i$ $(i = 1, \ldots, N)$ in Eq. (2) are the non-linear parameters of the exponential expansion. Also, in Eq. (2) the functions $Y_{LM}^{(\ell_1, \ell_2)}(n_1, n_2)$ are the bi-polar harmonics (see, e.g., [2]). The quantity $L$ is the total angular momentum of the considered bound state in the three-body system, while $M$ is the magnetic quantum number. In the absence of an external magnetic field, all considered bound state properties, including the total energies, cannot depend upon the numerical value of $M$. Therefore, without loss of generality we will assume that $M = 0$ in Eq. (2). The individual angular momenta $\ell_1$ and $\ell_2$ in Eq. (2) are integer, non-negative numbers and their sum equals $L$, since in this work we consider only bound states with natural (spatial) parity.

The variational expansion Eq. (2) and its various modifications (see, e.g., [1], [3]) are extensively used in bound state computations of many different three-body systems. Note that the first numerical computations to use the exponential variational expansion, Eq. (2), were performed in 1968 [4] by Delves and Kalotas for the ground $S(L = 0)$–state of the $pp\mu$ muonic molecular ion. Since that 1968 study [4] the overall efficiency of the exponential variational expansion Eq. (2) has been increased substantially. Currently, this expansion [1], [3] is one of the most effective methods specifically designed for high precision variational calculations of the bound state spectra in arbitrary three-body systems. The very high efficiency of this expansion arises from the advanced optimization strategy used to chose the non-linear parameters in Eq. (2). In general, such a strategy includes the two following stages: (1) construction of highly accurate “short-term” cluster wave function (so-called booster wave function) which includes $N_0 \approx 400 - 600$ exponential basis functions, and (2) optimization of the remaining part of the total wave function which includes $N - N_0 \geq 3000$ exponential basis functions. Optimization of the non-linear parameters in the short-term wave function is performed very carefully and accurately. Analogous optimization of 28 non-linear parameters at the second step of our procedure [1], [5] can be accurate only for relatively small dimensions $N \approx 800 - 1500$. At larger dimensions any careful optimization of non-linear parameters in the total wave function takes a very long time. In [5] we have developed an approximate optimization method for these parameters which was based on a separation of these 28 non-linear parameters into three groups: fast, intermediate and slow parameters depending on the rate of convergence of the optimization. The optimization was performed only for the fast and intermediate non-linear parameters. In general, this procedure works very well. This strategy was successfully used in applications to the Ps$^-$
and H\(^-\) ions, He atoms (ground 1\(^1\)S–state and excited 2\(^3\)S–state) and to many other three-body systems.

In this study our main goal is to consider the rotationally excited bound states, i.e. states with \(L \geq 1\) in three-body systems with arbitrary masses of three particles. To compute these states to high numerical accuracy below we have developed a different idea of approximate optimization of the non-linear parameters at large and very large dimensions. This idea can be illustrated by considering only one non-linear parameter (of 28 such parameters \([1]\)), e.g., the \(A_2\) parameter (all notations used here and below were defined in \([1]\)). In general, the optimal value of this parameter varies when the total number of basis functions increases. In other words, we have a \(A_2(N)\) function, where \(N = N_0 + (N - N_0)\) is the total number of basis functions in Eq.(2). Here we consider the situation when the booster function with \(N_0\) terms has been constructed already, and it does not change at the following steps. Suppose, for simplicity, that \(N_0 = 400\) and at the second stage we need to perform optimization of 28 non-linear parameters by using wave functions with \(N = 800, 1000, 1200\) and 1400 terms. After optimizations at each dimension we obtain four ‘optimal’ values for the \(A_2\) parameter, i.e. \(A_2(800), A_2(1000), A_2(1200)\) and \(A_2(1400)\). As follows from the results of numerical calculations, the overall variations of the \(A_2(N)\) values for \(N = 800, 1000, 1200\) and 1400 are typically relatively small. Therefore, we can determine the approximate limit of the \(A_2(N)\) function for \(N \to \infty\). The projected value \(A_2\), or \(A_2(\infty)\), can be used in actual calculations with large and very large number of basis functions. The same procedure is applied to the 27 remaining non-linear parameters used in our method as described in \([1, 5]\). This gives us the approximate optimal values of all 28 non-linear parameters \(A_1(\infty), A_2(\infty), B_1(\infty), B_2(\infty), \ldots\) needed at the second stage of our method. The overall accuracy achieved at the second stage of our procedure is even better than the approximate procedure in Ref.\([5]\) can provide. Note that in this method we do not neglect any of the non-linear parameters (compare with the ignorance of ‘slow’ non-linear parameters in \([5]\)).

To demonstrate the efficiency of our new procedure for construction of highly accurate wave functions, let us consider its application to the weakly bound \(P^*(L = 1)\)–states in the \(dd\mu, dt\mu\) and \(tt\mu\) muonic molecular ions. Here the notation \(L\) designates the total angular momentum of the three-body system, while the asterisk ‘*’ means that the wave function of this state equals zero for some configuration in relative coordinates \(r_{32}, r_{31}\) and \(r_{21}\). This
classification scheme originated from the one-electron hydrogen atom. In the alternative system of \((L, \nu)\)-notations this state is designated as the \((1,1)\)-state, where \(L = 1\) means ‘rotationally’ excited state and \(\nu = 1\) means ‘vibrationally’ excited state. The alternative classification system for bound states in three-body systems originated from the two-center \(\text{H}_2^+\) ion which is a pure adiabatic (or Born-Oppenheimer) system. Despite some differences in these classification schemes one easily finds a uniform correspondence between the explicit notations used to designate the same bound states in three-body systems. It is well known that the bound \(P^*(L = 1)\) states in the \(dd\mu\) and \(dt\mu\) ions are extremely weakly bound. In general, a state can be considered as weakly bound if its binding energy is \(\leq 1\%\) of its total energy \([7], [8]\); for the \(P^*(L = 1)\) state in the \(dt\mu\) ion the binding energy is less than \(0.01\%\) of its total energy. Highly accurate calculations of such states are very difficult to perform.

Note that each of the \(dd\mu\), \(dt\mu\) and \(tt\mu\) ions is a Coulomb three-body system with unit charges. The general theory of such systems was developed twenty years ago (see, e.g., \([7], [8]\) and references therein). In those works it was shown that the type of bound state spectra in an arbitrary \(a^+b^+\mu^-\) system is determined substantially by the lightest positive ion, e.g., by the \(a^+\) ion, if \(m_a \leq m_b\). Briefly, this means that the binding energies of the \(a^+b^+\mu^-\) and \(a^+a^+\mu^-\) ions are always very close to each other, while their total energies can be substantially different. Moreover, as follows from \([8]\), the binding energy of the \(a^+b^+\mu^-\) ion is always smaller than the binding energy of the \(a^+a^+\mu^-\) ion, if \(m_a \leq m_b\). In application to the muonic molecular ions mentioned above this means that the binding energies of the \(P^*(L = 1)\) states in the \(dd\mu\) and \(dt\mu\) ions are approximately equal to each other. This is a very interesting situation since the total energies of the \(P^*(L = 1)\) states in the \(dd\mu\) and \(dt\mu\) ions are substantially different from each other (the actual difference is \(\approx 60\) eV). Furthermore, since the \(P^*(L = 1)\) state in the \(dd\mu\) ion is weakly bound, then the analogous state in the \(dt\mu\) ion is even more weakly bound. On the other hand, since \(m_t > m_d\), then it is clear that the energy spectrum of the \(tt\mu\) ion is completely different from those of the \(dd\mu\) and \(dt\mu\) ions. In particular, the bound state spectra of the \(tt\mu\) ion contains six (not five!) bound states and the \(P^*(L = 1)\) state of the \(tt\mu\) ion is not weakly bound.

The results of numerical calculations of the \(P^*(L = 1)\) states in the \(dd\mu\), \(dt\mu\) and \(tt\mu\) muonic molecular ions can be found in Table I. In our calculations we have used the following
values of nuclear masses [9], [10]:

\[ m_\mu = 206.268262m_e \quad , \quad m_p = 1836.152701m_e \]  \tag{3}

\[ m_d = 3670.483014m_e \quad , \quad m_t = 5496.92158m_e \]

where \( m_e \) designates the electron mass. All computations are performed in muon-atomic units, where \( m_\mu = 1, \hbar = 1 \) and \( e = 1 \). Note that our highly accurate computations in this study are performed with the use of 84 - 104 decimal digits per computer word [11], [12]. The total energies are determined to the accuracy \( \approx 1 \cdot 10^{-20} - 1 \cdot 10^{-23} \) m.a.u. (or a.u. for atoms). For the purposes of reporting the results of our calculations in this paper, it was assumed that all particle masses and corresponding conversion factors (e.g., the factor \( R_y \) below) are exact. Such assumptions are always made in papers on highly accurate computations in few-body systems (see, e.g., [3], [13]). The known experimental uncertainties in particle masses and conversion factors can be taken into account at the last step of calculations, when the most accurate computation would simply be repeated with the use of particle masses and conversion factors of known or chosen accuracy and the resulting energies reported to to an accuracy commensurate with the accuracy of these masses and conversion factors. A primary motivation for, and advantage of, calculating wave functions of very high accuracy is that relatively small energy differences between states in a given system or between systems can be reliably detected and and calculated, after which the requisite conversion factor can be applied and account taken of its accuracy.

As follows from Table I the total energies obtained for these states are significantly more accurate than analogous energies determined in earlier studies. The \( P^*(L = 1) \)–states in the \( dd\mu \) and \( dt\mu \) ions are of great interest in some applications (see, e.g., [3], [14] and references therein). The binding \( \varepsilon \) and total \( E \) energies of the \( P^*(L = 1) \)–states in the \( dd\mu \) and \( dt\mu \) ions determined from the results shown in Table I are:

\[ E(dd\mu) = -0.4736867338427270 \pm 5 \cdot 10^{-16} \text{m.a.u} \quad , \quad \varepsilon(dd\mu) = -1.974988087997(3) \text{eV} \]  \tag{4}

\[ E(dt\mu) = -0.48199152997385 \pm 5 \cdot 10^{-14} \text{m.a.u} \quad , \quad \varepsilon(dt\mu) = -0.6603386865(3) \text{ eV} \]

where the conversion factor \( R_y = 27.2113961(\frac{m_\mu}{m_e}) \) was used. The binding energies are related to the total energies as \( \varepsilon(dd\mu) = [E(dd\mu) - E(d\mu)]R_y \) and \( \varepsilon(dt\mu) = [E(dt\mu) - E(t\mu)]R_y \), where \( E(d\mu) = -\frac{1}{2} \frac{m_am_\mu}{m_d+m_\mu} \) and \( E(t\mu) = -\frac{1}{2} \frac{m_tm_\mu}{m_t+m_\mu} \) are the total energies of the
ground states in the $d\mu$ and $t\mu$ muonic atoms, respectively. By performing such a re-
calculation from the total energy (expressed in $m.a.u.$) to the binding energy (expressed in
$eV$) we assume that the factor $Ry$ is exact.

Table II contains results of variational computations of the three $P(L = 1)$—states in the
non-symmetric $pd\mu, pt\mu$ and $dt\mu$ muonic molecular ions. These bound states are traditionally
difficult for highly accurate computations. Nevertheless, by using our approach described
above we have determined their total energies to very high accuracy, significantly exceeding
numerical accuracy achieved in earlier calculations. The total energies of three bound $P(L = 1)$—
states in the non-symmetric muonic molecular ions $pd\mu, pt\mu$ and $dt\mu$ are now known
with numerical uncertainties less than $1 \cdot 10^{-15} m.a.u.$ which is sufficient for all practically
important problems which include these ions.

To confirm the efficiency of our method we have also calculated the rotationally excited
$2^1P(L = 1)$— and $2^3P(L = 1)$—states in the $\infty He$, $^3He$ and $^4He$ helium atoms. The total
energies of these states in the $\infty He$, $^3He$ and $^4He$ helium atoms have been computed in a
number of earlier studies (see, e.g., [13], [15], [16]). Our values of the total energies (in
atomic units $\hbar = 1, m_e = 1, e = 1$) of these states can be found in Table III. In calculations
of the $^3He$ and $^4He$ atoms we have used the following values of nuclear masses [9], [10]

$$M_{3He^{2+}} = 5495.8852m_e, \quad M_{4He^{2+}} = 7294.2996m_e$$

Note that our calculations of the $2^1P(L = 1)$— and $2^3P(L = 1)$-states of the helium atoms
have been performed in atomic units. As follows from Table III our total energies determined
for these two states in the helium atoms are substantially more accurate than the total
energies known for these states from the literature.

In conclusion, the results of this study indicate that the exponential variational expa-
sion in relative coordinates, Eq.(2), appears to be the most appropriate expansion for high
precision variational calculations of the bound state spectra in non-relativistic three-body
systems. For an arbitrary Coulomb three-body system (with arbitrary particle masses
$m_1, m_2, m_3$) the approach based on Eq.(2) allows one to obtain extremely accurate (i.e.
essentially exact) numerical solutions for the ground and all excited states, including weakly
bound states and Rydberg states in two-electron atoms [17], [18]. The generalization of
Eq.(2) to the case of adiabatic (or two-center) systems can be found in [19]. To provide a
very high accuracy for the bound states in adiabatic systems, e.g., for $H_2^+$ ion, the non-linear
parameters $\alpha_i, \beta_i, \gamma_i$ in Eq. (2) must be complex, i.e. they must have non-zero imaginary parts. It is also important to note that numerical accuracy of such solutions can be made arbitrarily high, e.g., by using more advanced optimization strategies for actual non-nonlinear parameters. The highly accurate wave functions obtained in this study are needed to determine many bound state properties of muonic molecular ions to the accuracy which will be sufficient for current experimental capabilities. In particular, the knowledge of highly accurate variational wave functions is extremely important for weakly-bound $P^*(L = 1)$–states in the $dt\mu$ and $dd\mu$ muonic molecular ions. In addition, there is a need for the prediction of the lowest order relativistic, QED, and mass corrections to the total non-relativistic energy in arbitrary three-body systems and the computational results for such corrections depend sensitively on the accuracy of the “zeroth-order” wave function.

Acknowledgements

It is a pleasure to thank David H. Bailey (Lawrence Berkeley National Laboratory, Berkeley, California) for his valuable help and discussions and the University of Western Ontario for financial support.
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TABLE I: The total energies $E$ of the excited $P^*(L = 1)$–states (or $(1,1)$-states) in the $dd\mu, tt\mu$ 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).

| $N$ | $E(dd\mu; (1,1)–state)$ | $E(tt\mu; (1,1)–state)$ | $E(dt\mu; (1,1)–state)$ |
|-----|------------------------|------------------------|------------------------|
| 3300 | -0.473 686 733 842 725 810 43 | -0.489 908 667 504 942 696 78 | -0.481 991 529 973 471 68 |
| 3500 | -0.473 686 733 842 725 998 08 | -0.489 908 667 504 942 819 82 | -0.481 991 529 973 590 96 |
| 3700 | -0.473 686 733 842 726 125 12 | -0.489 908 667 504 942 935 53 | -0.481 991 529 973 677 08 |
| 3800 | -0.473 686 733 842 726 218 22 | -0.489 908 667 504 942 980 54 | -0.481 991 529 973 697 42 |
| 3840 | -0.473 686 733 842 726 242 81 | -0.489 908 667 504 942 990 80 | -0.481 991 529 973 715 97 |
| $A^a$ | -0.473 686 733 842 727 0(5) | -0.489 908 667 504 943 30(8) | -0.481 991 529 973 85(5) |
| $E^b$ | -0.473 686 733 842 720 3 [3] | -0.489 908 667 504 943 3 [1] | -0.481 991 529 971 713 [3] |

$^a$The expected energies with estimated uncertainties.

$^b$The best variational energies known from earlier calculations.

TABLE II: The total energies $E$ of the $P(L = 1)$–states (or $(1,0)$-states) in the $pd\mu, pt\mu$ 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).

| $N$ | $E(pd\mu; (1,0)–state)$ | $E(pt\mu; (1,0)–state)$ | $E(dt\mu; (1,0)–state)$ |
|-----|------------------------|------------------------|------------------------|
| 3300 | -0.490 664 169 479 316 12 | -0.499 492 029 991 533 40 | -0.523 191 456 315 954 69 |
| 3500 | -0.490 664 169 479 320 24 | -0.499 492 029 991 534 83 | -0.523 191 456 315 955 64 |
| 3700 | -0.490 664 169 479 323 29 | -0.499 492 029 991 535 83 | -0.523 191 456 315 956 51 |
| 3840 | -0.490 664 169 479 324 78 | -0.499 492 029 991 536 26 | -0.523 191 456 315 957 14 |
| $A^a$ | -0.490 664 169 479 327(1) | -0.499 492 029 991 539(1) | -0.523 191 456 315 960(1) |
| $E^b$ | -0.490 664 169 479 315 [1] | -0.499 492 029 991 513 [1] | -0.523 191 456 315 937 14 [1] |

$^a$The expected energies with estimated uncertainties.

$^b$The best variational energies known from earlier calculations.
TABLE III: The total energies $E$ (in atomic units $m_e = 1, \hbar = 1, e = 1$) for the $2^1P(L=1)-$ and $2^3P(L=1)-$states in the $^\infty$He atom. $N$ designates the number of basis functions used in Eq.(2).

| $N$  | $2^1P(L=1)-$state     | $2^3P(L=1)-$state     |
|------|-----------------------|-----------------------|
| 3500 | -2.123 843 086 498 101 358 895 90 -2.133 164 190 779 283 205 057 11 |
| 3800 | -2.123 843 086 498 101 358 970 11 -2.133 164 190 779 283 205 079 75 |
| 4000 | -2.123 843 086 498 101 359 030 07 -2.133 164 190 779 283 205 092 36 |
| 4200 | -2.123 843 086 498 101 359 074 18 -2.133 164 190 779 283 205 102 51 |

$A^a$ -2.123 843 086 498 101 359 20(5) -2.133 164 190 779 283 205 17(5)

$E^b$ -2.123 843 086 498 101 360(2) [16] -2.133 164 190 779 283 206(2) [16]

$E^b$ -2.123 843 086 498 093(2) [13] -2.133 164 190 779 273(5) [13]

$E^c(^3\text{He})$ -2.123 448 345 012 547 695 33 -2.132 787 874 710 055 466 03

$E^c(^4\text{He})$ -2.123 553 590 529 057 856 32 -2.132 880 642 105 551 984 62

$^a$The expected energies with estimated uncertainties.

$^b$The best variational energies known from earlier calculations.

$^c$Results obtained for $N = 3800.$