Calculations of the $1s_\mu 2s_e$-electron-excited $S(L=0)$ states in helium-muonic atoms

Alexei M. Frolov
Department of Chemistry, Queen's University, Kingston, Ontario, Canada K7L 3N6
(Received 30 May 2001; revised manuscript received 10 September 2001; published 15 January 2002)

The bound-state energies and other properties are determined to high accuracy for the ground and first electron-excited $S(L=0)$ states in the $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ helium-muonic atoms. Such highly accurate calculations are performed with the use of an advanced, recently developed, multibox variational approach. In particular the hyperfine splitting has been calculated for the $1s_\mu 2s_e$-electron-excited states in both helium-muonic atoms. The corresponding hyperfine splittings for these states are $\approx$520.786 MHz ($^3He^{2+}\mu^-e^-$) and $\approx$558.055 MHz ($^4He^{2+}\mu^-e^-$). The analogous splittings for the ground states are $\Delta\nu(^3He^{2+}\mu^-e^-)\approx 4166.393$ MHz and $\Delta\nu(^4He^{2+}\mu^-e^-)\approx 4464.555$ MHz, respectively.

DOI: 10.1103/PhysRevA.65.024701 PACS number(s): 36.10.Dr

In this Brief Report we report the results of highly accurate calculations for the bound, electron-excited $S(L=0)$ states (or $1s_\mu 2s_e$ states, for short) in the helium-muonic $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms. Such calculations are performed with the use of our recently developed, multibox variational approach [1]. Our main goal is to determine the bound-state properties and hyperfine splitting for these electron-excited states in both helium-muonic atoms. Note that recently significant progress has been made in our understanding of basic geometrical and dynamical properties of the $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms in their ground states [2–8]. In particular, in [8] the expectation values for the electron-nucleus $\langle\delta(\mathbf{r}_{e^-He})\rangle$ and electron-muonic delta functions $\langle\delta(\mathbf{r}_{e^-\mu^-})\rangle$ have been determined to very high accuracy. In fact, the absolute errors for these expectation values were less than 1×10^{-7} a.u. By using both $\langle\delta(\mathbf{r}_{e^-He})\rangle$ and $\langle\delta(\mathbf{r}_{e^-\mu^-})\rangle$ expectation values, we determined in [8] the hyperfine splitting for the ground states in both helium-muonic atoms. The appropriate computational results for the hyperfine splitting are 4166.392 MHz for the $^3He^{2+}\mu^-e^-$ atom and 4464.555 MHz for the $^4He^{2+}\mu^-e^-$ atom [8]. The absolute errors in both cases are less than 1 kHz. Moreover, these figures are very close to the known experimental values for these atoms, which equal 4166.41 MHz and 4464.95 MHz, respectively (see references and discussions in [2,4]).

However, the recent progress is quite modest for the bound, electron-excited $1s_\mu 2s_e$ states in the helium-muonic systems. Indeed, the total energies for these states are known only approximately [7], i.e., with relatively large errors. An analogous situation can be found for a number of bound-state properties in the $1s_\mu 2s_e$ states in the helium-muonic atoms. Furthermore, in [7] we estimated the hyperfine splitting for these excited states as 527.8 MHz ($^3He^{2+}\mu^-e^-$) and 570.3 MHz ($^4He^{2+}\mu^-e^-$). Our present results indicate clearly that these results from [7] were determined with absolute errors $\geqslant$ 10 MHz (see below). The main source of such large errors is obvious, since the expectation values of the electron-nucleus and muon-electron δ functions were computed [7] only approximately. Presently, our results for all bound-state properties in the helium-muonic atoms, including δ functions, have been improved significantly. Finally, now we can predict the hyperfine splittings for the electron-excited $1s_\mu 2s_e$ states in the helium-muonic atoms to the accuracy $\approx$0.5–1 kHz (comparable with the accuracy obtained for the ground states in these systems). In fact, for the electron-excited states the hyperfine splitting has never been measured. However, it can be done, e.g., by using the technique used for the ground $1s_\mu 1s_e(L=0)$ states.

The main computational problem here is related with the fact that our approach [8] was not very effective for the excited states. Later, however, an advanced, relatively simple and reliable approach has been developed and tested for many three-body systems [1]. This approach works very successfully for an arbitrary state (excited or ground) in various three-body systems, including so-called adiabatic systems such as the H_2^+ ion. Moreover, it was found that the later approach produces significantly more accurate wave functions than is possible by using competitive methods [1]. In particular, by using this approach we finally solved the long-standing problem of highly accurate determination of the weakly bound (1,1) states in the $dd\mu$ and $dt\mu$ muonic molecular ions [1]. Presently, the same approach [1] is applied to study the helium-muonic $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms in their $1s_\mu 2s_e$-electron-excited $S(L=0)$ states.

For the $S(L=0)$ states in an arbitrary Coulomb three-body system, the trial variational wave function is represented in the form (the general case is discussed in [1])

$$\psi_{LM}=(1+\kappa P_{12})\sum_{i=1}^{N} C_i \exp(-\alpha_i u_1-\beta_i u_2-\gamma_i u_3), \quad (1)$$

where C_i are the linear (or variational) parameters, α_i, β_i, and γ_i are the real nonlinear parameters. The parameter κ equals zero identically for nonsymmetric three-body systems. For symmetric systems $\kappa=1$ for the singlet states and $\kappa=-1$ for the triplet states. Such choices of κ correspond to the cases when the spatial part of the total wave functions is symmetric and antysymmetric, respectively. The operator P_{12} permutes the identical particles (1 and 2) in the symmetric systems. Also, in Eq. (1) u_1, u_2, and u_3 are the three perimetric coordinates (see, e.g., [1]). These three-coordinates are expressed as the linear combinations of the relative coordinates $u_i=\frac{1}{2}(r_{ik}+r_{ij}-r_{jk})$, where $(i,j,k)=(1,2,3)$. Here, $r_{ij}=|\vec{r}_i-\vec{r}_j|$ are the three interparticle distances ($r_{ij}=r_{ji}$). The inverse relation between u_1, u_2, u_3

and r_{32}, r_{31}, r_{21} takes a very simple form $r_{ij}=u_i+u_j$, where $i\neq j=(1,2,3)$. The use of three perimetric coordinates u_1, u_2, and u_3 instead of the relative r_{32}, r_{31}, r_{21} coordinates is an obvious advantage of the later approach [1]. This follows from the fact that the perimetric coordinates are truly independent, and each of them varies from 0 to $+\infty$. This means that all nonlinear parameters in Eq. (1) are positive real numbers. The optimization of such nonlinear parameters in Eq. (1) can be performed very effectively, since there are no additional conditions for these parameters. In contrast with this, if the relative coordinates are used in Eq. (1), then a number of additional conditions must be obeyed, which are needed to guarantee convergence of all essential integrals. Obviously, in this case the optimization of the nonlinear parameters cannot be very effective.

The main improvement in [1] has been done in the optimization of the nonlinear parameters in Eq. (1). Note that an actual variational (trial) wave function may include a few thousand nonlinear parameters (see, e.g., below). Obviously, their detail optimization cannot be completed at realistic times. In [8], for each of the considered systems, we optimized carefully only a small part Ψ_1 of the total wave function. Usually, such a small (or cluster) part contains only a few hundred nonlinear parameters. This is the first step of the procedure [8] that generates the so-called booster function $\Psi_1(N_0)$, where N_0 is the number of basis functions used to construct Ψ_1. Note that in the present case each of the basis functions contains only three nonlinear parameters. For constructing the second stage function $\Psi_2(N-N_{ij})$ in [8] we used a quasirandom choice [9,10] of the nonlinear parameters from one parallelotop (or box). The boundaries of such a parallelotop are chosen from the results of separate calculations and later they never changed. Obviously, in this case the second-stage wave function $\Psi_2(N-N_0)$ is not an optimal variational supplement to the initial booster function $\Psi_1(N_0)$.

In contrast with this, in [1] the choice of nonlinear parameters in the variational wave function is performed from a few different parallelotops (or boxes). The boundaries of these boxes are the real nonlinear parameters of the method. By varying these and a few additional scaling parameters one can obtain significantly better (i.e., lower) variational energies, than have been determined for the considered three body systems with the use of any other method [1]. This approach has been called [1] the multibox strategy for choosing the nonlinear parameters in the three-body bound-state wave functions. In fact, in [1] the three parallelotops have been used for each of the considered systems. It can be shown that now the second-stage wave function $\Psi_2(N-N_0)$ is an optimal supplement to the given booster function $\Psi_1(N_0)$. Note also, that the procedure proposed in [1] works very well even in the case when $N_0=0$, i.e., when no booster function $\Psi_1(N_0)$ has been constructed.

To illustrate the efficiency of this approach presently we performed highly accurate, variational calculations for the $2\ ^3S(L=0)$ state in the $^\infty$He atom. The total energies for this system (in atomic units $m_c=1$, $\hbar=1$, and $e=1$) can be found in Table I. Presently, for simplicity, we apply the same three-box version of the procedure [1]. The total number of nonlinear parameters in this version equals 28. These 28 nonlinear parameters have been optimized with the use of 1000 basis functions in each of the trial wave functions. The observed convergence for the variational results on N is extremely high. Finally, we could determine at least four additional significant figures for the total energy of the $2^3S(L=0)$ state in the $^\infty$He atom in comparison with the results of previous calculations (except [1] where the same method was used). In fact, our present approach [1] allows one to reproduce as many exact significant figures in the total energy as needed. Below, the same approach is used to perform highly accurate calculations for the $1s_\mu 2s_e$-electron-excited $S(L=0)$ states in the helium-muonic atoms.

TABLE I. The convergence of the total energies E in atomic units for the $2\ ^3S(L=0)$ state in the $^\infty$He atom.

N[a]	E
1000	−2.175 229 378 236 791 305 733 900
1800	−2.175 229 378 236 791 305 738 718
2000	−2.175 229 378 236 791 305 738 805
2250	−2.175 229 378 236 791 305 738 866
2400	−2.175 229 378 236 791 305 738 891
E[b]	−2.175 229 378 236 791 305 738 4

[a]The number of basis functions used in calculations.
[b]The best results determined in previous calculations [1].

The results of numerical calculations for the ground and first electron-excited $S(L=0)$ states of the helium-muonic atoms are presented in Tables II–IV. Table II contains variational energies for the both $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms in the ground and first electron-excited $S(L=0)$ states. Our present calculations have been performed in atomic units ($\hbar=1$, $m_e=1$, and $e=1$). In these units the following values for the particle masses [11,12]

$$m_\mu=206.768\,262, \quad M_{^3He^{2+}}=5495.8852,$$

$$M_{^3He^{2+}}=7294.2996$$

were used in calculations. The numerical values for other physical constants used in our present calculations (for more detail, see [8]) have also been chosen from [11,12]. To recalculate the energies from a.u. to MHz, the conversion factor $6.579\,683\,920\,61\times10^9$ [11] has been used.

The energies from Table II are significantly more accurate than the values from previous calculations for the helium-muonic atoms. In particular, the energies obtained for $N=700$ basis functions are better than the corresponding energies from [8] computed with $N=2500$ basis functions. In fact, by using the method [1] one can easily increase the overall accuracy and determine the next six to ten significant figures for the total energies in both helium-muonic atoms. However, this step will certainly require extensive computational resources. For our present purposes, however, it is important to note that a very high convergence rate for results presented in Table II allows us to stabilize 20–21 significant figures in the final energies. The convergence for the

TABLE II. The convergence of the total energies in atomic units for the first electron-excited $1s_\mu 2s_e$ states (*) and ground $1s_\mu 1s_e$ states in the helium-mounic atoms.

N[a]	$(^3He^{2+}\mu^- e^-)$*	$(^4He^{2+}\mu^- e^-)$*
700	−398.66739108745739419922	−402.26230156525181323033
1000	−398.66739108745739433625	−402.26230156525181346636
2100	−398.66739108745739439414	−402.26230156525181353478
2300	−398.66739108745739439590	−402.26230156525181353673
2500	−398.66739108745739439767	−402.26230156525181353867
	−398.66739108745739[b]	−402.2623015652484[b]
N[a]	$^3He^{2+}\mu^- e^-$	$^4He^{2+}\mu^- e^-$
700	−399.04233683286253333860	−402.63726303513545316784
1000	−399.04233683286253433727	−402.63726303513545383910
2100	−399.04233683286253474368	−402.63726303513545399718
2300	−399.04233683286253475716	−402.63726303513545400209
2500	−399.04233683286253476960	−402.63726303513545400481
	−399.04233683286252384[b]	−402.63726303513544403[b]

[a]The number of basis functions used in calculations.
[b]The best results determined in previous calculations [1].

electron-muon and electron-nucleus δ-function expectation values is shown in Table III. However, in contrast with the energy, there is no bound principle for the expectation values of δ functions. This means that the observed convergence for the δ functions differs qualitively from the convergence for the energies shown in Table II. The expectation values for some selected geometrical and dynamical properties [13] can be found in Table IV (for the excited states in the helium-muonic atoms). The presently obtained values are also significantly more accurate than values known from previous calculations (see, e.g., [7]).

By using the numerical values for the expectation values of the δ functions presented in Table III, one can evaluate the hyperfine splitting for the $1s_\mu 2s_e$-electron-excited and $1s_\mu 1s_c$ ground states in the helium-muonic atoms. The formulas for the hyperfine splitting in the $S(L=0)$ states of the helium-muonic atoms takes the form (for more details see, e.g., [4], [8], and also [14])

$$\Delta\nu(^3He^{2+}\mu^{-1}e^{-1}) = 10\,671.885\,079\,542\langle\delta(\mathbf{r}_{e^-\mu^-})\rangle + 2553.907\,751\,447\,6\langle\delta(\mathbf{r}_{e^-\mathrm{He}})\rangle\ \mathrm{MHz}, \quad (2)$$

$$\Delta\nu(^4He^{2+}\mu^- e^-) = 14\,229.180\,061\,055\langle\delta(\mathbf{r}_{e^-\mu^-})\rangle\ \mathrm{MHz},$$

where $\langle\delta(\mathbf{r}_{e^-\mu^-})\rangle$ and $\langle\delta(\mathbf{r}_{e^-\mathrm{He}})\rangle$ are the expectation values for the electron-muonic and electron-nucleus δ functions, respectively. The expectation values of all δ functions in Eqs. (2) are expressed in atomic units.

TABLE III. Convergence of the expectation values of electron-muon and electron-nucleus δ function in atomic units for the ground $1s_\mu 1s_e$ states and first electron-excited $1s_\mu 2s_e$ states (*) in the helium-muonic atoms.

$\langle\delta(\vec{r}_{e^-\mu})\rangle$	$^3He^{2+}\mu^- e^-$	$^4He^{2+}\mu^- e^-$	$(^3He^{2+}\mu^- e^-)$*	$(^4He^{2+}\mu^- e^-)$*
700	3.136822003×10^{-1}	3.137605001×10^{-1}	3.920926498×10^{-2}	3.921904111×10^{-2}
1000	3.136822039×10^{-1}	3.137604985×10^{-1}	3.920926450×10^{-2}	3.921904512×10^{-2}
2100	3.136822638×10^{-1}	3.137605176×10^{-1}	$3.9209272050\times10^{-2}$	3.921905192×10^{-2}
2300	3.136822683×10^{-1}	3.137605208×10^{-1}	$3.9209272609\times10^{-2}$	3.921905287×10^{-2}
2500	3.136822749×10^{-1}	3.137605249×10^{-1}	$3.9209273406\times10^{-2}$	3.921905359×10^{-2}
$\langle\delta(\vec{r}_{e^-\mathrm{He}})\rangle$	$^3He^{2+}\mu^- e^-$	$^4He^{2+}\mu^- e^-$	$(^3He^{2+}\mu^- e^-)$*	$(^4He^{2+}\mu^- e^-)$*
700	3.206114051×10^{-1}	3.206317249×10^{-1}	4.007557170×10^{-2}	4.007810900×10^{-2}
1000	3.206114583×10^{-1}	3.206317390×10^{-1}	4.007557843×10^{-2}	4.007810779×10^{-2}
2100	3.206115016×10^{-1}	3.206317709×10^{-1}	4.007558304×10^{-2}	4.007811562×10^{-2}
2300	3.206115015×10^{-1}	3.206317724×10^{-1}	4.007558297×10^{-2}	4.007811613×10^{-2}
2500	3.206115086×10^{-1}	3.206317726×10^{-1}	4.007558391×10^{-2}	4.007811668×10^{-2}

TABLE IV. The expectation values (in atomic units) of some properties for the first electron-excited S states ($L=0$) of the $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms. Below, the subscript 3 designates the helium nucleus, 2 stands for muon, and 1 denotes the electron.

System	$^3He^{2+}\mu^-e^-$	$^4He^{2+}\mu^-e^-$
$\langle r_{21}^{-1}\rangle$	0.249 959 239 476 657	0.249 969 739 782 088 733
$\langle r_{31}^{-1}\rangle$	0.249 961 061 388 004	0.249 971 551 933 312
$\langle r_{32}^{-1}\rangle$	398.542 409 645 807	402.137 314 883 210
$\langle \delta(\vec{r}_{32})\rangle$	2.0149939956×10^7	2.0700138478×10^7
$\langle \delta(\vec{r}_{321})\rangle$	8.0173240×10^5	8.2372867×10^5
$\langle -\frac{1}{2}\nabla_1^2\rangle$	0.124 961 160 140 246	0.124 971 647 880 655
$\langle -\frac{1}{2}\nabla_2^2\rangle$	$7.94\ 180\ 263\ 037\ 479\times10^4$	$8.08\ 572\ 101\ 067\ 646\times10^4$
$\langle (r_{31}r_{32})^{-1}\rangle$	99.6 200 394 831 515 5	100.522 844 889 408 4
$\langle (r_{31}r_{21})^{-1}\rangle$	0.249 000 723 411 012 4	0.249 029 798 384 398 0

Finally, the corresponding hyperfine splittings for the electron-excited $1s_\mu 2s_e$ states are $\approx$520.786 MHz ($^3He^{2+}\mu^-e^-$) and $\approx$558.055 MHz ($^4He^{2+}\mu^-e^-$). The analogous splittings for the ground $1s_\mu 1s_e$ states are $\Delta\nu(^3He^{2+}\mu^-e^-)\approx4166.393$ MHz and $\Delta\nu(^4He^{2+}\mu^-e^-)\approx4464.555$ MHz respectively. These values are very accurate (their uncertainties are less than 1 kHz). For the electron-excited $1s_\mu 2s_e$ states these values correct our previous results for the hyperfine splittings in both helium-muonic atoms by $\approx$7 MHz ($^3He^{2+}\mu^-e^-$ atom) and by $\approx$12 MHz ($^4He^{2+}\mu^-e^-$ atom), respectively. The computational results for the ground states are very close to the experimentally known values $\Delta\nu(^3He^{2+}\mu^-e^-)\approx4166.41$ MHz and $\Delta\nu(^4He^{2+}\mu^-e^-)\approx4464.95$ MHz, respectively (see, e.g., discussion in [8] and references therein). The future experimental figures for the electron-excited $1s_\mu 2s_e$ states in both helium-muonic atoms are also expected to be close to the presently computed values. Further deviations for the helium-muonic atoms ($\approx$0.02–0.5 MHz) can be explained by considering the relativistic and quantum-electrodynamics (radiative) corrections [15,16]. Analysis of such corrections require a separate discussion. Now, we want to note only that the results of these high-precision measurements of the hyperfine splitting for both the helium-muonic atoms $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ (in their ground and electron-excited states) are of paramount importance for providing further progress in theoretical studies of such systems. Hopefully, our work will stimulate further experimental activity to perform high-precision measurements for the hyperfine splitting and other properties in the helium-muonic atoms.

It is a pleasure to thank the Natural Sciences and Engineering Research Council of Canada for financial support.

[1] A. M. Frolov, Phys. Rev. E **64**, 036704 (2001).
[2] S. D. Lakdawala and P. J. Mohr, Phys. Rev. A **22**, 1572 (1980); **24**, 2224 (1981).
[3] K. N. Huang and V. W. Hughes, Phys. Rev. A **20**, 706 (1979); **21**, 1071(E) (1980); **26**, 2330 (1982).
[4] R. J. Drachman, J. Phys. B **14**, 2733 (1981); **16**, L749 (1983).
[5] M. K. Chen and C. S. Hsue, J. Phys. B **22**, 3951 (1989); Phys. Rev. A **40**, 5520 (1989); **42**, 1830(E) (1990); **45**, 1479 (1992).
[6] M. K. Chen, J. Phys. B **22**, 4041 (1990); **26**, 2263 (1993).
[7] V. H. Smith, Jr. and A. M. Frolov, J. Phys. B **28**, 1357 (1995); **29**, 5969 (1996).
[8] A. M. Frolov, Phys. Rev. A **61**, 022509 (2000); Phys. Rev. E **62**, 8740 (2000).
[9] A. J. Thakkar and V. H. Smith, Jr., Phys. Rev. A **15**, 1 (1977).
[10] A. M. Frolov and V. D. Efros, Pis'ma Zh. Eksp. Teor. Fiz. **39**, 544 (1984) [JETP Lett. **39**, 449 (1984)]; J. Phys. B **18**, L265 (1985).
[11] E. R. Cohen and B. N. Taylor, Phys. Today **53** (8), BG11 (2000).
[12] *CRC Handbook of Chemistry and Physics*, 78th ed., edited by D. R. Lide (CRC Press, Boca Raton, FL, 1998).
[13] Highly accurate expectation values for other bound-state properties in the helium-muonic atoms (the ground and first electron-excited states) can be obtained from the author.
[14] C. L. Schwartz, Phys. Rev. **97**, 380 (1955).
[15] S. J. Brodskiy and G. W. Erickson, Phys. Rev. **148**, 26 (1966).
[16] E. Borie, Z. Phys. A **291**, 107 (1979).