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Bound state properties of the ground states in the DT^{+} and T_2^{+} ions

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Recently developed multibox approach [A.M. Frolov, Phys. Rev. E **64**, 036704 (2001)] is used to construct highly accurate, bound state wave functions for the ground states in the heavy adiabatic ions DT^{+} and T_2^{+}. The computed variational energies and bound state properties have significantly higher accuracy than results known from earlier computations. Nevertheless, the computed and predicted nucleus-nucleus cusp and nucleus-nucleus δ function differ significantly even for the highly accurate wave functions used in this study.

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In this paper we report highly accurate results for the ground states in the heavy adiabatic ions DT^{+} and T_2^{+}. These ions are of great interest in various applications that are mainly related with the nuclear (d,t) fusion and β^{-} decay of tritium nuclei. Computation of the corresponding final state probabilities requires the knowledge of the initial bound state wave functions. Presently, to determine the bound state spectra in these systems we apply the exponential variational expansion in the relative coordinates combined with our recently developed multibox approach for choosing the nonlinear parameters [1]. Note that this approach does not use any of the Born-Oppenheimer (or adiabatic) approximations [2]. In general, all nonadiabatic methods are not very successful for performing highly accurate, bound state calculations in the heavy adiabatic ions, such as DT^{+} and T_2^{+}. In particular, the observed convergence rate and numerical stability of the computed results are significantly lower for heavy adiabatic ions, than for light adiabatic ions, e.g., for the H_2^{+} and HD^{+} ions. A closely related problem is to explain the observed huge differences between computed and expected nuclear-nuclear contact properties [3] in the heavy adiabatic ions. For instance, it was found in Ref. [4] that the computed and actual values for the tritium-tritium δ function in the T_2^{+} ion differ from each other by ≈ 33 orders of magnitude. Analogous deviations were also detected for the nuclear-nuclear cusp and three-particle δ function. In fact, for the heavy adiabatic ions such deviations are maximal. Note that all other bound state properties in the adiabatic three-body ions can be determined to a high accuracy. Such properties include energies, all electron-nuclear expectation values, and many nuclear-nuclear expectation values. But the presence of unexplained and very large differences between the computed and actual nuclear-nuclear contact properties [3] devaluates our approach [5] developed originally for the adiabatic ions.

Unfortunately, at the present time we cannot explain why the exponential variational expansion produces such poor results for the contact nuclear-nuclear properties in the adiabatic systems. In fact, this question requires a further investigation. But, in this study we provide some arguments that can be useful for choosing the correct explanation. Indeed, it is shown below that by increasing the accuracy of trial wave functions one can drastically improve the observed agreement between the computed and predicted contact nucleus-nucleus properties. This indicates clearly that currently observed deviations for the contact properties are not fundamental and can be eliminated completely by developing the next generation of more effective and better convergent variational methods.

Presently, we want to improve significantly the overall accuracy of the variational wave functions used for bound state calculations of the adiabatic ions. This means that such wave functions must provide highly accurate results not only for the bound state energies, but also for other bound state properties in the heavy adiabatic ions DT^{+} and T_2^{+}. In fact, it is shown below that the main troubles for these ions are related with the contact nuclear-nuclear properties, rather than with the highly accurate energy determination. Note that the considered DT^{+} and T_2^{+} ions are the Coulomb three-body systems with unit charges. The nonrelativistic Hamiltonian for an arbitrary Coulomb three-body system can be written in the following form:

$$H=-\frac{1}{2m_1}\nabla_1^2-\frac{1}{2m_2}\nabla_2^2-\frac{1}{2m_3}\nabla_3^2+\frac{q_3q_2}{r_{32}}+\frac{q_3q_1}{r_{31}}+\frac{q_2q_1}{r_{21}}, \tag{1}$$

where atomic units ($\hbar=1, e=1$ and $m_e=1$) are used. In this equation q_1, q_2, q_3 are the particle charges, while m_1, m_2, m_3 are their masses. In fact, in all formulas below the subscripts 1 and 2 represent the two heavy nuclei, while the subscript 3 corresponds to the electron (light particle). Furthermore, in this study only atomic units are used. In atomic units for the considered adiabatic ions we have $q_1=q_2=+1$, $q_3=e^{-}=-1$, $m_3=m_e=1$ and $\min(m_1,m_2)\gg m_3=1$. Presently, for the nuclei of hydrogen isotopes the following masses $m_d=3670.483014m_e$ and $m_t=5496.92158m_e$ are used [6].

Our main computational goal in this study is to determine (to a high accuracy) the bound states of the corresponding Schrödinger equation $(H-E)\Psi=0$, where H is the Hamiltonian from Eq. (1) and $E(E<0)$ is its eigenvalue. The determined wave functions are used to perform highly accurate computations of various bound state properties. Presently, to determine the bound state energies and corresponding wave functions we apply an improved version of the exponential variational expansion [1]. The general form of such an expansion is discussed in Ref. [1]. Below, however, we restrict ourselves to the study of the ground $S(L=0)$ states in the

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DT^{+} and T_2^{+} ions. For these states the exponential variational expansion can be written in the form

$$\Psi = \frac{1}{2}(1+\kappa\hat{P}_{21})\sum_{i=1}^{N} C_i \exp(-\alpha_i u_1 - \beta_i u_2 - \gamma_i u_3) \times \exp(\imath\,\delta_i u_1 + \imath\, e_i u_2 + \imath\, f_i u_3), \tag{2}$$

where u_1, u_2, and u_3 are the truly independent perimetric coordinates $(0 \leqslant u_i < +\infty)$. These three coordinates are simply related to the three relative (or interparticle) coordinates $r_{ij} = |\vec{r}_i - \vec{r}_j|$:

$$u_i = \frac{1}{2}(r_{ik} + r_{ij} - r_{jk}),$$

where $r_{ij} = r_{ji}$ and $i \neq j \neq k = (1,2,3)$ [1]. In Eq. (2) the operator $\hat{P}_{21}$ is the permutation of the two identical (1 and 2) particles in the symmetric systems, where $\kappa = \pm 1$, otherwise $\kappa = 0$ (e.g., for the DT^{+} ion). In fact, for the ground state of the T_2^{+} ion $\kappa = +1$. Also, in Eq. (2) $\imath$ is the imaginary unit, C_i are the linear (variational) parameters, and $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i$, and f_i are the $6N$ nonlinear parameters ($i = 1, \ldots, N$) and N is the total number of basis functions used in calculations. The simple conditions $\alpha_i > 0, \beta_i > 0$, and $\gamma_i > 0$ (for $i = 1, \ldots, N$) must be obeyed to guarantee the convergence of all integrals needed in computations. In actual computations the central part of the solution is an optimal choice of these $6N$ nonlinear parameters $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i$, and f_i ($i = 1, \ldots, N$) in the trial wave functions in Eq. (2). Recently, we proposed (see, e.g., Ref. [1] and references therein) a few different strategies for optimization of these nonlinear parameters. In particular, in this study, we apply our multibox strategy, which was developed in Ref. [1] and effectively used for highly accurate calculations in various three-body systems.

The basic ideology of the multibox approach is described in detail in Ref. [1]. This work also contains a brief history of its invention. Presently, we do not want to repeat all arguments used in Ref. [1] to explain numerous advantages of the multibox approach. Note only, that this approach has been developed to perform high precision, variational, bound state calculations for arbitrary three-body systems. In this approach the nonlinear parameters $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i$, and f_i ($i = 1, 2, \ldots, N$) in Eq. (2) are chosen quasirandomly from a few (up to 10) different six-dimensional boxes $\mathcal{B}_1, \mathcal{B}_2, \ldots, \mathcal{B}_{10}$. Since these $6N$ parameters $[\alpha_i, \beta_i, \gamma_i, \delta_i, e_i$, and f_i $(i = 1, 2, \ldots, N)]$ are not varied in the procedure, they are not real nonlinear parameters of the method. These parameters are usually called either the lattice points, or quadrature points. In contrast with $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i$, and f_i ($i = 1, 2, \ldots, N$), the geometrical sizes and positions of the mentioned six-dimensional boxes $\mathcal{B}_1, \mathcal{B}_2, \ldots, \mathcal{B}_{10}$ are optimized, i.e., they are the actual nonlinear parameters of the method. Furthermore, there are also a few scaling parameters, which are optimized for each step (or each pass) of the procedure. These parameters are used to find a proper balance between different parts of the trial function [1].

Let us present the following simplified version of the procedure. The simplification means the use of the three-box version and restriction to the four scaling parameters. This means that only three six-dimensional boxes $\mathcal{B}_1, \mathcal{B}_2$ and $\mathcal{B}_3$ are used in our present calculations. The choice of the nonlinear parameters in Eq. (2) proceeds as follows. Let i be the number (or index) of the basis function in Eq. (2) $(1 \leqslant i \leqslant N)$ and $k = \mathrm{mod}(i,3) + 1$, where $\mathrm{mod}(i,3)$ designates the modular division (i.e., an integer remainder after division of i by 3). Now, the parameters $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i$, and f_i are chosen quasirandomly from the six intervals $[A_1^{(k)}, A_2^{(k)}], [B_1^{(k)}, B_2^{(k)}], [G_1^{(k)}, G_2^{(k)}], [D_1^{(k)}, D_2^{(k)}], [E_1^{(k)}, E_2^{(k)}]$, and $[F_1^{(k)}, F_2^{(k)}]$:

$$\alpha_i = \left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{2} \right\rangle\right\rangle (A_2^{(k)} - A_1^{(k)}) + A_1^{(k)}, \tag{3}$$

$$\beta_i = \left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{3} \right\rangle\right\rangle (B_2^{(k)} - B_1^{(k)}) + B_1^{(k)}, \tag{4}$$

$$\gamma_i = \left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{5} \right\rangle\right\rangle (G_2^{(k)} - G_1^{(k)}) + G_1^{(k)}, \tag{5}$$

$$\delta_i = \left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{7} \right\rangle\right\rangle (D_2^{(k)} - D_1^{(k)}) + D_1^{(k)}, \tag{6}$$

$$e_i = \left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{11} \right\rangle\right\rangle (E_2^{(k)} - E_1^{(k)}) + E_1^{(k)}, \tag{7}$$

$$f_i = \left\langle\left\langle \frac{1}{2} i(i+1)\sqrt{13} \right\rangle\right\rangle (F_2^{(k)} - F_1^{(k)}) + F_1^{(k)}, \tag{8}$$

where $k = 1,2,3$ and the symbol $\langle\langle \cdots \rangle\rangle$ designates the fractional part of a real number. As we mentioned above, the boundaries of six mentioned intervals, i.e., $A_1^{(k)}, A_2^{(k)}, \ldots, F_1^{(k)}, F_2^{(k)}$ are the actual nonlinear parameters of the method. The total number of actual nonlinear parameters used in this stage of the procedure equals 36 ($2 \times 6 \times 3$ for the considered three-box version). In fact, such a choice of the $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i$, and f_i parameters in Eq. (2) represents the first (or main) stage of the procedure. For many Coulomb three-body adiabatic systems one pass of the first stage already produces very accurate results.

The second stage is essentially a scaling of the lattice points chosen in the first step. The scaling itself is performed as follows. The families of the parameters $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i$, and f_i (which correspond to the same k) are multiplied by the positive factor λ_k $(k = 1,2,3)$. Then, this parameter λ_k is also varied. The total number of such additional parameters equals 3 (3×1). Also, one additional variational parameter is used to perform a scaling for all lattice points in Eq. (2). Finally, this method produces a properly balanced wave function that represents the considered bound state very accurately. Note that the total number of actual nonlinear parameters in this version of the procedure equals 40.

TABLE I. The convergence of the total energies in atomic units for the ground states in the T_2^+ and DT^+ ions.

N [a]	T_2^+	DT^+
400	−0.599 506 910 077 21	−0.599 130 660 648 8
500	−0.599 506 910 108 40	−0.599 130 662 613 5
600	−0.599 506 910 111 33	−0.599 130 662 806 9
1400 [b]	−0.599 506 910 111 54	−0.599 130 662 855 0
1600 [b]	−0.599 506 910 111 54	−0.599 130 662 855 0
∞ [c]	−0.599 506 910 111 54	−0.599 130 662 855 0
	−0.599 506 909 80 [d]	−0.599 130 661 5 [d]

[a] The number of basis functions used in calculations.

[b] For this case the nonlinear parameters were not optimized.

[c] The asymptotic value ($N=\infty$) of energy determined by using the formula $E(N_i)=E(\infty)+A/N_i^{\gamma}$.

[d] The best results determined in previous calculations [4,10].

In fact, we can say that six intervals (which correspond to the same k) $[A_1^{(k)},A_2^{(k)}]$,$[B_1^{(k)},B_2^{(k)}]$,$[G_1^{(k)},G_2^{(k)}]$, $[D_1^{(k)},D_2^{(k)}]$,$[E_1^{(k)},E_2^{(k)}]$, and $[F_1^{(k)},F_2^{(k)}]$ form one six-dimensional box (or parallelotop) $\mathcal{B}_k$. The first three such intervals must always be positive, while the last three can be arbitrary. Note also that, the high efficiency of our present strategy for choosing the lattice points in Eq. (2) is based on the fact that in Eqs. (3)–(8) any additional condition for the $A_1^{(k)},A_2^{(k)},\ldots,F_2^{(k)}$ points is not used. In particular, either $A_1^{(k)}\leqslant A_2^{(k)}$, or $A_1^{(k)}\geqslant A_2^{(k)}$. The same is true for the $B_1^{(k)},B_2^{(k)},\ldots,F_1^{(k)},F_2^{(k)}$ points. Furthermore, for any k the relative position of the interval $[A_1^{(k)},A_2^{(k)}]$ with respect to the intervals $[A_1^{(k-1)},A_2^{(k-1)}]$ and $[A_1^{(k+1)},A_2^{(k+1)}]$ can be arbitrary. This is also true for the $[B_1^{(k)},B_2^{(k)}],\ldots,[F_1^{(k)},F_2^{(k)}]$ intervals. The results of calculations for different systems indicate clearly that such a freedom in choosing the lattice points is one of the main advantages of our present approach. In fact, this allows the generation of extremely accurate variational wave functions for different systems (see results below).

Our present procedure can be modified easily to the case when the original variational expansion [e.g., Eq. (2)] includes some cluster (or booster) functions. Such functions are often used in calculations to accelerate convergence of the whole method. For instance, if one booster function is used, then the index i in Eqs. (3)–(8) changes from N_0+1 to N. Here N_0 is the number of basis functions in the booster functions, while N is the total number of basis functions used. The cases when three-, four-, and many-cluster functions are included in calculations can be considered in analogous manner. In any case, our presently developed multibox approach produces a variationally optimal, orthogonal complement to the original cluster wave function. In other words, by using our present procedure one can obtain the best (in the variational sense) correction to the short-term (or cluster) wave function known from separate computations.

The variational energies obtained with the use of exponential expansion Eq. (2) can be found in Table I. To perform our present calculations for the T_2^+ ion we used the booster wave function that contains 200 exponential basis functions. This booster wave function have been determined in a series of separate computations for the H_2^+ ion ($m_p=1836.152701m_e$). The corresponding variational energy for the H_2^+ ion is -0.5971390630234 a.u. [$N=200$ in Eq. (2)]. This is the most compact and accurate short-term wave function known for this ion. In fact, our present approach has been tested fully for the H_2^+ ion. The energy computed with $N=1800$ basis wave functions in Eq. (2) is $-0.597\,139\,063\,123\,405\,07$ a.u., i.e., it is one of the best variational results known for this system (see, e.g., Ref. [7]). The bound state properties for the H_2^+ ion coincide very well with the results obtained in Refs. [4,8,9]. Our results for the light adiabatic ions will be published elsewhere. For the T_2^+ ion we used essentially the same approach. The variational energies computed with the $N=400$–600, 1400, and 1600, and 600 basis functions can be found in Table I. The forty nonlinear parameters of the present methods (see above) have been varied for each N. The observed convergence for the energies E upon the number (N) of basis functions used [i.e., $E(N)$] is significantly faster than in the case, when these nonlinear parameters are varied only for one value of N. It can be illustrated by representing the dependence $E(N)$ in a simple asymptotic form $E(N)=E(\infty)+A/N^{\gamma}$, where the positive constant γ can be used as a numerical indicator of the convergence rate. From Table I one finds in this formula $\gamma\approx 11.0$. However, if the nonlinear parameters are varied only for one value of N, then the parameter γ decreases to ≈ 7.5. Finally, the computed variational energy $-0.599\,506\,910\,111\,54$ a.u. for the ground state of the T_2^+ ion is much more accurate than our previous value [4] (at least fourteen decimal figures here are stable).

For the DT^+ ion the procedure was essentially the same, but in this case the short term booster wave function has not been used. Nevertheless, the computed variational energies for the DT^+ ion also converge very fast when the number of basis functions N grows. Our best variational energy $-0.599\,130\,662\,855\,0$ a.u. for the ground state in the DT^+ ion is also most accurate computed value. Note, that already for $N=500$ functions in Eq. (2) the energy from Table I is significantly better than the appropriate energy from Ref. [10]. The fact that Eq. (2) can produce the lower bound state energies than values determined in Ref. [10] for the DT^+ ion was quite unexpected. Indeed, the numerical value of tritium nuclear mass used in Ref. [10] is larger than ours. Moreover, as we mentioned above, the variational expansions in the relative (or perimetric) coordinates [e.g., Eq. (2)] work significantly better for light adiabatic ions, rather than for the considered DT^+ and T_2^+ ions. On the contrary, the method used in Ref. [10] was specifically designed for purely adiabatic systems. Note also, that due to the very restricted computer resources, in this study we could not apply the more effective four-, five-, and six-box versions of our present method. However, as follows from Table I, our three-box approach is quite effective even for the heavy adiabatic ions DT^+ and T_2^+.

It should be mentioned that such very fast convergence can be observed only for the bound state energies. Numerical results for other bound state properties (see below) computed

TABLE II. The expectation values (in atomic units) of some properties $\langle X\rangle$ for the ground states in the T_2^+ and DT^+ adiabatic ions. Below, the subscript 3 designates the electron, 2 stands for the tritium nucleus, while 1 mean deuterium nucleus in the DT^+ ion and tritium nucleus in the T_2^+ ion.

$\langle X\rangle$	$t^+t^+e^-$	$d^+t^+e^-$	$\langle X\rangle$	$t^+t^+e^-$	$d^+t^+e^-$
$\langle r_{21}^{-2}\rangle$	0.246 808 951 8	0.246 346 97	$\langle r_{21}^{-1}\rangle$	0.494 949 541 9	0.494 269 271 7
$\langle r_{31}^{-2}\rangle$	1.435 633 793 3	1.434 312 47	$\langle r_{31}^{-1}\rangle$	0.846 981 681 1	0.846 195 194 9
$\langle r_{32}^{-2}\rangle$		1.433 821 04	$\langle r_{32}^{-1}\rangle$		0.846 335 402 0
$\langle r_{21}\rangle$	2.035 386 031 4	2.039 939 517 9	$\langle r_{21}^2\rangle$	4.173 214 426 2	4.195 439 299
$\langle r_{31}\rangle$	1.677 707 679 3	1.680 255 516 9	$\langle r_{31}^2\rangle$	3.485 248 902 1	3.497 361 208
$\langle r_{32}\rangle$		1.680 023 341 2	$\langle r_{32}^2\rangle$		3.496 476 880
$\langle r_{21}^3\rangle$	8.618 701 719 5	8.698 479 28	$\langle r_{21}^4\rangle$	17.927 967 28	18.179 373
$\langle r_{31}^3\rangle$	8.414 752 010 7	8.462 810 11	$\langle r_{31}^4\rangle$	22.885 378 11	23.070 722
$\langle r_{32}^3\rangle$		8.459 833 01	$\langle r_{32}^4\rangle$		23.060 545
$\langle (r_{31}r_{32})^{-1}\rangle$	0.614 265 774 11	0.613 216 778	$\langle \tau_{21}\rangle$	0.255 371 804 2	0.254 827 444
$\langle (r_{31}r_{21})^{-1}\rangle$	0.420 871 615 15	0.420 100 102	$\langle \tau_{31}\rangle$	0.508 819 321 0	0.509 076 474
$\langle (r_{32}r_{21})^{-1}\rangle$		0.420 161 323	$\langle \tau_{32}\rangle$		0.508 931 835
$\langle (r_{32}r_{31}r_{21})^{-1}\rangle$	0.307 061 035 4	0.306 471 673	$\langle f\rangle$	0.068 252 611 56	0.068 208 938 1
$\langle \vec{r}_{31}\cdot\vec{r}_{32}\rangle$	1.398 641 689	1.399 199 476			
$\langle \vec{r}_{21}\cdot\vec{r}_{31}\rangle$	2.086 607 213	2.098 161 733			
$\langle \vec{r}_{12}\cdot\vec{r}_{32}\rangle$		2.097 277 404			
$\langle -\frac{1}{2}\nabla_1^2\rangle$	4.389 953 849 08	0.394 773 61	$\langle \vec{\nabla}_1\cdot\vec{\nabla}_2\rangle$	8.181 998 028 9	7.297 674 5
$\langle -\frac{1}{2}\nabla_2^2\rangle$		0.394 727 55	$\langle \vec{\nabla}_1\cdot\vec{\nabla}_3\rangle$	0.597 909 669	0.597 797 598
$\langle -\frac{1}{2}\nabla_3^2\rangle$	0.597 909 669 26	0.597 337 079 9	$\langle \vec{\nabla}_2\cdot\vec{\nabla}_3\rangle$		0.596 876 562
$\langle \delta(\vec{r}_{21})\rangle$	0.4714×10^{-14}	0.6151×10^{-12}	$2\,\langle T\rangle$	1.119 013 820 22	1.119 826 132 49
$\langle \delta(\vec{r}_{31})\rangle$	0.208 151 37	0.207 880 0	$\langle V\rangle$	$-1.119\,013\,820\,22$	$-1.119\,826\,132\,52$
$\langle \delta(\vec{r}_{32})\rangle$		0.207 980 0	η	1.8411×10^{-15}	2.2286×10^{-12}
$\langle \delta(\vec{r}_{321})\rangle$	0.7631×10^{-14}	0.3114×10^{-11}	ε (eV)	$-2.710\,196\,635\,59$	$-2.7011\,895\,098\,0$
ν_{32}		$-0.999\,827\,313$	ν_{31} [a]	$-0.999\,818\,113\,1$	$-0.999\,727\,630\,5$
ν_{32} [a]		$-0.999\,818\,113\,1$	ν_{21}	122.7	161.4
ν_{31}	$-0.999\,819\,631$	$-0.999\,736\,577$	ν_{21} [a]	2748.460 790 0	2200.879 985 4

[a] The expected value determined by Eq. (10).

for different N oscillate around some values, but they do not converge in a rigorous sense. In fact, in many cases the amplitudes of such oscillations are relatively small and one can easily determine the final expectation values. However, the worst situation can be found for those properties that include the nuclear-nuclear δ function (i.e., nuclear-nuclear contact properties). The corresponding numerical results are discussed below. But it is quite clear that for adiabatic systems even very fast convergence for the energies does not indicate a high quality of the trial wave functions. In contrast with this, the expectation value of the nuclear-nuclear δ function can indicate, in general, the overall numerical accuracy of the wave function.

The numerical values for a number of geometrical and dynamical properties for the T_2^+ and DT^+ ions (in atomic units) can be found in Table II. Table II also contains the corresponding variational energies determined by using different numbers N of basis functions in Eq. (2). For most of the properties presented in Table II only stable figures from calculations with the higher N are shown. For the two-particle cusps and δ functions only the best results are given in Table II. The physical meaning for all of the expectation values in Table II is quite clear from the notations used (for more details, see also, Ref. [4]). In fact, here we have to make only a few following remarks. In all formulas given below and in Table II the subscripts 1 and 2 mean positively charged heavy nuclei ($m_1 \le m_2$), while the subscript 3 designates the electron ($m_3 = 1$). The notations $\delta_{32}, \delta_{31}, \delta_{21}$, and δ_{321} stand for the corresponding two- and three-particle δ functions, respectively. The two-body cusps are determined in a traditional manner [11,12]:

$$\nu_{ij} = \frac{\langle \delta(\mathbf{r}_{ij})(\partial/\partial r_{ij})\rangle}{\langle \delta(\mathbf{r}_{ij})\rangle}, \tag{9}$$

where $\delta_{ij}=\delta(\mathbf{r}_{ij})$ is the appropriate δ function and $(ij)=(32)$, (31), and (21). The exact value of ν_{ij} equals [11,12]

$$\nu_{ij}=q_i q_j \frac{m_i m_j}{m_j+m_j}, \tag{10}$$

where q_i and q_j are the charges and m_i and m_j the masses of the two (i and j) particles.

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

$$\tau_{ij}=\langle\cos(\mathbf{r}_{ik}\times\mathbf{r}_{jk})\rangle=\left\langle\frac{\mathbf{r}_{ik}\cdot\mathbf{r}_{jk}}{r_{ik}r_{jk}}\right\rangle, \tag{11}$$

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:

$$\langle f\rangle=\left\langle \psi\left|\frac{u_1}{r_{32}}\frac{u_2}{r_{31}}\frac{u_3}{r_{21}}\right|\psi\right\rangle$$
$$=\int\int\int|\psi(u_1,u_2,u_3)|^2 u_1u_2u_3\,du_1du_2du_3. \tag{12}$$

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

$$\tau_{21}+\tau_{32}+\tau_{31}=1+4\langle f\rangle \tag{13}$$

hold for arbitrary three-body system. For the T_2^+ symmetric ion we have $\tau_{32}=\tau_{31}$.

The virial factor η is determined as follows:

$$\eta=\left|1+\frac{\langle V\rangle}{2\langle T\rangle}\right|, \tag{14}$$

where $\langle T\rangle$ and $\langle V\rangle$ are the expectation values of the kinetic and potential energy, respectively. The deviation of the factor η from zero indicates, in principle, the quality of the wave function used. Note, however, that this statement is not true in those cases when the virial factor η is artificially improved (for more details, see, e.g., discussion in Ref. [4]). Table II also contains the appropriate binding energies ε that are given in eV (the conversion factor is 1a.u. $=27.211\,396\,1$ eV [6]). These values represent the differences between the total energies E and corresponding dissociation energies for the considered T_2^+ and DT^+ ions. The lowest-energy dissociation thresholds for these ions corresponds to the reactions $T_2^+=T+t^+$ and $DT^+=T+d^+$, respectively. Here, T designates the neutral tritium atom, while t^+ and d^+ are the two positively charged nuclei (tritium and deuterium, respectively).

The properties of the T_2^+ ion presented in Table II agree quite well with the less accurate results obtained in previous calculations [4]. Analogous properties for the DT^+ ions has never been determined. So, it is very important to note that some expectation values in Table II can be expressed as the linear combinations of other properties. Furthermore, such combinations can be transformed to a system of independent tests. For instance, for the three relative vectors $\vec{r}_{32},\vec{r}_{31}$, and $\vec{r}_{21}$ we have

$$\vec{r}_{32}-\vec{r}_{31}+\vec{r}_{21}=\vec{0}. \tag{15}$$

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

$$\vec{r}_{ik}\cdot\vec{r}_{jk}=\frac{1}{2}(r_{ik}^2+r_{jk}^2-r_{ij}^2) \tag{16}$$

hold for an arbitrary three-body system. For the appropriate expectation values one finds

$$\langle\vec{r}_{ik}\cdot\vec{r}_{jk}\rangle=\frac{1}{2}(\langle r_{ik}^2\rangle+\langle r_{jk}^2\rangle-\langle r_{ij}^2\rangle). \tag{17}$$

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

$$\vec{p}_i\cdot\vec{p}_j=\frac{1}{2}(p_k^2-p_i^2-p_j^2) \tag{18}$$

and

$$\langle\vec{p}_i\cdot\vec{p}_j\rangle=\frac{1}{2}(\langle p_k^2\rangle-\langle p_j^2\rangle-\langle p_i^2\rangle), \tag{19}$$

respectively $[(i,j,k)=(1,2,3)]$. Moreover, since $\vec{p}_i=(-\imath)\vec{\nabla}_i$, then one finds

$$\langle\vec{\nabla}_i\cdot\vec{\nabla}_j\rangle=-\left\langle-\frac{1}{2}\nabla_k^2\right\rangle+\left\langle-\frac{1}{2}\nabla_i^2\right\rangle+\left\langle-\frac{1}{2}\nabla_j^2\right\rangle, \tag{20}$$

where $(i,j,k)=(1,2,3)$. Here, the $\vec{\nabla}_i\cdot\vec{\nabla}_j$ operator is understood to act on its right. The expectation values form both sides of this equality can be found in Table II. Moreover, for the symmetric T_2^+ ion one easily finds that $\langle\vec{\nabla}_1\cdot\vec{\nabla}_3\rangle=\langle-\frac{1}{2}\nabla_3^2\rangle>0$ is always positive.

Now, let us discuss the computational results for the bound state properties presented in Table II. Consider first the DT^+ ion. For this system the important point to make is that, all electron-deuterium expectation values presented in Table II coincide almost exactly with the corresponding electron-tritium values. In other words, the differences between these two groups of properties are relatively small. Thus we arrive at the remarkable conclusion that the electron in the adiabatic DT^+ ion cannot essentially distinguish between the two heavy nuclei (d^+ and t^+). It can be shown that this statement is also true for an arbitrary adiabatic ion that contains two isotopic nuclei, i.e., two nuclei that have different masses, but the same electric charges. On the other hand, analogous results for the muonic molecular ions (see, e.g. Ref. [13]) indicate clearly that the negatively charged muon μ^- in such systems distinguishes quite well between the two different (isotopic) nuclei. Note, however, that the muonic molecular ions $p\mathrm{d}\mu,p\mathrm{t}\mu$, and $\mathrm{dt}\mu$ are not purely adiabatic systems. Furthermore, for the antiprotonic $\mathrm{d}^+\mathrm{t}^+p^-$ ion, the observed d^+p^- properties differ significantly from the corresponding $t^{+}p^{-}$ properties [14]. Obviously, in this case all three particle masses are comparable with each other.

Second we consider the computational results for the contact nuclear-nuclear properties. As we stressed above, the current accuracy which Eq. (2) can provide for the contact nuclear-nuclear properties in the adiabatic ions is very poor and obviously not sufficient for many experimental and theoretical problems. In general, the contact property X can be written in the form

$$\langle X\rangle = \langle \delta(\mathbf{r}_{ij})\hat{F}(\vec{x}_i,\vec{p}_j)\rangle, \tag{21}$$

where $\hat{F}$ is an arbitrary, in principle, operator that depends on the dynamical variables ($\vec{x}_i$ and $\vec{p}_j$) of the considered system. The δ functions and cusps introduced above are the two examples of quite simple contact operators. A large number of more complicated contact operators arise, e.g., when the nonrelativistic wave functions are used to determine the fourth- and higher-order relativistic corrections (upon the fine structure constant α) in few-body systems. In this case, such contact operators are also essentially singular [15].

As follows from Table II the accuracy of our present calculations for the T_2^+ ion is significantly higher than known from our earlier work [4]. This conclusion follows from the comparison of corresponding virial factors η. Based on these virial factors, we can say that our present bound state energies are $\approx 10^5$ times more accurate than energies determined in Ref. [4]. Note that our present nuclear-nuclear δ function computed for the T_2^+ ion (see Table II) is also $\approx 10^5$ times more accurate than such a δ function determined in Ref. [4]. This means a better agreement between the computed and expected values for the nuclear-nuclear δ function. It follows from here, that currently observed deviations for the nuclear-nuclear contact properties are not fundamental and can be eliminated in the future studies, e.g., by developing more effective and better convergent variational methods.

Note that the deuterium-tritium nuclear-nuclear δ function in the DT^+ ion (as well as in the DT molecule) is of interest for applications, since its value can be used to evaluate the nuclear fusion probability in various deuterium-tritium systems. In general, the expectation value of the nuclear-nuclear δ function determines the probability for the two nuclei to be very close to each other. The numerical value for such a close nuclear-nuclear distance R_0 depends significantly on the considered system. For instance, in atomic and molecular systems $R_{0,e} \approx \alpha a_0$ (i.e., $R_{0,e} \approx \Lambda$), where α is the fine structure constant, a_0 is the Bohr radius, and Λ is the Compton wavelength ($\approx 3.861\,592\,642 \times 10^{-11}$ cm). For muonic systems one finds $R_{0,\mu} \approx \alpha a_\mu = \Lambda/m_\mu \approx 1.87 \times 10^{-13}$ cm. Thus the deuterium-tritium δ function in the DT^+ ion determines the total probability to find both nuclei at the distances $R_{0,e} \approx \Lambda$. For the dtμ muonic molecular ion the deuterium-tritium δ function gives such a probability for distances that are approximately 200 times smaller ($R_{0,\mu} \approx \Lambda/m_\mu$). In fact, the nuclear (d,t) fusion occurs when the distance between the deuterium and tritium nuclei is less than $R_f \approx 5 \times 10^{-13}$ cm. This explains a principal difference in computation of the nuclear fusion probabilities for the DT^+ and dtμ ions. Indeed, in the last case $R_{0,\mu} < R_f$ and for computing the nuclear fusion probability one needs to know only the deuterium-tritium δ function and astrophysical factor for the (d,t) reaction. For the DT^+ ion we have $R_{0,e} \gg R_f$, and therefore, the analogous expression for the nuclear fusion probability must also include an additional penetration factor ($\approx 10^{-5}$).

Finally, one finds that the (d,t) fusion probability for the DT^+ ion (as well as for the DT molecule) is a very small value ($\approx 10^{-25} - 10^{-27}$ s^{-1} per DT molecule) at normal conditions. This means that the nuclear fusion in the DT^+ ions and DT molecules (at normal conditions) cannot be considered for actual thermonuclear applications. Note, however, that our method developed in this study can be modified to evaluate the rate of bound-free transitions and Compton scattering rate in the DT^+ ion and other similar one-electron adiabatic ions, e.g., $(^6\mathrm{LiD})^{3+}$. In turn, this simplifies significantly the evaluation of analogous values for the highly compressed ($\rho_0 \geq 150$ g cm^{-3}) mixtures of the lithium-6, deuterium, tritium, and helium-4. In general, the rates of bound-free and bound-bound transitions (along with the bremsstrahlung rate and corresponding rates for inverse processes) are of paramount importance for solving of the corresponding burn-up equations, i.e., to predict the thermonuclear ignition at actual conditions (for more details see, e.g., Refs. [16,17]).

The nuclear-nuclear cusps presented in Table II are significantly less accurate than other bound state properties from Table II. It should be mentioned, that the actual computational accuracy for the nuclear-nuclear cusps and δ functions has never been determined in molecular calculations. In fact, since Ref. [12] it was assumed that all computed nuclear-nuclear cusps for an arbitrary molecule are approximately equal to the expected values given by Eq. (9). Moreover, such an agreement can be improved, if the more accurate wave functions are used. This also was never tested numerically for adiabatic systems. Our present results indicate that all computed nuclear-nuclear cusps and δ functions in the DT^+ and T_2^+ ions have a very poor numerical accuracy. Also, the presently computed nuclear-nuclear cusp for the T_2^+ ion (see Table II) has the same accuracy as in Ref. [4]. In contrast with this, the electron-nucleus cusps and δ functions for an arbitrary adiabatic system can be determined quite accurately (see Table II). Note also, that for many nonadiabatic (or nonmolecular) Coulomb three-body systems the cusp conditions have been tested to a very high accuracy (see, e.g., Ref. [1] and references therein).

Thus in this study we considered the ground bound states in the heavy adiabatic ions T_2^+ and DT^+. The total energies of these states have been determined to a high accuracy by using the recently developed multibox approach [1]. A large number of bound state properties has also been computed for these two ions. For the nonsymmetric DT^+ ion the presented kinetic and geometrical properties have never been determined in earlier calculations. In contrast with the energies and other bound state properties, the problems related to the nuclear-nuclear contact properties remain unsolved. Presently, we cannot obtain such expectation values even approximately. For instance, the current deviation between the computed and expected tritium-tritium delta function in the T_2^+ ion can be evaluated as $\approx 10^{28}$. For the DT^+ ion such a deviation can also be evaluated as $\approx 10^{28}$. In conclusion, it should be mentioned that the more accurate determination of contact nuclear-nuclear properties must be a central problem for future studies of the Coulomb three-body adiabatic systems.

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