# Ground bound state in the fully adiabatic $^{\infty}H_2^+$ ion

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The fully adiabatic $^{\infty}H_2^+$ ion is considered by using the improved version of our multibox variational procedure [A.M. Frolov, Phys. Rev. E **64**, 036704 (2001)]. This procedure has been developed and successfully tested in highly accurate computations of bound-state spectra of various three-body systems. Note that our method is not based on the Born-Oppenheimer approximation, i.e., it is a nonadiabatic approach. In this study, we determine the ground-state energies of the adiabatic $HD^+$, $HT^+$, and $T_2^+$ ions with finite nuclear masses. The computed variational energies for the $HD^+$, $HT^+$, and $T_2^+$ ions are $-0.597\,897\,968\,645\,036\,508$ a.u., $-0.598\,176\,134\,669\,766\,232$ a.u., and $-0.599\,506\,910\,111\,541\,451\,13$ a.u., respectively. The ground-state energy and bound-state properties of $^{\infty}H_2^+$ ion are also presented. In general, the observed agreement between our variational energies and analogous energies determined with the use of pure adiabatic methods can be considered as very good.

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In this communication, we report the numerical results of highly accurate calculations for a number of adiabatic one-electron $H_2^+$-like ions. Our results also include the purely adiabatic $^{\infty}H_2^+$ ion with two infinitely heavy (i.e., immovable) nuclei. To determine the bound states in $HD^+$, $HT^+$, $T_2^+$, and $^{\infty}H_2^+$ ions, we apply the universal variational multibox approach developed in Ref. [1]. This approach was found to be very effective for a large number of three-body systems, including $Ps^-$ and $H^-$ ions [2], muonic molecular ions [3], helium-muonic ions [3], and various adiabatic ions [3,4]. The results obtained in these studies indicate clearly that the multibox approach developed in Ref. [1] is an universal variational method that can be used for high-precision bound-state computations of arbitrary three-body systems. Briefly, this means that by using the approach [1], one can determine numerically all bound states in such systems to very high accuracy.

Note that almost all applications of the approach [1] are related to the nonrelativistic Coulomb three-body systems in which $|\mathbf{p}_i| \ll m_i c$. In atomic units, $\hbar=1$, $m_e=1$, and $e=1$, 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 $m_1, m_2, m_3$ and $q_1, q_2, q_3$ are the particle masses and charges. Our present goal is to determine the solutions of the corresponding Schrödinger equation for the bound-state spectra $H\Psi=E\Psi$, where $E<0$. The approach [1] allows one to obtain such solutions to arbitrarily high, in principle, accuracy. Moreover, it was also shown [1–4] that such an accuracy does not depend on the particle masses or their charges.

The approach [1] is based on the use of exponential variational expansion in perimetric coordinates $u_1$, $u_2$, and $u_3$, which can be written in the form [1]

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

where $u_1$, $u_2$, and $u_3$ are the three truly independent and always positive perimetric coordinates ($0 \leqslant u_i < +\infty$ for $i=1,2,3$). These three are simply related to the three scalar relative (or interparticle) coordinates $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$:

$$u_i=\tfrac{1}{2}(r_{ik}+r_{ij}-r_{jk}), \quad \text{and} \quad r_{ij}=u_i+u_j, \tag{3}$$

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. In fact, the variational expansion, Eq. (2), corresponds to the case $L=0$, where $L$ is the total angular momentum of the considered system. Its generalization to the case of arbitrary $L$ can be found, e.g., in Ref. [1]. For nonsymmetric systems the factor $\kappa$ always equals zero, while for the systems with two identical particles, i.e., for $T_2^+$ and $^{\infty}H_2^+$ ions, $\kappa=\pm 1$. In fact, below, for all considered symmetric systems, we have $\kappa=1$. Note that all earlier versions of the variational expansion (2) [5–7] could not provide even approximate accuracy for the adiabatic systems (see results and discussion in Ref. [6]). Later, it was shown [4] that the modified variational expansion (2) can effectively be used in computations of the bound-state spectra in arbitrary three-body systems, including adiabatic systems.

In actual computations, the highly accurate trial functions $\Psi$ can be constructed, e.g., by using a complete optimization of the nonlinear parameters $\alpha_i$, $\beta_i$, $\gamma_i$, $\delta_i$, $e_i$, and $f_i$ ($i=1,\ldots,N$) in Eq. (2). However, this procedure is not very effective, if the total number of basis functions in Eq. (2) exceeds 500. In Ref. [1], we have developed an alternative approach with relatively small number of actual nonlinear parameters (28). In this study (as well as in Ref. [1]), the choice of the nonlinear parameters in Eq. (2) proceeds as follows. Let $i$ be the number (or index) of basis functions in Eq. (2) ($1 \leqslant i \leqslant N$) and $k=\mathrm{mod}(i,3)+1$, where mod($i$,3)

 

designates the modular division (i.e., an integer remainder after division of $i$ by 3). The number 3 corresponds to the three-box version that was used successfully in variational calculations of various three-body systems [1–4]. The same version is applied in all present calculations. Now, the parameters $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i, f_i$ 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 $[F_1^{(k)}, F_2^{(k)}]$:

$$\alpha_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{2}\rangle\rangle (A_2^{(k)} - A_1^{(k)}) + A_1^{(k)}, \tag{4}$$

$$\beta_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{3}\rangle\rangle (B_2^{(k)} - B_1^{(k)}) + B_1^{(k)}, \tag{5}$$

$$\gamma_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{5}\rangle\rangle (G_2^{(k)} - G_1^{(k)}) + G_1^{(k)}, \tag{6}$$

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

$$e_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{11}\rangle\rangle (E_2^{(k)} - E_1^{(k)}) + E_1^{(k)}, \tag{8}$$

$$f_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{13}\rangle\rangle (F_2^{(k)} - F_1^{(k)}) + F_1^{(k)}, \tag{9}$$

where $k=1,2,3$ and the symbol $\langle\langle \cdots \rangle\rangle$ designates the fractional part of a real number. As easy to understand 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 parameters in exponents (2) (i.e., $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i, f_i$, $i=1,\ldots,N$) are chosen quasirandomly and not varied in calculations. Note that the total number of actual nonlinear parameters used in this stage of the procedure equals 36 ($2\times6\times3$ for the considered three-box version).

The second stage of our procedure [1] 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 $\alpha_i, \beta_i, \gamma_i, \delta_i, e_i, f_i$ (which correspond to the same $k$) are multiplied by the positive factor $\lambda_k$ ($k=1,2,3$). Then, this parameter $\lambda_k$ is also varied. The total number of such additional parameters equals 3 ($3\times1$). 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 which represents the considered bound state very accurately. Note that the total number of actual nonlinear parameters in this version of the procedure equals 40. These 40 actual nonlinear parameters were optimized in calculations with relatively small number of basis functions used. For the considered adiabatic ions, we used $N=1000$, 1200, and 1500 in Eq. (2).

In fact, our present main interest is related to the adiabatic three-body systems with unit charges, i.e., to the $X^+Y^+Z^-$ ions, where $\min(m_X, m_Y) \gg m_Z$. In the Hamiltomian, Eq. (1), in this case we have $q_1=q_2=+1$, $q_3=-1$, $m_1 \gg m_3 (=1)$, and $m_2 \gg m_3$. Here the notations 1, 2, and 3 stand for the $X^+$, $Y^+$, and $Z^-$ particles, respectively. As mentioned above, recently, significant progress has been achieved in theoretical study of the bound-state spectra in such systems [3,4,8–12]. However, a few problems for the adiabatic three-body systems remain unsolved. The first group of unsolved problems is related to very poor numerical accuracy, which is currently observed in computations of the contact nuclear-nuclear properties. For instance, the best-to-date deviations between the predicted and computed nuclear-nuclear $\delta$ functions in the $H_2^+$-like ions exceed 23–30 orders of magnitude. Such huge deviations must be explained in the course of further studies (for more details, see Ref. [4]).

The second remaining problem is related to the use of nonadiabatic methods for computations of bound states in the fully adiabatic $^{\infty}H_2^+$ ion [13]. Both the nuclei in the one-electron $^{\infty}H_2^+$ ion are assumed to be infinitely heavy, and therefore, immovable. This ion was considered by Hylleraas [14] and others (see, e.g., Refs. [15–17] in terms of the rigorous Born-Oppenheimer approximation. In these papers, a number of adiabatic two-center expansions were developed and used. An accurate numerical result for the ground-state (adiabatic) energy in the $^{\infty}H_2^+$ ion can be found, e.g., in Ref. [17], $E=-0.602\,634\,2$ a.u. For our present purposes this result can be considered as the ''exact'' energy. Below, our goal is to approximate this Born-Oppenheimer energy to good accuracy by using the present nonadiabatic approach described above. In addition to the energy, we also want to obtain some expectation values for a number of bound-state properties in this ion.

Note that all earlier attempts to compute the ground state in the fully adiabatic $^{\infty}H_2^+$ ion by using various nonadiabatic procedures have failed, since even the best energies computed with these procedures were not sufficiently accurate. For instance, our best result for this ion was $E \approx -0.602\,45$ a.u. In fact, the energies obtained with the use of nonadiabatic methods for the $^{\infty}H_2^+$ ion were never published due to their very poor accuracy. Moreover, it is commonly assumed that (1) the bound states in this ion cannot be computed even approximately by using the nonadiabatic methods and (2) the nonzero ''correlation'' energy will always separate the exact adiabatic energy from the computed nonadiabatic energies. In general, by using only a few quite approximate energies, one cannot confirm such conclusions.

In general, the recent progress achieved for the adiabatic systems allows one to perform extremely accurate calculations for many adiabatic three-body systems [3,4], including the heavy adiabatic ions $DT^+$ and $T_2^+$ [4]. In terms of the nuclear masses, the $DT^+$ and $T_2^+$ ions are close to the limiting case of the fully adiabatic $^{\infty}H_2^+$ ion. However, the adiabatic (or Born-Oppenheimer) parameter $\tau$ [13] for an arbitrary $X^+X^+e^-$ ion is $\tau = \sqrt[4]{m_e/M_X} = 1/\sqrt[4]{M_X}$, rather than $1/M_X$. The numerical value of $\tau \approx 1.35\times10^{-2}$ for the $T_2^+$ ion is significantly larger than the inverse nuclear mass $1/M_X \approx 1.82\times10^{-4}$. In general, the adiabatic parameter $\tau$ determines the ability of heavy nuclei to move. This means that the positions of both tritium nuclei in heavy adiabatic $T_2^+$ ion are not really fixed, i.e., these nuclei are moving. This simplifies the highly accurate computations for the $T_2^+$ ion with the use of nonadiabatic methods. In contrast with this, the fully adiabatic $^{\infty}H_2^+$ ion is a system with the two infinitely heavy (i.e., fixed) nuclei. Obviously, the adiabatic pa-

TABLE I. The total energies $E$ (in atomic units $m_e=1$, $\hbar=1$, $e=1$) for the ground states of the adiabatic $HD^+$, $HT^+$, and $T_2^+$ ions. $N$ designates the number of basis functions used in Eq. (2). The binding energies $\varepsilon$ (in eV) are also presented.

| $N$ | $HD^+$ | $HT^+$ | $T_2^+$ |
|---|---|---|---|
| 2000 | −0.597897968645033686 | −0.598176134669761820 | −0.59950691011154144648 |
| 2600 | −0.597897968645036217 | −0.598176134669765745 | −0.59950691011154145069 |
| 3000 | −0.597897968645036428 | −0.598176134669766097 | −0.59950691011154145101 |
| 3500 | −0.597897968645036508 | −0.598176134669766232 | −0.59950691011154145113 |
| $E_p$[a] | −0.5978979686450 [12] | −0.5981761344 [10] | |
| $\varepsilon$ (eV) | −2.6676461793872477 | −2.6739843865228183 | −2.7101966441891162848 |

[a]$E_p$ are the best variational energies known from earlier calculation by other groups.

rameter in this case is zero, i.e., $\tau=0$. Formally, the nonadiabatic methods, including Eq. (2), cannot be applied to the $^{\infty}H_2^+$ ion.

This means that highly accurate computations of this ion can include a few additional troubles. In particular, we expected that there is a nonzero correlation energy, which will always separate our result from the value obtained by Wind [17]. Such a conclusion was essentially confirmed in our earlier computations performed for the ground state in the fully adiabatic $^{\infty}H_2^+$ ion. However, in those computations we used the nonlinear parameters optimized for the heavy $T_2^+$ ion. Later, all nonlinear parameters have been reoptimized for the adiabatic $^{\infty}H_2^+$ ion. Such a reoptimization of the nonlinear parameters has significantly increased the actual convergence of the computed variational energies. The quality of the variational wave functions has also been increased. Finally, by comparing our best results with the exact adiabatic energy [17], we can now make the correct conclusion about the overall accuracy of nonadiabatic variational expansion, Eq. (2), in the case of fully adiabatic $^{\infty}H_2^+$ ion. In particular, it is shown below that now the ground-state energy of the $^{\infty}H_2^+$ ion is reproduced quite accurately.

Note that the fully adiabatic $^{\infty}H_2^+$ ion is of a great interest in a number of applications, including the general theory of bound states in three-body systems with unit charges [18]. In this theory, the $^{\infty}H_2^+$ ion plays a very important role, being one of the three fundamental reference systems (as well as the $Ps^-$ and $^{\infty}H^-$ ions). Furthermore, the highly accurate variational solution obtained for this ion can be used for better understanding of the nuclear motion in heavy adiabatic ions and molecules. Note also, that for many years the fully adiabatic $^{\infty}H_2^+$ ion was a very important test system for various newly developed nonadiabatic methods and approaches. In general, the adiabatic $H_2^+$-like ions are of great interest in numerous actual applications. In particular, the laboratory sources of $H_2^+$ ions are currently available for research and cancer treatment (see, e.g., Ref. [19] and references therein). Astrophysical applications for $H_2^+$ ions are discussed in Refs. [20–22].

The computed energies for the considered adiabatic $HD^+$, $HT^+$, $T_2^+$, and $^{\infty}H_2^+$ ions are presented in Tables I and II. Table I contains highly accurate variational energies obtained for the adiabatic $HD^+$, $HT^+$, and $T_2^+$ ions. All nuclear masses in these ions are finite. In the present calculations for the nuclei of hydrogen isotopes we used the following masses $m_p=1836.152\,701m_e$, $m_d=3670.483\,014m_e$, and $m_t=5496.921\,58m_e$ [23]. The same nuclear masses were used in our earlier works (see, e.g., Refs. [3,4]). In fact, the energies from Table I are significantly more accurate than analogous results presented in Ref. [4]. The energies and other properties for the adiabatic $^1H_2^+$, $D_2^+$, and $DT^+$ ions have been determined in Ref. [3] (for the bound-state properties, see Ref. [4]). Table I also contains the energies ob-

TABLE II. The total energies $E$ and some bound-state properties $\langle X\rangle$ (in atomic units $m_e=1$, $\hbar=1$, $e=1$) for the ground states of the fully adiabatic $^{\infty}H_2^+$ ion. $N$ designates the number of basis functions used in Eq. (2).

| $N$ | $E$ | $\langle X\rangle$ | | $\langle X\rangle$ | |
|---|---|---|---|---|---|
| 2000 | −0.602 630 862 02 | $\langle r_{31}^{-1}\rangle$ | 0.852 928 72 | $\langle r_{31}^2\rangle$ | 3.389 218 78 |
| 2600 | −0.602 632 254 14 | $\langle r_{21}^{-1}\rangle$ | 0.500 006 51 | $\langle r_{21}^2\rangle$ | 3.999 907 06 |
| 3000 | −0.602 632 851 12 | $\langle r_{31}\rangle$ | 1.657 558 31 | $\langle -\frac{1}{2}\nabla_3^2\rangle$ | 0.602 631 12 |
| 3500 | −0.602 633 511 30 | $\langle \delta(\mathbf{r}_{31})\rangle$ | 0.210 046 | $\langle \cos(\mathbf{r}_{31}\mathbf{r}_{32})\rangle$ | 0.259 957 63 |
| $E$[a] | −0.6026342 | $\nu_{31}$[b] | −1.000 731 | $\langle \cos(\mathbf{r}_{31}\mathbf{r}_{21})\rangle$ | 0.507 261 48 |

[a]The "exact" adiabatic (or Born-Oppenheimer) energy of the $^{\infty}H_2^+$ ion from Ref. [17].
[b]The predicted value for the electron-nucleus cusp $\nu_{31}^{(b)}$ is −1.0 (see, e.g., Refs. [26,27]).

tained in earlier computations for $HD^+$ and $HT^+$ ions by other groups. This Table includes the binding energies of all considered ions (in eV). To compute the binding energies, the conversion factor 27.211 396 1 is used. To perform all our present calculations, we used the special FORTRAN pretranslator written by D.H. Bailey [24,25]. The variational energies presented in Table I determine the ''standard'' (or ''reference'') level of numerical accuracy, which is currently available for the adiabatic $H_2^+$-like ions with the finite nuclear masses.

In the case of fully adiabatic $^\infty H_2^+$ ion both the nuclei are assumed to be infinitely heavy. The variational energies computed for this system with the use of Eq. (2) are presented in Table II. A number of bound-state properties determined for this ion can also be found in Table II. Note that the nuclear-nuclear contact properties are not presented in Table II, since their exact values equal zero identically. Such contact properties usually include the nuclear-nuclear $\delta$ function, nuclear-nuclear cusp, triple $\delta$ function, etc.

In general, the observed convergence rate for the variational energies $E(N)$ is very high for the adiabatic $HD^+$, $HT^+$, and $T_2^+$ ions. This allows us to apply the three-box version of our procedure [1]. However, for the fully adiabatic $^\infty H_2^+$ ion, a few modifications have been made in the procedure. In particular, the explicit dependence of actual nonlinear parameters upon the total number of basis functions $N$ in Eq. (2) has been included in the consideration. Note that, in general, the optimized values of $A_1^{(k)}, A_2^{(k)}, \ldots, F_1^{(k)}, F_2^{(k)}$ parameters depend upon $N$. This means that the optimal values of such parameters determined for $N=N_1$ in Eqs. (3)–(8) are not optimal parameters in the calculations with for $N=N_2>N_1$. The reoptimization of all 40 nonlinear parameters is a very costly procedure for $N>2000$. An alternative idea is to guess an explicit form of the $N$ dependence for each of the actual nonlinear parameters. This idea can be very successful in highly accurate three-body calculations.

In the present case, the $N$ dependence of the six parameters $F_1^{(1)}$, $F_2^{(1)}$, $F_1^{(2)}$, $F_2^{(2)}$, $F_1^{(3)}$, and $F_2^{(3)}$ was crucial. The known optimal values of these parameters determined for $N=400,\ 500, \ldots, 1500$ allow us to produce some simple interpolational formulas for the $F_k^{(i)}(N)$ dependencies. The interpolated values of $F_1^{(1)}$, $F_2^{(1)}$, $F_1^{(2)}$, $F_2^{(2)}$, $F_1^{(3)}$, and $F_2^{(3)}$ parameters were used in actual calculations with the large number of basis functions $N$, where $N \geqslant 2000$. Finally, the overall accuracy obtained for the ground-state energy of the fully adiabatic $^\infty H_2^+$ ion has been drastically improved.

Thus, in this study we have performed the highly accurate calculations for a number of adiabatic ions $HD^+$, $HT^+$, and $T_2^+$ and for the fully adiabatic $^\infty H_2^+$ ion. Our present variational approach is completely nonadiabatic. Nevertheless, the obtained variational energies indicate clearly that this approach is a very powerful tool which can be useful in the study of various adiabatic atomic systems. It is shown that the fully adiabatic $^\infty H_2^+$ ion can be considered by using the same nonadiabatic methods that are successfully used for other three-body ions. In particular, our present computational results for the fully adiabatic $^\infty H_2^+$ ion can be recognized as sufficiently accurate. Obviously, further improvement of the variational energies is also possible.

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