Bound-state properties of negatively charged hydrogenlike ions

Alexei M. Frolov
Department of Chemistry, Queen's University, Kingston, Ontario, Canada K7L 3N6
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The results of high-precision, variational, bound-state calculations for the ground state in the negatively charged hydrogenlike ions $^{\infty}H^-$, T^-, D^-, $^1H^-$, and Mu^- are presented. The mass dependence for various properties is studied. The results are formulated in the form of relatively simple analytical expressions. The probabilities of finding the final He atom in its ground and low-lying excited states (after the nuclear β^- decay in the T^- ion) have been determined numerically. It is shown that the total ionization probability has a very large value ($\approx$30%). A possible explanation may include the spin conversion between the β^- particle and remaining ^{3}He atom. This means that the final ^{3}He atom can be found not only in its singlet states, but also in the triplet states. [S1050-2947(98)08512-6]

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In the present paper we report the results of highly accurate calculations for a number of the negatively charged hydrogenlike ions $^{\infty}H^-$, T^-, D^-, $^1H^-$ and Mu^-. As is known (see, e.g., [1]) these systems have very simple bound-state spectra that contain only the one bound (ground), singlet state with $L=0$ (or $1\ ^1S$ state, for short). The stability of the bound H^- ion (actually the $^{\infty}H^-$ ion) has been known since the first papers of Bethe [2] and Hylleraas [3]. The initial interest in the H^- ion was related to its astrophysical observations. It was shown that the H^- ions form intensively in the areas close to the sun's surface. These ions then absorb radiation coming from the center of the sun, and dissociate: $H^- \rightarrow H + e^-$ (photoeffect with dissociation). The emitted electrons will be recaptured again by the neutral H atoms (with the emission of radiation) and, in principle, these processes repeat many times. Actually, these two processes are mainly responsible for the opacity in the solar atmosphere (see, e.g., [4]). The same arguments can be used also for other stars with surface temperature $T \leqslant 9500$ K [5]. This explains why the H^- ion is of increasing interest for astrophysics. The existence of the bound $\mu^+ e^- e^-$ ion (abbreviated as Mu^-) has been known since [6,7] (see also [8]). Later, this system was created in the laboratory [9], but no properties were reported.

The main goal of the present study is to perform highly accurate variational calculations for the two-electron, H^--like systems with the real (i.e., finite) masses. First of all, we want to compute various geometrical and physical properties for these systems. Such properties are of interest for astrophysical applications. The second step is to propose simple interpolation formulas that can be applied to determine corrections related to the experimental errors in the nuclear mass values. Also, we determine the probabilities to find the final He atom in its ground and low-lying excited states (after the nuclear β^- decay in the T^- ion).

To perform the high precision variational calculations we use the exponential variational expansion in the relative coordinates. For the considered $1\ ^1S$ states it takes the form [10]

$$\Psi_{LM} = \frac{1}{2}(1+\hat{P}_{21}) \sum_{i=1}^{N} C_i \times \exp(-\alpha_i r_{32} - \beta_i r_{31} - \gamma_i r_{21}), \qquad (1)$$

where N is the total number of basis functions, C_i are the linear (or variational) parameters, α_i, β_i, and γ_i are the nonlinear parameters. The operator P_{21} is the permutation of the identical particles in the symmetric systems. The choice of the nonlinear parameters is based on the two-stage procedure developed in [10]. This means that the wave function is represented in the form of the highly accurate short-term (first stage or booster) wave function Ψ_1 and roughly optimized (or nonoptimized) long-term wave function Ψ_2.

In the present study the results for $N=200$ (see Table I)

TABLE I. The total energies (E) in atomic units ($m_e=1, \hbar=1, e=1$) for the ground states of the two-electron H^--like ions. N designates the number of basis functions used.

N	E ($^{\infty}H^-$)	E (T^-)	E (D^-)	E ($^1H^-$)	E (Mu^-)
200	−0.527 751 016 542 889	−0.527 649 048 201 512	−0.527 598 324 684 988	−0.527 445 881 112 677	−0.525 054 806 240 231
400	−0.527 751 016 543 776	−0.527 649 048 202 401	−0.527 598 324 685 880	−0.527 445 881 113 584	−0.525 054 806 242 950
500	−0.527 751 016 544 049	−0.527 649 048 202 672	−0.527 598 324 686 151	−0.527 445 881 113 853	−0.525 054 806 243 213
600	−0.527 751 016 544 166	−0.527 649 048 202 789	−0.527 598 324 686 267	−0.527 445 881 113 968	−0.525 054 806 243 315
700	−0.527 751 016 544 265	−0.527 649 048 202 887	−0.527 598 324 686 366	−0.527 445 881 114 067	−0.525 054 806 243 411
800	−0.527 751 016 544 302	−0.527 649 048 202 925	−0.527 598 324 686 403	−0.527 445 881 114 104	−0.525 054 806 243 451

TABLE II. The expectation values $\langle X_{ij}\rangle$ in atomic units ($m_e=1,\hbar=1,e=1$) of some properties for the ground states in the two-electron H^--like ions.

$\langle X_{ij}\rangle$	E ($^{\infty}H^-$)	E (T^-)	E (D^-)	E ($^1H^-$)	E (Mu^-)
$\langle r_{21}^{-2}\rangle$	0.155 104 151 84	0.155 033 945 09	0.154 999 029 82	0.154 894 130 69	0.153 255 571 63
$\langle r_{31}^{-2}\rangle$	1.116 662 822 24	1.116 240 173 5	1.116 029 957 0	1.115 398 286 4	1.105 512 211 1
$\langle r_{21}^{-1}\rangle$	0.311 021 502 219 1	0.310 952 489 018 9	0.310 918 161 829 4	0.310 815 007 479	0.309 199 388 980 8
$\langle r_{31}^{-1}\rangle$	0.683 261 767 654 0	0.683 125 292 712 5	0.683 057 405 601 2	0.682 853 384 854	0.679 654 500 734 0
$\langle r_{21}\rangle$	4.412 694 497 79	4.413 696 085 42	4.414 194 431 63	4.415 692 603 31	4.439 280 091 81
$\langle r_{31}\rangle$	2.710 178 278 34	2.710 818 805 09	2.711 137 506 35	2.712 095 626 51	2.727 182 982 39
$\langle r_{21}^{2}\rangle$	25.202 025 298 2	25.213 765 480 3	25.219 607 856 1	25.237 175 614 1	25.514 536 371 7
$\langle r_{31}^{2}\rangle$	11.913 699 681 6	11.919 727 619 1	11.922 727 398 3	11.931 747 760 0	12.074 193 988 0
$\langle r_{21}^{3}\rangle$	180.605 601 24	180.735 630 15	180.800 349 13	180.995 002 15	184.077 314 13
$\langle r_{31}^{3}\rangle$	76.023 097 561	76.083 393 736	76.113 405 589	76.203 674 315	77.633 690 344
$\langle r_{21}^{4}\rangle$	1 590.094 676	1 591.667 914	1 592.451 105	1 594.807 275	1 632.234 593
$\langle r_{31}^{4}\rangle$	645.144 578 9	645.844 998 2	646.193 695 3	647.242 776 2	663.917 866 2
$\langle (r_{31}\cdot r_{32})^{-1}\rangle$	0.382 627 890 337	0.382 460 806 219	0.382 377 710 308	0.382 128 051 445	0.378 227 084 382 6
$\langle (r_{31}\cdot r_{21})^{-1}\rangle$	0.253 077 567 071	0.252 967 450 107	0.252 912 685 611 9	0.252 748 147 338	0.250 177 168 402 0
τ_{31}	0.649 871 581 193 9	0.649 846 203 399 7	0.649 833 580 278 2	0.649 795 646 586	0.649 201 369 274 5
τ_{21}	−0.105 147 693 566 0	−0.105 097 200 234 2	−0.105 072 084 095 1	−0.104 996 606 303 1	−0.103 813 878 095 5
$\langle f\rangle$	0.048 648 867 205 47	0.048 648 801 641 27	0.048 648 769 115 32	0.048 648 671 717 35	0.048 647 215 113 36
$\langle \mathbf{r}_{31}\cdot\mathbf{r}_{32}\rangle$	−0.687 312 967 50	-0.687 155 121 08	−0.687 076 529 80	−0.686 840 047 056	−0.683 074 197 86
$\langle \mathbf{r}_{31}\cdot\mathbf{r}_{21}\rangle$	12.601 012 649 0	12.606 882 274 0	12.609 803 928 1	12.618 587 807 0	12.757 268 185 9
$\langle -\frac{1}{2}\nabla_1^2\rangle$	0.263 875 508 272 3	0.263 773 550 736	0.263 722 840 643 5	0.236 570 469 595	0.261 186 844 278 7
$\langle -\frac{1}{2}\nabla_3^2\rangle$	0.560 630 798 396 8	0.560 393 181 814 0	0.560 275 005 582 2	0.559 919 939 393 7	0.554 370 044 211 2
$\langle \boldsymbol{\nabla}_1\cdot\boldsymbol{\nabla}_2\rangle$	0.032 879 781 852 3	0.032 846 080 341 2	0.032 829 324 295 2	0.032 779 000 182 3	0.031 996 355 653 8
$\langle \boldsymbol{\nabla}_1\cdot\boldsymbol{\nabla}_3\rangle$	−0.288 535 344 662	−0.288 408 110 992	−0.288 344 833 865	−0.288 154 719 731	−0.285 184 111 019
$\langle \delta_{31}\rangle$	0.164 552 853	0.164 461 616	0.164 416 243	0.164 279 924	0.162 150 662
$\langle \delta_{21}\rangle$	$2.737\,987\,2\times10^{-3}$	$2.735\,840\,7\times10^{-3}$	$2.734\,773\,4\times10^{-3}$	$2.731\,567\,8\times10^{-3}$	$2.681\,676\times10^{-3}$
$\langle \delta_{321}\rangle$	$5.064\,44\times10^{-3}$	$5.057\,11\times10^{-3}$	$5.053\,56\times10^{-3}$	$5.042\,95\times10^{-3}$	$4.878\,89\times10^{-3}$
ν_{31}	−0.999 996 224 839	−0.999 814 281 493	−0.999 723 854 280	−0.999 451 881 287	−0.995 183 309 891
ν_{31}^{a}	−1.0	−0.999 818 113 084	−0.999 727 630 498	−0.999 455 679 433	−0.995 186 945 348
ν_{21}	0.500 039 796 232	0.500 039 898 808	0.500 039 796 232	0.500 039 741 09	0.500 039 116 850
ν_{21}^{a}	0.5	0.5	0.5	0.5	0.5
η	5.904×10^{-13}	6.003×10^{-13}	8.083×10^{-13}	8.359×10^{-13}	1.200×10^{-12}
ε	−0.755 143 903 364 662	−0.754 843 900 894 657	−0.754 694 721 939 902	−0.754 246 603 587 335	−0.747 261 225 195 369
$\mathcal{T}_{in}(K)$	8 763.028 2	8 752.615 5	8 757.815 7	8 752.615 5	8 671.554 0

[a]The exact two-particle *cusp* value.

correspond to the highly accurate short-term (or first stage) wave function Ψ_1. The maximal total number of basis functions in calculations equals 800 (see Table I). Table I contains only the found variational energies, while Table II includes various geometrical and physical properties. In both of these tables only atomic units are used: $m_e=1$, $e=1$, and $\hbar=1$. In Table II only stable figures from calculations with the higher values of N are presented. The nuclear masses of the hydrogen isotopes used in calculations have been chosen from [11]. Their numerical values are $m_p=1836.152\,701 m_e$, $m_d=3670.483\,014 m_e$, and $m_t=5496.921\,58 m_e$. The mass of the positively charged muonium μ^+ equals $m_\mu=206.768\,262 m_e$ [11]. The appropriate binding energies ε of the H^- ions are given in eV (1 Ry $=27.2113\,961$ eV). The results of previous variational calculations for $^{\infty}H^-$ can be found, e.g., in [12] (see also [1] and references therein).

The physical meaning for almost all of the expectation values given in Table II seems to be quite clear and we restrict ourselves only to a few remarks, as follows. Throughout the rest of this paper, subscripts 1 and 2 stand for the electrons, while 3 designates the nucleus. The expectation values of τ_{ij} are the two interparticle *cosine* functions:

$$\tau_{ij}=\langle\cos(\mathbf{r}_{ik}\cdot\mathbf{r}_{jk})\rangle=\left\langle\frac{\mathbf{r}_{ik}\cdot\mathbf{r}_{jk}}{r_{ik}r_{jk}}\right\rangle, \tag{2}$$

where $(i,j,k)=(1,2,3)$. The sum of these three τ_{ij} values is represented in the following form:

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

and

$$\tau_{21}+2\tau_{31}=1+4\langle f\rangle \tag{3}$$

for arbitrary nonsymmetric and symmetric three-body systems, respectively. The quantity $\langle f\rangle$ can be 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:

$$\langle f\rangle=\left\langle \psi\left|\frac{u_1}{r_{32}}\frac{u_2}{r_{31}}\frac{u_3}{r_{21}}\right|\psi\right\rangle$$
$$=\int\int\int |\psi(u_1,u_2,u_3)|^2 u_1u_2u_3du_1du_2du_3. \quad (4)$$

The value $\langle f\rangle$ can be calculated directly or by applying τ_{ij}. Their coincidence is an additional test to prove the correctness of our results. The virial factor η is determined as follows:

$$\eta=\left|1+\frac{\langle V\rangle}{2\langle T\rangle}\right|, \quad (5)$$

where $\langle T\rangle$ and $\langle V\rangle$ are the expectation values of the kinetic and potential energy, respectively. The parameter η indicates the quality of the wave function for Coulomb systems. The expected (exact) two-particle *cusp* values equal $\nu_{ij}=q_iq_j[(m_im_j)/(m_i+m_j)]$, where q_i,q_j are the particle's charges and m_i,m_j are their masses.

The so-called ionization temperature $\mathcal{T}_{in}=|\varepsilon|/k=11\,604.448|\varepsilon|$ is of great value in astrophysical applications. Here ε is the binding energy of the corresponding H^- ion (in eV) and k is the Boltzmann constant, $k^{-1}=11\,604.448$ K eV^{-1}, and finally, $\mathcal{T}_{in}$ is in K. The importance of the $\mathcal{T}_{in}$ follows from the fact that the ratio of the H^- ion concentration ($[H^-]$) to the concentration of hydrogen H atoms ([H]) takes the following general form:

$$\frac{[H^-]}{[H]}=AF(T)\exp\left(\frac{\mathcal{T}_{in}}{T}\right), \quad (6)$$

where $F(T)$ is a rational function of the temperature T in the solar atmosphere (i.e., in a corona [4]), and A is proportional to the electron concentration in the solar atmosphere. For instance, if all components (i.e., the H^- ions, H atoms, and electrons e^-) are considered as ideal gases (Saha approximation), one easily finds that in the last equation $F(T)=T^{-(3/2)}$.

As follows from Tables I and II, all negatively charged hydrogenic ions considered are typically weakly bound systems with two-body ($H+e^-$) cluster structure. Indeed, as follows from Table I the maximal ratio of the binding energies to the appropriate total energies does not exceed 2%. This means that any of the H^- ions is a weakly bound system, or, in other words, these ions are very close to their dissociation limit ($H^-=H+e^-$). But such a cluster structure cannot be seen easily from the geometrical properties shown in Table II. The reason is obvious: all electron-nuclear properties are averaged upon the two electrons (particles 1 and 2). If one electron (e.g., electron 1) is close to the nucleus and a second electron (electron 2) is far away from the nucleus, then the averaged electron-nuclear distance $\langle r_{31}\rangle$ (given in Table II) will not indicate anything typical for a weakly bound structure. Let x be the distance between the first electron and nucleus, while y is the distance between the second electron and nucleus. The two-body, cluster structure means $x\ll y$, and therefore, $y\approx\langle r_{21}\rangle$. Now, the numerical values of x and y can be evaluated from the two following equalities $x+y=2\langle r_{en}\rangle$ and $y=\langle r_{ee}\rangle$, where r_{ne} and r_{ee} are the electron-nucleus and electron-electron distances, respectively. Finally, by using the appropriate results from Table II one finds $r_{31}\approx 1$ (i.e., the value that can be found for the ground state in the neutral H atom), while $r_{32}\approx 4.4$, where 1 and 2 designate electrons, while 3 means the nucleus. In other words, the distance between one electron and the nucleus is roughly 4.4 times larger than this distance between the other electron and the nucleus. Note, however, that the evaluation made above assumes that we can distinguish electrons 1 and 2 in the H^- ion. This violates the principle of indistinguishability, and therefore all presented arguments cannot be taken very rigorously (for more detail see [13]).

Now, by using the results presented in Tables I and II we can derive simple interpolation formulas for the bound-state properties in the H^- ion. Such formulas are important for applications, since the nuclear masses are the subject of intensive experimental revision. For an arbitrary property $\langle X\rangle$ we can write the following general expression [14]:

$$\langle X(^M H^-)\rangle=\langle X(^\infty H^-)\rangle+\sum_k \frac{a_k(X)}{M^k}, \quad (7)$$

where M is the mass of the nucleus in the H^- ion and $a_k(X)$ are the unknown numerical coefficients. In general, the series in the last equation should be a Puiseux series in M^{-1} [14]. But the ground state in the $^\infty H^-$ ion is nondegenerate, and hence, all powers k in the last equation can be chosen as integer. Presently, we restrict ourselves to the quadratic formulas only, i.e., $k_{max}=2$ in the last equation, or, in other words,

$$\langle X(^M H^-)\rangle=\langle X(^\infty H^-)\rangle+\frac{a_1(X)}{M}+\frac{a_2(X)}{M^2}. \quad (8)$$

The coefficients $a_1(X)$ and $a_2(X)$ have been determined from the results given in Table II (for all systems). For instance, for the four following properties $X=E$ (the total energy), r_{31}, r_{21}^2, and δ_{31}, these coefficients can be found in Table III. Table III also includes the appropriate numerical results (predicted by using the last equation and found in direct computations) for the $\pi^+e^-e^-$ system ($m_\pi=273.126\,95\,m_e$). As follows from Table III the agreement between expected and computed results seems to be very good.

In conclusion, let us discuss some problems related to the nuclear β^- decay in the T^- ion. Our present goal is to evaluate the appropriate probabilities for the final ^{3}He atom to be found in one of its bound states. The process can be written symbolically in the form

$$^3H^-=\,^3He+e^-+18.57\ \text{keV}. \quad (9)$$

This problem was discussed in detail in [15]. The computational procedure used in [15] is based on the so-called sud-

TABLE III. The predicted and computed expectation values $\langle X_{ij}\rangle$ in atomic units ($m_e=1,\hbar=1,e=1$) of some properties for the ground states in the two-electron $\pi^+e^-e^-$ ion. $a_1(X)$ and $a_2(X)$ are the two coefficients in Eq. (8).

$\langle X_{ij}\rangle$	$a_1(X)$	$a_2(X)$	$\langle X_{ij}\rangle^{a}$	$\langle X_{ij}\rangle^{b}$
E	0.560 628 955 414 4	−0.648 887 973 485 1	−0.525 707 083 563	−0.525 707 095 013 630
$\langle r_{31}\rangle$	3.521 116 463 89	−1.051 078 371 547	2.723 056 056 06	2.723 056 055 69
$\langle r_{21}^2\rangle$	64.531 684 287 8	17.717 403 239 5	25.438 532 728 3	25.438 533 238 1
$\langle \delta_{31}\rangle$	−0.501 704 596 817	1.035 441 688 30	0.162 729 841	0.162 729 868

[a]The predicted value [see Eq. (8)].
[b]The computed (variational) value.

den approximation [16,17]. In the considered case the sudden approximation means that the emitted β^- particle leaves the maternal ion (atom) for a time $\tau\approx a_0/v_\beta = a_0/c\,\sqrt{1+(m_ec^2/E_\beta)}$ (where E_β is the kinetic energy of the emitted β^- particle), which is significantly shorter than the typical atomic time $t_a=a_0/(\alpha c)$. Here and below a_0 is the Bohr radius and α is the fine-structure constant ($\approx\frac{1}{137}$). The condition $\tau\ll t_a$ can be rewritten in the different form

$$\sqrt{1+\frac{m_ec^2}{E_\beta}}\ll\frac{1}{\alpha}$$

or

$$E_\beta\gg\alpha^2m_ec^2=0.027\,211\,396\,1\ \text{keV}=1\ \text{Ry}. \tag{10}$$

The last condition is obviously obeyed for the β^- decay in the T^- ion.

In [15] it was shown that in the sudden approximation the appropriate probability can be represented in the following form:

$$P_{g,n^1S}=\left|\langle\Psi_{H^-}(r_{32},r_{31},r_{21})|\Phi_{\,^3He;n^1S}(r_{32},r_{31},r_{21})\rangle\right|^2, \tag{11}$$

where $\Psi_{H^-}(r_{32},r_{31},r_{21})$ is the wave function of the ground state in the H^- ion, while $\Phi_{\,^3He;n^1S}(r_{32},r_{31},r_{21})$ is the ''final'' wave function of the $(n-1)$th excited $^1S(L=0)$ state in the ^{3}He atom. The case $n=1$ corresponds to the ground state in the ^{3}He atom. In the present study we have determined the probability for the final ^{3}He atom to be in its ground $1^1S(L=0)$ state as $P\approx(0.479\,518\,28)^2=0.229\,937\,64$. The analogous probability for the first excited $2^1S(L=0)$ state of the ^{3}He atom is $\approx(0.684\,597\,7)^2\approx0.468\,674\,04$, while for the second excited $3^1S(L=0)$ state such a probability equals $\approx(0.011\,620\,4)^2\approx0.001\,35$, and for the third excited $4^1S(L=0)$ state $P\approx(0.045\,872)^2\approx0.002\,1$. Thus, the helium-3 atom produced after β^- decay in the T^- ion can be found in its first excited state ($\approx$47%) or in its ground state ($\approx$23%). In our present computations both initial and final nuclei are assumed to be infinitely heavy.

Let us compare the found figures with the known results for the β^- decay from the ground state of the tritium (T) atom [15]. In the last case, the final $^3He^+$ ion can be found mainly in the ground ($\approx$70%) or first excited (25%) states. For other excited states the appropriate probabilities are relatively small (for details see [15]). For the β^- decay in the T^- ion these figures are $\approx$23% for the ground state of the ^{3}He atom and $\approx$47% for its first excited state. The principal difference between β^- decay from the T^- ion and T atom can be explained from the fact that the T^- ion has a very diffuse, weakly bound structure, while the final (neutral) ^{3}He atom is quite compact. The question about atomic ionization stimulated by the β^- decay is even more interesting. Its probability P_i can be found as the difference between the unit and the total probability for the remaining atom (or ion) to be bound (i.e., the sum of all bound-state probabilities). This gives $P_i\approx3\%$ for the β^- decay in the T atom, and almost $\approx$30% for the β^- decay in the T^- ion. Such a remarkably large deviation needs a separate investigation, but here we want to make only the following remark. The traditional arguments related to the weakly bound structure of the H^- ion cannot explain satisfactorily the difference in 10 times between these two cases. For instance, the β^- decay of the tritium atom in its highly excited, weakly bound (Rydberg) states also gives only 2–4 % for the total ionization probability. From our present point of view the $\approx$70% probability for the T^- ion includes only those bound-state probabilities where the final states (in the ^{3}He atom) are singlets. But it is easy to understand that the corresponding (bound) triplet states of the final ^{3}He atom must also be included in the consideration. The triplet states arise as the result of spin-spin (or spin exchange) interactions between atomic electrons and moving β^- particle (i.e., fast electron). This means that the spin state of the emitted β^- particle changes also (spin conversion). But in terms of the sudden (two-electron) approximation used above, the appropriate probabilities cannot be evaluated even approximately, since in this method all of them equal zero identically. If the total probability of finding the final ^{3}He atom in triplet states is $\approx$15–20 %, then the total ionization probability equals $\approx$10–15 %, which is only 3–5 times larger than the values known from other β^- decaying atomic and ionic systems.

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