Bound state properties of four-body muonic quasi-atoms

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Abstract

Total energies and various bound state properties are determined for the ground states in all six four-body muonic $a^+b^+\mu^-e^-$ quasi-atoms. These quasi-atoms contain two nuclei of hydrogen isotopes p^+, d^+, t^+, one negatively charged muon μ^- and one electron e^-. In general, each of the four-body muonic $a^+b^+\mu^-e^-$ quasi-atoms, where $(a,b) = (p,d,t)$, can be considered as the regular one-electron (hydrogen) atom with the complex nucleus $a^+b^+\mu^-$ which has a finite number of bound states. Furthermore, all properties of such quasi-nuclei $a^+b^+\mu^-$ are determined from highly accurate computations performed for the three-body muonic ions $a^+b^+\mu^-$ with the use of pure Coulomb interaction potentials between particles. It is shown that the bound state spectra of such quasi-atoms are similar to the spectrum of the regular hydrogen atoms, but there are a few important differences. Such differences can be used in future experiments to improve the overall accuracy of current evaluations of various properties of hydrogen-like systems, including the lowest-order relativistic and QED corrections.

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I.   INTRODUCTION

Recently, by performing variational calculations of the bound states in three-body muonic molecular ions [1] we have re-discovered a new class of four-body systems which are of interest in some applications. The existence of these neutral four-body atomic systems follows from the analysis of actual experimental conditions which can be found in liquid hydrogen/deuterium. Indeed, in actual experiments with muons it is hard to imagine a positively charged muonic molecular ion, e.g., the $(pd\mu)^+$ ion, which moves as a separate and stable system in liquid hydrogen/deuterium with the density $\rho \approx 0.213 \; g \cdot cm^{-3}$. It is clear that such system will take an additional electron e^- from surrounding atoms/molecules and form the neutral muonic quasi-atom $pd\mu e$. Later such a four-body quasi-atom $pd\mu e$ will react with a protium/deuterium molecule and form a stable six-body quasi-molecule $(pd\mu)pe_2$ or $(pd\mu)de_2$. All transformations of muonic four-body quasi-atoms and six-body quasi-molecules occur on a time scale of $\tau \approx 1 \cdot 10^{-10} \; sec$ which is significantly shorter than the muon life time $\tau_\mu \approx 2 \cdot 10^{-6} \; sec$ and/or the reaction time for the nuclear $(p, d)-$reaction. This means that the muonic quasi-atoms $pd\mu e$, $pd\mu e$, $dt\mu e$, etc, and muonic quasi-molecules $(pd\mu)pe_2$ and $(pd\mu)de_2$ can be observed in actual experiments. Therefore, it is interesting to investigate the properties of such systems. In this study we determine the bound state properties of the four-body $ab\mu e$ quasi-atoms and discuss some interesting experiments for these systems.

In atomic units $\hbar = 1, m_e = 1, e = 1$ the Hamiltonian of the four-body $pd\mu e$ quasi-atom is:

$$H = -\frac{1}{2m_p}\Delta_1 - \frac{1}{2m_d}\Delta_2 - \frac{1}{2m_\mu}\Delta_3 - \frac{1}{2}\Delta_4 + \frac{1}{r_{12}} - \frac{1}{r_{13}} - \frac{1}{r_{14}} - \frac{1}{r_{23}} - \frac{1}{r_{24}} + \frac{1}{r_{34}} \quad (1)$$

where the notation 1 designates the protium nucleus (p or ^{1}H), the notation 2 (or +) means the deuterium (d) nucleus, while 3 and 4 stand for the negatively charged muon μ^- and electron e^-, respectively. This system of notations will be used everywhere below in this study. Note that the three heavy particles p^+, d^+ and μ^- in this system have very large masses in comparison with the electron mass m_e (in atomic units $m_e = 1$) and opposite electric charges. Therefore, we can expect that inside of the $pd\mu e$ quasi-atom these three heavy particles (p^+, d^+ and μ^-) will form a separate three-body cluster $pd\mu$ which is spatially compact and has a positive electric charge +1. The fourth particle (electron e^-) moves at

very large distances from this central, heavy cluster. If a_0 is the Bohr radius, then the radius of the electron orbit in the $pd\mu e$ quasi-atom is $R_e \approx a_0$, while the spatial radius of the central heavy cluster is $R_\mu \approx \left(\frac{m_e}{m_\mu}\right) a_0 \approx \left(\frac{1}{206.768262}\right) a_0 \ll a_0$. Analogous relations between radii of the electron and muonic orbits can be found in other four-bound quasi-atoms $ab\mu e$. In fact, all bound state properties in the four-bound quasi-atoms $ab\mu e$ can be separated into two different groups: electronic properties and muonic properties. Sometimes, it is convenient to split the muonic properties into two additional subgroups: muonic and nuclear properties. The reason for such a separation is obvious, since each of the nuclear masses M_p, M_d, M_t is substantially larger than the muon mass $m_\mu = 206.768262 m_e$.

II.   TOTAL ENERGIES

Based on the cluster structure of the four-body quasi-atom $pd\mu e$ we can predict that this quasi-atom is a bound four-body system which is very similar to the regular hydrogen atom. Moreover, the binding state energy of this quasi-atom must be very close to the total energy of the one-electron hydrogen atom. For instance, the binding energy of the ground $1S(L = 0)-$state in the $pd\mu e$ atom must be close to -0.5 $a.u.$, while the analogous energy of the $2S(L = 0)-$state (electron state) in the $pd\mu e$ quasi-atom must be close to -0.125 $a.u.$, etc. In general, the total energy of the bound state with the principal quantum number n in the $pd\mu e$ quasi-atom is approximately equal to

$$E \approx E(pd\mu) + E(\mathrm{H}) \approx -106.012527069515844 - \frac{1}{2n^2} \quad a.u. \tag{2}$$

Thus, the ground state ($n = 1$) in this four-body quasi-atom $pd\mu e$ has the total energy $E \approx$ -106.512 527 069 515 844(2) $a.u.$ [1]. Analogous relations can be found for other $ab\mu e$ quasi-atoms.

In reality, the value of E given by Eq.(2) must be corrected, since the masses of the deuterium and protium nuclei and μ^- muon are finite. In this study we shall assume that $m_p = 1836.152701 \ m_e$, $m_d = 3670.483014 \ m_e$, $m_t = 5496.92158 \ m_e$ and $m_\mu = 206.768262$ m_e. These masses are often used in accurate computations of the muonic molecular ions. With these masses the total energy of the four-body quasi-atom $pd\mu e$ is $E \approx$ -106.512 439 401 $a.u.$, i.e. it is slightly above the value -106.512 527 069 52 $a.u.$ mentioned above. It is clear that the non-relativistic energy E from Eq.(2) is only an approximation to the exact

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total energy of the $pd\mu e$ quasi-atom, since this value of E does not include all contributions from the lowest-order relativistic and QED corrections. A large number of other corrections, e.g., the finite-size corrections, corrections on nuclear interactions, etc, to the total energy have been ignored as well.

The total energy E given by Eq.(2) corresponds to the case when the central quasi-nucleus (or heavy three-body cluster) $pd\mu$ is in its ground $S(L = 0)-$state. However, this three-body quasi-nucleus $pd\mu$ can also be detected in its bound $P(L = 1)-$state with the total energy -101.453 777 548 914 a.u. [1]. In this case the total energy of the $pd\mu e$ quasi-atom with the central nucleus in its bound $P(L = 1)-$state is $\approx$ -101.953 777 548 914 a.u., i.e. it is substantially different from the value $E \approx$ -106.512 439 401 a.u. mentioned above for the ground state and the main difference arises from the energy of the central quasi-nucleus $pd\mu$.

As is well known the six muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$ have 22 bound states (see, e.g., [1] and references therein). These are the $S(L = 0)-, P(L = 1)-, D(L = 2)-$ and $F(L = 3)-$states, where the notation L designates the total angular momentum of this three-body ion $ab\mu$, where $(a, b) = (p, d, t)$. Nine of these bound states are the $S(L = 0)-$states, nine $P(L = 1)-$states, three $D(L = 2)-$states and one $F(L = 3)-$state. The four-body muonic quasi-atoms which contain two nuclei of hydrogen isotopes can be considered as a family of similar one-electron (or hydrogen-like) atoms. One of the six muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$ plays the role of the nucleus in each of these atoms. In general, such a nucleus can be either in the ground $S(L = 0)-$state, or in one of its 'rotationally' and/or 'vibrationally' $(L, \nu)-$excited states. Here to designate the excited states in the $ab\mu$ ion we use the $(L, \nu)-$notation, where L denotes the rotational state, while ν stands for the vibrational state.

All bound states properties, including the lowest order relativistic and QED corrections, determined for such hydrogen-like quasi-atoms substantially depend upon the hydrogen-isotope composition and excitation of the central three-body 'nucleus' $ab\mu$. The spectra of the excited states is very well known for each of the six muonic molecular ions $ab\mu$. Therefore, the $ab\mu e$ quasi-atoms with different hydrogen isotopes $a = (p, d, t)$ and $b = (p, d, t)$ can be considered as model hydrogen-like atoms. The 'nuclear' spectra in such atoms are known to very high accuracy. This allows one to consider possible interactions between 'atomic' and 'nuclear' bound states in the $ab\mu e$ quasi-atoms. Note again that all 'nuclear' properties of

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the $ab\mu$ quasi-nucleus can be obtained from highly accurate Coulomb calculations performed for three-body systems.

In general, the electron motion in the $ab\mu e$ quasi-atom is well separated from the motion of the three heavy particles $a^+ b^+ \mu^-$. For instance, the expectation values of the kinetic energies of the electron and muon in the $ab\mu e$ quasi-atom differ by a factor of 50 - 100. However, as is well known (see, e.g., [2], [3] and references therein) the 'vibrationally' excited $P(L = 1)-$states (or (1,1)-states) in the $dd\mu$ and $dt\mu$ three-body ions are very weakly bound. The binding energies of the three-body ions $dd\mu$ and $dt\mu$ in their excited (1,1)-states are $\approx$ -1.9749881 eV and $\approx$ -0.6603387 eV, respectively [1]. These 'nuclear' binding energies are comparable with the corresponding atomic energies. In such cases one can certainly observe a strong interference between the 'nuclear' and 'atomic' bound states. In reality, for bound states with very weakly bound nuclei (or quasi-nuclei) we cannot discuss their nuclear and electron spectra separately. The analysis of atomic systems with weakly bound nuclei is very complex, but its results are of great interest in a number of applications.

III. VARIATIONAL WAVE FUNCTIONS

To determine the total energies and bound state properties one needs to construct approximate wave functions for the four-body quasi-atoms. In this study these wave functions are approximated by the variational expansion written in the basis of the six-dimensional (or four-body) gaussoids of relative (or inter-particle) scalar coordinates r_{ij}. This variational expansion was originally proposed 30 years ago in [4] for accurate variational calculations of the few-nucleon nuclei and $\Lambda-$nuclei. For the bound $S(L = 0)-$states the variational anzatz of fully correlated six-dimensional (or four-body) gaussoids is written in the form [4]

$$\Psi_{L=0} = (1 + \delta_{ab}\epsilon_{ab}\mathcal{P}_{ab}) \sum_{k=1}^{N} C_k \cdot exp(-\alpha_{12}^{(k)}r_{12}^2 - \alpha_{13}^{(k)}r_{13}^2 - \alpha_{23}^{(k)}r_{23}^2 - \alpha_{14}^{(k)}r_{14}^2 - \alpha_{24}^{(k)}r_{24}^2 - \alpha_{34}^{(k)}r_{34}^2) \quad (3)$$

where C_k are the linear coefficients (or linear variational parameters), while $\alpha_{ij}^{(k)}$ are the optimized non-linear parameters. The notation $\epsilon_{ab}\mathcal{P}_{ab}$ means the appropriate symmetrizer (or antisymmetrizer), i.e. a projection operator which produces the wave function with the correct permutation symmetry in those cases when $a = b$. This case is designated in Eq.(3) with the use of the delta-function. The operator $\mathcal{P}_{ab}$ is the pair-permutation operator for all coordinates, i.e. for the spatial, spin, iso-spin, etc, coordinates.

By using some effective strategies for optimization of the non-linear parameters $\alpha_{ij}^{(k)}$ in Eq.(3) one can obtain very accurate variational wave functions with relatively small number of terms $N \approx 400$ - 600 in Eq.(3). The generalization of the variational expansion, Eq.(3), to the bound states $L \geq 1$ is straightforward. It is clear that for the quasi-atoms $ab\mu e$ with the 'rotationally' excited 'nuclei' $ab\mu$ the minimal number of terms in Eq.(3) must be larger to achieve better overall accuracy. However, in this study we shall not discuss numerical computations of bound states with $L \geq 1$ and restrict ourselves to the analysis of the bound $S(L = 0)-$states.

IV.   BINDING ENERGIES AND OTHER BOUND STATE PROPERTIES

As we have shown above the total energy of the $pd\mu e$ atom is approximately equal to the sum of the total energies of the hydrogen atom and $pd\mu$ ion, i.e. $E(pd\mu e) \approx E(pd\mu) + E(\mathrm{H}; n\ell)$, where n and ℓ are the principal and angular quantum numbers of the hydrogen atom. The corresponding binding energy is the difference between this value and the total energy of the three-body $pd\mu$ ion. This means that the binding energy of the ground state of the four-body atom $pd\mu e$ approximately equals to the total energy of the ground state of the hydrogen atom which equals -0.5 $a.u.$ In other words, the total energy of the ground state in the four-body $pd\mu e$ system approximately equals the sum of total energies of the three-body muonic molecular ion $pd\mu$ and the ground state energy of the 'hydrogen' atom, i.e. -0.5 $a.u.$ The use of the finite masses for different hydrogen isotopes p, d, t and muon μ slightly decreases the 'expected' value of the total energy.

Other bound state properties of the $ab\mu e$ quasi-atoms computed with our approximate wave functions, e.g., the $\langle r_{ij} \rangle, \langle r_{ij}^2 \rangle, \langle \delta(\mathbf{r}_{ij}) \rangle$ expectation values, coincide well either with the known properties of the hydrogen atom (in those cases, when one of the indexes i or j designates the electron), or with the bound state properties known for the three-body muonic molecular ion $ab\mu$ (see, e.g., [1] and references therein). The expectation values of some of the operators computed numerically for the four-body $pd\mu e, pt\mu e$ and $dt\mu e$ quasi-atoms can be found in Table II. They can be compared directly with the expectation values obtained earlier for the three-particle $pd\mu$ ion and for the one-electron hydrogen atom. In general, such a comparison is of great interest, since it allows to compare directly the overall qualities of the different variational wave functions. On the other hand, it is very interesting

to find the electronic properties of the four-body $ab\mu e$ quasi-atoms which are substantially different from the known properties of the hydrogen atoms.

The expectation values of different bound state properties determined to high numerical accuracy allow one to estimate a large number of fundamental atomic properties which can be directly measured in actual experiments. Here by 'fundamental property' we shall understand some combination of atomic expectation values which determine the results of direct experimental observations. In other words, any fundamental property leads to some experimental effects. Below, we discuss only the two following effects: (a) the evaluation of the field component of the total isotope shift for the $ab\mu e$ quasi-atoms, and (b) the hyperfine structure splittings in these quasi-atoms. As is well known (see, e.g., [5], [6] and references therein) the field shift is related to the extended nuclear charge distribution which produces the non-Coulomb field at distances close to the nucleus. It is clear that the largest deviations between the Coulomb and actual potentials can be found close to the atomic nucleus, i.e. for distances $r \approx r_e \ll \Lambda \ll a_0$, where $r_e = \alpha^2 a_0$ is the classical electron radius and $\Lambda = \alpha a_0$ is the Compton wave length. Here and below, $\alpha = 7.297352568 \cdot 10^{-3}$ is the fine structure constant and $a_0 \approx 5.29177249 \cdot 10^{-11}$ m is the Bohr radius. Now note that all 'nuclei' in $ab\mu e$ quasi-atoms are three-body muonic molecular ions $ab\mu$ with the spatial radius $a_\mu \approx a_0/m_\mu \gg r_e = \alpha^2 a_0$. Therefore, we can predict that the field component of the total isotope shift in the $ab\mu e$ quasi-atoms must be relatively large. Furthermore, this component of the total isotope shift will be substantially $a-$ and $b-$ dependent, since the spatial radius of the $ab\mu e$ quasi-atom depends upon the two nuclei of the hydrogen isotopes a and b.

Another interesting problem is to predict the hyperfine structure splitting of the four-body $pd\mu e$ and other similar quasi-atoms. Later the computed hyperfine structure splitting must be compared with the corresponding experimental results. For instance, consider the hyperfine structure splitting of the four-body $pd\mu e$ quasi-atom. The central quasi-particle, i.e. the $pd\mu$ ion, has two bound states with different angular momenta. These states are also bound in the analogous $pt\mu$ and $pp\mu$ ions. In each of the $dd\mu$ and $dt\mu$ ions one finds five bound states: two $S(L = 0)-$states, two $P(L = 1)-$states and one $D(L = 2)-$state). The heaviest $tt\mu$ ion has six bound states: two $S(L = 0)-$states, two $P(L = 1)-$states, one $D(L = 2)-$state and $F(L = 3)-$state). We can define the angular moment L of the central 'nucleus' $ab\mu$ and the magnetic moment $\mathbf{S}$ (or 'spin', for short)

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associated with L. The 'nuclear' spin $\mathbf{S}$ of the $ab\mu$ quasi-nucleus is combined with the electron spin $\mathbf{s}_e$ and this produces the hyperfine structure splitting of the four-body $ab\mu e$ quasi-atom. By determining the expectation values of the corresponding delta-functions and a few other properties one can evaluate the hyperfine structure splitting in all six four-body $ab\mu e$ systems, where $(a, b) = (p, d, t)$, and then to compare the predicted hyperfine structure splittings with the actual experimental values.

V.   CONCLUSIONS

We have discussed the bound state spectra and properties of the muonic four-body quasi-atoms $ab\mu e$, where $(a, b) = (p, d, t)$. The energy spectra of such four-body quasi-atoms are of interest in some applications. Briefly, an arbitrary bound state in the four-body muonic quasi-atom $ab\mu e$ is represented as a motion of the negatively charged electron e^- in the field of a compact 'central cluster' $ab\mu$ which has positive electric charge $+1$. The spatial radius of the central cluster in the $ab\mu e$ quasi-atom is in ≈ 206.77 times smaller than the actual radius of the electron orbit $r_e \approx a_0$, where a_0 is the Bohr (atomic) radius. The study of bound state spectra in four-body muonic quasi-atoms $ab\mu e$ may lead to some important results and conclusions which can also be useful in applications to other atomic and quasi-atomic systems. In reality, for each four-body muonic quasi-atoms $ab\mu e$ we know the bound state spectra of its central quasi-nucleus $ab\mu$. Moreover, the probabilities of all possible electromagnetic transitions in this quasi-nucleus $(ab\mu)$ can be determined to very good accuracy. This simplifies the analysis of many related phenomena, including internal transitions of radiation, in the four-body quasi-atom $ab\mu e$.

There are a number of other problems which are of special interest in various applications. In particular, the problems related with accurate computations of some bound state properties for the four-body muonic quasi-atoms $ab\mu e$. Such properties include the lowest order relativistic and QED corrections. There is a great interest to determine such corrections from direct calculations and compare them with the results of approximate evaluations based on the one-electron model of the $ab\mu e$ quasi-atom. In general, the theoretical and experimental analysis of four-body quasi-atoms $ab\mu e$ is a very interesting problem. Analysis and solutions of this problem will certainly lead to a substantial improvement of our current knowledge

about the bound state spectra in four-body systems with arbitrary particle masses.

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TABLE I: The total non-relativistic energies E of the ground states of the six four-body muonic quasi-atoms $ab\mu e$ (in atomic units). N designates the total number of basis functions used in Eq.(3).

$E(N)$	$pd\mu e$	$pt\mu e$	$dt\mu e$
$E(N = 400)$	-106.51220095	-107.99440514	-111.86416935
$E(N = 600)$	-106.51221589	-107.99447566	-111.86417390
$E(N)$	$pp\mu e$	$dd\mu e$	$tt\mu e$
$E(N = 400)$	-102.72325941	-110.31674273	-113.47253968

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 of the $pd\mu e$ and $pt\mu e$ ions. Below, the notations 1 and 2 designate the two heavy hydrogen nuclei, while 3 stands for the negatively charged muon and 4 denotes the electron.

$\langle X_{ij} \rangle$	$pd\mu e$	$pt\mu e$	$\langle X_{ij} \rangle$	$pd\mu e$	$pt\mu e$
$\langle r_{12}^{-2} \rangle$	6844.241	7006.672	$\langle r_{12}^{-1} \rangle$	76.31734	77.53007
$\langle r_{13}^{-2} \rangle$	38979.32	37946.94	$\langle r_{13}^{-1} \rangle$	132.5684	130.9652
$\langle r_{23}^{-2} \rangle$	52479.23	56036.31	$\langle r_{23}^{-1} \rangle$	155.7732	161.5537
$\langle r_{14}^{-2} \rangle$	1.998033	1.999259	$\langle r_{14}^{-1} \rangle$	0.999936	1.000105
$\langle r_{24}^{-2} \rangle$	1.997728	1.998940	$\langle r_{24}^{-1} \rangle$	0.999946	1.000120
$\langle r_{34}^{-2} \rangle$	1.996369	1.997399	$\langle r_{34}^{-1} \rangle$	0.999893	1.000065
$\langle r_{12} \rangle$	0.01499605	0.01468559	$\langle r_{12}^{2} \rangle$	$0.2532887 \cdot 10^{-3}$	$0.2420306 \cdot 10^{-3}$
$\langle r_{13} \rangle$	0.01185618	0.01190350	$\langle r_{13}^{2} \rangle$	$0.1879009 \cdot 10^{-3}$	$0.1878566 \cdot 10^{-3}$
$\langle r_{23} \rangle$	0.01009683	0.00968241	$\langle r_{23}^{2} \rangle$	$0.1379205 \cdot 10^{-3}$	$0.1264102 \cdot 10^{-3}$
$\langle r_{14} \rangle$	1.49881976	1.49871404	$\langle r_{14}^{2} \rangle$	2.9900765	2.9899082
$\langle r_{24} \rangle$	1.49879648	1.49868607	$\langle r_{24}^{2} \rangle$	2.9899945	2.9898139
$\langle r_{34} \rangle$	1.49881730	1.49870839	$\langle r_{34}^{2} \rangle$	2.9900578	2.9898811
$\langle -\frac{1}{2}\nabla_1^2 \rangle$	11997.3637	12048.5840	$\langle \delta_{12} \rangle$	204.556	111.396
$\langle -\frac{1}{2}\nabla_2^2 \rangle$	15710.1876	17057.8313	$\langle \delta_{13} \rangle$	$1.03470 \cdot 10^6$	$9.996883 \cdot 10^5$
$\langle -\frac{1}{2}\nabla_3^2 \rangle$	19683.9060	20227.9869	$\langle \delta_{23} \rangle$	$1.52440 \cdot 10^6$	$1.66268 \cdot 10^6$
$\langle -\frac{1}{2}\nabla_4^2 \rangle$	0.50000887	0.50017715	$\langle \delta_{14} \rangle$	0.312824	0.315269
$\langle \delta_{24} \rangle$	0.311171	0.313777	$\langle \delta_{34} \rangle$	0.307469	0.307219