Bound state spectra and properties of the five- and six-body muonic ions and quasi-molecules.

Alexei M. Frolov

ITAMP, Harvard-Smithonian Center for Astrophysics,

MS 14, 60 Garden Street, Cambridge MA 02138-1516, USA and

Department of Applied Mathematics

University of Western Ontario, London, Ontario N6H 5B7, Canada

(Dated: October 8, 2018)

Abstract

The ground bound states in the five-body muonic ions \(ab\mu e_2\) (or \((ab\mu e_2)^-\)), where \((a,b) = (p,d,t)\), are considered for the first time. As follows from accurate numerical computations of these five-body ions they are similar to the negatively charged hydrogen ion \(H^-\) with a three-particle central quasi-nucleus \(ab\mu\) (or \((ab\mu)^+\)). These five-body ions play some role in the muon-catalyzed fusion of nuclear reaction in liquid deuterium and/or deuterium-tritium mixtures. We also discuss the bound states in the six-body \(abc\mu e_2\) quasi-molecules, where \((a,b,c) = (p,d,t)\). These six-body, two-electron quasi-molecules are of great interest for muon-catalyzed nuclear fusion, since in liquid deuterium and/or deuterium-tritium mixture more than 99 % of all muon-catalyzed reactions of the \((dd)^-\) and \((dt)^-\)-fusion occur in such six-body quasi-molecules: \(dd\mu e_2,ddd\mu e_2\) and \(dt\mu e_2\).

PACS number(s): 36.10.Dr

*E–mail address: afrolov@uwo.ca
I. INTRODUCTION

The goal of this study is to analyze the bound state spectra and internal structure of a number of five- and six-body species which contain one negatively charged muon $\mu^-$ and two bound electrons $e^-$. These compounds are formed when fast negatively charged muons $\mu^-$ slow down in liquid deuterium (hydrogen) and during the following chain of reactions of muon-catalyzed fusion. In various papers published since the end of 1950’s (see, e.g., [1] - [5]) it was assumed that the reactions of the nuclear $(d,d)$- and $(d,t)$-fusion
\[ d + d = ^3\text{He} + n + 3.270\text{MeV} \quad ; \quad d + d = t + p + 4.033\text{MeV} \quad (1) \]
\[ d + t = ^4\text{He} + n + 17.590\text{MeV} \quad (2) \]
proceed in the three-particle muonic molecular ions $dd\mu$ and $dt\mu$, respectively (see, e.g., [6]). It is clear that the actual fusion rates substantially depend upon the quantum numbers of actual bound state(s) in three-body muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$. The total energies of all 22 bound states in six muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$ can be found in [7]. In reality, it is difficult to imagine that such compact ions can exist as bare positively charged quasi-particles at very low temperatures which can be found in liquid hydrogen, or in liquid deuterium. In general, all three-particle muonic molecular ions will attract a number of electrons from surrounding molecules. In addition to this, the positively charged $dd\mu$ and $dt\mu$ ions and neutral hydrogen-like $dd\mu e$ and $dt\mu e$ atoms will interact with the atoms of deuterium, tritium and hydrogen molecules from liquid deuterium and/or deuterium-tritium mixture. Such interactions will lead, in principle, to the formation of a number of four-, five- and six-particle atomic and molecular muonic systems, i.e. systems which include one negatively charged muon $\mu^-$, two bound electrons $e^-$ and two (or three) nuclei of hydrogen isotopes.

In this study we consider the five-particle atomic ions, such as $pd\mu e_2, dd\mu e_2, dt\mu e_2$, etc, and six-body neutral quasi-molecules, such as $pdt\mu e_2$ and $ddt\mu e_2$. Based on our current knowledge of internal structures of various few-body atoms and ions we can predict that all five-body, two-electron $(ab\mu e_2)^-$ ions are similar to the negatively charged hydrogen ion $\text{H}^-$, which has only one stable (ground) electronic $1^1S$-state. Here and everywhere below the letters $a, b$ and $c$ designate the nuclei of hydrogen isotopes. In contrast with this, the internal structure of the six-body quasi-molecules $pdt\mu e_2, ddt\mu e_2$ is similar to the structure
of the neutral two-electron H$_2$ molecule. As was found in actual experiments more than 99 % of all (dd$\rightarrow$ and (dt$\rightarrow$-fusion reactions in liquid deuterium and/or deuterium-tritium mixture occur in such six-body quasi-molecules: pdt$\mu e_2$, ddd$\mu e_2$ and ddt$\mu e_2$ (see, e.g., [6] and references therein). In this study we investigate the basic properties and internal structure of these six-body quasi-molecules abc$\mu e_2$. It should be mentioned here that none of these five- and six-body muonic ions and quasi-molecules have been considered earlier.

Our goal below is to perform variational computations of the ground $S(L = 0)$-states in the five-body ions ab$\mu e_2 = (ab\mu e_2)^-$, where (a, b) = (p, d, t), and in the six-body abc$\mu e_2$ quasi-molecules, where (a, b, c) = (p, d, t). Briefly, we consider the bound ground $S(L = 0)$-states in a number of five- and six-body two-electron systems each of which contains one negatively charged muon $\mu^-$, two electrons $e^-$ and two (or three) bare nuclei of hydrogen isotopes, i.e. the nuclei of protium $p$, deuterium $d$ and/or tritium $t$. In our computations we determine the total energies and basic geometrical and physical properties of these ions and quasi-molecules. All calculations in this work have been performed with the use the following particle masses:

$$m_\mu = 206.768262 m_e, \quad M_p = 1836.152701 m_e$$
$$M_d = 3670.483014 m_e, \quad M_t = 5496.92158 m_e$$

where $m_e$ is the electron’s mass. The same set of particle masses has been used in our calculations of the three-body muonic molecular ions [7]. In this study we apply the atomic units in which $\hbar = 1, e = 1$ and $m_e = 1$. Our goal below is to determine the accurate solutions of the non-relativistic Schrödinger equation for the discrete spectrum $H \Psi = E \Psi$ (where $E < 0$). The non-relativistic Hamiltonians of the five- and six-body systems considered in this study are

$$H_5 = -\frac{\hbar^2}{2m_e} \left[ \nabla_1^2 + \nabla_2^2 + \frac{m_e}{m_\mu} \nabla_\mu^2 + \frac{m_e}{M_a} \nabla_a^2 + \frac{m_e}{M_b} \nabla_b^2 \right] + \sum_{i=2}^{5} \sum_{j=1}^{4} \frac{q_i q_j e^2}{r_{ij}},$$

and

$$H_6 = -\frac{\hbar^2}{2m_e} \left[ \nabla_1^2 + \nabla_2^2 + \frac{m_e}{m_\mu} \nabla_\mu^2 + \frac{m_e}{M_a} \nabla_a^2 + \frac{m_e}{M_b} \nabla_b^2 + \frac{m_e}{M_c} \nabla_c^2 \right] + \sum_{i=2}^{6} \sum_{j=1}^{5} \frac{q_i q_j e^2}{r_{ij}},$$

respectively. Here and everywhere below in this study we assume that the indexes 1 and 2 designate the two bound electrons, the index 3 stands for the negatively charged muon $\mu^-$,
while indexes 4, 5 and 6 denote the two (or three) heavy hydrogen nuclei. In atomic units the explicit forms of these two Hamiltonians, Eqs. (4) - (5), are drastically simplified, since in this case in Eqs. (4) - (5) we have \( e^2 = 1, \hbar^2 = 1 \) and \( m_e = 1 \).

This paper has the following structure. Variational computations of the five-body ions \( ab\mu e_2 \), where \((a,b) = (p,d,t)\), are considered in the next Section. Here we also compare some of the bound state properties of these ions with the known expectation values for the negatively charged hydrogen ion(s) \( H^- \) \[8\]. Numerical calculations of the total energies and a few other bound state properties of the six-body quasi-molecules \( abc\mu e_2 \), where \((a, b, c) = (p, d, t)\), are performed in Section III. Comparison of these properties with the known properties of the \( \text{H}_2 \) molecule can also be found in Section III. Concluding remarks can be found in the last Section.

II. NEGATIVELY CHARGED FIVE-BODY MUONIC IONS

As mentioned above the energy spectrum of each of the five-body negatively charged ions \( ab\mu e_2 \), where \((a, b) = (p, d, t)\), contains only one bound electron state, which is the ground \( 1^1S \) state. The five-body negatively charged ion \( ab\mu e_2 \) includes the central heavy nucleus \( ab\mu \) which is positively charged and two bound electrons. This follows from the fact that the radius of the central nucleus is in \( \approx \left( \frac{m_u}{m_e} \right) \approx 206.768 \) times smaller than the radius of the \( 1s \)–electron orbit in the hydrogen atom. It should be mentioned that each of the three-body \((ab\mu)^+\) ions has a few different bound states, e.g., each of the \( p\mu, pd\mu \) and \( pt\mu \) ions has two bound states, each of the \( dd\mu \) and \( dt\mu \) ions has five bound states, etc (for more detail, see \[7\]). Therefore, in experiments we can expect the appearance of a few different series of bound states in the five- and six-body muonic systems \( ab\mu e_2 \) and \( abc\mu e_2 \), respectively. In general, each bound state in the three-particle quasi-nucleus \((ab\mu)^+\) generates one separate series of bound states in the \( ab\mu e_2 \) and \( abc\mu e_2 \) systems. Below, such series of bound states are called the fundamental series of bound states. As follows from here the bound state spectra of the \( ab\mu e_2 \) \((= (ab\mu e_2)^-)\) ions is represented as a combination of a few fundamental series. If the particles \( a \) and \( b \) are the bare nuclei of the hydrogen isotopes, then each fundamental series of bound states in the \( ab\mu e_2 \) ion contains only one bound \( 1^1S \)–state.

To determine the accurate solutions of the non-relativistic Schrödinger equation \( H\Psi = E\Psi \) (where \( E < 0 \)) in this study we apply the variational expansion of the wave function \( \Psi \)
written in multi-dimensional gaussoids in the relative coordinates \( r_{ij} = | \mathbf{r}_i - \mathbf{r}_k | = r_{kj} \). The symbol \( \mathbf{r}_i \) designates the Cartesian coordinates of the \( i \)-th particle. Each of these gaussoids explicitly depends upon a complete set of the relative coordinates \( r_{ij} \). For the five-particle \( ab\mu e_2 \) ions one finds ten relative coordinates \( r_{ij} = r_{12}, r_{13}, r_{14}, r_{15}, r_{23}, \ldots, r_{45} \). Formally, only nine of these relative coordinates are truly independent, but this fact does not complicate analytical operations and numerical computations with the use of multi-dimensional gaussoids (in contrast with the basis of linear exponents).

The variational expansion of the ground state wave function of the \( ab\mu e_2 \) ion, where \( a \neq b \), written in multi-dimensional gaussoids takes the form:

\[
\Psi = \sum_{i=1}^{N_A} C_i (1 + \hat{P}_{12})(1 + \hat{P}_{45}) \exp\left( - \sum_{(jk)} \alpha_{ij}^{(i)} r_{jk}^2 \right)
\]

where \( N_A \) is the total number of basis functions used in variational computations, \( C_i \) are the linear parameters of this variational expansion, while \( \alpha_{ij}^{(i)} \) are the non-linear parameters which must be varied in actual calculations. The internal sum in the exponent in Eq.(6) is calculated over all possible pairs of particles, i.e. \((jk) = (12), (13), \ldots, (45)\), where we used the fact that the \((jk)\) and \((kj)\) permutations are identical, i.e., \((jk) = (kj)\). Note that the wave functions, Eq.(6), corresponds to the spatial part of the total wave function. Indeed, this wave function does not contain any spin functions, but it has the correct permutation symmetry in respect to the two electron coordinates (particles 1 and 2 in our notation).

In the \( pp\mu e_2, dd\mu e_2 \) and \( tt\mu e_2 \) ions we have an additional pair of indistinguishable particles. Antisymmetrization of the total wave functions for such ions is slightly complicated. For the spatial part of the total wave function of the \( aa\mu e_2 \) ion we can write in our notations:

\[
\Psi = \sum_{i=1}^{N_A} C_i (1 + \hat{P}_{12})(1 + \hat{P}_{45}) \exp\left( - \sum_{(jk)} \alpha_{ij}^{(i)} r_{jk}^2 \right)
\]

where \( \Psi \) is the spatial part of the total wave function of this ion. Since the spin part of the total wave function is a spatial constant, then the spatial wave function \( \Psi \) can be considered as the total wave function of the \( aa\mu e_2 \) ion. The basis wave function \( \psi_i \) in Eq.(6) is written in the form

\[
\psi_i = \exp\left( -\alpha_{12}^{(i)} r_{12}^2 - \alpha_{13}^{(i)} r_{13}^2 - \alpha_{14}^{(i)} r_{14}^2 - \alpha_{15}^{(i)} r_{15}^2 - \alpha_{23}^{(i)} r_{23}^2 - \alpha_{24}^{(i)} r_{24}^2 - \alpha_{25}^{(i)} r_{25}^2 - \alpha_{34}^{(i)} r_{34}^2 - \alpha_{35}^{(i)} r_{35}^2 - \alpha_{45}^{(i)} r_{45}^2 \right)
\]
Correspondingly, the $\hat{P}_{12}\psi_i$ function takes the from:

$$\hat{P}_{12}\psi_i = \exp(-\alpha_{12}r_{12}^2 - \alpha_{13}r_{13}^2 - \alpha_{23}r_{13}^2 - \alpha_{24}r_{14}^2 - \alpha_{25}r_{15}^2 - \alpha_{13}r_{23}^2 - \alpha_{14}r_{24}^2 - \alpha_{15}r_{25}^2)$$  \hspace{1cm} (9)

As follows from these two formulas the $\hat{P}_{12}\psi_i$ function can be obtained from the $\psi_i$ function by replacing the corresponding non-linear parameters in the exponent of the $\psi_i$ basis function. The $\hat{P}_{45}\psi_i$ and $\hat{P}_{12}\hat{P}_{45}\psi_i$ functions are determined analogously:

$$\hat{P}_{45}\psi_i = \exp(-\alpha_{12}r_{12}^2 - \alpha_{13}r_{13}^2 - \alpha_{15}r_{15}^2 - \alpha_{14}r_{14}^2 - \alpha_{23}r_{23}^2 - \alpha_{24}r_{24}^2 - \alpha_{25}r_{25}^2)$$  \hspace{1cm} (10)

and

$$\hat{P}_{12}\hat{P}_{45}\psi_i = \exp(-\alpha_{12}r_{12}^2 - \alpha_{13}r_{13}^2 - \alpha_{15}r_{15}^2 - \alpha_{14}r_{14}^2 - \alpha_{23}r_{23}^2 - \alpha_{24}r_{24}^2 - \alpha_{14}r_{25}^2)$$  \hspace{1cm} (11)

By performing a careful optimization of all ten non-linear parameters in each basis function $\psi_i$, where $i = 1, \ldots, N$, one finds an accurate approximation (for relatively large $N$) to the spatial part of the actual wave function of an arbitrary $ab\mu e_2$ ion, where $(a, b) = (p, d, t)$. Results of our calculations of the five-body negatively charged ions $ab\mu e_2 = (ab\mu e_2)^-$ can be found in Table I. Table I contains the total energies of the $ab\mu e_2$ ions. As follows from a comparison of the total energies from Tables I and II all five-particle ions considered in this study are stable. A number of bound state properties of these ions (expectation values) can be found in Table III. All these properties and energies are expressed in atomic units. Note that almost all electronic properties of the five-body $ab\mu e_2$ ions coincide very well with the expectation values known for the negatively charged hydrogen ion(s) $H^-$. (see Table IV). This indicates clearly that the electronic structure of the five-body $ab\mu e_2$ ions is similar to the electronic structure of the two-electron $H^-$ ion(s).

III. SIX-BODY MUONIC QUASI-MOLECULES

The neutral six-body systems $pdt\mu e_2, ddt\mu e_2, ddd\mu e_2$ and $dtt\mu e_2$, etc, include two heavy positively charged quasi-nucleus, e.g., $dt\mu$ (or $(dt\mu)^+$) and $d$ (or $d^+$), and two bound electrons $e^-$. Therefore, the internal structure of these six-body muonic systems must be similar
to the two-electron hydrogen $H_2$ molecule. To respect this fact below we shall call and consider these six-body systems as ‘quasi-molecules’. As mentioned above the radius of the three-particle ‘muonic’ quasi-nucleus $(dt\mu)^+$ (and analogous $(pd\mu)^+, (pt\mu)^+, (dd\mu)^+$, etc quasi-nuclei) is in $\approx \left( \frac{m_\mu}{m_e} \right) \approx 206.768$ times smaller than atomic radius of the hydrogen atom which equals $a_0 = \frac{\hbar^2}{m_e e^2} \approx 5.292 \cdot 10^{-9} \, \text{cm}$ (Bohr radius). In this Section we use the same system of notations as above, i.e. the indexes 1 and 2 mean the electrons $e^-$, the index 3 stands for the negatively charged muon $\mu^-$, while three other indexes (4, 5 and 6) designate three nuclei of hydrogen isotopes. Note that our notation $abc\mu e_2$ used here contains some uncertainty, since the heaviest quasi-nucleus (or quasi-nucleus which includes the $\mu^-$-muon) can be either $ab\mu$, or $ac\mu$, or $bc\mu$. Below, we assume that the $bc\mu$ (or $(bc\mu)^+$) quasi-nucleus always include the two heaviest nuclei of hydrogen isotopes. This means that the $pdt\mu e_2$ system contains the two quasi-nuclei: three-particle $(dt\mu)^+$ ion and one bare proton $p^+$ (it cannot be the $(pt\mu)^+$ ion and bare $d^+$ nuclei, or the $(pd\mu)^+$ ion and bare $t^+$ nuclei). The two-electron systems, which can be designated as $dpt\mu e_2$ and $tdp\mu e_2$, with the two other pairs of possible quasi-nuclei: $(pt\mu)^+ + d^+$ and $(pd\mu)^+ + t^+$ are also stable (or quasi-stable), but the absolute values of their total energies are smaller than the total energy of the $p(dt)\mu e_2$ system and they are not considered in this study. In other words, our notation $abc\mu e_2$ always means that the inequality $M_a \leq M_b \leq M_c$ is obeyed for three nuclear masses of the hydrogen isotopes $a, b, c$.

For the non-symmetric six-body quasi-molecules, e.g., for $pdt\mu e_2$, the trial variational wave function of the correct permutation symmetry takes the form

$$\Psi = \sum_{i=1}^{N_A} C_i (1 + \hat{P}_{12}) \exp\left( - \sum_{(jk)} \alpha_{jk} (i) r_{jk}^2 \right)$$

(12)

while for the ‘partially’ symmetric quasi-molecules, e.g., for $ddt\mu e_2$, we can write

$$\Psi = \sum_{i=1}^{N_A} C_i (1 + \hat{P}_{12})(1 + \hat{P}_{45}) \exp\left( - \sum_{(jk)} \alpha_{jk} (i) r_{jk}^2 \right)$$

(13)

where the internal sum is taken over all 15 permutations of particles $(jk) = (kj)$ = (12), (13), (14), ..., (45), (46) and (56). Note again that for an arbitrary six-body system we have fifteen relative coordinates $r_{ij}$, but in our three-dimensional space only twelve of them are truly independent. Nevertheless, as it was shown in [9] one can operate with the variational expansion, Eq.(13), by assuming that all fifteen relative coordinates are indepen-
dent of each other and all variational parameters $\alpha_{jk}^{(i)}$ can be varied without any additional restriction.

As follows from Eqs. (12) and (13) the explicit construction of the trial wave functions for both these cases is relatively simple. A real complication can be found for the $ppp\mu e_2$, $ddd\mu e_2$ and $ttt\mu e_2$ quasi-molecules which contain three identical hydrogen nuclei. In these cases we cannot represent the actual wave function as a single product of the spatial and spin functions. The actual wave functions of these six-body quasi-molecules must be represented as finite sums of products of the different spatial and spin functions. To illustrate this fact let us consider the six-body $ppp\mu e_2$ quasi-molecule. To produce the trial wave function of the correct permutation symmetry we can act as for the three-electron Li-atom [10], [11]. This means that we write the explicit expression for the wave function in the form

$$\Psi = \sum_{i=1}^{N_4} C_i (1 + \hat{P}_{12}) A_{456} \left\{ \exp\left( - \sum_{(jk)} \alpha_{jk}^{(i)} r_{jk}^2 \right) \phi_S(456) \right\}$$

where $A_{456}$ is the complete antisymmetrizer for three particles with indexes (or numbers) 4, 5 and 6, i.e. $A_{456} = 1 - \hat{P}_{45} - \hat{P}_{46} - \hat{P}_{56} + \hat{P}_{456} + \hat{P}_{465} + \hat{P}_{546}$, where $\hat{P}_{jk}$ and $\hat{P}_{ijk}$ are the permutations of the two and three identical particles, respectively. The notation $\phi_S(456)$ stands for the spin function(s) of the three protons. Below we designate single-proton spin function in the following way: spin-up function is the $\alpha-$function, while spin-down function is the $\beta-$function (see, e.g., [10], [12]). In these notations one finds the following spin functions for three-proton system: $\phi_S^{(1)}(456) = \alpha \beta \alpha - \beta \alpha \alpha$ and $\phi_S^{(2)}(456) = 2 \alpha \alpha \beta - \beta \alpha \alpha - \alpha \beta \alpha$, where spin-up (or spin-down) function located at the first place (in each product of three spin functions) correspond to the first proton, or particle with the index 4, at the second place represents the second proton with index 5 and at the third place means the proton with the index 6. Such a system of numbering particles by their location in the formula is called the ‘indexacion by location’. This means that the notation $\alpha \beta \alpha$ designates the $\alpha_4 \beta_5 \alpha_6$ spin function, while the analogous $\alpha \alpha \beta$ function denotes the $\alpha_4 \alpha_5 \beta_6$ spin function, etc. To determine all matrix elements of the Hamiltonian and overlap matrices in their final forms we need to perform integration over spin variables of all particles, including two electrons and three protons. Details of such an integration and explicit forms of the arising spatial projectors can be found in [7]. Note that in calculations of the total energy and for large number of bound state properties of the $ppp\mu e_2$, $ddd\mu e_2$ and $ttt\mu e_2$ quasi-molecules we can use only one spin functions, e.g., $\phi_S^{(1)}(456)$. The spatial projector in this case is
\[ \mathcal{P} = \frac{1}{12} (2 + 2 \hat{P}_{45} - \hat{P}_{46} - \hat{P}_{56} - \hat{P}_{456} - \hat{P}_{546}) \]

In general, the use of only one spin function substantially simplifies all numerical computations.

Results of our calculations of the six-body \( \text{pdt} \mu \text{e}_2 \) and \( \text{ddt} \mu \text{e}_2 \) quasi-molecules in their ground \( S(L = 0) \)-states can be found in Tables I (total energies) and III (properties).

Again, we have to note that, e.g., the three-particle \( \text{dt} \mu \) ion (or \( \text{dt} \mu^+ \) ion) have five bound states (for more detail, see [11]) and each of these bound states generates a separate series of electron bound states in the \( \text{ddt} \mu \text{e}_2 \) quasi-molecules (the ‘fundamental series’, see above). In addition to this there is a number of electron excited states and many ‘vibrational’ and ‘rotational’ states in each of these six-body quasi-molecules. Moreover, for the \( \text{abc} \mu \text{e}_2 \) quasi-molecule, where \( a \neq b \neq c \), one finds three different series of bound state spectra, since one of the central heavy nucleus can be either \( \text{ab} \mu^+ \), or \( \text{ac} \mu^+ \), or \( \text{bc} \mu^+ \). These series of bound states form the exchange series of the bound state spectra. The difference between the fundamental and exchange series of bound states is obvious, since the fundamental series of bound stateis related to the internal structure of the heaviest quasi-nucleus \( \text{bc} \mu^+ \), while the exchange series are related with the different combinations of hydrogen isotopes in the two heavy quasi-nuclei. It is clear that there is no exchange series of the bound state spectra in the five-body \( \text{ab} \mu \text{e}_2 \) ions. For the six-body \( \text{pdt} \mu \text{e}_2 \) quasi-molecule one finds three different exchange series of bound states, while for the \( \text{ddt} \mu \text{e}_2 \) system there are two ‘exchange’ series of bound states. The total number of different series of bound electronic states (fundamental + exchange) equals nine for the \( \text{pdt} \mu \text{e}_2 \) quasi-molecule and ten for the \( \text{ddt} \mu \text{e}_2 \) quasi-molecule.

As mentioned above in this study for each \( \text{abc} \mu \text{e}_2 \) system we investigate the ground \( S(L = 0) \)-state only. This bound state has the lowest energy among all possible bound states. The computed total energies for all ten \( \text{abc} \mu \text{e}_2 \) systems are presented in Table I in atomic units. Table III contains some bound state properties of the six-body \( \text{pdt} \mu \text{e}_2 \) quasi-molecule which must be compared with the bound state (electronic) properties of the two-electron hydrogen \( ^1\text{H}_2 \) (or \( \text{ppee} \)) molecule (see Table IV). As follows from such a comparison the basic electronic properties of the six-body \( \text{pdt} \mu \text{e}_2 \) quasi-molecule (and, in general, any six-body \( \text{abc} \mu \text{e}_2 \) system) are very similar to the analogous properties of the two-center \( \text{H}_2 \) molecules. Therefore, the electronic structures of these two classes of few-body systems are also similar. This fact must simplify future analysis of the six-body \( \text{abc} \mu \text{e}_2 \) systems which contain three nuclei of the hydrogen isotopes.
IV. CONCLUSION

We have considered the bound state spectra of the five- and six-body two-electron muonic systems $ab\mu e_2$ [or $(ab\mu e_2)^-\]$ and $abc\mu e_2$ which includes the two bound electrons, one negatively charged muon $\mu^-$ and two (or three) nuclei of hydrogen isotopes, i.e., protium $p$, deuterium $d$ and tritium $t$. Analysis of the bound state properties leads us to the conclusion about similarity between the internal structures of the five-body, two-electron ions $ab\mu e_2$ [or $(ab\mu e_2)^-\]$ and the two-electron $H^-$ ion (three-body system). In particular, this fact follows from an accurate coincidence of a number of basic geometrical and physical properties of the five-body, two-electron ions $ab\mu e_2$ with the analogous propeties of the three-body hydrogen ion $H^-$. Such a similarity allows one to predict that each of the $(ab\mu e_2)^-\]$ ions has only one bound electron state per one bound state of the central $(ab\mu)^+\$ ion.

The bound state spectra in the six-body $abc\mu e_2$ quasi-molecules are also considered. It is shown that the internal structure of each of these six-body quasi-molecules is similar to the electronic structure of the two-center hydrogen $H_2$ molecule. In contrast with the five-body $(ab\mu e_2)^-\]$ ions, each of the six-body quasi-molecules $abc\mu e_2$ has many dozens of electron bound states. Classification of these bound states is a complex problem, which can be solved by considering separation of the bound state spectra into different series of bound states, e.g., into the fundamental and exchange series. Accurate and complete analysis of the bound state spectra in the six-body $abc\mu e_2$ quasi-molecules will require a number of years. In addition to this, now we can determined a large number of expectation values (i.e. bound state properties) of these quasi-molecules to a good accuracy.

In conclusion, we note again that the direct numerical calculations of the bound state spectra in the five- and six-body two-electron muonic systems $ab\mu e_2$ [or $(ab\mu e_2)^-\]$ and $abc\mu e_2$ is a new and significant step in our understanding of the internal structre of these systems and processes in them. In one short paper it is impossible to answer all important questions. The next goal in studies of five- and six-body two-electron muonic systems $ab\mu e_2$ [or $(ab\mu e_2)^-\]$ and $abc\mu e_2$ is to increase the overall accuracy of numerical computations of bound states in these ions and/or quasi-molecules. In addition to this, we need to determine more bound state properties, including the expectation values of all interparticle delta-functions, triple delta-functions, etc. These values are needed to predict the actual rates of different processes, e.g., nuclear fusion rate(s), in different five- and six-body two-electron muonic
systems. In particular, the study of the six-body $abc\mu e_2$ quasi-molecules which contain either the $dt\mu$ quasi-nucleus, or $dd\mu$ quasi-nucleus in their weakly bound states (the excited $L$-states, or (1,1)-states) is of great theoretical interest, since in these quasi-nucleus we can observe a strong mixture of the ‘nuclear’ and electron bound states. In other words, the electron and nuclear motions in such six-body systems cannot be separated from each other and must be considered together. Even classification of such ‘mixed’ bound states is a very interesting problem.

V. ACKNOWLEDGMENTS

This work was supported in part by the NSF through a grant for the Institute for Theoretical Atomic, Molecular, and Optical Physics (ITAMP) at Harvard University and the Smithsonian Astrophysical Observatory. Also, I wish to thank James Babb (ITAMP, Cambridge, MA) and Leonid I. Menshikov (Kurchatov Institute, Moscow, Russia) for stimulating discussions.

[1] Ya.B. Zeldovich and A.D. Sakharov, JETP 32, 947 (1957) [Sov. Phys. JETP 5, 775 (1957)].
[2] L.W. Alvarez, H. Bradner, F.S. Crawford, Jr., J.A. Crawford, P. Falk-Vairant, M.L. Good, J.D. Gow, A.H. Rosenfeld, F. Solmitz, M.L. Stevenson, H.K. Ticho, and R.D. Tripp, Phys. Rev. 105, 1127 (1957).
[3] Ya.B. Zeldovich and S.S. Gershtein, Usp. Fiz. Nauk 71 581 (1960) [Sov. Phys. Usp. 3, 593 (1961)].
[4] S.E. Jones, Nature 321 127 (1986).
[5] K. Langanke and C.A. Barnes, Nucleosynthesis in the Big Bang and in Stars, in Advances in Nuclear Physics (eds. J.W. Negie and E. Wogt, Spinger Verlag, Berlin, 1998), Chpt. 5.
[6] L.I. Menshikov and L.N. Somov, Sov. Phys. Usp. 33, 616 (1990).
[7] A.M. Frolov and David M. Wardlaw, Europ. Phys. Journal D 63, 339 (2011); ibid, 66, 212 (2012).
[8] A.M. Frolov, Europ. Phys. Journal D 69, 132 (2015).
[9] N.N. Kolesnikov and V.I. Tarasov, Yad. Fiz. 35, 609 (1982), [Sov. J. Nucl. Phys. 35, 354
[10] S. Larsson, Phys. Rev. 169, 49 (1968).

[11] A.M. Frolov and D.M. Wardlaw, Phys. Rev. A Phys. Rev. A 78, 042506 (2008); JETP 138, 5 (2010).

[12] L.D. Landau and E.M. Lifshitz, Quantum Mechanics: Non-Relativistic Theory, (3rd. ed. Pergamon Press, New York (1976)).
TABLE I: Total energies in atomic units (in a.u.) of the ground $S(L = 0)$—states in the five-body hydrogen-muonic ions $(ab\mu e)_2^-$ and six-body quasi-molecules $abc\mu e_2$.

| $N$  | $pd\mu e_2$ | $pt\mu e_2$ | $dt\mu e_2$ |
|------|-------------|-------------|-------------|
| 200  | -106.53518185 | -108.01709125 | -111.88679470 |

| $N$  | $pp\mu e_2$ | $dd\mu e_2$ | $tt\mu e_2$ |
|------|-------------|-------------|-------------|
| 200  | -102.7500577 | -110.34333639 | -113.49897897 |

| $N$  | $pdt\mu e_2$ | $ppd\mu e_2$ | $ppt\mu e_2$ |
|------|-------------|-------------|-------------|
| 200  | -112.47480351 | -107.12363558 | -108.60558047 |

| $N$  | $ddt\mu e_2$ | $pdd\mu e_2$ | $ptt\mu e_2$ |
|------|-------------|-------------|-------------|
| 200  | -112.47116785 | -110.94095171 | -114.10055093 $^{(a)}$ |

| $N$  | $ppp\mu e_2$ | $ddd\mu e_2$ | $ttt\mu e_2$ |
|------|-------------|-------------|-------------|
| 200  | -103.33587577 | -110.92797031 | -114.07956931 |

$^{(a)}$ The total energy of the ground bound state of the $dtt\mu e_2$ system is -114.10115887 a.u.

TABLE II: Total energies in atomic units (in a.u.) of the ground $S(L = 0)$—states of the three-body muonic molecular ions $ab\mu$ (or $(ab\mu)^+$). Numerical values of all total energies have been taken from [7], where all particle masses are exactly the same as they used in this study.

| $N$  | $pp\mu$ | $dd\mu$ | $tt\mu$ |
|------|---------|---------|---------|
| $E$  | -102.2235035785787 | -109.8169263959981 | -112.9728490317648 |

| $N$  | $pd\mu$ | $pt\mu$ | $dt\mu$ |
|------|---------|---------|---------|
| $E$  | -106.0125270695158 | -107.4947026128185 | -111.3643469153818 |
TABLE III: The expectation values of a number of properties (in a.u.) of the ground $S(L = 0)$−states in some five-body $(ab\mu e_2)^-$ ions and six-body $abc\mu e_2$ quasi-molecules.

| ion/molecule | $\langle r_{pp}^{-2} \rangle$ | $\langle r_{pp}^{-1} \rangle$ | $\langle r_{pp} \rangle$ | $\langle r_{pp}^2 \rangle$ |
|--------------|-------------------------------|------------------------------|-------------------|-------------------|
| $pd\mu e_2$  | 52465.736                    | 155.77373                   | 0.01009561        | 0.000137855       |
| $dd\mu e_2$  | 48961.114                    | 150.62685                   | 0.01025263        | 0.001390777       |
| $pdt\mu e_2$ | 47948.92                     | 149.4191                    | 0.0102416          | 0.00013845        |

| ion/molecule | $\langle r_{de}^{-2} \rangle$ | $\langle r_{de}^{-1} \rangle$ | $\langle r_{de} \rangle$ | $\langle r_{de}^2 \rangle$ |
|--------------|-------------------------------|------------------------------|-------------------|-------------------|
| $pd\mu e_2$  | 1.1008758                    | 0.68634114                   | 2.5693953          | 9.8722965         |
| $dd\mu e_2$  | 1.1104775                    | 0.68433819                   | 2.6485125          | 10.895838         |
| $pdt\mu e_2$ | 1.488335                     | 0.8834730                    | 1.606050           | 3.248165          |

| ion/molecule | $\langle r_{ee}^{-2} \rangle$ | $\langle r_{ee}^{-1} \rangle$ | $\langle r_{ee} \rangle$ | $\langle r_{ee}^2 \rangle$ |
|--------------|-------------------------------|-------------------------------|-------------------|-------------------|
| $pd\mu e_2$  | 0.1612780                    | 0.3201021                   | 4.1271305          | 20.8879           |
| $dd\mu e_2$  | 0.1573468                    | 0.3142697                   | 4.2891434          | 23.0935           |
| $pdt\mu e_2$ | 0.507390                     | 0.574317                    | 2.220188           | 5.85409           |

| ion/molecule | $\langle \frac{1}{2}P_{p}^2 \rangle$ | $\langle \frac{1}{2}P_{h}^2 \rangle$ | $\langle \frac{1}{2}P_{p}^2 \rangle$ | $\langle \frac{1}{2}P_{d}^2 \rangle$ |
|--------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| $pd\mu e_2$  | 0.263352470                    | 19683.345                      | 15710.399                      | 11997.327                      |
| $dd\mu e_2$  | 0.263570803                    | 20880.742                      | 16204.694                      | 16204.694                      |
| $pdt\mu e_2$ | 0.22206238                     | 21510.84                      | 23875.25                      | 21291.87                       |

(a) The $\langle \frac{1}{2}P_{l}^2 \rangle$ expectation value for the $pdt\mu e_2$ quasi-molecule is $\approx 20357.74$. 
TABLE IV: The expectation values of a number of properties (in a.u.) of the ground states in the H$^-$ ion (or $\infty$H$^-$ ion) and $^1$H$_2$ (or ppee) molecule. The notation $e$ stands for the electron(s), while $N$ designates the heavy nucleus (or nuclei).

| ion/molecule | $\langle r_{Ne}^{-2}\rangle$ | $\langle r_{Ne}^{-1}\rangle$ | $\langle r_{Ne}\rangle$ | $\langle r_{Ne}^2\rangle$ |
|-------------|------------------|------------------|------------------|------------------|
| H$^-$       | 1.1166282452542572 | 0.6832617676515272224 | 2.7101782784444203653 | 11.91369678051262274 |
| $^1$H$_2$   | 1.5730801         | 0.9017345         | 1.5751544         | 3.146458         |

| ion/molecule | $\langle r_{ee}^{-2}\rangle$ | $\langle r_{ee}^{-1}\rangle$ | $\langle r_{ee}\rangle$ | $\langle r_{ee}^2\rangle$ |
|-------------|------------------|------------------|------------------|------------------|
| H$^-$       | 0.15510415256242466 | 0.311021502214300052 | 4.4126944979917277211 | 25.202025291240331897 |
| $^1$H$_2$   | 0.5050168         | 0.5793405         | 2.2012319         | 0.5803927         |

| ion/molecule | $\langle r_{NN}^{-2}\rangle$ | $\langle r_{NN}^{-1}\rangle$ | $\langle r_{NN}\rangle$ | $\langle r_{NN}^2\rangle$ |
|-------------|------------------|------------------|------------------|------------------|
| $^1$H$_2$   | 0.497428         | 0.699864         | 1.450543         | 2.135437         |

(a) The $\langle \frac{1}{2}P_e^2 \rangle$ expectation value for the $\infty$H$^-$ ion (computed with the same wave function) is $\approx 0.2638755082721885983$ a.u.