Internal structure and positron annihilation in the four-body MuPs system

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Abstract

A large number of bound state properties of the four-body muonium-positronium system MuPs (or $\mu^+e^-e^+$) are determined to high accuracy. Based on these expectation values we predict that the weakly-bound four-body MuPs system has the ‘two-body’ cluster structure Mu + Ps. The two neutral clusters Mu ($\mu^+e^-$) and Ps ($e^+e^-$) interact with each other by the attractive van der Waals forces. By using our expectation values of the electron-positron delta-functions we evaluated the half-life $\tau_a$ of the MuPs system against annihilation of the electron-positron pair: $\tau_a = \frac{1}{\Gamma} \approx 4.076453 \cdot 10^{-10}$ sec. The hyperfine structure splitting of the ground state in the MuPs system evaluated with our expectation values is $\Delta \approx 23.064(5) \, MHz$. 

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In this study we consider bound state properties of the four-body muonium-positronium system MuPs, or $\mu^+ e^- e^+ e^-$. The fact that this system is bound is known since the middle of 1980’s when it was shown that the negatively charged Mu$^-$ (or $\mu^+ e^- e^- e^+$) is bound [1] (calculations) and [2] (experiment). The goal of this study is to perform highly accurate computations of the ground bound $^1S(L = 0)$−state in the MuPs system, which is, in fact, the only bound state in this four-body system. The non-relativistic Hamiltonian of the four-body $\mu^+ e^- e^+ e^+$ system is written in the form (in atomic units $\hbar = 1$, $m_e = 1$, $e = 1$):

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

where the notation 1 designates the positively charged muon $\mu^+$, the notation 2 (or +) means the positron, while 3 and 4 (or -) stand for electrons. The same system of notations is used everywhere below in this study.

By solving the corresponding Schrödinger equation $H\Psi = E\Psi$ for bound states ($E < 0$) one can determine the total energy and wave function of the bound (ground) $S(L = 0)$−state in the MuPs system. In general, to determine the bound state spectra in four-body MuPs system in this study we apply the variational expansion written in the basis of four-dimensional gaussoids, where each basis function depends upon the relative (or interparticle) coordinates $r_{ij} = |r_i - r_j| = r_{ji}$ and $r_i$ ($i = 1, 2, 3, 4$) are the Cartesian coordinates of the particle $i$. This expansion was proposed more than 35 years ago (see, e.g., [4] and earlier references therein) to solve some nuclear and hypernuclear few-body problems. Since the middle of 1980’s the same expansion was also used to determine some bound states in different Coulomb few-body systems. In the case of four-body Coulomb systems this variational expansion takes the form

$$\Psi = \sum_{k=1}^{N} C_k \exp(-\alpha_{12}^{(k)} r_{12}^2 - \alpha_{13}^{(k)} r_{13}^2 - \alpha_{14}^{(k)} r_{14}^2 - \alpha_{23}^{(k)} r_{23}^2 - \alpha_{24}^{(k)} r_{24}^2 - \alpha_{34}^{(k)} r_{34}^2)$$

where $C_k$ are the linear variational parameters of this expansion ($k = 1, \ldots, N$), while $\alpha_{ij}^{(k)}$ are the non-linear parameters of the variational expansion, Eq.(2). In applications to actual four-body systems the trial wave function, Eq.(2), must be symmetrized (or anti-symmetrized) in respect to possible presence of identical particles. In particular, in the MuPs system we have two identical electrons (particles 3 and 4).

In general, the overall efficiency of the variational expansion, Eq.(2), depends upon algorithms which are used to optimize the non-linear parameters in Eq.(2). Recently, for
four-body systems we have developed a number of algorithms which are very effective and produce fast optimization. The accuracy of the constructed wave functions is usually high and very high for the total energies. The expectation values of various geometrical and dynamical properties are also determined to relatively high numerical accuracy. However, some troubles can be found in computations of the expectation values of some delta-functions, cusp values and a few other similar properties.

Results of our calculations of the ground state in the MuPs system are shown in Table I. All calculations have been performed in atomic units and include the total energies and some other bound state properties of this system computed for different values of \( N \) in Eq. (2). In our calculations we have used the following values of \( N = 600, 800, 1000 \) and \( 1500 \). The mass of the positive charged muon \( \mu^+ \) used in our calculations equals \( m_\mu = 206.768262 \ m_\text{e} \). Note that our current wave functions are significantly more accurate than analogous functions used in earlier studies. As follows from the results shown in Table I the internal structure of the MuPs system is represented as a two-body cluster \( \text{Mu} \leftrightarrow \text{Ps} \) which is formed from the muonium atom \( \text{Mu} \) (or \( \mu^+ e^- \)) and neutral positronium \( \text{Ps} \) (\( e^- e^+ \)) weakly interacting with each other. In general, such an interaction of these two neutral clusters is represented by the van der Waals attracting force(s) which is sufficient to bind the whole four-body system together. The competing ‘ionic’ model of MuPs fails to predict correctly many properties from Table I. In this ionic model the MuPs system is represented as a motion of the positron \( e^+ \) in the field of the central, heavy ion \( \mu^+ e^- \) which is negatively charged. In this model actual distances from the positron to the central cluster/ion are significantly larger than the radius of this central ion \( \text{Mu}^- \).

The expectation values of different operators are used to determine the properties which can later be measured in actual experiments. For instance, let us consider annihilation of electron-positron pair in the MuPs system. This process can be observed experimentally. It is clear that the largest annihilation rate corresponds to the two-photon annihilation. The formula for the two-photon annihilation width (or rate) \( \Gamma_{2\gamma}(\text{MuPs}) \) is

\[
\Gamma_{2\gamma}(\text{MuPs}) = 2\pi\alpha^4 a_0^{-1} \left[ 1 - \frac{\alpha}{\pi} \left( 5 - \frac{\pi^2}{4} \right) \right] \langle \delta(r_{+-}) \rangle = 100.3456053781 \cdot 10^9 \langle \delta(r_{+-}) \rangle \ \text{sec}^{-1}
\]

where \( \langle \delta_{+-} \rangle \) is the expectation value of the electron-positron delta-function determined for the ground bound state in the MuPs system. Here and below the indexes ‘+’ and ‘−’ designate the positron and electron, respectively. Analogous formula for the three-photon annihilation
rate $\Gamma_3\gamma(\text{MuPs})$ takes the form

$$\Gamma_3\gamma(\text{MuPs}) = 2\frac{4(\pi^2 - 9)}{3}\alpha^5ca_0^{-1}\langle\delta(r_{+-})\rangle = 2.718545954 \cdot 10^8\langle\delta(r_{+-})\rangle \text{ sec}^{-1}$$ (4)

In these formulas and everywhere below $\alpha$ is the fine structure constant, $c$ is the speed of light in vacuum and $a_0$ is the Bohr radius. Below, the numerical values of these constants have been taken from [5].

The rates of the four- and five-photon annihilations of the electron-positron pairs in the MuPs system are uniformly related with the $\Gamma_2\gamma(\text{MuPs})$ and $\Gamma_3\gamma(\text{MuPs})$ rates, respectively. The approximate relations are written in the two following forms [6]

$$\Gamma_4\gamma(\text{MuPs}) \approx 0.274\left(\frac{\alpha}{\pi}\right)^2\Gamma_2\gamma(\text{MuPs}) \approx 1.478364 \cdot 10^{-6} \cdot \Gamma_2\gamma(\text{MuPs})$$ (5)

and

$$\Gamma_5\gamma(\text{MuPs}) \approx 0.177\left(\frac{\alpha}{\pi}\right)^2\Gamma_3\gamma(\text{MuPs}) \approx 9.550018 \cdot 10^{-7} \cdot \Gamma_3\gamma(\text{MuPs})$$ (6)

By using the expectation value of the $\delta(r_{+-})$—function from Table I we can evaluate these annihilation rates: $\Gamma_2\gamma = 2.4495957 \cdot 10^9 \text{ sec}^{-1}$, $\Gamma_3\gamma = 6.6364027 \cdot 10^6 \text{ sec}^{-1}$, $\Gamma_4\gamma = 3.621394 \cdot 10^3 \text{ sec}^{-1}$ and $\Gamma_5\gamma = 6.337777 \text{ sec}^{-1}$. Now, one can evaluate the total annihilation rate of the MuPs system by the following sum $\Gamma \approx \Gamma_2\gamma + \Gamma_3\gamma + \Gamma_4\gamma + \Gamma_5\gamma \approx \Gamma_2\gamma + \Gamma_3\gamma \approx 1006.174599735 \cdot 10^8\langle\delta_{+-}\rangle \text{ sec}^{-1} \approx 2.4531127 \cdot 10^9 \text{ sec}^{-1}$. In other words, the knowledge of accurate values of the $\Gamma_2\gamma$ and $\Gamma_3\gamma$ annihilation rates is sufficient to predict half-life of the MuPs system against positron annihilation $\tau = \frac{1}{\Gamma} \approx 4.076453 \cdot 10^{-10} \text{ sec}$.

In addition to the few-photon annihilation discussed above in the four-body MuPs system the electron-positron pair can annihilate with the emission of one and zero photons. The corresponding annihilation rates are very small, but in some theoretical considerations one- and zero-photon annihilations play a noticeable role. An approximate formula for zero-photon annihilation rate $\Gamma_0\gamma$ takes the form (see, e.g., [3]):

$$\Gamma_0\gamma = \xi\frac{147\sqrt{3}\pi^3}{2} \cdot \alpha^{12}(ca_0^{-1}) \cdot \langle\delta_{\mu+\mu-}\rangle = 5.0991890 \cdot 10^{-4} \cdot \xi \cdot \langle\delta_{\mu+\mu-}\rangle \text{ sec}^{-1}$$ (7)

where $\langle\delta_{\mu+\mu-}\rangle$ is the expectation value of the four-particle delta-function in the ground state of muonium-positronium (MuPs). The numerical value of $\langle\delta_{\mu+\mu-}\rangle$ is the probability to find all four particles in one small volume with the spatial radius $\alpha a_0$. The unknown (dimensionless) factor $\xi$ has the numerical value close to unity. The expectation value of
the four-particle delta-function determined in our calculations is \( \approx 1.80154 \cdot 10^{-4} \) (in a.u.). From here one finds that \( \Gamma_{0\gamma}(\text{MuPs}) \approx 9.1864 \cdot 10^{-8} \xi \, \text{sec}^{-1} \).

One-photon annihilation rate can be evaluated by using the fact that in the lowest-order approximation the one-photon annihilation of the electron-positron pair in MuPs can be considered as a regular two-photon annihilation, but one of the two emitted photons is absorbed either by the remaining electron \( e^- \), or by the muon \( \mu^+ \). This leads to the two different one-photon annihilation rates which are designated below as \( \Gamma^{(1)}_{1\gamma} \) and \( \Gamma^{(2)}_{1\gamma} \), respectively. In the case of absorption by an electron the probability of this process is given by the formula

\[
\Gamma^{(1)}_{1\gamma} = \frac{64\pi^2}{27} \cdot \alpha^8 (ca_0^{-1}) \cdot \langle \delta_{++-} \rangle = 1.066420947 \cdot 10^3 \cdot \langle \delta_{++-} \rangle \, \text{sec}^{-1},
\]

where \( \langle \delta_{++-} \rangle \) is the expectation value of the triple electron-positron-electron delta-function determined for the ground state of the MuPs system. Its numerical value is the probability to find all three particles inside of a sphere which has spatial radius \( R \approx \alpha a_0 \approx \frac{a_0}{137} \). Our best numerical treatment to-date for the \( \langle \delta_{++-} \rangle \) value gives \( \approx 3.67540 \cdot 10^{-4} \), and therefore, \( \Gamma^{(1)}_{1\gamma} \approx 3.9195 \cdot 10^{-1} \, \text{sec}^{-1} \) for the bound (ground) state in the MuPs system.

Analysis of the second one-photon annihilation of the \((e^+, e^-)\)-pair in the MuPs system is more complicated (see discussion in [3]). An approximate expression for the \( \Gamma^{(2)}_{1\gamma} \) is written in the form which is similar to Eq.(8)

\[
\Gamma^{(2)}_{1\gamma} = \chi \frac{64\pi^2}{27} \cdot \alpha^8 (ca_0^{-1}) \cdot \langle \delta_{\mu++-} \rangle = 1.066420947 \cdot 10^3 \cdot \langle \delta_{\mu++-} \rangle \, \text{sec}^{-1},
\]

where \( \langle \delta_{\mu++-} \rangle \) is the expectation value of the triple muon-electron-positron delta-function determined for the ground state of the MuPs system and factor \( \chi \) is a numerical factor which approximately equals to the factor \( \xi \) in Eq.(7). To produce more accurate formulas for \( \Gamma^{(2)}_{1\gamma} \) and exact expressions for the factors \( \xi \) in Eqs.(7) and \( \chi \) in Eq.(9) one needs to perform an additional analysis.

For the muonium-positronium system MuPs there is a possibility to observe an interesting process which is called the muon-positron conversion. In general, the muon decay is written in the form \( \mu^+ = e^+ + \nu_e + \bar{\nu}_\mu \), where the notation \( \nu_e \) stands for the electron neutrino, while the notation \( \bar{\nu}_\mu \) designates the muonic anti-neutrino. The decay equation for the positively charged muon re-written from the left-to-right represents a creation (or synthesis) of the \( \mu^+ \) muon, i.e. \( e^+ + \nu_e + \bar{\nu}_\mu = \mu^+ \). Since the MuPs system already contains a positron \( e^+ \), then
these two processes (muonic decay and muon synthesis) can proceed instantly and we can observe a ‘self-transition’ of MuPs into MuPs. In our earlier paper [7] we have evaluated the probability to observe the muon-positron conversion as one event for $\approx 1 \cdot 10^8$ of MuPs systems. This means that currently we cannot observe the muon-positron conversion in MuPs, since the probability of conversion is extremely small and it is still very difficult to create even one MuPs system. However, in the future this situation can be changed and one can study the muon-positron conversion in the MuPs system experimentally.

In conclusion, let us determine the hyperfine structure splitting in the MuPs system. Such structure arise from interaction between the spin-vectors of the positron and muon. The hyperfine structure splitting in the MuPs system is written in the form

$$a = \frac{8\pi\alpha^2}{3}\mu_B^2 \frac{g_\mu}{m_\mu} \frac{g_e}{m_e} \cdot \langle \delta_{\mu^+e^+} \rangle = 14229.1255 \cdot \langle \delta_{\mu^+e^+} \rangle$$

(10)

where $\alpha$ is the fine structure constant, $\mu_B$ is the Bohr magneton (exactly equals 0.5 in atomic units), $\langle \delta_{\mu^+e^+} \rangle$ is the expectation value of the muon-positron delta-function. Also in Eq.(10) the notations $m_\mu$ and $m_e$ stand for the mass-at-rest for the muon and positron, respectively, while the factors $g_+ = -2.0023193043718$ and $g_\mu = -2.0023318396$ are the hyromagnetic ratios. By using the expectation value of the muon-positron delta-function $\langle \delta_{\mu^+e^+} \rangle \approx 1.620893 \cdot 10^{-3}$ a.u. from Table I, one finds that the value $a$ in Eq.(10) equals $a \approx 23.064 \text{ MHz}$. This coincides the energy difference between the hyperfine structure states with $J = 0$ and $J = 1$, where the notation $J$ stands the total spin of the muon-positron pair in the MuPs system.

We have considered the bound state properties of the MuPs system ($\mu^+e^-e^+$, or muonium-positronium). As follows from our computational results of bound state properties the internal structure of the MuPs system is represented to very good accuracy as a two-body cluster $\text{Mu} + \text{Ps}$. The two neutral systems $\text{Mu} (\mu^+e^-)$ and $\text{Ps} (e^+e^-)$ interact with each other by the attractive van der Waals forces. By using our results from accurate computations we determine a few annihilation rates of the electron-positron pair in the MuPs system. Numerical values of the two-, three-, four- and five-photon annihilation rates of the MuPs system are determined to high numerical accuracy. The rate of zero-photon annihilation $\Gamma_0(\text{MuPs})$ and first one-photon annihilation rate $\Gamma_1^{(1)}(\text{MuPs})$ have been evaluated approximately. Another interesting property which we also determine in this study is the hyperfine structure splitting between singlet $J = 0$ and triplet $J = 1$ spin states of the muon-positron pair in MuPs. By using our expectation value of the $\mu^+ - e^+$ delta-function we have found
that the hyperfine splitting $\Delta$ in the ground state of the MuPs system is $\approx 23.064(5) \, MHz$. The values ($\Gamma_2\gamma, \Gamma_3\gamma, \Gamma$ and $\Delta$) can be determined in this study can directly be measured in future experiments.

Results of our study indicate clearly that many bound state properties, including properties which can be measured in modern experiments have now been determined to very good accuracy. The next step is to perform an experiment to create the actual MuPs system, observe its decay and measure some of the properties. Further changes in theoretical values will be small and even negligible. Without actual experiments it is hard to expect to make any visible progress in this area.

[1] A.M. Frolov, Z. für Phys. 2, 61 (1986).
[2] Y. Kuang, K.P. Arnold, F. Chmely et al, Phys. Rev. A 39, 6109 (1989).
[3] A.M. Frolov and D.M. Wardlaw, Phys. Lett. A 374, 1732 (2010).
[4] N.N. Kolesnikov and V.I. Tarasov, Yad. Fiz. 35, 609 (1982), [Sov. J. Nucl. Phys. 35, 354 (1982)].
[5] CRC Handbook of Chemistry and Physics, 95th Edition, Ed. W.M. Haynes, (CRC Press, Taylor & Francis Group, Boca Raton, Florida, 2015).
[6] G.P. Lepage, P.B. Mackenzie, K.H. Streng and P.M. Zerwas, Phys. Rev. A 28, 3090 (1983).
[7] A.M. Frolov, Phys. Lett. A, 376, 1451 (2012).
TABLE I: The expectation values of a number of bound state properties in atomic units of the MuPs system \((\mu^+e^-e^+)\). The notation \(\mu\) designates the positively charged muon, while the notations \(e^-\) and \(e^+\) denote the electron and positron, respectively.

| \(N\)  | \(E\)        | \(\langle r_{\mu-e^+}^{-2}\rangle\) | \(\langle r_{\mu-e^+}^{-1}\rangle\) | \(\langle r_{\mu-e^+}\rangle\) | \(\langle r_{\mu-e^+}^{2}\rangle\) | \(\langle r_{\mu-e^+}^{3}\rangle\) | \(\langle r_{\mu-e^+}^{4}\rangle\) |
|--------|--------------|---------------------------------------|---------------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 600    | -0.78631700815 | 0.1708476 | 0.3460479 | 3.678243   | 16.41074 | 86.4005 | 527.295 |
| 800    | -0.78631706515 | 0.1708477 | 0.3460481 | 3.678240   | 16.41068 | 86.3994 | 527.272 |
| 1000   | -0.78631706573 | 0.1708476 | 0.3460482 | 3.678237   | 16.41065 | 86.3986 | 527.257 |
| 1500   | -0.78631706673 | 0.1708476 | 0.3460483 | 3.678236   | 16.41063 | 86.3984 | 527.251 |

| \(N\)  | \(\langle \frac{1}{2}p_{e^-}^2\rangle\) | \(\langle r_{e^-e^-}^{-2}\rangle\) | \(\langle r_{e^-e^-}^{-1}\rangle\) | \(\langle r_{e^-e^-}\rangle\) | \(\langle r_{e^-e^-}^{2}\rangle\) | \(\langle r_{e^-e^-}^{3}\rangle\) | \(\langle r_{e^-e^-}^{4}\rangle\) |
|--------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 600    | 0.32338448362 | 0.3485124 | 0.4178999 | 3.4882569 | 15.666223 | 85.1136 | 539.805 |
| 800    | 0.32338468807 | 0.3485146 | 0.4179002 | 3.4882549 | 15.666187 | 85.1129 | 539.790 |
| 1000   | 0.32338474500 | 0.3485150 | 0.4179003 | 3.4882533 | 15.666160 | 85.1124 | 539.781 |
| 1500   | 0.32338474874 | 0.3485151 | 0.4179005 | 3.4882530 | 15.666155 | 85.1121 | 539.778 |

| \(N\)  | \(\langle \frac{1}{2}p_{\mu}^2\rangle\) | \(\langle r_{e^-\mu}^{-2}\rangle\) | \(\langle r_{e^-\mu}^{-1}\rangle\) | \(\langle r_{e^-\mu}\rangle\) | \(\langle r_{e^-\mu}^{2}\rangle\) | \(\langle r_{e^-\mu}^{3}\rangle\) | \(\langle r_{e^-\mu}^{4}\rangle\) |
|--------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 600    | 0.13668660960 | 1.1945831 | 0.7257294 | 2.3260105 | 7.9172577 | 35.9559 | 204.728 |
| 800    | 0.13668676776 | 1.1945864 | 0.7257297 | 2.3260092 | 7.9172364 | 35.9555 | 204.719 |
| 1000   | 0.13668681862 | 1.1945869 | 0.7257298 | 2.3260078 | 7.9172134 | 35.9551 | 204.712 |
| 1500   | 0.13668681473 | 1.1945871 | 0.7257299 | 2.3260075 | 7.9172127 | 35.9550 | 204.708 |

| \(N\)  | \(\langle \delta(r_{e^-e^-})\rangle\) | \(\langle \delta(r_{\mu-e^+})\rangle\) | \(\langle \delta(r_{\mu-e^-})\rangle\) | \(\langle \delta(r_{e^-e^-})\rangle\) | \(\langle \delta(r_{e^-e^-})\rangle\) | \(\langle \delta(r_{e^-e^-})\rangle\) | \(\langle \delta(r_{e^-e^-})\rangle\) |
|--------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 600    | 0.024383813 | 0.001624112 | 0.17419597 | 8.59175-10^{-4} | 3.68481-10^{-4} | 7.1599-10^{-3} | 1.75700-10^{-4} |
| 800    | 0.024409132 | 0.001623304 | 0.17426468 | 8.58962-10^{-4} | 3.66965-10^{-4} | 7.2092-10^{-3} | 1.81837-10^{-4} |
| 1000   | 0.024411665 | 0.001620911 | 0.17426917 | 8.58744-10^{-4} | 3.67365-10^{-4} | 7.1895-10^{-3} | 1.79864-10^{-4} |
| 1500   | 0.024411589 | 0.001620893 | 0.17426911 | 8.56456-10^{-4} | 3.67540-10^{-4} | 7.1890-10^{-3} | 1.80154-10^{-4} |