Weakly bound states of $dt\mu$ muonic molecular ion in quantum electrodynamics

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Abstract. The energy spectrum of ground and excited bound states of muonic molecule $dt\mu$ is calculated on the basis of stochastic variational method. The basis wave functions of the muonic molecule are taken in the Gaussian form. The matrix elements of the Hamiltonian are calculated analytically. For numerical calculation, a computer code is written in the MATLAB system. As a result, the numerical energy levels of ground and excited states of the muonic molecule $dt\mu$ are obtained.

1. Introduction
The investigation of the energy spectra of hydrogen muonic molecules is important for muonic catalysis of nuclear fusion reactions [1, 2, 3]. A calculation of fine and hyperfine structure of muonic molecular ions with the account of higher order QED corrections allows us to predict the rates of reactions of their formation and other parameters of the $\mu$CF cycle. Energies of weakly bound states of mesomolecular ions $dd\mu$ and $dt\mu$ are important for calculation the rates of their resonant formation.

Muonic molecules $pt\mu$, $pd\mu$, and $dt\mu$ consist of various isotopes of hydrogen, which results in a different structure of energy levels. In our work we investigate P-states of the molecule $dt\mu$ ($L = 1$). There are several different approaches to the classification of bound states in mesomolecular ions. One of them originates from adiabatic approach and involves a pair of quantum numbers $J$ and $\nu$, where $J$ is rotational quantum number and $\nu$ is vibrational quantum number [4, 5]. For example ground state in this approach is designated as $(0,0)$, while the excited $P^*(L = 1)$-state becomes $(1,1)$. Aside from the states with "normal" spacial parity $(-1)^L$ described above there are metastable states with $L = 1$ and "odd" spacial parity $(-1)^{L+1}$ [6]. Such states have also been investigated in this work.

2. General formalism
To calculate the energy spectrum of ground and excited bound states of muonic molecule $dt\mu$ we use stochastic variational method [7]. The trial wave function of the muonic molecule in this approach has the Gaussian form. The Gaussian-type basis function with non-zero angular momentum for nonidentical particles has the following general form:

$$\Phi_{LS}(x, A) = e^{-\frac{1}{2}Ax}x^L\chi_{SMS}.$$ (1)
where \( x = (x_1, \ldots, x_{N-1}) \) are Jacobi coordinates, \( A \) is a \((N-1) \times (N-1)\) positive-defined matrix of nonlinear variational parameters, \( \chi_{SM} \) is the spin function,

\[
\theta_L(x) = \left[ \begin{array}{c} \mathbb{Y}_{l1}(x_1) \mathbb{Y}_{l2}(x_2) \mathbb{Y}_{l3}(x_3) \end{array} \right]_{LM},
\]

where \( \mathbb{Y}_{lm}(x) = r^{l} \mathbb{Y}_{lm}(x) \). For \( S \)-states the coordinate part of the wave function for three nonidentical particles takes the form:

\[
\phi_{00}(\rho, \lambda, A) = e^{-\frac{1}{2} \left[ A_{11}\rho^2 + A_{22}\lambda^2 + 2A_{12}(\rho\lambda) \right]} (\epsilon \rho),
\]

\[
\phi_{01}(\rho, \lambda, A) = e^{-\frac{1}{2} \left[ A_{11}\rho^2 + A_{22}\lambda^2 + 2A_{12}(\rho\lambda) \right]} (\epsilon \lambda),
\]

\[
\phi_{11}(\rho, \lambda, A) = e^{-\frac{1}{2} \left[ A_{11}\rho^2 + A_{22}\lambda^2 + 2A_{12}(\rho\lambda) \right]} (\epsilon [\rho \times \lambda]),
\]

where \( \rho \) and \( \lambda \) denote two Jacobi coordinates, two indices denote excitations associated with variables \( \rho \) and \( \lambda \). In the case of three nonidentical particles in \( P \)-state \((L = 1, \text{where } L \text{ is total angular momentum of particles})\) there are three possible wave functions:

\[
< \phi'|\phi >_{00} = \frac{8\pi^3}{\det(B)^{3/2}},
\]

Let us calculate firstly the overlap matrix elements. For the ground state we have obtained:

\[
\sum_{pol.} \epsilon_i^* \epsilon_j = \frac{3}{4\pi} \delta_{ij}.
\]

The integral for the wave function (4) has the form:

\[
< \phi'|\phi >_{10} = \int d\rho d\lambda e^{-\frac{1}{2} \left[ B_{11}\rho^2 + B_{22}\lambda^2 + 2B_{12}(\rho\lambda) \right]} (\epsilon \rho) (\epsilon \rho).
\]

After the analytical integration over Jacobi coordinates we obtain:

\[
< \phi'|\phi >_{10} = \frac{1}{3} \int d\rho d\lambda e^{-\frac{1}{2} \left[ B_{11}\rho^2 + B_{22}\lambda^2 + 2B_{12}(\rho\lambda) \right]} \frac{3}{4\pi} \delta_{ij} \rho_i \rho_j = \frac{6\pi^2 B_{22}}{(\det(B)^{5/2})},
\]

For the wave function (5) the integration can be performed in a similar manner with the following result:

\[
< \phi'|\phi >_{01} = \frac{6\pi^2 B_{11}}{(\det(B)^{5/2})}.
\]
After an analytical integration matrix elements of kinetic energy operator take the form:

$$\sum_{pol.} \epsilon_i^* \epsilon_j |\vec{\rho} \times \lambda_i||\vec{\rho} \times \lambda_j| = \frac{3}{4\pi} ((\vec{\rho} \times \lambda))^2 = \frac{3}{4\pi} \rho^2 \lambda^2 \sin^2 \theta_{\rho \lambda}$$ (12)

After that an analytical integration gives:

$$< \phi' | \phi >^{1^{1}} = -\frac{12\pi^2}{(\det B)^{5/2}}. \quad (13)$$

We also calculate "off-diagonal" matrix elements of the form $$< \phi_0 | \phi >$$:

$$< \phi' | \phi >^{(01|10)} = -\frac{6\pi^2 B_{12}}{(\det B)^{5/2}}. \quad (14)$$

For the calculation of matrix elements of the Hamiltonian we use explicit expressions for potential and kinetic energy operators. In Jacobi coordinates the kinetic energy operator has the form

$$\hat{T} = -\frac{\hbar^2}{2\mu_1} \Delta_\rho - \frac{\hbar^2}{2\mu_2} \Delta_\lambda,$$ (15)

where $$\mu_1 = \frac{m_1 m_3}{m_1 + m_2}, \quad \mu_2 = \frac{(m_1 + m_2) m_3}{m_1 + m_2 + m_3}$$. Acting by the Laplace operators $$\Delta_\rho$$ and $$\Delta_\lambda$$ on the wave function (4) we obtain:

$$\Delta_\rho \phi_{10}(\rho, \lambda, A) = e^{-\frac{1}{2} B_{12} \rho^2 + A_{12} \lambda^2 + 2 A_{12} (\rho \lambda)} \left( A_{12}^2 \lambda^2 (\epsilon_\rho) + 2 A_{12} [-(\epsilon_\lambda) + A_{11} (\lambda \rho) (\epsilon_\rho)] + A_{11} (\epsilon_\rho) [-5 + A_{11} \rho^2] \right),$$ (16)

$$\Delta_\lambda \phi_{10}(\rho, \lambda, A) = e^{-\frac{1}{2} B_{12} \rho^2 + A_{12} \lambda^2 + 2 A_{12} (\rho \lambda)} \left( A_{12}^2 \lambda^2 + A_{12}^2 \rho^2 + A_{22} (-3 + 2 A_{12} (\lambda \rho)) \right).$$ (17)

After an analytical integration matrix elements of kinetic energy operator take the form:

$$< \phi' | \hat{T} | \phi >^{(00,10,01,11,01|10)} = -\frac{6\pi^2}{(\det B)^{5/2}} \left\{ \frac{\hbar^2}{2\mu_1} I_{\rho}^{00,10,01,11,01|10} + \frac{\hbar^2}{2\mu_2} I_{\lambda}^{00,10,01,11,01|10} \right\}, \quad (18)$$

$$I_{\rho}^{00} = A_{12}^2 B_{11} - 2 A_{12} A_{12} B_{12} + A_{11} (B_{12}^2 + (A_{11} - B_{11}) B_{22}), \quad (19)$$

$$I_{\lambda}^{00} = A_{12}^2 B_{22} - 2 A_{22} A_{12} B_{12} + A_{22} (B_{12}^2 + (A_{22} - B_{22}) B_{11}), \quad (20)$$

$$I_{\rho}^{10} = 5 A_{12} B_{12} [B_{12}^2 + (A_{11} - B_{11}) B_{22}] - 2 A_{12} B_{12} (B_{12}^2 + 5 A_{11} B_{22} - B_{11} B_{22}) + A_{12}^2 (2 B_{12}^2 + 3 B_{11} B_{22}), \quad (21)$$

$$I_{\lambda}^{10} = 5 A_{12}^2 B_{22} + A_{22} B_{22} (-10 A_{12} B_{12} + 3 B_{12}^2 - 3 B_{11} B_{22}) + A_{22}^2 (2 B_{12}^2 + 3 B_{11} B_{22}), \quad (22)$$

$$I_{\rho}^{01} = 5 A_{12}^2 B_{11} + A_{12} B_{11} (-10 A_{12} B_{12} + 3 B_{12}^2 - 3 B_{22} B_{11}) + A_{12}^2 (2 B_{12}^2 + 3 B_{22} B_{11}), \quad (23)$$

$$I_{\lambda}^{01} = 5 A_{22} B_{11} [B_{12}^2 + (A_{22} - B_{22}) B_{11}] - 2 A_{12} B_{12} (B_{12}^2 + 5 A_{22} B_{11} - B_{22} B_{11}) + A_{12}^2 (2 B_{12}^2 + 3 B_{22} B_{11}), \quad (24)$$

$$I_{\rho}^{11} = A_{12}^2 B_{11} - 2 A_{11} A_{12} B_{12} + A_{11} (B_{12}^2 + (A_{11} - B_{11}) B_{22}), \quad (25)$$

$$I_{\lambda}^{11} = A_{12}^2 B_{22} - 2 A_{22} A_{12} B_{12} + A_{22} (B_{12}^2 + (A_{22} - B_{22}) B_{11}), \quad (26)$$

$$< \phi' | \hat{T} | \phi >^{(01|10)} = -B_{12} (2 A_{12} B_{12} (4 A_{11} + B_{11}) + 5 A_{11} B_{12}^2 + 5 A_{12} B_{11}) - \quad (27)$$
The potential energy of Coulomb interaction between three particles has the form:

\[ \langle \phi|V|\phi \rangle = \epsilon_{1}e_{2} + \frac{\epsilon_{1}\epsilon_{3}}{|\rho|} + \frac{\epsilon_{2}\epsilon_{3}}{|\lambda - m_{3}^{12}\rho|}. \]  

(29)

where \( \rho_{12} = r_{1} - r_{2} = \rho, \rho_{13} = r_{1} - r_{3} = \lambda + \frac{m_{1}^{12}\rho}{m_{3}^{12}}, \rho_{23} = r_{2} - r_{3} = \lambda - \frac{m_{1}^{12}\rho}{m_{3}^{12}}. \) \( \epsilon_{1}, \epsilon_{2}, \epsilon_{3} \) are the charges of particles. To perform the integration for the second and third terms we introduce a new variable \( k_{13,23}^{18} = \lambda \pm \frac{m_{13}^{12}}{m_{3}^{12}}\rho. \) After the integration we obtain the following analytical expressions for matrix elements of potential energy:

\[ I_{12}^{01} = \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{B_{22}\det B}}, \quad I_{13,23}^{01} = \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{F_{1}^{13,23}(B_{22}F_{1}^{13,23} - (F_{2}^{13,23})^{2})}}, \]

(30)

\[ I_{12}^{01} = \frac{4\sqrt{2}\pi^{5/2}}{(\det B)^{2}}, \quad I_{13,23}^{01} = \frac{4\sqrt{2}\pi^{5/2}}{(\det B)^{2}} \left\{ \frac{2\sqrt{F_{1}^{13,23} + (3B_{22}F_{1}^{13,23} - F_{2}^{13,23})^{2}}}{(F_{1}^{13,23})^{3/2}} \left( \frac{m_{2}^{13,23}}{m_{3}^{12}} \right) \pm \frac{4F_{1}^{13,23}m_{2}^{13,23}}{\sqrt{F_{1}^{13,23}}} \right\}, \]

(31)

\[ I_{12}^{11} = \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{B_{22}(\det B)^{2}}}, \quad I_{13,23}^{11} = \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{F_{1}^{13,23}(B_{22}F_{1}^{13,23} - (F_{2}^{13,23})^{2})}}, \]

(32)

\[ I_{12}^{(010)} = \frac{4\sqrt{2}\pi^{5/2}B_{12}}{\sqrt{B_{22}(\det B)^{2}}}, \quad I_{13,23}^{(010)} = \frac{4\sqrt{2}\pi^{5/2}B_{12}}{\sqrt{F_{1}^{13,23}(B_{22}F_{1}^{13,23} - (F_{2}^{13,23})^{2})}}, \]

(33)

\[ F_{1}^{13,23} = B_{11} + B_{22} \frac{m_{2}^{13,23}}{m_{3}^{12}} \pm 2B_{12} \frac{m_{2}^{13,23}}{m_{3}^{12}}, \quad F_{2}^{13,23} = B_{12} \pm B_{22} \frac{m_{2}^{13,23}}{m_{3}^{12}}. \]

(34)

To increase the accuracy of our calculations we have to consider relativistic, vacuum polarization corrections [8, 9, 10]. The interaction operator containing these corrections in three-body bound state can be written in muon atomic units as follows:

\[ \Delta V = -\frac{\alpha^{2}}{8} \sum_{i=1}^{3} \frac{p_{i}^{4}}{m_{i}^{3}} - \frac{\pi \alpha}{2} \sum_{i,j=1; i \neq j}^{3} \epsilon_{i} \epsilon_{j} \left( \frac{1}{m_{i}^{2}} + \frac{1}{m_{j}^{2}} \right) \delta(r_{ij}) \]

(35)
To obtain numerical value of such correction one has to use first order perturbation theory (PT) with a variational wave functions. In first order PT the average value of operator $\Delta V$ is the following:

$$< \Delta V > = \frac{1}{2} \frac{\sum_{i,j=1}^{K} c_i c_j \langle \Delta V \phi_j \rangle}{\sum_{i,j=1}^{K} c_i c_j |(A_{i1}+A_{i1})(A_{i2}+A_{i2})-(A_{i1}+A_{i2})|^2|^{3/2}},$$

where $c_i$, $c_j$ are linear variational parameters, $K$ is a number of basis functions. The matrix elements $\langle \Delta V \phi_j \rangle$ determine the value of corrections in the energy spectrum. Let us present the matrix elements of some operators entering in $\Delta V$:

$$< \phi_i | \delta(r_{12}) | \phi_j > = \langle \delta(\rho) >= \int d\rho d\lambda \delta(\rho) e^{-\frac{1}{2}B_{11}\rho^2+B_{22}\lambda^2+2B_{12}(\rho\lambda)} =$$

$$= 4\pi \int \lambda^2 d\lambda \delta(\rho)e^{-\frac{1}{2}B_{22}\lambda^2} = \frac{(2\pi)^{3/2}}{(B_{22})^{3/2}},$$

$$< \phi_i | \delta(r_{13}) | \phi_j > = \frac{(2\pi)^{3/2}}{(B_{11}-2B_{12}\frac{m_1}{m_2} + B_{22}(\frac{m_2}{m_1})^2)^{3/2}},$$

$$< \phi_i | \delta(r_{23}) | \phi_j > = \frac{(2\pi)^{3/2}}{(B_{11} + 2B_{12}\frac{m_1}{m_2} + B_{22}(\frac{m_2}{m_1})^2)^{3/2}},$$

$$< \phi_i | p^4_{1} | \phi_j > = \frac{15(2\pi)^{3}}{(\text{det } B)^{1/2}} \left[ (A_{i1} - 2 \frac{m_1}{m_1 + m_2} A_{i1} + (\frac{m_1}{m_1 + m_2})^2 A_{i2}) \text{det}(A^i) + \right.$$}

$$\left. + \left( A_{i1} - 2 \frac{m_1}{m_1 + m_2} A_{i1} + \left( \frac{m_1}{m_1 + m_2} \right)^2 A_{i2} \right) \text{det}(A^i) \right]^2,$$

$$< \phi_i | p^4_{2} | \phi_j > = \frac{15(2\pi)^{3}}{(\text{det } B)^{1/2}} \left[ (A_{i1} - 2 \frac{m_2}{m_1 + m_2} A_{i1} + (\frac{m_2}{m_1 + m_2})^2 A_{i2}) \text{det}(A^i) + \right.$$}

$$\left. + \left( A_{i1} - 2 \frac{m_2}{m_1 + m_2} A_{i1} + \left( \frac{m_2}{m_1 + m_2} \right)^2 A_{i2} \right) \text{det}(A^i) \right]^2,$$

$$< \phi_i | p^4_{3} | \phi_j > = \frac{15(2\pi)^{3}}{(\text{det } B)^{1/2}} [A^i_{22} \text{det } A^i + A^i_{22} \text{det } A^i]^2,$$

$$< \phi_i | \rho \phi_j > = \frac{1}{2} \frac{\sum_{i,j=1}^{K} c_i c_j \langle \rho \phi_j \rangle}{\sum_{i,j=1}^{K} c_i c_j |(A_{i1}+A_{i1})(A_{i2}+A_{i2})-(A_{i1}+A_{i2})|^2|^{3/2}},$$

$$< \phi_i | \rho \phi_j > = \frac{8(2\pi)^{5/2}}{[\text{det } B]^2 \sqrt{B_{22}}} \left[ (A_{i1} + \frac{m_1 - m_2}{m_1 + m_2} A_{i1} - \right.$$}

$$\left. - \frac{m_1 m_2}{(m_1 + m_2)^2} A_{i2}) \text{det}(A^i) + (A_{i1} + \frac{m_1 - m_2}{m_1 + m_2} A_{i1} - \right.$$}

$$\left. - \frac{m_1 m_2}{(m_1 + m_2)^2} A_{i2}) \text{det}(A^i) \right]$$

$$< \phi_i | \rho \phi_j > = \frac{8(2\pi)^{5/2}}{[\text{det } B]^2 \sqrt{B_{22}}} \left[ (A_{i1} + \frac{m_1 - m_2}{m_1 + m_2} A_{i1} - \right.$$}

$$\left. - \frac{m_1 m_2}{(m_1 + m_2)^2} A_{i2}) \text{det}(A^i) + (A_{i1} + \frac{m_1 - m_2}{m_1 + m_2} A_{i1} - \right.$$}

$$\left. - \frac{m_1 m_2}{(m_1 + m_2)^2} A_{i2}) \text{det}(A^i) \right]$$

$$< \phi_i | \rho \phi_j > = \frac{8(2\pi)^{5/2}}{[\text{det } B]^2 \sqrt{B_{22}}} \left[ (A_{i1} + \frac{m_1 - m_2}{m_1 + m_2} A_{i1} - \right.$$}

$$\left. - \frac{m_1 m_2}{(m_1 + m_2)^2} A_{i2}) \text{det}(A^i) + (A_{i1} + \frac{m_1 - m_2}{m_1 + m_2} A_{i1} - \right.$$}

$$\left. - \frac{m_1 m_2}{(m_1 + m_2)^2} A_{i2}) \text{det}(A^i) \right].$$
$$< \phi_i | \frac{1}{r_{23}} \left( p_2 p_3 + \frac{r_{23} (r_2 \cdot p_2) r_3}{r_{23}^2} \right) | \phi_j > = \frac{8 (2 \pi)^{5/2}}{(\det B)^2} \left[ B_{11} + 2 \frac{m_1}{m_1 + m_2} B_{12} + \left( \frac{m_1}{m_1 + m_2} \right)^2 B_{22} \right] \times$$
$$\times \left[ \left( \frac{m_2}{m_1 + m_2} A_{22}^i - A_{12}^i \right) \det(A^j) + \left( \frac{m_2}{m_1 + m_2} A_{22}^j - A_{12}^j \right) \det(A^i) \right], \quad (49)$$

where $B = A^i + A^j$. Using these analytical expressions we obtain total numerical value of correction in the energy spectrum of $td\mu$ (-0.0000220101) in muon atomic units.

3. Conclusion
As it is previously mentioned we use stochastic variational method to calculate energies of muonic molecule $dt\mu$. The matrix of variational parameters in the framework of stochastic variational method is generated randomly, which prevents convergence of the result to a local minimum and eliminates the possibility of obtaining an incorrect result. Moreover, according to the Mini-Max theorem in variational calculation the energies for excited states can be obtained along with the ground state energies.

For direct numerical calculation, a computer code was written in the MATLAB system to solve the three-body Coulomb problem based on the Schrodinger equation. The Varga-Suzuki program [7] written in Fortran is taken as the basis. Overlap, kinetic energy and potential energy matrix elements are inserted into the program. We have also changed the function that generates random numbers. For variational parameters the stochastic optimization procedure is used. As a result, the numerical values of energies of ground and excited states of the muonic molecule $dt\mu$ are obtained in muon atomic units: $E^{dt\mu}_{tot}(0,0)=-0.538594971$, $E^{dt\mu}_{tot}(0,1)=-0.488056287$, $E^{dt\mu}_{tot}(1,0)=-0.523191450$, $E^{dt\mu}_{tot}(1,1)=-0.481772186$, $E^{dt\mu}_{tot}((-1)^L+1)=-0.123867812$.

Along with total energy $E_{tot}$ of a particular state of mesomolecular ion one can introduce so-called "binding energy" $\epsilon_{bind} = -2Ry(E_{tot} + \frac{m_r}{2m_{dt\mu}})$ (in eV), where $m_r$ is reduced mass of a two-particle bound state of muon and triton, $n$ is the principle quantum number of such bound state. For $(1,0)$ and $(1,1)$ states $n = 1$, while for the "odd" parity metastable P-state $n = 2$ [5, 6]. For a given total energy of a particular state of a mesomolecular ion the sign of $\epsilon_{bind}$ defines whether the state of two clusters (deuteron and muonic tritium atom) is bound or not.

All energies are in a good agreement with [4, 5]. The noticeable difference for $(0,1)$ and $(1,1)$ states is connected with a smaller basis size and a need for a more careful parameters optimization procedure. The results for the "odd" parity state coincide with [6]. It is worth mentioning that in our calculations we use double precision while in [4] quadruple precision is being used. This fact also contributes to the difference of results.

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