Hyperfine structure of muonic mesomolecules $td\mu$, $tp\mu$, $dp\mu$ in variational method

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Abstract. The hyperfine structure of energy levels of muonic molecules $td\mu$, $tp\mu$ and $dp\mu$ is calculated on the basis of stochastic variational method. The basis wave functions are taken in the Gaussian form. The matrix elements of the Hamiltonian are calculated analytically. Vacuum polarization, relativistic and nuclear structure corrections are taken into account to increase the accuracy. For numerical calculation, a computer code is written in the MATLAB system. Numerical values of energy levels of hyperfine structure in muonic molecules $td\mu$, $tp\mu$ and $dp\mu$ are obtained.

1 Introduction

The interest in hydrogen mesomolecular ions is primarily connected with muonic catalysis of nuclear fusion reactions [1]. Precise calculation of fine and hyperfine structure of muonic molecular ions with the inclusion of higher order QED corrections allows us to predict the rates of reactions of their formation and other parameters of the μ CF cycle.

We use stochastic variational method [2–4] to calculate energy spectra of hydrogen mesomolecular ions numerically. Variational method allows us to determine energies of three-body systems with very high accuracy. Random generation of variational parameters prevents possible convergence of the method to a local minimum and gives a much higher flexibility when applied to different three-body systems. In case of hydrogen mesomolecular ions the choice of variational method is also motivated by comparable masses of all three particles, which does not allow us to use adiabatic approximation effectively.

In this work not only do we calculate ground state energies and hyperfine structure of $td\mu$, $tp\mu$ and $dp\mu$ mesomolecular ions but also include important QED corrections to increase the accuracy. We calculate relativistic, vacuum polarization and nuclear structure corrections to the ground state energy as well as vacuum polarization and Zemach corrections to the hyperfine splitting. Inclusion of these corrections is crucial in achieving precise results. In all formulas throughout the paper we use muon-atomic units ($e = m_\mu = \hbar = 1$).

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2 General formalism

To calculate ground state energy and hyperfine structure in muonic molecules $\text{td}\mu$, $\text{tp}\mu$ and $\text{dp}\mu$ we use stochastic variational method [4]. The trial wave function of muonic molecule in this approach has Gaussian form. The Gaussian-type basis function with non-zero angular momentum for nonidentical particles is the following:

$$\begin{aligned}\phi_L(\mathbf{x}, A) &= e^{-\frac{1}{2}\bar{\mathbf{x}}A\mathbf{x}}\theta_L(\mathbf{x}), \\ \theta_L(\mathbf{x}) &= [[[\mathbb{Y}_{l_1}(\mathbf{x}_1)\mathbb{Y}_{l_2}(\mathbf{x}_2)]_{L_{12}}\mathbb{Y}_{l_3}(\mathbf{x}_3)]_{L_{123}}\dots]_{LM},\end{aligned}\quad (1)$$

where $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_{N-1})$ are the Jacobi coordinates, A is a $(N-1) \times (N-1)$ positive-defined matrix of variational parameters, $\mathbb{Y}_{lm}(\mathbf{x}) = r^l Y_{lm}(\mathbf{x})$. In the case of three nonidentical particles in S -state ($L = 0$, where L is total angular momentum of particles) basis functions take the form:

$$\phi_0(\boldsymbol{\rho}, \boldsymbol{\lambda}, A) = e^{-\frac{1}{2}[A_{11}\rho^2 + A_{22}\lambda^2 + 2A_{12}(\boldsymbol{\rho}, \boldsymbol{\lambda})]}, \quad (2)$$

where $\boldsymbol{\rho}$ and $\boldsymbol{\lambda}$ denote two Jacobi coordinates. Knowing the basis functions we can now perform analytical calculation of matrix elements of the Hamiltonian, which is an advantage of the Gaussian basis. The overlap matrix element has the form:

$$\langle \phi'_0 | \phi_0 \rangle = \frac{8\pi^3}{(\det B)^{3/2}}. \quad (3)$$

where elements of matrix B are expressed in terms of matrix A as $B_{ij} = A'_{ij} + A_{ij}$. For the calculation of matrix elements of the Hamiltonian we use explicit expressions for potential and kinetic energy operators. In nonrelativistic approximation the Hamiltonian of the molecule without the account of hyperfine structure has the following form in Jacobi coordinates:

$$\hat{H} = -\frac{\hbar^2}{2\mu_1}\Delta_\rho - \frac{\hbar^2}{2\mu_2}\Delta_\lambda + \frac{e_1 e_2}{|\boldsymbol{\rho}|} + \frac{e_1 e_3}{|\boldsymbol{\lambda} + \frac{m_2}{m_{12}}\boldsymbol{\rho}|} + \frac{e_2 e_3}{|\boldsymbol{\lambda} - \frac{m_1}{m_{12}}\boldsymbol{\rho}|}, \quad (4)$$

where $\mu_1 = \frac{m_1 m_2}{m_1 + m_2}$, $\mu_2 = \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3}$, $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2 = \boldsymbol{\rho}$, $\mathbf{r}_{13} = \mathbf{r}_1 - \mathbf{r}_3 = \boldsymbol{\lambda} + \frac{m_2}{m_{12}}\boldsymbol{\rho}$, $\mathbf{r}_{23} = \mathbf{r}_2 - \mathbf{r}_3 = \boldsymbol{\lambda} - \frac{m_1}{m_{12}}\boldsymbol{\rho}$, e_1, e_2, e_3 are charges of the particles. Matrix elements of kinetic energy have the following analytical form:

$$\langle \phi'_0 | \hat{T} | \phi_0 \rangle = -\frac{24\pi^3}{(\det B)^{5/2}} \left\{ \frac{\hbar^2}{2\mu_1} I_\rho + \frac{\hbar^2}{2\mu_2} I_\lambda \right\}, \quad (5)$$

$$I_\rho = A_{12}^2 B_{11} - 2A_{11}A_{12}B_{12} + A_{11}(B_{12}^2 + (A_{11} - B_{11})B_{22}), \quad (6)$$

$$I_\lambda = A_{12}^2 B_{22} - 2A_{22}A_{12}B_{12} + A_{22}(B_{12}^2 + (A_{22} - B_{22})B_{11}). \quad (7)$$

For potential energy matrix elements we present the following analytical expressions:

$$\langle \phi'_0 | \hat{V} | \phi_0 \rangle = e_1 e_2 I_{12} + e_1 e_3 I_{13} + e_2 e_3 I_{23}. \quad (8)$$

$$I_{12} = \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{B_{22}\det B}}, \quad I_{13,23} = \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{F_1^{13,23}(B_{22}F_1^{13,23} - (F_2^{13,23})^2)}}, \quad (9)$$

$$F_1^{13,23} = B_{11} + B_{22} \frac{(m_{2,1}^{13,23})^2}{m_{12}^2} \mp 2B_{12} \frac{m_{2,1}^{13,23}}{m_{12}}, \quad F_2^{13,23} = B_{12} \mp B_{22} \frac{m_{2,1}^{13,23}}{m_{12}}, \quad (10)$$

where to get the expressions for F_1^{13} and F_2^{13} one should choose m_2 and the first sign in (10) and to obtain F_1^{23} and F_2^{23} m_1 and the second sign in (10) must be chosen.

To further increase the accuracy of our calculation we take into account various QED corrections. Let us start with relativistic corrections. The explicit expression for relativistic corrections can be obtained from the Breit Hamiltonian for two interacting particles. In case of hydrogen mesomolecular ions Breit corrections have the form [5, 6]:

$$V_B = -\frac{\alpha^2}{8} \sum_{i=1}^3 \frac{\mathbf{p}_i^4}{m_i^3} - \frac{\pi\alpha^2}{2} \sum_{i,j=1;i \neq j}^3 e_i e_j \left(\frac{1}{m_i^2} + \frac{1}{m_j^2} \right) \delta(\mathbf{r}_{ij}) - \frac{\alpha^2}{2} \sum_{i,j=1;i \neq j}^3 \frac{e_i e_j \left(\mathbf{p}_i \mathbf{p}_j + \frac{\mathbf{r}_{ij}(\mathbf{r}_{ij} \cdot \mathbf{p}_i) \mathbf{p}_j}{r_{ij}^2} \right)}{m_i m_j r_{ij}}, \quad (11)$$

where $\mathbf{p}_i$ are momentums of the particles, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ are interparticle coordinates. Averaging over basis functions gives the following analytical expressions for matrix elements:

$$\begin{aligned} \langle \phi_i | \mathbf{p}_1^4 | \phi_j \rangle &= \frac{15(2\pi)^3}{(\det B)^{7/2}} \left[\left(A_{11}^j + 2 \frac{m_1}{m_1 + m_2} A_{12}^j + \left(\frac{m_1}{m_1 + m_2} \right)^2 A_{22}^j \right) \times \right. \\ &\quad \left. \times \det(A^i) + \left(A_{11}^i + 2 \frac{m_1}{m_1 + m_2} A_{12}^i + \left(\frac{m_1}{m_1 + m_2} \right)^2 A_{22}^i \right) \det(A^j) \right]^2, \end{aligned} \quad (12)$$

$$\begin{aligned} \langle \phi_i | \mathbf{p}_2^4 | \phi_j \rangle &= \frac{15(2\pi)^3}{(\det B)^{7/2}} \left[\left(A_{11}^j - 2 \frac{m_2}{m_1 + m_2} A_{12}^j + \left(\frac{m_2}{m_1 + m_2} \right)^2 A_{22}^j \right) \times \right. \\ &\quad \left. \times \det(A^i) + \left(A_{11}^i - 2 \frac{m_2}{m_1 + m_2} A_{12}^i + \left(\frac{m_2}{m_1 + m_2} \right)^2 A_{22}^i \right) \det(A^j) \right]^2, \end{aligned} \quad (13)$$

$$\langle \phi_i | \mathbf{p}_3^4 | \phi_j \rangle = \frac{15(2\pi)^3}{(\det B)^{7/2}} [A_{22}^j \det A^i + A_{22}^i \det A^j]^2, \quad (14)$$

$$\begin{aligned} \langle \phi_i | \frac{1}{r_{12}} \left(\mathbf{p}_1 \mathbf{p}_2 + \frac{\mathbf{r}_{12}(\mathbf{r}_{12} \cdot \mathbf{p}_1) \mathbf{p}_2}{r_{12}^2} \right) | \phi_j \rangle &= \frac{8(2\pi)^{5/2}}{[\sqrt{B_{22}}(\det B)^2]} \left[\left(A_{11}^i + \frac{m_1 - m_2}{m_1 + m_2} A_{12}^i - \right. \right. \\ &\quad \left. \left. - \frac{m_1 m_2}{(m_1 + m_2)^2} A_{22}^i \right) \det(A^j) + \left(A_{11}^j + \frac{m_1 - m_2}{m_1 + m_2} A_{12}^j - \frac{m_1 m_2}{(m_1 + m_2)^2} A_{22}^j \right) \det(A^i) \right], \end{aligned} \quad (15)$$

$$\begin{aligned} \langle \phi_i | \frac{1}{r_{13}} \left(\mathbf{p}_1 \mathbf{p}_3 + \frac{\mathbf{r}_{13}(\mathbf{r}_{13} \cdot \mathbf{p}_1) \mathbf{p}_3}{r_{13}^2} \right) | \phi_j \rangle &= \frac{8(2\pi)^{5/2}}{\left[(\det B)^2 \sqrt{B_{11} - 2 \frac{m_2}{m_1 + m_2} B_{12} + \left(\frac{m_2}{m_1 + m_2} \right)^2 B_{22}} \right]} \times \\ &\quad \times \left[\left(\frac{m_1}{m_1 + m_2} A_{22}^i + A_{12}^i \right) \det(A^j) + \left(\frac{m_1}{m_1 + m_2} A_{22}^j + A_{12}^j \right) \det(A^i) \right], \end{aligned} \quad (16)$$

$$\begin{aligned} \langle \phi_i | \frac{1}{r_{23}} \left(\mathbf{p}_2 \mathbf{p}_3 + \frac{\mathbf{r}_{23}(\mathbf{r}_{23} \cdot \mathbf{p}_2) \mathbf{p}_3}{r_{23}^2} \right) | \phi_j \rangle &= \frac{8(2\pi)^{5/2}}{\left[(\det B)^2 \sqrt{B_{11} + 2 \frac{m_1}{m_1 + m_2} B_{12} + \left(\frac{m_1}{m_1 + m_2} \right)^2 B_{22}} \right]} \times \\ &\quad \times \left[\left(\frac{m_2}{m_1 + m_2} A_{22}^i - A_{12}^i \right) \det(A^j) + \left(\frac{m_2}{m_1 + m_2} A_{22}^j - A_{12}^j \right) \det(A^i) \right]. \end{aligned} \quad (17)$$

Now let us consider another important QED correction - one-loop vacuum polarization correction. The potential in this case takes the form:

$$V_{VP} = \frac{\alpha}{3\pi} \sum_{i,j=1;i \neq j}^3 \frac{e_i e_j}{r_{ij}} \int_1^\infty d\xi \rho(\xi) e^{-2\gamma \xi r_{ij}}, \quad (18)$$

where $\gamma = \frac{m_e}{m_\mu \alpha}$, $\rho(\xi) = \sqrt{\xi^2 - 1}(2\xi^2 + 1)/\xi^4$. Analytical expression for matrix elements is the following:

$$\begin{aligned} \langle \phi_i | \frac{1}{r_{12}} \int_1^\infty d\xi \frac{\sqrt{\xi^2 - 1}(2\xi^2 + 1)}{\xi^4} e^{-2\frac{m_e}{m_\mu \alpha} \xi r_{12}} | \phi_j \rangle = & \frac{\sqrt{2}\pi^{7/2}}{4M^{5/2}B_{22}^{3/2}} \times \\ \times \left[8\pi M^{3/2} G_{3,4}^{2,1} \left(\frac{\gamma^2}{M} \middle| \begin{matrix} 0, \frac{1}{2}, \frac{3}{2} \\ 0, 0, \frac{1}{2}, \frac{1}{2} \end{matrix} \right) + \sqrt{\pi}(4\sqrt{\pi}M^{3/2} G_{3,4}^{2,1} \left(\frac{\gamma^2}{M} \middle| \begin{matrix} 0, \frac{1}{2}, \frac{5}{2} \\ 0, 1, \frac{1}{2}, \frac{1}{2} \end{matrix} \right) + 8\gamma^3 + 12\gamma M) \right], \end{aligned} \quad (19)$$

$$\begin{aligned} \langle \phi_i | \frac{1}{r_{13,23}} \int_1^\infty d\xi \frac{\sqrt{\xi^2 - 1}(2\xi^2 + 1)}{\xi^4} e^{-2\frac{m_e}{m_\mu \alpha} \xi r_{13,23}} | \phi_j \rangle = & \\ = \frac{\sqrt{2}\pi^{7/2}}{4(L^{13,23})^{5/2}(F_1^{13,23})^{3/2}} \times \left[8\pi(L^{13,23})^{3/2} G_{3,4}^{2,1} \left(\frac{\gamma^2}{L^{13,23}} \middle| \begin{matrix} 0, \frac{1}{2}, \frac{3}{2} \\ 0, 0, \frac{1}{2}, \frac{1}{2} \end{matrix} \right) + \right. & (20) \\ \left. + \sqrt{\pi}(4\sqrt{\pi}(L^{13,23})^{3/2} G_{3,4}^{2,1} \left(\frac{\gamma^2}{L^{13,23}} \middle| \begin{matrix} 0, \frac{1}{2}, \frac{5}{2} \\ 0, 1, \frac{1}{2}, \frac{1}{2} \end{matrix} \right) + 8\gamma^3 + 12\gamma L^{13,23}) \right], \end{aligned}$$

$$L = \frac{B_{22}F_1^{13,23} - (F_2^{13,23})}{2F_1^{13,23}}, \quad M = \frac{\det B}{2B_{22}}, \quad (21)$$

where G is the Meijer G-function.

It is important to also include nuclear structure correction, which in case of mesomolecular ions has the form:

$$V_{\text{str}} = -\frac{2}{3}\pi(e_1e_3)r_{1e}^2\delta^3(\mathbf{r}_{13}) - \frac{2}{3}\pi(e_2e_3)r_{2e}^2\delta^3(\mathbf{r}_{23}), \quad (22)$$

where indices 1, 2 denote nuclei of hydrogen isotopes, r_{1e} , r_{2e} are charge radii of the corresponding nuclei of hydrogen isotopes, index 3 denotes the muon. This correction can be obtained using the following expansion of electric form-factor:

$$G_E(k^2)|_{k^2 \rightarrow 0} = G_E(0) + \frac{dG_E(k^2)}{dk^2} \bigg|_{k^2=0} k^2 + \dots = 1 - \frac{1}{6}r_E^2 k^2 + \dots \quad (23)$$

The calculation of the matrix elements of $\delta^3(\mathbf{r}_{ij})$ will be presented explicitly in the next section. To calculate QED corrections numerically we use first order perturbation theory. General expression for an arbitrary potential:

$$\langle V \rangle = \frac{\sum_{i,j=1}^K c_i c_j \langle \phi_i | V | \phi_j \rangle}{\sum_{i,j=1}^K c_i c_j \frac{8\pi^3}{[(A_{11}^i + A_{11}^j)(A_{22}^i + A_{22}^j) - (A_{12}^i + A_{12}^j)^2]^{3/2}}}, \quad (24)$$

where V is an arbitrary potential, c_i , c_j are linear variational parameters, K is the number of basis functions. All numerical results for ground state energy and corrections after variational calculation are presented in Table 1 in lines 1 through 4. Results from paper [3] are presented in Table 1 in parentheses for comparison.

3 Hyperfine structure

Now let us calculate matrix elements of the hyperfine part of the Hamiltonian. The potential of hyperfine structure of $L = 0$ state, which is a part of the Breit Hamiltonian, can be written in the following simple form for three interacting particles with spins S_1 , S_2 , S_3 respectively [7–9]:

$$\Delta V^{hfs} = a(\mathbf{S}_1\mathbf{S}_2) + b(\mathbf{S}_1\mathbf{S}_3) + c(\mathbf{S}_2\mathbf{S}_3), \quad (25)$$

$$a = -\frac{2\pi\alpha^2 g_1 g_2}{3m_p^2} \delta^3(\mathbf{r}_{12}), \quad b = \frac{2\pi\alpha^2 g_1 g_3}{3m_p} \delta^3(\mathbf{r}_{13}), \quad c = \frac{2\pi\alpha^2 g_2 g_3}{3m_p} \delta^3(\mathbf{r}_{23}),$$

where g_1, g_2, g_3 are gyromagnetic factors, indices 1,2 denote nuclei of hydrogen isotopes, index 3 denotes muon. Averaging procedure for such potential involves both averaging over radial and spin basis functions. Analytical integration of radial matrix elements of $\delta(\mathbf{r}_{ij})$ can be performed as follows:

$$\begin{aligned} \langle \delta^3(\mathbf{r}_{12}) \rangle &= \langle \delta(\rho) \rangle = \int \int d\rho d\lambda \delta(\rho) e^{-\frac{1}{2}[B_{11}\rho^2 + B_{22}\lambda^2 + 2B_{12}(\rho\lambda)]} = \\ &= 4\pi \int \lambda^2 d\lambda \delta(\rho) e^{-\frac{1}{2}B_{22}\lambda^2} = \frac{(2\pi)^{3/2}}{(B_{22})^{3/2}}. \end{aligned} \quad (26)$$

$$\langle \delta^3(\mathbf{r}_{13}) \rangle = \frac{(2\pi)^{3/2}}{(B_{11} - 2B_{12}\frac{m_2}{m_1} + B_{22}(\frac{m_2}{m_1})^2)^{3/2}}, \quad (27)$$

$$\langle \delta^3(\mathbf{r}_{23}) \rangle = \frac{(2\pi)^{3/2}}{(B_{11} + 2B_{12}\frac{m_1}{m_2} + B_{22}(\frac{m_1}{m_2})^2)^{3/2}}. \quad (28)$$

To perform averaging over spin functions Wigner - Eckart theorem [10] can be used with success. General formulas for spin averaging for any S_1, S_2 and S_3 take the form:

$$\langle S'_{12}, S | (S_1 S_2) | S_{12}, S \rangle = \overline{(S_1 S_2)}_{S_{12}} \delta_{S_{12} S'_{12}}, \quad (29)$$

$$\begin{aligned} \langle S'_{12}, S | (S_1 S_3) | S_{12}, S \rangle &= \sqrt{(2S'_{12} + 1)(2S_{12} + 1)(2S_1 + 1)(S_1 + 1)S_1} \sqrt{(2S_3 + 1)} \times \\ &\times \sqrt{(S_3 + 1)S_3} (-1)^{S_{12}^{max} + S_{12}^{min} + S_1 + S_2 + S_3 + 1} \left\{ \begin{matrix} S_{12} & S_3 & S \\ S_3 & S'_{12} & 1 \end{matrix} \right\} \left\{ \begin{matrix} S_1 & S'_{12} & S_2 \\ S_{12} & S_1 & 1 \end{matrix} \right\}, \end{aligned} \quad (30)$$

$$\begin{aligned} \langle S'_{12}, S | (S_2 S_3) | S_{12}, S \rangle &= \sqrt{(2S'_{12} + 1)(2S_{12} + 1)(2S_2 + 1)(S_2 + 1)S_2} \sqrt{(2S_3 + 1)} \times \\ &\times \sqrt{(S_3 + 1)S_3} (-1)^{2S_{12}^{max} + S_1 + S_2 + S_3 + 1} \left\{ \begin{matrix} S_{12} & S_3 & S \\ S_3 & S'_{12} & 1 \end{matrix} \right\} \left\{ \begin{matrix} S_2 & S'_{12} & S_1 \\ S_{12} & S_2 & 1 \end{matrix} \right\}. \end{aligned} \quad (31)$$

In the case of $S_1 = S_2 = S_3 = 1/2$ the energy matrix has the form:

$$\begin{pmatrix} \frac{1}{4}a + \frac{1}{4}b + \frac{1}{4}c & 0 & 0 \\ 0 & \frac{1}{4}a - \frac{1}{2}b - \frac{1}{2}c & \frac{\sqrt{3}}{4}b - \frac{\sqrt{3}}{4}c \\ 0 & \frac{\sqrt{3}}{4}b - \frac{\sqrt{3}}{4}c & -\frac{3}{4}a \end{pmatrix}. \quad (32)$$

After the matrix diagonalization we obtain the following eigenvalues:

$$\lambda_{1,2} = -\frac{1}{4}(a + b + c) \pm \frac{1}{2} \sqrt{a^2 + b^2 + c^2 - ab - bc - ac}, \quad \lambda_3 = \frac{1}{4}(a + b + c). \quad (33)$$

These eigenvalues are energies of hyperfine structure levels with respect to the total energy of ground state. In case of $S_1 = S_2 = S_3 = 1/2$, as it was already mentioned, we have 3 hyperfine levels. In the case of $S_1 = 1, S_2 = S_3 = 1/2$ the energy matrix is the following:

$$\begin{pmatrix} \frac{1}{2}a + \frac{1}{2}b + \frac{1}{4}c & 0 & 0 & 0 \\ 0 & \frac{1}{2}a - \frac{5}{6}b - \frac{5}{12}c & \frac{\sqrt{2}}{3}b - \frac{\sqrt{2}}{3}c & 0 \\ 0 & \frac{\sqrt{2}}{3}b - \frac{\sqrt{2}}{3}c & -a + \frac{1}{3}b - \frac{1}{12}c & 0 \\ 0 & 0 & 0 & -a - b + \frac{1}{4}c \end{pmatrix}. \quad (34)$$

After the matrix diagonalization the following eigenvalues are obtained:

$$\lambda_1 = \frac{1}{4}(-4a - 4b + c), \quad \lambda_2 = \frac{1}{4}(2a + 2b + c), \quad (35)$$

$$\lambda_{3,4} = \frac{1}{4}(\mp \sqrt{9a^2 - 14ab - 4ac + 9b^2 - 4bc + 4c^2} - a - b - c). \quad (36)$$

For $S_1 = 1$, $S_2 = S_3 = 1/2$ spin configuration we get 4 hyperfine levels. To calculate hyperfine structure of muonic molecular ions $\text{td}\mu$, $\text{tp}\mu$, $\text{dp}\mu$ we use first order perturbation theory with a variational wave function obtained in variational calculation. For instance, to calculate $\langle \delta(\mathbf{r}_{12}) \rangle$ matrix element in first order perturbation theory one has to use the following expression:

$$\langle \delta(\mathbf{r}_{12}) \rangle = \frac{\sum_{i,j=1}^K c_i c_j \frac{(2\pi)^{3/2}}{(A_{22}^i + A_{22}^j)^{3/2}}}{\sum_{i,j=1}^K c_i c_j \frac{8\pi^3}{[(A_{11}^i + A_{11}^j)(A_{22}^i + A_{22}^j) - (A_{12}^i + A_{12}^j)^2]^{3/2}}}. \quad (37)$$

Other matrix elements are evaluated in a similar way. Thus we obtain numerical values of a , b and c coefficients and energies of hyperfine structure levels of $\text{td}\mu$, $\text{tp}\mu$, $\text{dp}\mu$ mesomolecular ions.

To obtain a more precise result we include vacuum polarization and nuclear structure corrections to hyperfine structure. The potential of one loop vacuum polarization correction to the hyperfine structure has the form:

$$\Delta V_{VP}^{hfs} = a_{VP}(\mathbf{S}_1 \mathbf{S}_2) + b_{VP}(\mathbf{S}_1 \mathbf{S}_3) + c_{VP}(\mathbf{S}_2 \mathbf{S}_3), \quad (38)$$

$$\begin{aligned} a_{VP} &= -\frac{2\alpha^2 g_1 g_2}{3m_p^2} \frac{\alpha}{3\pi} \int_1^\infty \rho(\xi) d\xi \left[\pi \delta(\mathbf{r}_{12}) - \frac{\gamma^2 \xi^2}{r_{12}} e^{-2\gamma \xi r_{12}} \right], \\ b_{VP} &= \frac{2\alpha^2 g_1 g_3}{3m_p m_3} \frac{\alpha}{3\pi} \int_1^\infty \rho(\xi) d\xi \left[\pi \delta(\mathbf{r}_{13}) - \frac{\gamma^2 \xi^2}{r_{13}} e^{-2\gamma \xi r_{13}} \right], \\ c_{VP} &= \frac{2\alpha^2 g_2 g_3}{3m_p m_3} \frac{\alpha}{3\pi} \int_1^\infty \rho(\xi) d\xi \left[\pi \delta(\mathbf{r}_{23}) - \frac{\gamma^2 \xi^2}{r_{23}} e^{-2\gamma \xi r_{23}} \right]. \end{aligned}$$

Integration over the Jacobi coordinates can be performed analytically. Thus we obtain the following integral expressions for vacuum polarization correction to the hyperfine structure:

$$\begin{aligned} I_{VP,hfs}^{12} &= \int_1^\infty \rho(\xi) d\xi \left[\frac{2\sqrt{2}\pi^{5/2}}{B_{22}^{3/2}} - \right. \\ &\quad \left. \frac{8\pi^2 \gamma^2 \xi^2 \left(\sqrt{2\pi} \sqrt{B_{11} - \frac{B_{12}^2}{B_{22}}} - 2\pi \gamma \xi e^{\frac{2B_{22}\gamma^2 \xi^2}{B_{11}B_{22} - B_{12}^2}} \operatorname{erfc} \left(\sqrt{2\pi} \gamma \xi \sqrt{\frac{B_{22}}{B_{11}B_{22} - B_{12}^2}} \right) \right)}{(B_{11}B_{22} - B_{12}^2)^{3/2}} \right], \end{aligned} \quad (39)$$

$$\begin{aligned} I_{VP,hfs}^{13,23} &= \int_1^\infty \rho(\xi) d\xi \left[\frac{2\sqrt{2}\pi^{5/2}}{(F_1^{13,23})^{3/2}} - \frac{8\pi^2 \gamma^2 \xi^2}{(F_1^{13,23} B_{22} - (F_2^{13,23})^2)^{3/2}} \left(\sqrt{2\pi} \sqrt{B_{22} - \frac{(F_2^{13,23})^2}{F_1^{13,23}}} - \right. \right. \\ &\quad \left. \left. - 2\pi \gamma \xi e^{\frac{2F_1^{13,23} \gamma^2 \xi^2}{F_1^{13,23} B_{22} - (F_2^{13,23})^2}} \operatorname{erfc} \left(\sqrt{2\pi} \gamma \xi \sqrt{\frac{F_1^{13,23}}{F_1^{13,23} B_{22} - (F_2^{13,23})^2}} \right) \right) \right], \end{aligned} \quad (40)$$

Table 1. Numerical results for hydrogen mesomolecular ions. Numerical values for ground state and hyperfine structure as well as QED corrections are presented. In parenthesis numerical results from [3] are presented

Contribution	$pd\mu$	$tp\mu$	$td\mu$
Total energy, μ a.u.	-0.51271179025 (-0.51271179248)	-0.51988008423 (-0.51988008570)	-0.53859497060 (-0.53859497171)
Breit correction, μ a.u.	-0.00004680312	-0.00004243284	-0.00002662515
VP correction, μ a.u.	-0.00111191215	-0.00043309998	-0.00123291439
Structure correction, μ a.u.	0.00002808260	0.00003032453	0.00004789756
Total energy + corrections, μ a.u.	-0.51384242292	-0.52032529252	-0.53980661258
λ_1 , MHz	-2.3086×10^7 (-2.3097×10^7)	-3.1823×10^7 (-3.1839×10^7)	-3.6021×10^7 (-3.6038×10^7)
VP correction to λ_1 , MHz	-0.0047×10^7	-0.0067×10^7	-0.0087×10^7
Zemach correction to λ_1 , MHz	-0.0019×10^7	-0.0010×10^7	-0.0073×10^7
λ_1 + corrections, MHz	-2.3152×10^7	-3.1900×10^7	-3.6181×10^7
λ_2 , MHz	-2.1213×10^7 (-2.1222×10^7)	1.6774×10^6 (1.6797×10^6)	-3.4422×10^7 (-3.4439×10^7)
VP correction to λ_2 , MHz	-0.0043×10^7	0.0039×10^6	-0.0083×10^7
Zemach correction to λ_2 , MHz	0.0048×10^7	0.0974×10^6	0.0161×10^7
λ_2 + corrections, MHz	-2.1208×10^7	1.7787×10^6	-3.4344×10^7
λ_3 , MHz	9.3013×10^6 (9.3058×10^6)	1.5073×10^7 (1.5080×10^7)	1.5977×10^7 (1.5985×10^7)
VP correction to λ_3 , MHz	0.0186×10^6	0.0031×10^7	0.0039×10^7
Zemach correction to λ_3 , MHz	0.0567×10^6	-0.0044×10^7	0.0171×10^7
λ_3 + corrections, MHz	9.3766×10^6	1.506×10^7	1.6187×10^7
λ_4 , MHz	1.2514×10^7 (1.2519×10^7)	—	1.8911×10^7 (1.8920×10^7)
VP correction to λ_4 , MHz	0.0025×10^7	—	0.0045×10^7
Zemach correction to λ_4 , MHz	-0.0032×10^7	—	-0.0091×10^7
λ_4 + corrections, MHz	1.2507×10^7	—	1.8865×10^7

where $\text{erfc}(z)$ is the complementary error function. Another important correction to the hyperfine structure of the same order is the well-known Zemach correction. For mesomolecular ions we obtain the following formula for this correction:

$$\Delta V_{str,2\gamma}^{hfs} = b_{str}(\mathbf{S}_1\mathbf{S}_3) + c_{str}(\mathbf{S}_2\mathbf{S}_3), \quad (41)$$

$$b_{str} = \frac{2\alpha^2 g_1 g_3}{3m_p} \delta(\mathbf{r}_{13}) \frac{8\alpha m_3}{\pi} \int_0^\infty \frac{dk}{k^2} \left[\frac{G_E^1(k^2) G_M^1(k^2)}{G_M^1(0)} - 1 \right], \quad (42)$$

$$c_{str} = \frac{2\alpha^2 g_2 g_3}{3m_p} \delta(\mathbf{r}_{23}) \frac{8\alpha m_3}{\pi} \int_0^\infty \frac{dk}{k^2} \left[\frac{G_E^2(k^2) G_M^2(k^2)}{G_M^2(0)} - 1 \right]. \quad (43)$$

All numerical values that are calculated in this work are presented in Table 1.

4 Summary and conclusion

For numerical calculation a computer code is written in the MATLAB system to solve the three-body Coulomb problem based on the Schrödinger equation. The Varga-Suzuki program [4] written in Fortran is taken as the basis. Overlap matrix elements, matrix elements of kinetic and potential energies are inserted into the program. The random number generation algorithm has been changed. For variational parameters the stochastic optimization procedure is being used. As a result, the numerical values of the ground state energy as well as energy levels of hyperfine structure of $\text{td}\mu$, $\text{tp}\mu$, $\text{dp}\mu$ are obtained. In first order perturbation theory relativistic, vacuum polarization and nuclear structure corrections to the ground state energy are calculated for $\text{td}\mu$, $\text{tp}\mu$ and $\text{dp}\mu$ hydrogen mesomolecular ions. Vacuum polarization and Zemach corrections are taken into account in the hyperfine structure of mesomolecular ions. All energies are in agreement with [3, 11, 12]. The values of ground state energies coincide with the results from paper [3] in 8 digits. In our method we can obtain up to 10 precise digits in ground state energy value which gives us 3 precise digits in hyperfine structure values. The difference in precision with [3] is connected with smaller basis size in our work and lower convergence rate of the Gaussian basis compared with exponential basis that is used in [3]. It is also worth mentioning that in our calculations we use double precision while in [3] quadruple precision is being used. This fact also contributes to differences in results.

This work is supported by Russian Science Foundation (Grant 18-12-00128).

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