

Hyperfine structure of muonic molecular ions $\text{td}\mu$, $\text{tp}\mu$, $\text{dp}\mu$

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Abstract. The hyperfine structure of energy levels of muonic molecules $\text{td}\mu$, $\text{tp}\mu$ and $\text{dp}\mu$ 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. For numerical calculation, a computer code is written in the MATLAB system. Numerical values of energy levels of hyperfine structure in muonic molecules $\text{td}\mu$, $\text{tp}\mu$ and $\text{dp}\mu$ are obtained.

1. Introduction

The study of the energy spectra of hydrogen muonic molecules is important for 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 μCF cycle. In our work we investigate hyperfine structure of S-states with $L = 0$. Muonic molecules $\text{td}\mu$, $\text{tp}\mu$ and $\text{dp}\mu$ consist of various isotopes of hydrogen with different spins which results in different number of hyperfine structure levels. In $\text{tp}\mu$ all spins are equal to $1/2$ and it has 3 hyperfine energy levels. In $\text{td}\mu$ and $\text{dp}\mu$ deuteron has spin 1 which gives 4 hyperfine energy levels in the ground state of these mesomolecular ions. 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 ν , where J is rotational quantum number and ν is vibrational quantum number [2, 3]. Ground state in this approach is designated as $(0,0)$.

2. General formalism

To calculate the bound state energies and their 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 the Gaussian form. The Gaussian-type basis function with non-zero angular momentum for nonidentical particles is the following:

$$\phi_{LS}(\mathbf{x}, A) = e^{-\frac{1}{2}\tilde{\mathbf{x}}A\mathbf{x}}\theta_L(\mathbf{x}), \quad \theta_L(\mathbf{x}) = [([\mathbb{Y}_{l_1}(\mathbf{x}_1)\mathbb{Y}_{l_2}(\mathbf{x}_2)]_{L_{12}}\mathbb{Y}_{l_3}(\mathbf{x}_3)]_{L_{123}\dots}]_{LM}, \quad (1)$$

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, $\mathbb{Y}_{l_m}(\mathbf{x}) = r^l Y_{lm}(\mathbf{x})$. 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:

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

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:

$$\langle \phi' | \phi \rangle^{00} = \frac{8\pi^3}{(\det B)^{3/2}}. \quad (3)$$

where the matrix elements of matrix B are expressed in terms of matrix A: $B_{ij} = A'_{ij} + A_{ij}$. 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 particles. Matrix elements of kinetic energy have the following analytical form:

$$\langle \phi' | \hat{T} | \phi \rangle^{00} = -\frac{24\pi^3}{(\det B)^{5/2}} \left\{ \frac{\hbar^2}{2\mu_1} I_\rho^{00} + \frac{\hbar^2}{2\mu_2} I_\lambda^{00} \right\}, \quad (5)$$

$$I_\rho^{00} = A_{12}^2 B_{11} - 2A_{11} A_{12} B_{12} + A_{11} (B_{12}^2 + (A_{11} - B_{11}) B_{22}), \quad (6)$$

$$I_\lambda^{00} = A_{12}^2 B_{22} - 2A_{22} A_{12} B_{12} + A_{22} (B_{12}^2 + (A_{22} - B_{22}) B_{11}). \quad (7)$$

For potential energy matrix elements we have:

$$\langle \phi' | \hat{V} | \phi \rangle^{00} = e_1 e_2 I_{12}^{00} + e_1 e_3 I_{13}^{00} + e_2 e_3 I_{23}^{00}. \quad (8)$$

$$I_{12}^{00} = \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{B_{22}} \det B}. \quad (9)$$

To obtain $I_{13,23}^{00}$ one has to introduce a new variable $\mathbf{k}^{13,23} = \boldsymbol{\lambda} \pm \frac{m_2^{13,23}}{m_{12}} \boldsymbol{\rho}$.

$$I_{13,23}^{00} = \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{F_1^{13,23} (B_{22} F_1^{13,23} - (F_2^{13,23})^2)}}, \quad (10)$$

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

Now let us calculate matrix elements of the hyperfine part of Hamiltonian. The potential of hyperfine structure of $L = 1$ state, which is a part of the well-known Breit Hamiltonian, can be written in the following simple form for three interacting particles with spins S_1, S_2, S_3 respectively:

$$\Delta V^{hfs} = a(\mathbf{S}_1 \mathbf{S}_2) + b(\mathbf{S}_1 \mathbf{S}_3) + c(\mathbf{S}_2 \mathbf{S}_3), \quad (12)$$

$$a = \frac{2\pi\alpha}{3m_1 m_2} \frac{(1 + \kappa_1)}{S_1} \frac{(1 + \kappa_2)}{S_2} \delta(\mathbf{r}_{12}),$$

$$b = \frac{2\pi\alpha}{3m_1 m_3} \frac{(1 + \kappa_1)}{S_1} \frac{(1 + \kappa_3)}{S_3} \delta(\mathbf{r}_{13}),$$

$$c = \frac{2\pi\alpha}{3m_2m_3} \frac{(1 + \kappa_2)}{S_2} \frac{(1 + \kappa_3)}{S_3} \delta(\mathbf{r}_{23}).$$

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:

$$\begin{aligned} \langle \delta(\mathbf{r}_{12}) \rangle &= \langle \delta(\rho) \rangle = \int \int d\rho d\lambda \delta(\rho) e^{-\frac{1}{2}[B_{11}\rho^2 + B_{22}\lambda^2 + 2B_{12}(\rho\lambda)]} = \\ &= 4\pi \int \lambda^2 d\lambda \delta(\rho) e^{-\frac{1}{2}B_{22}\lambda^2} = \frac{(2\pi)^{3/2}}{(B_{22})^{3/2}}. \end{aligned} \quad (13)$$

$$\langle \delta(\mathbf{r}_{13}) \rangle = \frac{(2\pi)^{3/2}}{(B_{11} - 2B_{12}\frac{m_2}{m_1} + B_{22}(\frac{m_2}{m_1})^2)^{3/2}}, \quad (14)$$

$$\langle \delta(\mathbf{r}_{23}) \rangle = \frac{(2\pi)^{3/2}}{(B_{11} + 2B_{12}\frac{m_1}{m_2} + B_{22}(\frac{m_1}{m_2})^2)^{3/2}}. \quad (15)$$

To perform averaging over spin functions Wigner - Eckart theorem [5] can be used with success. General formulas for spin averaging for any S_1 , S_2 and S_3 take the form:

$$\langle S'_{12}, S | (\mathbf{S}_1 \mathbf{S}_2) | S_{12}, S \rangle = \overline{(S_1 S_2)}_{S_{12}} \delta_{S_{12} S'_{12}}, \quad (16)$$

$$\begin{aligned} \langle S'_{12}, S | (\mathbf{S}_1 \mathbf{S}_3) | S_{12}, S \rangle &= \sqrt{(2S'_{12} + 1)(2S_{12} + 1)(2S_1 + 1)(S_1 + 1)S_1} \sqrt{(2S_3 + 1)(S_3 + 1)S_3} \times \\ &\times (-1)^{S_{12}^{max} + S_{12}^{min} + S + S_1 + S_2 + S_3 + 1} \begin{Bmatrix} S_{12} & S_3 & S \\ S_3 & S'_{12} & 1 \end{Bmatrix} \begin{Bmatrix} S_1 & S'_{12} & S_2 \\ S_{12} & S_1 & 1 \end{Bmatrix}, \end{aligned} \quad (17)$$

$$\begin{aligned} \langle S'_{12}, S | (\mathbf{S}_2 \mathbf{S}_3) | S_{12}, S \rangle &= \sqrt{(2S'_{12} + 1)(2S_{12} + 1)(2S_2 + 1)(S_2 + 1)S_2} \sqrt{(2S_3 + 1)(S_3 + 1)S_3} \times \\ &\times (-1)^{2S_{12}^{max} + S + S_1 + S_2 + S_3 + 1} \begin{Bmatrix} S_{12} & S_3 & S \\ S_3 & S'_{12} & 1 \end{Bmatrix} \begin{Bmatrix} S_2 & S'_{12} & S_1 \\ S_{12} & S_2 & 1 \end{Bmatrix}. \end{aligned} \quad (18)$$

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

$$\begin{pmatrix} \frac{1}{4}a + \frac{1}{4}b + \frac{1}{4}c & 0 & 0 \\ 0 & \frac{1}{4}a - \frac{1}{2}b - \frac{1}{2}c & \frac{\sqrt{3}}{4}b - \frac{\sqrt{3}}{4}c \\ 0 & \frac{\sqrt{3}}{4}b - \frac{\sqrt{3}}{4}c & -\frac{3}{4}a \end{pmatrix}. \quad (19)$$

After the diagonalization we obtain the following eigenvalues:

$$\lambda_{1,2} = -\frac{1}{4}(a + b + c) \pm \frac{1}{2}\sqrt{a^2 + b^2 + c^2 - ab - bc - ac}, \quad \lambda_3 = \frac{1}{4}(a + b + c). \quad (20)$$

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:

$$\begin{pmatrix} \frac{1}{2}a + \frac{1}{2}b + \frac{1}{4}c & 0 & 0 & 0 \\ 0 & \frac{1}{2}a - \frac{5}{6}b - \frac{5}{12}c & \frac{\sqrt{2}}{3}b - \frac{\sqrt{2}}{3}c & 0 \\ 0 & \frac{\sqrt{2}}{3}b - \frac{\sqrt{2}}{3}c & -a + \frac{1}{3}b - \frac{1}{12}c & 0 \\ 0 & 0 & 0 & -a - b + \frac{1}{4}c \end{pmatrix}. \quad (21)$$

After the diagonalization eigenvalues are:

$$\lambda_1 = \frac{1}{4}(-4a - 4b + c), \quad \lambda_2 = \frac{1}{4}(2a + 2b + c), \quad (22)$$

$$\lambda_{3,4} = \frac{1}{4}(\mp \sqrt{9a^2 - 14ab - 4ac + 9b^2 - 4bc + 4c^2} - a - b - c). \quad (23)$$

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 using first order perturbation theory one has to use the following expression:

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

where c_i , c_j are linear variational parameters, K is a number of basis functions. 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.

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. Matrix elements of the wave function normalization, kinetic and potential energies are inserted into the program. Changed the way to set the function of generating random numbers. For variational parameters the stochastic optimization procedure is being used. As a result, the numerical values of energy levels of hyperfine structure of $\text{td}\mu$, $\text{tp}\mu$, $\text{dp}\mu$ are obtained in muon atomic units. All energies are in agreement with [3]. The difference for hyperfine splitting energies is connected with a smaller basis size and lower accuracy for the value of ground state total energy. It is worth mentioning that in our calculations we use double precision while in [3] quadruple precision is being used. This fact also contributes to difference of results.

3. References

- [1] Gershtein, S.S. Muon catalysis and nuclear breeding / S.S. Gershtein, Yu.V. Petrov, L.I. Ponomarev // Sov. Phys. Usp. – 1990. – Vol. 33(8). – P. 3-46.
- [2] Frolov, A.M. Bound state spectra of three-body muonic molecular ions / A.M. Frolov, D.M. Wardlaw // Eur. Phys. J. – 2011. – Vol. 63. – P. 339-350.
- [3] Frolov, A.M. On the bound states in the muonic molecular ions / A.M. Frolov // Eur. Phys. J. – 2012. – Vol. 66. – P. 212-223.
- [4] Varga, K. Solution of few-body problems with the stochastic variational method I. Central forces with zero orbital momentum / K. Varga, Y. Suzuki // Comp. Phys. Comm. – 1997. – Vol. 106. – P. 157-168.
- [5] Landau, L.D. Quantum Mechanics: Non-Relativistic Theory / L.D. Landau, E.M. Lifshitz. – Pergamon Press, 1977. – 688 p.

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