Hyperfine structure of excited states of hydrogen mesomolecules

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The investigation of energy spectra of hydrogen muonic molecules is important for muonic catalysis of nuclear fusion reactions. A calculation of fine and hyperfine structure of muonic molecular ions as well as higher order QED corrections allows us to predict the rates of reactions of their formation and other parameters of the μCF cycle.

The aim of this work is to study hyperfine splitting of excited states of three-particle $td\mu$, $dp\mu$ and $tp\mu$ muonic molecular ions on the basis of variational approach.

Tasks:

1. Analytical calculation of matrix elements of the hyperfine structure potential for $L=1$ state;

2. Writing computer code to solve bound state problem for three particles using stochastic variational method with correlated Gaussian basis;

3. Calculation of the energy of the excited $L=1$ state of $td\mu$, $dp\mu$ and $tp\mu$ muonic molecular ions and their hyperfine structure.
GENERAL FORMALISM

Let us consider a system of 3 particles with masses $m_1$, $m_2$ and $m_3$ and charges $z_1$, $z_2$ and $z_3$ respectively. The Schrodinger equation in the Jacobi coordinates has the form:

$$H \Psi = E \Psi$$

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} - T_{cm} - \sum_{i<j}^{N} V_{ij} \quad V_{ij} \text{ – two-body interaction potentials}$$

In variational method the wave function of the system is presented as follows

$$\Psi = \sum_{i=1}^{K} c_i \psi(x, A_i)$$

An upper bound for the energy of the ground state is given by the lowest eigenvalue of the generalized eigenvalue problem:

$$HC = E_K BC$$

$$H_{ij} = \langle \psi(x, A_i) \mid H \mid \psi(x, A_j) \rangle$$

$$B_{ij} = \langle \psi(x, A_i) \mid \psi(x, A_j) \rangle$$
In variational approach with correlated Gaussian basis wave functions have the form:

$$ \Psi(x, A) = G_A(x) \theta_L(x), $$

$$ G_A(x) = e^{-\tilde{A}x/2}, $$

$$ \tilde{A} = \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} A_{ij} x_i \cdot x_j. $$

$$ x = (x_1, \ldots, x_{N-1}) - \text{Jacobi coordinates} $$

$$ x_N - \text{center of mass coordinate} $$

The angular part of the basis wave function has the following form:

$$ \theta_L(x) = \left[ \left[ \nabla_{l_1} (x_1) \nabla_{l_2} (x_2) \right]_{l_{42}} \nabla_{l_3} (x_3) \right]_{l_{123}} \cdots \right]_{LM}. $$

The diagonal elements of the (N-1)×(N-1) dimensional symmetric, positive definite matrix $A$ correspond to the nonlinear parameters of Gaussian expansion, and the off-diagonal elements connect different relative coordinates thus representing the correlations between particles.
We use the following order of particles:

\[ 1 \quad 2 \quad 3 \quad 1 \quad 2 \quad 3 \quad 1 \quad 2 \quad 3 \]

\( t \quad d \quad \mu \), \( d \quad p \quad \mu \) and \( p \quad t \quad \mu \).

The Jacobi coordinates are related to the relative particle coordinates as follows:

\[ \rho = r_1 - r_2 \]

\[ \lambda = \frac{r_1 m_1 + r_2 m_2}{m_1 + m_2} - r_3 \]

\[ R = 0 \]

For the interparticle coordinates:

\[ r_{12} = r_1 - r_2 = \rho \]

\[ r_{13} = r_1 - r_3 = \lambda + \frac{m_2}{m_1 + m_2} \rho \]

\[ r_{23} = r_2 - r_3 = \lambda - \frac{m_1}{m_1 + m_2} \rho \]
EXCITED STATE L=1

\[ \psi_{10}(\rho, \lambda, A) = e^{-\frac{1}{2}[A_{11}\rho^2 + A_{12}\lambda^2 + 2A_{12}(\rho \cdot \lambda)]]} (\varepsilon \rho), \]

\[ \psi_{01}(\rho, \lambda, A) = e^{-\frac{1}{2}[A_{11}\rho^2 + A_{12}\lambda^2 + 2A_{12}(\rho \cdot \lambda)]]} (\varepsilon \lambda). \]

Matrix elements of kinetic energy:

\[ <\phi' | \hat{T} | \phi >^{10,01,11,(01||00)} = -\frac{6\pi^2}{(\det B)^{7/2}} \left\{ \frac{\hbar^2}{2\mu_1} I_{\rho}^{10,01,11,(01||00)} + \frac{\hbar^2}{2\mu_2} I_{\lambda}^{10,01,11,(01||00)} \right\}, \]

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

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

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

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

\[ I_{\rho}^{11} = A_{12}B_{11} - 2A_{11}A_{12}B_{12} + A_{11}[B_{12}^2 + (A_{11} - B_{11})B_{22}], \]

\[ I_{\lambda}^{11} = A_{22}B_{12} - 2A_{22}A_{12}B_{12} + A_{22}[B_{12}^2 + (A_{22} - B_{22})B_{11}], \]

\[ I_{\rho}^{(0||10)} = -B_{12}[-2A_{12}B_{12}(4A_{11} + B_{11}) + 5A_{11}B_{12}^2 + 5A_{12}B_{11}] - B_{22}(A_{11} - B_{11})(5A_{11}B_{12} - 2A_{12}B_{11}), \]

\[ I_{\lambda}^{(0||10)} = 5A_{12}B_{12}B_{22} - A_{22}(2A_{12}B_{11}B_{22} + 8A_{12}B_{12}^2 + 3B_{11}B_{12}B_{22} - 3B_{12}^3) + 5A_{22}B_{11}B_{12}. \]

Overlap matrix elements:

\[ <\phi' | \phi >^{01} = \frac{6\pi^2B_{11}}{(\det B)^{5/2}}, \]

\[ <\phi' | \phi >^{11} = \frac{12\pi^2}{(\det B)^{5/2}}, \]

\[ <\phi' | \phi >^{(0||10)} = -\frac{6\pi^2B_{12}}{(\det B)^{5/2}}. \]
EXCITED STATE L=1

Matrix elements of potential energy:

\[
\langle \phi' | \hat{V} | \phi \rangle^{10,01,11,(01||10)} = e_1 e_2 I_{12}^{10,01,11,(01||10)} + e_1 e_3 I_{13}^{10,01,11,(01||10)} + e_2 e_3 I_{23}^{10,01,11,(01||10)},
\]

\[
I_{12}^{10} = \frac{4\sqrt{2}\pi^{3/2} \sqrt{B_{22}}}{(\det B)^{2}}, \quad I_{13,23}^{10} = \frac{2\sqrt{2}\pi^{3/2} (3B_{11}B_{22} - B_{12})^2}{(B_{22})^{3/2} (\det B)^2},
\]

\[
I_{12}^{01} = \frac{2\sqrt{2}\pi^{3/2} (3B_{11}B_{22} - B_{12})^2}{(B_{22})^{3/2} (\det B)^2}, \quad I_{13,23}^{01} = \frac{2\sqrt{2}\pi^{3/2}}{[B_{22}F_1^{13,23} - (F_2^{13,23})^2]^2} \left\{ 2\sqrt{F_1^{13,23}} + \right.
\]

\[
\left. + \frac{(3B_{22}F_1^{13,23} - (F_2^{13,23})^2)}{(F_1^{13,23})^{3/2}} \left( \frac{m_{2,1}^{13,23}}{m_{12}^{13,23}} \right)^2 \pm \frac{4F_2^{13,23}}{m_{2,1}^{13,23}} \right\},
\]

\[
I_{12}^{11} = \frac{8\sqrt{2}\pi^{3/2}}{\sqrt{B_{22} (\det B)^2}}, \quad I_{13,23}^{11} = \frac{8\sqrt{2}\pi^{3/2}}{\sqrt{F_1^{13,23} [B_{22}F_1^{13,23} - (F_2^{13,23})^2]^2}}, \quad I_{12}^{(01||10)} = - \frac{4\sqrt{2}\pi^{3/2} B_{12}}{\sqrt{B_{22} (\det B)^2}},
\]

\[
I_{13,23}^{(01||10)} = - \frac{2\sqrt{2}\pi^{3/2}}{[B_{22}F_1^{13,23} - (F_2^{13,23})^2]^2} \left\{ 2\frac{F_2^{13,23}}{\sqrt{F_1^{13,23}}} + \frac{m_{2,1}^{13,23}}{m_{12}^{13,23}} \frac{(3B_{22}F_1^{13,23} - (F_2^{13,23})^2)}{(F_1^{13,23})^{3/2}} \right\}.
\]

\[
F_1^{13,23} = B_{11} + B_{22} \left( \frac{m_{2,1}^{13,23}}{m_1 + m_2} \right)^2 + 2B_{12} \frac{m_{2,1}^{13,23}}{m_1 + m_2}, \quad F_2^{13,23} = B_{12} + 2B_{22} \frac{m_{2,1}^{13,23}}{m_1 + m_2}.
\]
Hyperfine structure of L=1 energy level has the following 5 contributions:

1) $-\frac{2\pi \alpha^2}{3m_im_j} z_iz_j g_ig_j \left( S_i \cdot S_j \right) \delta^3(r_{ij})$

2) $-\frac{z_iz_j \alpha^2}{2m_i^2 r_{ij}^3} \left[ \frac{1}{s_i} - 1 + \frac{m_i}{s_im_j} + \frac{\kappa_i}{s_i} \left( 1 + \frac{m_i}{m_j} \right) \right] \left( L_{ij} \cdot S_i \right)$.  

3) $-\frac{z_iz_j \alpha^2(1+\kappa_j)}{2s_j m_im_j r_{ij}^3} \left[ 1 + \frac{(1+\kappa_j-S_j)m_i}{m_j(1+\kappa_j)} \right] \left( L_{ij} \cdot S_j \right)$

4) $\frac{z_iz_j \alpha^2(1+\kappa_i)(1+\kappa_j)}{2s_is_j m_im_j r_{ij}^3} \left[ (S_i \cdot S_j) - 3(S_i \cdot n_{ij})(S_j \cdot n_{ij}) \right]$.

5) $z_iz_j T^2(j) \cdot T^2(i)$

For P - states we have basis functions $(\epsilon \cdot \rho)$ and $(\epsilon \cdot \lambda)$, thus the following matrix elements should be calculated: $\langle \psi_\rho | V | \psi_\rho \rangle; \langle \psi_\rho | V | \psi_\lambda \rangle; \langle \psi_\lambda | V | \psi_\rho \rangle, \langle \psi_\lambda | V | \psi_\lambda \rangle$.

Let us write wave functions in the following notation: $|SLF\rangle$, where

$S_1 + S_2 = S_{12}$;

$S_{12} + S_3 = S$;

$S + L = F$.  

\[ \langle S'LF| (S_i \cdot S_j) \delta^3(r_{ij})|SLF \rangle = \sum_{S_z'S_z' L_z F_z} C(S'S_z'L_zF_z F_z) C(S S_z L_z F_z) \times \]

\[ \langle LL_{Z'}| \delta^3(r_{ij})|LL_Z \rangle \langle S'S_z'| (S_i \cdot S_j)|SS_z \rangle = \delta_{SS'} \langle L| \delta^3(r_{ij})|L \rangle \langle S|(S_i \cdot S_j)|S \rangle. \]

All possible integrals of \( \delta^3(r_{ij}) \):

a) \( r_{12} = \rho \), \( \langle L_\rho| \delta^3(\rho)|L_\rho \rangle = \langle L_\rho| \delta^3(\rho)|L_\lambda \rangle = \langle L_\lambda| \delta^3(\rho)|L_\rho \rangle = 0. \)

\[ \langle L_\lambda| \delta^3(\rho)|L_\lambda \rangle = \int d\rho \int d\lambda \, \delta^3(\rho) (\epsilon \cdot \lambda)(\epsilon \cdot \lambda) e^{-\frac{1}{2}[B_{11}\rho^2 + B_{22}\lambda^2 + 2B_{12}(\rho \cdot \lambda)]} \]

\[ = \int d\lambda \, (\epsilon \cdot \lambda)(\epsilon \cdot \lambda) e^{-\frac{1}{2}[B_{22}\lambda^2]} = \int d\lambda \, \lambda^2 e^{-\frac{1}{2}[B_{22}\lambda^2]} = \frac{3\sqrt{\pi}}{\sqrt{2}B_{22}^{5/2}}. \]

b) \( r_{13} = \lambda + \frac{m_2}{m_1 + m_2} \rho \), \( \lambda + \frac{m_2}{m_1 + m_2} \rho = k_{13}, \lambda_{13} = k_{13} - \frac{m_2}{m_1 + m_2} \rho. \)

\[ \langle L_\rho| \delta^3(k_{13})|L_\rho \rangle = \int d\rho \int dk \, \delta^3(k_{13}) e^{-\frac{1}{2}[F_{13}^1 \rho^2 + B_{22}k^2 + 2F_{13}^1 \rho \cdot k]} (\epsilon \cdot \rho)(\epsilon \cdot \rho) \]

\[ = \int d\rho \rho^2 e^{-\frac{1}{2}[F_{13}^1 \rho^2]} = \frac{3\sqrt{\pi}}{\sqrt{2}(F_{13}^1)^{5/2}}. \]
\[ \langle L_\rho | \delta^3(k_{13}) | L_\lambda \rangle = \langle L_\lambda | \delta^3(k_{13}) | L_\rho \rangle = \iint d\rho \, dk \, \delta^3(k_{13}) e^{-\frac{1}{2} [F_{1}^{13} \rho^2 + B_{22} k^2 + 2F_{2}^{13}(\rho \cdot k)]} (\varepsilon \cdot \rho)(\varepsilon \cdot k) - \frac{m_2}{m_1 + m_2} \iint d\rho \, dk \, \delta^3(k_{13}) e^{-\frac{1}{2} [F_{1}^{13} \rho^2 + B_{22} k^2 + 2F_{2}^{13}(\rho \cdot k)]} (\varepsilon \cdot \rho)(\varepsilon \cdot \rho) = \]

\[ -\frac{m_2}{m_1 + m_2} \langle L_\rho | \delta^3(k_{13}) | L_\rho \rangle; \ -\langle L_\lambda | \delta^3(k_{13}) | L_\lambda \rangle = \left( \frac{m_2}{m_1 + m_2} \right)^2 \langle L_\rho | \delta^3(k_{13}) | L_\rho \rangle. \]

c) \( r_{23} = \lambda - \frac{m_1}{m_1 + m_2} \rho. \)

\[ \langle L_\rho | \delta^3(k_{23}) | L_\rho \rangle = \iint d\rho \, dk \, \delta^3(k_{23}) e^{-\frac{1}{2} [F_{1}^{23} \rho^2 + B_{22} k^2 + 2F_{2}^{23}(\rho \cdot k)]} (\varepsilon \cdot \rho)(\varepsilon \cdot \rho) \]

\[ = \int d\rho \, \rho^2 e^{-\frac{1}{2} F_{1}^{23} \rho^2} = \frac{3\sqrt{\pi}}{\sqrt{2}(F_{1}^{23})^{\frac{5}{2}}}; \]
\[ \langle L_\rho | \delta^3(k_{13}) | L_\lambda \rangle = \langle L_\lambda | \delta^3(k_{13}) | L_\rho \rangle = -\frac{m_2}{m_1 + m_2} \langle L_\rho | \delta^3(k_{13}) | L_\rho \rangle; \quad -\langle L_\lambda | \delta^3(k_{13}) | L_\lambda \rangle = \left(\frac{m_2}{m_1 + m_2}\right)^2 \langle L_\rho | \delta^3(k_{13}) | L_\rho \rangle. \]

\[
\langle L_\rho | \delta^3(k_{23}) | L_\rho \rangle = \frac{3\sqrt{\pi}}{\sqrt{2}(F_{1}^{23})^2};
\]

c) \[ r_{23} = \lambda - \frac{m_1}{m_1 + m_2} \rho. \]

\[ \langle L_\rho | \delta^3(k_{23}) | L_\lambda \rangle = \langle L_\lambda | \delta^3(k_{23}) | L_\rho \rangle = \frac{m_1}{m_1 + m_2} \langle L_\rho | \delta^3(k_{23}) | L_\rho \rangle; \]

\[ \langle L_\lambda | \delta^3(k_{23}) | L_\lambda \rangle = \left(\frac{m_1}{m_1 + m_2}\right)^2 \langle L_\rho | \delta^3(k_{23}) | L_\rho \rangle. \]
\[
\langle S'LF| (L_{ij} \cdot S_{i,j})|SLF \rangle = (-1)^{L+S_{\text{max}}+F} \binom{S'}{L} \binom{L}{S} \binom{F}{1} \langle L || L_{ij} || L \rangle \langle S' || S_{ij} || S \rangle.
\]

\[
\frac{1}{r_{ij}^3} \left[ (S_i \cdot S_j) - 3(S_i \cdot n_{ij})(S_j \cdot n_{ij}) \right]
\]

\[
M_{ij} = -\frac{3}{r_{ij}} T_0^2(S_iS_j) \cdot T_0^2(n_{ij}),
\]

where \(T_0^2(S_iS_j) = \frac{1}{\sqrt{6}} \left( 3S_i^2S_j^2 - (S_i \cdot S_j) \right); \ T_0^2(n_{ij}) = \frac{1}{\sqrt{6}} (3(n_{ij}^2)^2 - 1).\)

\[
\langle LS'F|M_{ij}|LSF \rangle = (-1)^{L+S_{\text{max}}+F} \binom{S'}{L} \binom{L}{S} \binom{F}{2} \langle L || T_0^2(n_{ij}) || L \rangle \cdot \langle S' || T_0^2(S_iS_j) || S \rangle
\]
MATRIX ELEMENTS FOR HFS, CONTRIBUTION 5)

\[ z_i z_j T^2(j) \cdot T^2(i), \]

if i or j – nuclei

\[ T^2_q(i) = \int \sqrt{\frac{4\pi}{5}} r'^2 Y^2_q(\theta', \varphi') \rho(r') d^3r', \]

if i or j – muon

\[ T^2_q(i) = \sqrt{\frac{4\pi}{5}} \frac{1}{r^3} Y^2_q(\theta, \varphi). \]

\[ \langle LS'F|T^2(3) \cdot T^2(1,2)|LSF\rangle = (-1)^{L+S_{\text{max}}} \quad ^{+F} \times \]

\[ \left\{ S' \quad L \quad F \right\}\langle L||T^2(3)||L\rangle\langle S'||T^2(1,2)||S\rangle \]
The program is based on the Fortran program by K. Varga and Y. Suzuki;

A number of changes is made compared to the Fortran program, including the ability to calculate states with nonzero \( L \), more convenient generation of variational parameters and various optimization changes;

The main results of the calculation include energies of ground and excited states along with variational wave functions for each state. The program is capable of calculating \( L=0 \) and \( L=1 \);

For L=1 state hyperfine structure of $td\mu$ diagonalized energy matrix has the following form (all values are presented in muon atomic units):

\[
\begin{pmatrix}
0.0000606677 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0.\\
0. & 0.0000606575 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0.\\
0. & 0. & 0.0000543327 & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0.\\
0. & 0. & 0. & 0.0000543302 & 0. & 0. & 0. & 0. & 0. & 0. & 0.\\
0. & 0. & 0. & 0. & -0.000031384 & 0. & 0. & 0. & 0. & 0. & 0.\\
0. & 0. & 0. & 0. & 0. & -0.0000313817 & 0. & 0. & 0. & 0. & 0.\\
0. & 0. & 0. & 0. & 0. & 0. & -0.0000261379 & 0. & 0. & 0. & 0.\\
0. & 0. & 0. & 0. & 0. & 0. & 0. & -0.0000261372 & 0. & 0. & 0.\\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & -0.0000229046 & 0. & 0.\\
0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & 0. & -0.0000229036 & 0.
\end{pmatrix}
\]

Total energy of the L=1 state from variational calculation is (in muon atomic units):

\[-0.523191450430718\]
THANK YOU FOR YOUR ATTENTION