САМАРСКИЙ УНИВЕРСИТЕТ
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Hyperfine structure of mesomolecules pdμ, ptμ, dtμ in variational method

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INTRODUCTION AND OVERVIEW

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.

- *Korobov V.I., Puzynin I.V. and Vinitsky S.I. Physics Letters B* ***196*** *(1987) 272-276.*
- *Frolov A.M. and Wardlaw D.M. Eur. Phys. J. D* ***63*** *(2011) 339–350.*
- *Aznabayev D.T., Bekbaev A. K., Ishmukhamedov I. S., and Korobov V. I. Physics of Particles and Nuclei Letters* ***12*** *(2015) 689–694.*

PURPOSE

The aim of this work is to study hyperfine splitting of three-particle tdμ, dpμ and tpμ muonic molecular ions on the basis of variational approach.

Tasks:

1. Analytical calculation of diagonal and off-diagonal matrix elements of kinetic energy, potential energy and overlap for basis functions;

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 ground state of tdμ, dpμ and tpμ 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:

$$H\Psi = E\Psi$$

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} - T_{cm} - \sum_{i<j}^{N} V_{ij} \qquad V_{ij} - \text{ two-body interaction potentials}$$

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

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

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

$$HC = E_K BC$$

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

$$B_{ij} = \langle \psi(\mathbf{x}, A_i) \,|\, \psi(\mathbf{x}, A_j) \rangle$$

GAUSSIAN BASIS FUNCTIONS

In variational approach with correlated Gaussian basis wave functions have the form:

$$\Psi(\mathbf{x}, A) = G_A(\mathbf{x})\theta_L(\mathbf{x}),$$

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

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

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

x_N – center of mass coordinate

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

$$\theta_L(\mathbf{x}) = [[[\mathbb{Y}_{l_1}(\mathbf{x}_1)\mathbb{Y}_{l_2}(\mathbf{x}_2)]_{L_{12}}\ \mathbb{Y}_{l_3}(\mathbf{x}_3)]_{L_{123}} \ldots]_{LM} .$$

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.

JACOBI COORDINATES

We use the following order of particles:

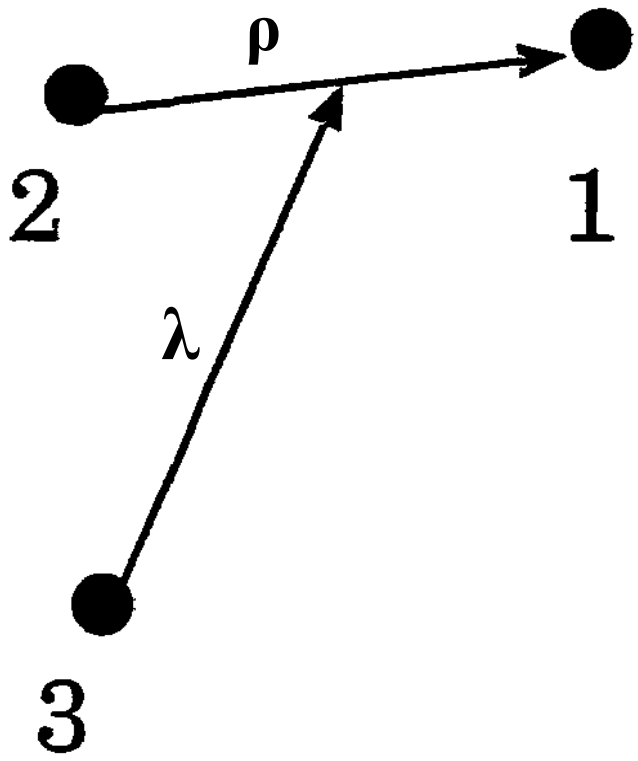
$$1\ 2\ 3 \qquad 1\ 2\ 3 \qquad 1\ 2\ 3$$
$$t\,d\,\mu, \quad d\,p\,\mu \ \text{and} \ p\,t\,\mu.$$

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

$$\boldsymbol{\rho} = \mathbf{r}_1 - \mathbf{r}_2$$

$$\boldsymbol{\lambda} = \frac{\mathbf{r}_1 m_1 + \mathbf{r}_2 m_2}{m_1 + m_2} - \mathbf{r}_3$$

$$\mathbf{R} = 0$$



For the interparticle coordinates:

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2 = \boldsymbol{\rho}$$

$$\mathbf{r}_{13} = \mathbf{r}_1 - \mathbf{r}_3 = \boldsymbol{\lambda} + \frac{m_2}{m_1 + m_2}\boldsymbol{\rho}$$

$$\mathbf{r}_{23} = \mathbf{r}_2 - \mathbf{r}_3 = \boldsymbol{\lambda} - \frac{m_1}{m_1 + m_2}\boldsymbol{\rho}$$

GROUND STATE L=0

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

Kinetic energy operator:

$$\hat{T} = -\frac{\hbar^2}{2\mu_1}\nabla^2_{\boldsymbol{\rho}} - \frac{\hbar^2}{2\mu_2}\nabla^2_{\boldsymbol{\lambda}}$$

where:

$$\mu_1 = \frac{m_1 m_2}{m_1 + m_2}, \qquad \mu_2 = \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3}$$

Matrix elements of kinetic energy:

$$<\phi' | \hat{T} | \phi>^{00} = \frac{24\pi^3}{\det B^{2.5}}\{\frac{\hbar^2}{2\mu_1} I_\rho^{00} + \frac{\hbar^2}{2\mu_2} I_\lambda^{00}\}$$

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

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

$$B_{ij} = A_{ij} + A'_{ij}$$

GROUND STATE L=0

Potential energy operator:

$$V = \frac{e_1 e_2}{|\boldsymbol{\rho}|} + \frac{e_1 e_3}{|\boldsymbol{\lambda} + \frac{m_2}{m_1 + m_2}\boldsymbol{\rho}|} + \frac{e_2 e_3}{|\boldsymbol{\lambda} - \frac{m_2}{m_1 + m_2}\boldsymbol{\rho}|}$$

Matrix elements of potential energy:

$$<\phi' |\hat{V}| \phi> = e_1 e_2 I_{12}^{00} + e_1 e_3 I_{13}^{00} + e_2 e_3 I_{23}^{00}$$

$$I_{12}^{00} = \frac{8\sqrt{2}\pi^{2.5}}{\sqrt{B_{22}}\det B}$$

$$I_{13,23}^{00} = \frac{8\sqrt{2}\pi^{2.5}}{\sqrt{F_1^{13,23}}(B_{22}F_1^{13,23} - (F_2^{13,23})^2)}$$

$$F_1^{13,23} = B_{11} + B_{22}\left(\frac{m_{2,1}^{13,23}}{m_1 + m_2}\right)^2 \mp 2B_{12}\frac{m_{2,1}^{13,23}}{m_1 + m_2}$$

$$F_2^{13,23} = B_{12} \mp 2B_{22}\frac{m_{2,1}^{13,23}}{m_1 + m_2}$$

Overlap matrix elements:

$$<\phi' | \phi>^{00} = \frac{8\pi^3}{\det B^{1.5}}$$

HYPERFINE STRUCTURE

Hyperfine structure can be described with the following interaction potential:

$$\Delta V^{hfs} = a(\boldsymbol{S_1 S_2}) + b(\boldsymbol{S_1 S_3}) + c(\boldsymbol{S_2 S_3}),$$

$$a = -\frac{2\pi\alpha^2 e_1 e_2 g_1 g_2}{3m_p^2}\delta(\boldsymbol{r_{12}})$$

$$b = \frac{2\pi\alpha^2 e_1 e_3 g_1 g_3}{3m_p}\delta(\boldsymbol{r_{13}})$$

$$c = \frac{2\pi\alpha^2 e_2 e_3 g_2 g_3}{3m_p}\delta(\boldsymbol{r_{23}})$$

Where indices 1, 2 denote nuclei of hydrogen isotopes, index 3 denotes muon.

MATRIX ELEMENTS FOR HFS

$$\left\langle \delta(\mathbf{r_{12}}) \right\rangle = \sum_{i,j=1}^{K} c_i c_j \frac{(2\pi)^{3/2}}{(B_{22})^{3/2}}$$

$$\left\langle \delta(\mathbf{r_{13}}) \right\rangle = \sum_{i,j=1}^{K} c_i c_j \frac{(2\pi)^{3/2}}{(B_{11} - 2B_{12}\frac{m_2}{m_{12}} + B_{22}\left(\frac{m_2}{m_{12}}\right)^2)^{3/2}}$$

$$\left\langle \delta(\mathbf{r_{23}}) \right\rangle = \sum_{i,j=1}^{K} c_i c_j \frac{(2\pi)^{3/2}}{(B_{11} + 2B_{12}\frac{m_1}{m_{12}} + B_{22}\left(\frac{m_1}{m_{12}}\right)^2)^{3/2}}$$

$$m_{12} = m_1 + m_2$$

$$B_{11} = A_{11}^i + A_{11}^j$$

$$B_{12} = A_{12}^i + A_{12}^j$$

$$B_{22} = A_{22}^i + A_{22}^j$$

AVERAGING OVER SPIN FUNCTIONS

Averaging over spin functions can be performed using the following relations:

$$< S_{12'}, S \,|\, (\mathbf{S_1}\mathbf{S_2}) \,|\, S_{12}, S >= \overline{(S_1 S_2)}_{S_{12}} \delta_{S_{12} S_{12'}},$$

$$< S_{12'}, S \,|\, (\mathbf{S_1}\mathbf{S_3}) \,|\, S_{12}, S >= \sqrt{(2S_{12'}+1)(2S_{12}+1)(2S_1+1)(S_1+1)S_1}\sqrt{(2S_3+1)(S_3+1)S_3} \times$$

$$\times (-1)^{S_{12}^{max}+S_{12}^{min}+S+S_1+S_2+S_3+1} \begin{Bmatrix} S_{12} & S_3 & S \\ S_3 & S_{12'} & 1 \end{Bmatrix} \begin{Bmatrix} S_1 & S_{12'} & S_2 \\ S_{12} & S_1; & 1 \end{Bmatrix},$$

$$< S_{12'}, S \,|\, (\mathbf{S_2}\mathbf{S_3}) \,|\, S_{12}, S >= \sqrt{(2S_{12'}+1)(2S_{12}+1)(2S_2+1)(S_2+1)S_2}\sqrt{(2S_3+1)(S_3+1)S_3} \times$$

$$\times (-1)^{2S_{12}^{max}+S+S_1+S_2+S_3+1} \begin{Bmatrix} S_{12} & S_3 & S \\ S_3 & S_{12'} & 1 \end{Bmatrix} \begin{Bmatrix} S_2 & S_{12'} & S_1 \\ S_{12} & S_2 & 1 \end{Bmatrix}.$$

ENERGY MATRIX

After averaging over spin functions energy matrix takes form:

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

All particles have spins 1/2

After diagonalization eigenvalues can be obtained:

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

$$\lambda_3 = \frac{1}{4}(a+b+c)$$

ENERGY MATRIX

After averaging over spin functions energy matrix takes form:

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

Particles have spins 1, 1/2, 1/2

After diagonalization eigenvalues can be obtained:

$$\lambda_1 = -a-b+\frac{1}{4}c$$

$$\lambda_2 = \frac{1}{4}(2a+2b+c)$$

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

ADDITIONAL CORRECTIONS, VACUUM POLARIZATION

To improve the accuracy of our calculations we take into account vacuum polarization corrections:

$$\Delta V_{VP}^{hfs} = a_{VP}(\boldsymbol{S_a S_b}) + b_{VP}(\boldsymbol{S_a S_\mu}) + c_{VP}(\boldsymbol{S_b S_\mu}),$$

$$a_{VP} = -\frac{2\alpha^2 e_a e_b g_a g_b}{3 Z_a Z_b m_p^2}\frac{\alpha}{3\pi}\int_1^\infty \rho(\xi)d\xi\left[\pi\delta(\boldsymbol{r_{ab}}) - \frac{\gamma^2\xi^2}{r_{ab}}e^{-2\gamma\xi r_{ab}}\right],$$

$$b_{VP} = \frac{2\alpha^2 e_a e_\mu g_a g_\mu}{3 Z_a m_p m_\mu}\frac{\alpha}{3\pi}\int_1^\infty \rho(\xi)d\xi\left[\pi\delta(\boldsymbol{r_{a\mu}}) - \frac{\gamma^2\xi^2}{r_{a\mu}}e^{-2\gamma\xi r_{a\mu}}\right],$$

$$c_{VP} = \frac{2\alpha^2 e_b e_\mu g_b g_\mu}{3 Z_b m_p m_\mu}\frac{\alpha}{3\pi}\int_1^\infty \rho(\xi)d\xi\left[\pi\delta(\boldsymbol{r_{b\mu}}) - \frac{\gamma^2\xi^2}{r_{b\mu}}e^{-2\gamma\xi r_{b\mu}}\right],$$

Where indices a, b correspond to nuclei of hydrogen isotopes, μ corresponds to muon.

ADDITIONAL CORRECTIONS, NUCLEAR STRUCTURE

Nuclear structure corrections of the leading order take the form:

$$\Delta V^{hfs}_{str,2\gamma} = a_{str}(\boldsymbol{S_a S_b}) + b_{str}(\boldsymbol{S_a S_\mu}) + c_{str}(\boldsymbol{S_b S_\mu}),$$

$$a_{str} = \frac{2\alpha^2 (e_a e_b)^2 g_a g_b}{3 Z_a Z_b m_p^2} \delta(\boldsymbol{r_{ab}}) \frac{8\alpha m_a}{\pi} \int_0^\infty \frac{dk}{k^2} \times$$

$$\times \left[\frac{4 G_E^a G_M^a G_E^b G_M^b + 3 (G_E^a)^2 (G_E^b)^2 - 3 G_E^a G_M^a (G_E^b)^2 - 3 G_E^b G_M^b (G_E^a)^2 - 3}{G_M^a(0) G_M^b(0)} - \right.$$

$$\left. -4 + \frac{3}{G_M^a(0)} + \frac{3}{G_M^b(0)} \right].$$

$$b_{str} = \frac{2\alpha^2 (e_a e_\mu)^2 g_a g_\mu}{3 Z_a m_p m_\mu} \delta(\boldsymbol{r_{a\mu}}) \frac{8\alpha m_\mu}{\pi} \int_0^\infty \frac{dk}{k^2} \left[\frac{G_E^a(k^2) G_M^a(k^2)}{G_M^a(0)} - 1 \right],$$

$$c_{str} = \frac{2\alpha^2 (e_b e_\mu)^2 g_b g_\mu}{3 Z_b m_p m_\mu} \delta(\boldsymbol{r_{b\mu}}) \frac{8\alpha m_\mu}{\pi} \int_0^\infty \frac{dk}{k^2} \left[\frac{G_E^b(k^2) G_M^b(k^2)}{G_M^b(0)} - 1 \right],$$

THE PROGRAM

- For the numerical calculation of energy levels of three-particle Coulomb bound states the code in MATLAB is written. The program uses stochastic variational approach with random optimization procedure for nonlinear variational parameters;

- 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;

- We are now working on calculation of L=1 hyperfine structure.

K. Varga, Y. Suzuki// Computer Physics Communications **106** (1997) 157-168

NUMERICAL RESULTS

For ground state and hyperfine structure of tdμ, dpμ and tpμ the following numerical results are obtained:

Contribution	$pd\mu$	$tp\mu$	$td\mu$
Total energy μ a.u.	-0.51271179025 (-0.51271179248)	-0.51988008423 (-0.51988008570)	-0.53859497060 (-0.53859497171)
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)
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)
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)
λ_4, MHz	1.2514×10^7 (1.2519×10^7)	—	1.8911×10^7 (1.8920×10^7)

A. M. Frolov // Eur. Phys. J. D. — 2012. — Vol. 66. — P. 212—223.

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THANK YOU FOR YOUR ATTENTION

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