САМАРСКИЙ УНИВЕРСИТЕТ
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Hyperfine structure of excited states of hydrogen mesomolecules

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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 excited states of three-particle tdμ, dpμ and tpμ 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 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:

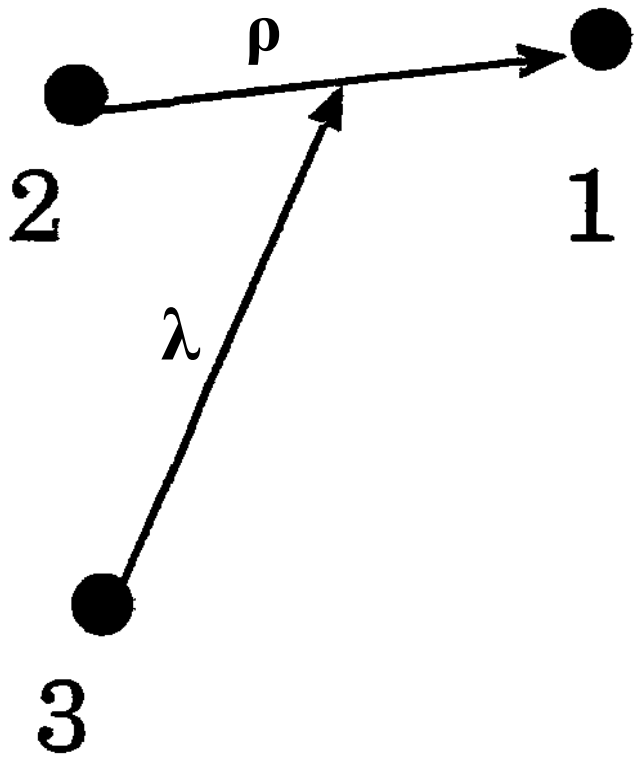
$$\overset{1\ 2\ 3}{t\,d\,\mu}, \quad \overset{1\ 2\ 3}{d\ p\,\mu} \ \text{and} \ \overset{1\ 2\ 3}{p\,t\,\mu}.$$

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:

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

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

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

EXCITED STATE L=1

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

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

Matrix elements of kinetic energy:

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

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

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

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

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

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

$$I_\rho^{(01|10)}=-B_{12}[-2A_{12}B_{12}(4A_{11}+B_{11})+5A_{11}B_{12}^2+5A_{12}^2B_{11}]-B_{22}(A_{11}-B_{11})(5A_{11}B_{12}-2A_{12}B_{11}),$$

$$I_\lambda^{(01|10)}=5A_{12}^2B_{12}B_{22}-A_{22}(2A_{12}B_{11}B_{22}+8A_{12}B_{12}^2+3B_{11}B_{12}B_{22}-3B_{12}^3)+5A_{22}^2B_{11}B_{12}.$$

Overlap matrix elements:

$$<\phi'|\phi>^{01}=\frac{6\pi^2B_{11}}{(\det B)^{5/2}},\ <\phi'|\phi>^{11}=\frac{12\pi^2}{(\det B)^{5/2}},\ <\phi'|\phi>^{(01|10)}=-\frac{6\pi^2B_{12}}{(\det B)^{5/2}}.$$

EXCITED STATE L=1

Matrix elements of potential energy:

$$<\phi'|\hat{V}|\phi>^{10,01,11,(01|10)} = e_1e_2I_{12}^{10,01,11,(01|10)} + e_1e_3I_{13}^{10,01,11,(01|10)} + e_2e_3I_{23}^{10,01,11,(01|10)},$$

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

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

$$+\frac{(3B_{22}F_1^{13,23} - (F_2^{13,23})^2)}{(F_1^{13,23})^{3/2}}\frac{(m_{2,1}^{13,23})^2}{m_{12}^2} \pm \frac{4F_2^{13,23}}{\sqrt{F_1^{13,23}}}\frac{m_{2,1}^{13,23}}{m_{12}}\Big\},$$

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

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

$$F_1^{13,23} = B_{11} + B_{22}\left(\frac{m_{2,1}^{13,23}}{m_1+m_2}\right)^2 \mp 2B_{12}\frac{m_{2,1}^{13,23}}{m_1+m_2},\ F_2^{13,23} = B_{12} \mp 2B_{22}\frac{m_{2,1}^{13,23}}{m_1+m_2}.$$

HYPERFINE STRUCTURE

Hyperfine structure of L=1 energy level has the following 5 contributions:

1) $-\frac{2\pi\alpha^2}{3\,m_i m_j} z_i z_j g_i g_j \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j\right)\delta^3\left(\boldsymbol{r}_{ij}\right)$

2) $-\frac{z_i z_j \alpha^2}{2m_i^2 r_{ij}^3}\left[\frac{1}{S_i} - 1 + \frac{m_i}{S_i m_j} + \frac{\varkappa_i}{S_i}\left(1 + \frac{m_i}{m_j}\right)\right]\left(\boldsymbol{L}_{ij} \cdot \boldsymbol{S}_i\right).$

3) $-\frac{z_i z_j \alpha^2(1+\varkappa_j)}{2S_j m_i m_j r_{ij}^3}\left[1 + \frac{(1+\varkappa_j - S_j)m_i}{m_j(1+\varkappa_j)}\right]\left(\boldsymbol{L}_{ij} \cdot \boldsymbol{S}_j\right)$

4) $\frac{z_i z_j \alpha^2(1+\varkappa_i)(1+\varkappa_j)}{2S_i S_j m_i m_j r_{ij}^3}\left[\left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j\right) - 3\left(\boldsymbol{S}_i \cdot \boldsymbol{n}_{ij}\right)\left(\boldsymbol{S}_j \cdot \boldsymbol{n}_{ij}\right)\right]$

5) $z_i z_j T^2(j) \cdot T^2(i)$

For P – states we have basis functions $(\boldsymbol{\varepsilon} \cdot \boldsymbol{\rho})$ and $(\boldsymbol{\varepsilon} \cdot \boldsymbol{\lambda})$, 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

$$S_1 + S_2 = S_{12};$$

$$S_{12} + S_3 = S;$$

$$S + L = F.$$

MATRIX ELEMENTS FOR HFS, CONTRIBUTION 1)

$$\langle S'LF|(\boldsymbol{S}_i\cdot\boldsymbol{S}_j)\delta^3(\boldsymbol{r}_{ij})|SLF\rangle=\sum_{S_z'S_zL_z} C(S'S_z'L\;L_zF\;F_z)C(S\;S_zL\;L_zF\;F_z)\times$$

$$\langle LL_Z|\delta^3(\boldsymbol{r}_{ij})|LL_Z\rangle\langle S'S_z'|(\boldsymbol{S}_i\cdot\boldsymbol{S}_j)|SS_z\rangle=\delta_{SS'}\langle L|\delta^3(\boldsymbol{r}_{ij})|L\rangle\langle S|(\boldsymbol{S}_i\cdot\boldsymbol{S}_j)|S\rangle.$$

All possible integrals of $\delta^3(\mathbf{r}_{ij})$:

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

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

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

b) $\boldsymbol{r}_{13}=\boldsymbol{\lambda}+\frac{m_2}{m_1+m_2}\boldsymbol{\rho},\boldsymbol{\lambda}+\frac{m_2}{m_1+m_2}\boldsymbol{\rho}=\boldsymbol{k}_{13},\boldsymbol{\lambda}_{13}=\boldsymbol{k}_{13}-\frac{m_2}{m_1+m_2}\boldsymbol{\rho}.$

$$\langle L_\rho|\delta^3(\boldsymbol{k}_{13})|L_\rho\rangle=\iint d\boldsymbol{\rho}\;d\boldsymbol{k}\,\delta^3(\boldsymbol{k}_{13})e^{-\frac{1}{2}[F_1^{13}\rho^2+B_{22}k^2+2F_2^{13}(\boldsymbol{\rho}\cdot\mathbf{k})]}(\boldsymbol{\varepsilon}\cdot\boldsymbol{\rho})(\boldsymbol{\varepsilon}\cdot\boldsymbol{\rho})$$

$$=\int d\rho\,\rho^2\rho^2e^{-\frac{1}{2}[F_1^{13}\rho^2]}=\frac{3\sqrt{\pi}}{\sqrt{2}(F_1^{13})^{\frac{5}{2}}};$$

MATRIX ELEMENTS FOR HFS, CONTRIBUTION 1)

$$\langle L_\rho|\delta^3(\boldsymbol{k}_{13})|L_\lambda\rangle = \langle L_\lambda|\delta^3(\boldsymbol{k}_{13})|L_\rho\rangle = \iint d\boldsymbol{\rho}\ d\boldsymbol{k}\,\delta^3(\boldsymbol{k}_{13})e^{-\frac{1}{2}\left[F_1^{13}\rho^2+B_{22}k^2+2F_2^{13}(\boldsymbol{\rho}\cdot\boldsymbol{k})\right]}(\boldsymbol{\varepsilon}\cdot\boldsymbol{\rho})(\boldsymbol{\varepsilon}\cdot\boldsymbol{k}) - \frac{m_2}{m_1+m_2}\iint d\boldsymbol{\rho}\ d\boldsymbol{k}\,\delta^3(\boldsymbol{k}_{13})e^{-\frac{1}{2}\left[F_1^{13}\rho^2+B_{22}k^2+2F_2^{13}(\boldsymbol{\rho}\cdot\boldsymbol{k})\right]}(\boldsymbol{\varepsilon}\cdot\boldsymbol{\rho})(\boldsymbol{\varepsilon}\cdot\boldsymbol{\rho}) =$$

$$-\frac{m_2}{m_1+m_2}\langle L_\rho|\delta^3(\boldsymbol{k}_{13})|L_\rho\rangle;\ -\langle L_\lambda|\delta^3(\boldsymbol{k}_{13})|L_\lambda\rangle = \left(\frac{m_2}{m_1+m_2}\right)^2\langle L_\rho|\delta^3(\boldsymbol{k}_{13})|L_\rho\rangle.$$

c) $\boldsymbol{r}_{23} = \boldsymbol{\lambda} - \frac{m_1}{m_1+m_2}\boldsymbol{\rho}.$

$$\langle L_\rho|\delta^3(\boldsymbol{k}_{23})|L_\rho\rangle = \iint d\boldsymbol{\rho}\ d\boldsymbol{k}\,\delta^3(\boldsymbol{k}_{23})e^{-\frac{1}{2}\left[F_1^{23}\rho^2+B_{22}k^2+2F_2^{23}(\boldsymbol{\rho}\cdot\boldsymbol{k})\right]}(\boldsymbol{\varepsilon}\cdot\boldsymbol{\rho})(\boldsymbol{\varepsilon}\cdot\boldsymbol{\rho})$$

$$= \int d\rho\,\rho^2\rho^2 e^{-\frac{1}{2}\left[F_1^{23}\rho^2\right]} = \frac{3\sqrt{\pi}}{\sqrt{2}(F_1^{23})^{\frac{5}{2}}};$$

MATRIX ELEMENTS FOR HFS, CONTRIBUTION 1)

$$\langle L_\rho|\delta^3(\boldsymbol{k}_{13})|L_\lambda\rangle = \langle L_\lambda|\delta^3(\boldsymbol{k}_{13})|L_\rho\rangle = -\frac{m_2}{m_1+m_2}\langle L_\rho|\delta^3(\boldsymbol{k}_{13})|L_\rho\rangle;\ -\langle L_\lambda|\delta^3(\boldsymbol{k}_{13})|L_\lambda\rangle =$$

$$\left(\frac{m_2}{m_1+m_2}\right)^2\langle L_\rho|\delta^3(\boldsymbol{k}_{13})|L_\rho\rangle.$$

c) $\boldsymbol{r}_{23} = \boldsymbol{\lambda} - \frac{m_1}{m_1+m_2}\boldsymbol{\rho}.$

$$\langle L_\rho|\delta^3(\boldsymbol{k}_{23})|L_\rho\rangle = \frac{3\sqrt{\pi}}{\sqrt{2}(F_1^{23})^{\frac{5}{2}}};$$

$$\langle L_\rho|\delta^3(\boldsymbol{k}_{23})|L_\lambda\rangle = \langle L_\lambda|\delta^3(\boldsymbol{k}_{23})|L_\rho\rangle = \frac{m_1}{m_1+m_2}\langle L_\rho|\delta^3(\boldsymbol{k}_{23})|L_\rho\rangle;$$

$$\langle L_\lambda|\delta^3(\boldsymbol{k}_{23})|L_\lambda\rangle = \left(\frac{m_1}{m_1+m_2}\right)^2\langle L_\rho|\delta^3(\boldsymbol{k}_{23})|L_\rho\rangle.$$

MATRIX ELEMENTS FOR HFS, CONTRIBUTION 2),3),4)

$$\langle S'LF|(\boldsymbol{L}_{ij}\cdot\boldsymbol{S}_{i,j})|SLF\rangle = (-1)^{L+S_{max}+F}\begin{Bmatrix} S' & L & F \\ L & S & 1 \end{Bmatrix}\langle L\,||L_{ij}||\,L\rangle\langle S'\,||S_{ij}||\,S\rangle.$$

$$\frac{1}{r_{ij}^3}\left[(\boldsymbol{S}_i\cdot\boldsymbol{S}_j)-3(\boldsymbol{S}_i\cdot\boldsymbol{n}_{ij})(\boldsymbol{S}_j\cdot\boldsymbol{n}_{ij})\right]$$

$$M_{ij} = -\frac{3}{r_{ij}}T^2(S_iS_j)\cdot T^2(n_{ij}),$$

where $T_0^2(S_iS_j) = \frac{1}{\sqrt{6}}\left(3S_i^zS_j^z-(\boldsymbol{S}_i\cdot\boldsymbol{S}_j)\right)$; $T_0^2(n_{ij}) = \frac{1}{\sqrt{6}}(3\,(n_{ij}^z)^2-1)$.

$$\langle LS'F|M_{ij}|LSF\rangle = (-1)^{L+S_{max}+F}\begin{Bmatrix} S' & L & F \\ L & S & 2 \end{Bmatrix}\langle L\,||T^2(n_{ij})\,||\,L\rangle\cdot\langle S'\,||T^2(S_iS_j)\,||\,S\rangle$$

MATRIX ELEMENTS FOR HFS, CONTRIBUTION 5)

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

if i or j – nuclei

$$T_q^2(i) = \int \sqrt{\frac{4\pi}{5}} r'^2 Y_q^2(\theta', \varphi') \rho(\boldsymbol{r}') d^3 r',$$

if i or j – muon

$$T_q^2(i) = \sqrt{\frac{4\pi}{5}} \frac{1}{r^3} Y_q^2(\theta, \varphi).$$

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

$$\begin{Bmatrix} S' & L & F \\ L & S & 2 \end{Bmatrix} \langle L||T^2(3)||L\rangle \langle S'||T^2(1,2)||S\rangle$$

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;

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

NUMERICAL RESULTS

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

0.0000606677	0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.0000606575	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.0000543327	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.0000543302	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	-0.000031384	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	-0.0000313817	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	-0.0000261379	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	-0.0000261372	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.	-0.0000229046	0.
0.	0.	0.	0.	0.	0.	0.	0.	0.	-0.0000229036

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

-0.523191450430718

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THANK YOU FOR YOUR ATTENTION

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