

## Energy levels in muonic helium

A.V. Eskin<sup>1</sup>, V.I. Korobov<sup>1,2</sup>, A.P. Martynenko<sup>1</sup>, V.V. Sorokin<sup>1</sup>

<sup>1</sup>Samara National Research University, Moskovskoe Shosse 34, Samara, Russia, 443086

<sup>2</sup>Joint Institute of Nuclear Research, BLTP, Dubna, Moscow region, Russia, 141980

**Abstract.** The energy spectrum of bound states and hyperfine structure of muonic helium is calculated on the basis of stochastic variational method. The basis wave functions of the muonic molecule 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. As a result, the numerical values of bound state energies and hyperfine structure for muonic helium are obtained.

### 1. Introduction

The problems of bound states of three-particle systems occupy a special position in quantum mechanics [1-2]. This problem can be solved using different methods such as the perturbation theory [3] or the variational approach [1-2]. Even in the non-relativistic spinless approximation, they are difficult to study and, as a rule, do not allow an analytical solution characteristic of the two-body problem. The study of the energy spectra of mesomolecules is of interest in connection with the phenomenon of muon catalysis of nuclear fusion reactions. The calculation of various energy levels of mesomolecules allows to predict the rate of reactions of their formation [4]. In our work, we use a stochastic variational method to calculate the energy of a three-particle bound state with high accuracy [1-2]. The wave function of the muon molecule in this approach is Gaussian. This choice of basis allows analytically calculating the matrix elements of the Hamiltonian. For the direct numerical calculation of energy levels based on the Schrödinger equation, a computer code was written in the MATLAB system. The program allows not only to find the values of the energy of the bound state, but also to perform the refinement cycles, which increase the accuracy of the previously calculated energies. As a result, the numerical values of the hyperfine structure of mesomolecules were obtained.

### 2. Calculation of matrix element operators in the case of the ground state

In the framework of the variational method, the trial function for a system of particles can be written in the following form:

$$\Psi = \sum_{i=1}^K c_i \psi_{SM_S}(x, A_i). \quad (1)$$

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

$$HC = E_K BC, \quad H_{ij} = \langle \psi_{SM_S}(x_i, A_i) | H | \psi_{SM_S}(x_j, A_j) \rangle, \quad B_{ij} = \langle \psi_{SM_S}(x_i, A_i) | \psi_{SM_S}(x_j, A_j) \rangle. \quad (2)$$

The trial function  $\psi_{SM_S}(x_i, A_i)$  of the muonic molecule in this approach has the Gaussian form. The Gaussian-type basis function with non-zero angular momentum for nonidentical particles can be written as follows:

$$\varphi_{LS}(\mathbf{x}, A) = e^{-\frac{1}{2}\tilde{\mathbf{x}}A\mathbf{x}}\theta_L(\mathbf{x}), \quad (3)$$

where  $\mathbf{x} = (x_1, \dots, x_{N-1})$  – are Jacobi coordinates,  $A$  is a  $(N-1) \times (N-1)$  positive-defined matrix of variational parameters,  $\tilde{\mathbf{x}}A\mathbf{x} = \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} A_{ij}x_i \cdot x_j$

$$\theta_L(\mathbf{x}) = \left[ \left[ \left[ Y_{l_1}(x_1)Y_{l_2}(x_2) \right]_{L_{12}} Y_{l_3}(x_3) \right]_{L_{123}} \dots \right]_{LM}, \quad (4)$$

where  $Y_{lm}(\mathbf{x}) = r^l Y_{lm}(\mathbf{x})$ . In the case of three nonidentical particles the wave function for ground state has a form:

$$\varphi_{00}(\boldsymbol{\rho}, \boldsymbol{\lambda}, A) = e^{-\frac{1}{2}[A_{11}\boldsymbol{\rho}^2 + A_{22}\boldsymbol{\lambda}^2 + 2A_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})]}, \quad (5)$$

where  $\boldsymbol{\rho}$  and  $\boldsymbol{\lambda}$  are the Jacobi coordinates of three particles which are related with the particle radius vectors:

$$\boldsymbol{\rho} = \mathbf{r}_1 - \mathbf{r}_2, \quad \boldsymbol{\lambda} = \frac{\mathbf{r}_1 m_1 + \mathbf{r}_2 m_2}{m_1 + m_2} - \mathbf{r}_3. \quad (6)$$

The matrix element for the normalization condition has the form:

$$\langle \varphi' | \varphi \rangle = \iint d\boldsymbol{\rho} d\boldsymbol{\lambda} e^{-\frac{1}{2}[B_{11}\boldsymbol{\rho}^2 + B_{22}\boldsymbol{\lambda}^2 + 2e^{-\frac{1}{2}[A_{11}\boldsymbol{\rho}^2 + A_{22}\boldsymbol{\lambda}^2 + 2A_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})]}]_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})]} = \frac{8\pi^3}{(\det B)^{3/2}}, \quad (7)$$

where the matrix  $B = A + A'$ .

Similarly calculation can be made for the matrix elements of the kinetic energy:

$$\begin{aligned} \langle \varphi' | \hat{T} | \varphi \rangle &= -\frac{24\pi^3}{(\det B)^{5/2}} \left[ \frac{\hbar^2}{2\mu_1} I_\rho + \frac{\hbar^2}{2\mu_2} I_\lambda \right], \quad (8) \\ I_\rho &= A_{12}^2 B_{11} - 2A_{11}A_{12}B_{12} + A_{11}(B_{12}^2 + (A_{11} - B_{11})B_{22}), \\ I_\lambda &= A_{12}^2 B_{22} - 2A_{22}A_{12}B_{12} + A_{22}(B_{12}^2 + (A_{22} - B_{22})B_{11}), \\ \mu_1 &= \frac{m_1 m_2}{m_1 + m_2}, \quad \mu_2 = \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3}. \end{aligned}$$

In the case of potential energy the matrix elements have the following form:

$$\begin{aligned} \langle \varphi' | \hat{V} | \varphi \rangle &= e_1 e_2 I_{12} + e_1 e_3 I_{13} + e_2 e_3 I_{23}, \quad (9) \\ I_{12} &= \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{B_{22} \det B}}, \quad I_{13} = \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{F_1^{13}(B_{22}F_1^{13} - (F_1^{13})^2)}}, \quad I_{23} = \frac{8\sqrt{2}\pi^{5/2}}{\sqrt{F_1^{23}(B_{22}F_1^{23} - (F_1^{23})^2)}}, \\ F_1^{13} &= B_{11} + B_{22} \left( \frac{m_2}{m_{12}} \right)^2 - 2B_{12} \frac{m_2}{m_{12}}, \quad F_1^{23} = B_{11} + B_{22} \left( \frac{m_1}{m_{12}} \right)^2 + 2B_{12} \frac{m_1}{m_{12}}, \\ F_2^{23} &= B_{12} - B_{22} \frac{m_2}{m_{12}}, \quad F_2^{13} = B_{12} + B_{22} \frac{m_1}{m_{12}}, \quad m_{12} = m_1 + m_2. \end{aligned}$$

### 3. The hyperfine structure of three-particle bound state

Consider a system of three charged particles of different masses with spins  $S_1, S_2$  и  $S_3$ . The various possible values of the total spin  $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3$  system set the levels of the hyperfine structure of the ground state. For definiteness, we choose all spins equal to 1/2. The arguments and formulas below are also valid for any other values of the particle spins.

In the leading order, the contribution to the hyperfine structure of the spectrum has the following general form:

$$\Delta V^{hfs} = a(\mathbf{S}_1 \mathbf{S}_2) + b(\mathbf{S}_1 \mathbf{S}_3) + c(\mathbf{S}_2 \mathbf{S}_3), \quad (10)$$

$$a = \frac{2\pi\alpha}{3m_1 m_2} \frac{1 + \kappa_1}{S_1} \frac{1 + \kappa_2}{S_2} \langle \delta(\mathbf{r}_{12}) \rangle, \quad (11)$$

$$b = \frac{2\pi\alpha}{3m_1 m_3} \frac{1 + \kappa_1}{S_1} \frac{1 + \kappa_3}{S_3} \langle \delta(\mathbf{r}_{13}) \rangle, \quad (12)$$

$$c = \frac{2\pi\alpha}{3m_2m_3} \frac{1 + \kappa_2}{S_2} \frac{1 + \kappa_3}{S_3} \langle \delta(\mathbf{r}_{23}) \rangle, \quad (13)$$

where  $\langle \delta(\mathbf{r}_{ij}) \rangle$  denotes averaging over basic functions. Let us show how this averaging is performed using the matrix element  $\langle \delta(\mathbf{r}_{12}) \rangle$  as an example.

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2 = \boldsymbol{\rho}, \quad (14)$$

$$\mathbf{r}_{13} = \mathbf{r}_1 - \mathbf{r}_3 = \boldsymbol{\lambda} + \frac{m_2}{m_{12}} \boldsymbol{\rho}, \quad (15)$$

$$\mathbf{r}_{23} = \mathbf{r}_2 - \mathbf{r}_3 = \boldsymbol{\lambda} - \frac{m_1}{m_{12}} \boldsymbol{\rho}. \quad (16)$$

Then for the first matrix element we have:

$$\langle \delta(\mathbf{r}_{12}) \rangle = \langle \delta(\boldsymbol{\rho}) \rangle = \iint d\rho d\lambda \delta(\boldsymbol{\rho}) e^{-\frac{1}{2}(B_{11}\rho^2 + B_{22}\lambda^2 + 2B_{12}(\boldsymbol{\rho}\boldsymbol{\lambda}))} = \frac{(2\pi)^{\frac{3}{2}}}{(B_{22})^{\frac{3}{2}}}, \quad (17)$$

where  $B_{22} = A_{22}^i + A_{22}^j$ . When calculating the specific contribution of the matrix element, it is necessary to divide it by the normalization factor. Similar expressions can be obtained for other matrix elements:

$$\langle \delta(\mathbf{r}_{13}) \rangle = \frac{(2\pi)^{3/2}}{\left( B_{11} - 2B_{12} \frac{m_2}{m_{12}} + B_{22} \left( \frac{m_2}{m_{12}} \right)^2 \right)^{3/2}}, \quad (18)$$

$$\langle \delta(\mathbf{r}_{23}) \rangle = \frac{(2\pi)^{3/2}}{\left( B_{11} + 2B_{12} \frac{m_1}{m_{12}} + B_{22} \left( \frac{m_1}{m_{12}} \right)^2 \right)^{3/2}}. \quad (19)$$

Next, it is necessary to perform averaging of the potential (10) over the spin functions. This can be done using the formalism of irreducible tensor operators and the Eckart-Wigner theorem [5]. The general formulas of matrix elements are as follows:

$$\langle S'_{12}, S | (\mathbf{S}_1 \mathbf{S}_2) | S_{12}, S \rangle = \overline{S_1 S_2 S_{12}} \delta_{S_{12} S'_{12}}, \quad (20)$$

$$\begin{aligned} \langle S'_{12}, S | (\mathbf{S}_1 \mathbf{S}_3) | S_{12}, S \rangle &= \sqrt{(2S'_{12} + 1)(2S_{12} + 1)(2S_2 + 1)(S_2 + 1)S_2} \times \sqrt{(2S_3 + 1)(S_3 + 1)S_3} \\ &\times (-1)^{S_{12}^{max} + S_{12}^{min} + S + S_1 + S_2 + S_3 + 1} \times \begin{Bmatrix} S_{12} & S_3 & S \\ S_3 & S'_{12} & 1 \end{Bmatrix} \begin{Bmatrix} S_1 & S'_{12} & S_2 \\ S_{12} & S_1 & 1 \end{Bmatrix}, \end{aligned} \quad (21)$$

$$\begin{aligned} \langle S'_{12}, S | (\mathbf{S}_2 \mathbf{S}_3) | S_{12}, S \rangle &= \sqrt{(2S'_{12} + 1)(2S_{12} + 1)(2S_2 + 1)(S_2 + 1)S_2} \times \sqrt{(2S_3 + 1)(S_3 + 1)S_3} \\ &\times (-1)^{2S_{12}^{max} + S + S_1 + S_2 + S_3 + 1} \times \begin{Bmatrix} S_{12} & S_3 & S \\ S_3 & S'_{12} & 1 \end{Bmatrix} \begin{Bmatrix} S_2 & S'_{12} & S_1 \\ S_{12} & S_2 & 1 \end{Bmatrix}. \end{aligned} \quad (22)$$

In the case of particles with spin 1/2, we obtain the energy matrix. After its diagonalization we obtain the following eigenvalues:

$$\lambda_1 = -\frac{1}{4}(a + b + c) + \frac{1}{2}\sqrt{a^2 + b^2 + c^2 - ab - bc - ac}, \quad (23)$$

$$\lambda_2 = -\frac{1}{4}(a + b + c) - \frac{1}{2}\sqrt{a^2 + b^2 + c^2 - ab - bc - ac}, \quad (24)$$

$$\lambda_3 = \frac{1}{4}(a + b + c). \quad (25)$$

#### 4. Stochastic variational method

There are two options in solving the problem using the stochastic variational method. Create a new basis or increase an existing one:

- 1) Increase dimension of basis.

Assuming that the basis already contains N-1 elements, we will create K new elements and find the energy values for the new basis, which contains the i-th new element and N-1 previously specified elements. The basic element for which the lowest energy is obtained is selected as a new element of the N basis and is stored in it. The dimension of the basis becomes equal to N.

- 2) "Stripping" of this basis, to improve energy.

In this case, the dimension of the basis remains unchanged, and some  $k$ -th elements are replaced with new ones. Further, the problem is solved by analogy with method 1. At the same time, it is checked whether the new elements provide better energy in comparison with the initial state. Such a replacement can be performed for all elements of the basis.

In both cases 1 and 2, one can observe the convergence of the energy value. Thus, at each step  $N$  ( $N = 1 \dots N_{\max}$ ), based on randomly defined nonlinear parameters, several future basis functions are compiled, and their “practicality” is determined by the amount of energy obtained by adding each to the common basis, as a result the most suitable.  $N_{\max}$  will be the finite dimension of the basis.

This method has several unique features: it is completely based on the analytical calculation of most types of particle interaction, which implies high accuracy and speed of calculations. The calculation method is quite universal and does not require changes depending on whether the system contains a strong, electromagnetic or other type of interaction between particles. And most importantly, the wave function is obtained in a compact analytical form, and can immediately be used to find any physical properties.

Using the MATLAB system we obtained the wave functions of muonic helium atom for the ground and excited states and calculated the matrix elements determining the hyperfine structure of the energy spectrum.

## 5. References

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