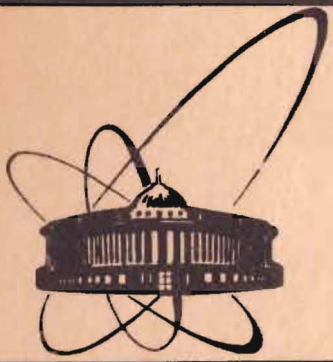

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SCHRÖDINGER EQUATION FOR A THREE-PARTICLE SYSTEM IN SPHEROIDAL COORDINATES

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1. INTRODUCTION

The three-body problem takes a kew position in the theoretical study of muon catalysis [1]. Different methods exist for a numerical solving of the problem. One of them is the adiabatic representation in the three-body problem [2]. In this approach, with the help of continuous analog of Newton method [3] we have (ref. [4,5]) first calculated the energy of a weakly bound rotational-vibrational state ($J = 1$, $v = 1$) of mesic molecule $dt\mu$ with accuracy ~0.001 eV. Moreover, in this case a high rate of resonance formation of mesic molecule $dt\mu$ was first predicted in ref. [6]. However, in view of the importance of the problem, it is necessary to develop other, alternative methods and, in particular, an approach, which does not require any standard separation of variables.

In the first paper [7] we introduced new variables in the three-body problem. Their advantage is that they correctly describe adiabatic character of motion of nuclei in a mesic molecule and provide a suitable representation for the asymptotic of solutions in all three channels of disintegration of a three-particle system (a,b,c) into subsystem (ac)+b, a+(bc) and (ab)+c. In this way, new coordinates establish a clear relation between all three sets of Jacobi variables and prolate spheroidal coordinates used in adiabatic representation [8] as well as with the Fock coordinates on a 3-d sphere [9] and different types of hyperspherical coordinates [10,11].

In this paper the three-body problem in the total-angular-momentum J representation [12] is formulated as a 3-d spectral problem in new variables [7] parametrized in prolate spheroidal coordinates. We have determined the boundary conditions on solutions of the discrete spectrum and have derived the corresponding Rayleigh-Ritz variational functional. Such an approach does not require the separation of variables and essentially enlarges the class of solvable three-body problems of quantum mechanics. In this case we are able to apply some variational-difference methods [13,14] for solving the 3-d spectral problem. These methods in a number of 2-d spectral problems of quantum mechanics [15] nuclear physics [16] and classical electrodynamics [17] have provided a higher accuracy of calculations and shortened computer time as compared with other approach.

2. COORDINATE SYSTEM

Let us consider a system of three particles **a**, **b**, and **c** with charges and masses (eZ_a, M_a), (eZ_b, M_b), and $(-e, M_c)$, respectively. We assume particle **c** to be a negative muon; particles **a** and **b**, nuclei of hydrogen or helium isotopes, and $Z_a M_a \geq Z_b M_b$. Such a system of three particles in a bound state is called the mesic molecule.

In the c.m.s. of the mesic molecule we introduce the Jacobi variables: radius-vector $\vec{R} = \{R\Theta\Phi\}$ connecting nuclei **a** and **b** and radius-vector $\vec{r}_{c0} = \{x_{c0} y_{c0} z_{c0}\}$ connecting the c.m. of nuclei (c.m.n.) with muon. In this case the Hamiltonian of the mesic molecule has the form $(\hbar = e = 1)$

$$H = -\frac{1}{2m_0}\Delta_{\vec{r}_{c0}} - \frac{1}{2M_0}\Delta_{\vec{R}} - \frac{Z_a}{|\vec{r}_{c0} + \gamma_a \vec{R}|} - \frac{Z_b}{|\vec{r}_{c0} + \gamma_b \vec{R}|} + \frac{Z_a Z_b}{R} \qquad (1)$$

$$m_0^{-1} = M_c^{-1} + (M_a + M_b)^{-1}, \quad M_0^{-1} = M_a^{-1} + M_b^{-1},$$

$$\gamma_a = M_b/(M_a + M_b), \quad \gamma_b = -M_a/(M_a + M_b), \qquad (2)$$

where m_0 and M_0 are reduced masses of the muon and nuclei, and $\gamma_a R$ and $\gamma_b R$ are distances from nuclei to their c.m.

It is convenient to describe the motion of muon in the body-fixed coordinate system constructed on spherical unit vectors of vector R:

$$\vec{e}_x = \vec{e}_\Theta, \quad \vec{e}_y = \vec{e}_\Phi, \quad \vec{e}_z = \vec{e}_R \qquad (3)$$

since in this case its potential energy does not depend on angles Θ and Φ*. Instead of $\vec{r}_{c0}$ we introduce the radius-vector $\vec{r}_c = \{x_c y_c z_c\}$ [7]:

$$\{\vec{r}_c\}_i = \hat{D}_{ij}(\Theta\Phi)\{\vec{r}_{c0}\}_j (R/2)^{-1} \quad i,j = 1,2,3. \qquad (4)$$

Components of $\vec{r}$ are given in the body fixed coordinate system (3) which is usually used in passing to the prolate spheroidal coordinates [2,12] $\{\xi\eta\phi\}$:

$$\xi = (r_{a0} + r_{b0})/R, \quad \eta = (r_{a0} - r_{b0})/R. \qquad (5)$$

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* The unit vectors $\vec{e}_x$, $\vec{e}_y$, $\vec{e}_z$ depend on angles Θ and Φ and form a right triple. The corresponding rotation matrix $\hat{D}(\Theta\Phi)$ is given in [2,12] and differs from the standard one by a cyclic permutation of rows.

Here ϕ is the angle of rotation about the major axis of the ellipse directed along axis $\vec{e}_R$, r_{a0} and r_{b0} are distances from nuclei to the muon. Note that nuclei **a** and **b** are placed at focal ellipse points $\{\xi = 1, \eta = -1\}$ and $\{\xi = 1, \eta = 1\}$, respectively. Owing to the scale transformation (dividing by R/2) the position of nuclei in both the coordinate systems (4) and (5) is fixed, i.e., is independent of R. This means that the beginning of vector $\vec{r}_c$ can be chosen equally well in the c.m.n. and in the geometrical centre of nuclei (g.c.n.))

$$\vec{r} = \vec{r}_c + \kappa \vec{e}_R, \quad \kappa = \gamma_a + \gamma_b, \qquad (6)$$

where $-\kappa \geq 0$ is the distance between those centres, or in one of the nuclei

$$\vec{r}_a = \vec{r}_c + 2\gamma_a \vec{e}_R, \quad \vec{r}_b = \vec{r}_c + 2\gamma_b \vec{e}_R. \qquad (7)$$

The volume element and operators $\nabla_{\vec{r}_{c0}}$ and $\nabla_{\vec{R}}$ are defined in terms of the coordinates $\{\vec{R}, \vec{r}_c\}$ by the relations

$$d\tau = 1/8\, R^5 dR \sin\Theta d\Theta\, d\Phi\, dr_c,$$

$$\nabla_{\vec{r}_{c0}} = (R/2)^{-1}\nabla_r = (R/2)^{-1}\nabla_r = (R/2)^{-1}\{\vec{e}_\Theta \frac{\partial}{\partial x} + e_\Phi \frac{\partial}{\partial y} + e_R \frac{\partial}{\partial z}\},$$

$$\nabla_{\vec{R}} = \frac{\vec{e}_\Theta}{R}\left(\frac{\partial}{\partial\Theta} - i\mathcal{L}_y\right) + \frac{\vec{e}_\Phi}{R}\left(\frac{1}{\sin\Theta}\frac{\partial}{\partial\Phi} + i\mathcal{L}_x - i\,\mathrm{ctg}\,\Theta\,\mathcal{L}_z\right) + \qquad (8)$$

$$+ e_R\left(\frac{\partial}{\partial R} - \frac{(r_c \cdot \nabla_{r_c})}{R}\right),$$

where

$$\vec{\mathcal{L}} = -i[\vec{r}_c \times \nabla_{\vec{r}_c}] = \vec{e}_\Theta \mathcal{L}_x + \vec{e}_\Phi \mathcal{L}_y + \vec{e}_R \mathcal{L}_z$$

is the muon angular momentum reckoned from c.m.n., projections of $\vec{\mathcal{L}}$ and $\vec{\ell} = -i[\vec{r} \times \nabla_{\vec{r}}]$ onto the axis $\vec{e}_R$ being equal, i.e., $\mathcal{L}_z = \ell_z$. The total angular momentum of mesic molecule is a sum of the angular momentum of relative motion of nuclei $\vec{L} = -i[\vec{R} \times \nabla_{\vec{R}}]$ and $\vec{\mathcal{L}}$

$$\vec{J} = \vec{L} + \vec{\mathcal{L}} = \vec{e}_\Theta\left(\frac{i}{\sin\Theta}\frac{\partial}{\partial\Phi} + \mathrm{ctg}\,\Theta\,\mathcal{L}_z\right) + \vec{e}_\Phi\left(-i\frac{\partial}{\partial\Theta}\right) + \vec{e}_R \mathcal{L}_z, \qquad (9)$$

i.e., $J_z = \mathcal{L}_z$.

The Hamiltonian (2) in coordinates $\{\vec{R}, \vec{r}_c\}$ has the form*

$$H = -\frac{1}{2M_0}\frac{1}{R^2}\frac{\partial}{\partial R}R^2\frac{\partial}{\partial R} + \frac{1}{2M_0}\frac{2}{R^2}(\vec{r}_c\cdot\nabla_{\vec{r}_c})(1+R\frac{\partial}{\partial R}) -$$

$$-\frac{1}{2m_0}(1+\frac{m_0}{4M_0}r_c^2)\frac{4}{R^2}\Delta_{\vec{r}_c} + V - \frac{2\vec{\mathcal{L}}\cdot\vec{J}}{2M_0R^2} + \frac{\vec{J}^2}{2M_0R^2}. \qquad (10)$$

Here

$$\vec{J}^2 = -[\frac{1}{\sin\Theta}\frac{\partial}{\partial\Theta}\sin\Theta\frac{\partial}{\partial\Theta} + (\frac{1}{\sin\Theta}\frac{\partial}{\partial\Theta} - i\,\mathrm{ctg}\Theta\,\mathcal{L}_z)^2] + \mathcal{L}_z^2 \qquad (10a)$$

is the square of the total angular momentum of the mesic molecule,

$$-\frac{2\vec{\mathcal{L}}\cdot\vec{J}}{2M_0R^2} = -\frac{\mathcal{L}_+J_- + \mathcal{L}_-J_+ + 2\mathcal{L}_z^2}{2M_0R^2} \qquad (10b)$$

is the Coriolis-interaction operator,

$$\mathcal{L}_\pm = e_\pm\cdot\mathcal{L} = \mathcal{L}_\pm \pm i\mathcal{L}_\perp, \quad e_\pm = e_\Theta \pm ie_\Phi,$$

$$J_\pm = e_\pm\cdot J = \pm\frac{\partial}{\partial\Theta} + \frac{i}{\sin\Theta}\frac{\partial}{\partial\Phi} + \mathrm{ctg}\Theta\,\mathcal{L}_z \qquad (10c)$$

are spherical components of $\vec{\mathcal{L}}$ and $\vec{J}$, and

$$V = \frac{1}{R}[-\frac{2Z_a}{|\vec{r}_c + 2\gamma_a\vec{e}_R|} - \frac{2Z_b}{|\vec{r}_c + 2\gamma_b\vec{e}_R|} + Z_aZ_b] \qquad (10d)$$

is the potential energy of mesic molecule.

Coordinates (4) of the vector $\vec{r}_c=\{x_c y_c z_c\}$ are connected with spheroidal coordinates (5) of the vector $\vec{r}=\{x\,y\,z\}$ with the origin in g.c.n. (see formula (6)) as follows**

$$x_c = x = \zeta\cos\phi, \quad y_c = y = \zeta\sin\phi, \quad z_c = z - \kappa,$$

$$\zeta = [(\xi^2-1)(1-\eta^2)]^{1/2}, \quad z = \xi\eta, \qquad (11)$$

$$dr_c = dr = (\xi^2-\eta^2)\,d\xi\,d\eta\,d\phi.$$

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* In deriving (10) we used the relation:

$$r_c^2\Delta_{\vec{r}_c} = (\vec{r}_c\cdot\nabla_{\vec{r}_c})^2 + (\vec{r}_c\cdot\nabla_{\vec{r}_c}) + [\vec{r}_c\times\nabla_{\vec{r}_c}]^2$$

** Here $\{\zeta\phi z\}$ are cylindrical coordinates of the vector $\vec{r}$.

Here the usual dependence on the dimensional parameter $R/2$ is absent therefore the structure of Hamiltonian in coordinates $\{\vec{R},\vec{r}_c\}$ and in the spheroidal ones is the same.

The Schrödinger equation for the mesic-molecule wave function $\Psi(\xi\eta R\phi\Theta\Phi)$ in units $e=h=m_0=1$ has the standard form

$$(H-E)\,\Psi(\xi\eta R\phi\Theta\Phi) = 0. \qquad (12)$$

$$H = -\frac{1}{2M}\frac{1}{R^2}\frac{\partial}{\partial R}R^2\frac{\partial}{\partial R} + \frac{1}{M}\frac{1}{R^2}(\vec{r}_c\cdot\nabla_{\vec{r}})(1+R\frac{\partial}{\partial R}) -$$

$$-\frac{2}{R^2}\rho\,\Delta_{\vec{r}} + V + \frac{J^2-2\mathcal{L}_z^2}{2MR^2} - \frac{\mathcal{L}_+J_- + \mathcal{L}_-J_+}{2MR^2}, \qquad (12a)$$

where

$$(\vec{r}_c\cdot\nabla_{\vec{r}}) = \frac{1}{\xi^2-\eta^2}[(\xi-\kappa\eta)(\xi^2-1)\frac{\partial}{\partial\xi} + (\eta-\kappa\xi)(1-\eta^2)\frac{\partial}{\partial\eta}],$$

$$\rho = (1+\frac{1}{4M}r_c^2) = (1+\frac{1}{4M}(\xi^2+\eta^2-1-2\kappa\xi\eta+\kappa^2)),$$

$$\Delta_{\vec{r}} = \Delta_{\xi\eta} + \frac{1}{\zeta^2}\frac{\partial^2}{\partial\phi^2}, \quad \zeta^2 = (\xi^2-1)(1-\eta^2),$$

$$\Delta_{\xi\eta} = \frac{1}{\xi^2-\eta^2}[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}], \quad \mathcal{L}_z = -i\frac{\partial}{\partial\phi},$$

$$\mathcal{L}_\pm = e^{\pm i\phi}[\pm\mathcal{L}_{\xi\eta} + i\frac{z_c}{\zeta}\frac{\partial}{\partial\phi}], \quad z_c = \xi\eta - \kappa, \qquad (12b)$$

$$\mathcal{L}_{\xi\eta} = \frac{\zeta}{\xi^2-\eta^2}[(\eta-\kappa\xi)\frac{\partial}{\partial\xi} - (\xi-\kappa\eta)\frac{\partial}{\partial\eta}],$$

$$V = \frac{1}{R}[-\frac{2Z_a}{\xi+\eta} - \frac{2Z_b}{\xi-\eta} + Z_aZ_b].$$

Here E is the energy of mesic molecule in the c.m.s., $M=M_0/m_0$ is the reduced mass of nuclei, the operators J^2 and $J_\pm$ are defined by (10a), (10c)*. The range of definition of indepen-

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* The operators $J_\pm$ differ from the standard lowering $\tilde{J}_+$ and raising $\tilde{J}_-$ operators. Indeed, latter ones are defined in the coordinate system turned by angle ϕ around our axis $\vec{e}_R$: $\tilde{J}_\pm = \tilde{e}_\pm\cdot J = e^{\mp i\phi}J_\pm$, $\tilde{e}_\pm = e^{\mp i\phi}e_\pm$. Then the operator J^2 is expressed by the known formula $J^2 = \frac{1}{2}(\tilde{J}_+\tilde{J}_- + \tilde{J}_-\tilde{J}_+) + J_z^2$.

dent variables $\{\xi\eta R\phi\Theta\Phi\}$ will be divided into two subranges $\Omega \times \Omega_{\phi\Theta\Phi}$

$$\Omega = \{1 \le \xi < \infty, \quad -1 \le \eta \le 1, \quad 0 \le R < \infty\},$$

$$\Omega_{\phi\Theta\Phi} = \{0 \le \phi \le 2\pi, \quad 0 \le \Theta \le \pi, \quad 0 \le \Phi \le 2\pi\}. \tag{13}$$

The volume element is of the form

$$d\tau = \frac{1}{8} R^5 (\xi^2 - \eta^2) d\xi\, d\eta\, dR\, d\phi \sin\Theta\, d\Theta\, d\Phi. \tag{14}$$

The binding energy $-\epsilon_{JV}$ (eV) of the mesic molecule in the state $|n\rangle$ with respect to the meson motion (usually, the ground state $n = 1$ is of interest) is expressed in terms of the total energy E as follows

$$\epsilon_{Jv} = (E - E_{na})\, m_0 2Ry, \tag{15}$$

where $E_{na} = -(Z_a^2/2n^2)(m_a/m_0)$ is the energy of the muonic atom with reduced mass $m_a : m_a^{-1} = M_a^{-1} + M_b^{-1}$, $Ry = 13.6058$ eV. Since $m_0 \rho^{-1} \xrightarrow[r_a^{-1}R \to \infty]{} m_a$ the units $e = h = m_a = 1$ are sometimes used. In this case ρ should be changed to ρ_a [2]:

$$\rho_a = i + \frac{1}{4M}(\xi^2 + \eta^2 - 2 - 2\kappa(\xi\eta + 1)) \tag{16}$$

and $M = M_0/m_0$ to $M = M_0/m_a$. Then

$$\epsilon_{Jv} = (E - E_{na})\, m_a 2Ry, \tag{17}$$

where $E_{na} = -Z_a^2/(2n^2)$.

3. THE SCHRÖDINGER EQUATION OF A THREE-PARTICLE SYSTEM IN THE REPRESENTATION OF TOTAL ANGULAR MOMENTUM

The Hamiltonian (12a) commutes with three operators: J^2, $J_z = -i\frac{\partial}{\partial\Phi}$ and the operator of total inversion of coordinates P_{tot} ($\xi \to \xi, \eta \to \eta$, $R \to R$, $\phi \to \pi - \phi$, $\Theta \to \pi - \Theta$, $\Phi \to \pi + \Phi$). The eigenfunctions of these operators

$$J^2 D^{J\lambda}_{mm_J} = J(J+1) D^{J\lambda}_{mm_J}, \quad J_z D^{J\lambda}_{mm_J} = m_J D^{J\lambda}_{mm_J}$$

$$P_{tot}\, D^{J\lambda}_{mm_J} = \lambda D^{J\lambda}_{mm_J}, \quad \lambda = \sigma_{yz}(-1)^J, \quad \sigma_{yz} = \pm 1 \tag{18}$$

are symmetrized and normalized Wigner D-functions

$$D^{J\lambda}_{mm_J} = D^{J\lambda}_{mm_J}(\Phi\Theta\phi) = \left[\frac{2J+1}{16\pi^2(1+\delta_{m0})}\right]^{1/2}$$

$$[(-1)^m D^J_{mm_J}(\Phi\Theta 0)\, e^{im\phi} + \sigma_{yz} D^J_{-mm_J}(\Phi\Theta 0)\, e^{-im\phi}]. \tag{18a}$$

The quantum number m is an eigenvalue of the operator of projection J onto the z-axis of the body-fixed coordinate system

$$J_z = \frac{e^{im\phi}}{\sqrt{2\pi}} = m\frac{e^{im\phi}}{\sqrt{2\pi}},$$

$\sigma_{yz} = \pm 1$ is an eigenvalue of the operator P_{yz} of reflection in the (yz) plane: P_{yz} ($\phi \to \pi - \phi$):

$$P_{yz}\, \Phi_m(\phi) = \sigma_{yz}\, \Phi_m(\phi),$$

$$\Phi_m(\phi) = \left[\frac{1}{2\pi(1+\delta_{m0})}\right]^{1/2} [(-1)^m e^{im\phi} + \sigma_{yz} e^{-im\phi}].$$

At the total inversion of coordinates the direction of z-axis becomes opposite.

In the total angular momentum representation the mesic-molecule wave function is specified by three quantum numbers $\{Jm_J\lambda\}$ and can be represented in the form

$$\Psi^{J\lambda}_{m_J} = \Psi^{J\lambda}_{m_J}(\xi\eta R\phi\Theta\Phi) = \sum_{m=0}^{J} D^{J\lambda}_{mm_J}(\Phi\Theta\phi)\, F^{J\lambda}_m(\xi\eta R). \tag{19}$$

The eigenvalues $\lambda = +1$ of operator P_{tot} determine the sign of a rotational state with given J.

In case of identical nuclei ($Z_a = Z_b$, $\kappa = 0$) Hamiltonian (12a) commutes also with the inversion operator of the muon coordinates P_μ ($\xi \to \xi$, $\eta \to -\eta$, $\phi \to \pi + \phi$) and the wave function (19) is characterized by eigenvalues p of this operator

$$P_\mu\, \Psi^{J\lambda}_{m_J p} = p \Psi^{J\lambda}_{m_J p}.$$

The values $p \equiv g = +1$ correspond to even states, and $p \equiv u = -1$ to odd ones.

The operators P_{tot} and P_μ are connected with the inversion operator of nuclei P_n ($\xi \to \xi$, $\eta \to -\eta$, $R \to R$, $\phi \to -\phi$, $\Theta \to \pi - \Theta$, $\Phi \to \pi + \Phi$) by $P_{tot} = P_\mu P_n$ therefore, the eigenvalues p_n of the

operator P_n are also expressed through λ and p:

$$P_n \Psi^{J\lambda}_{m_J p} = p_n \Psi^{J\lambda}_{m_J p} = \lambda p \Psi^{J\lambda}_{m_J p} .$$

The values $p_n \equiv s = +1$ correspond to symmetric states, and $p_n \equiv a = -1$ to antisymmetric ones.

According to the Pauli principle, $p_n = (-1)^I$ where I is the total spin of nuclei. Then there holds the constraint on possible combinations of quantum numbers $\lambda = \sigma_{yz}(-1)^J$ and $p \equiv (g,u) = \pm 1$ at fixed I : $(-1)^{J+I} = \sigma_{yz} p$.

Thus, the parity p of the rotational state $|J m_J \lambda p\rangle$ turns out to be uniquely connected with the parity of the total spin ofnuclei I. A definite (g,u) -parity of the wave function $\Psi^{J\lambda}_{m_J p}$ allows one to narrow its domain of definition (13) with respect to $\eta: \Omega \to \Omega_p = \{1 \le \xi < \infty,\ 0 \le \eta \le 1,\ 0 \le R < \infty\}$.

The substitution of expansion (19) into eq.(12) and averaging over $D^{J\lambda}_{mm_J}$ in $\Omega_{\phi\theta\Phi}$ leads, for a given set $\{Jm_J\lambda\}$ to the system of $J+1^J$ equations for $F^{J\lambda}_m \equiv F^{J\lambda}_m(\xi\eta R)$ in the region Ω:

$$H^{J\lambda}_{m\,m-1} F^{J\lambda}_{m-1} + (H^{J\lambda}_{mm} - E) F^{J\lambda}_m + H^{J\lambda}_{m\,m+1} F^{J\lambda}_{m+1} = 0, \qquad (20)$$

where

$$H^{J\lambda}_{mm} = \gamma^{J\lambda}_{mm} \{ T + V^J_{mm} \} .$$

$$\gamma^{J\lambda}_{mm} = \begin{cases} 1, & \text{at } m=0,\ \lambda = +(-1)^J, \text{ or at } m \neq 0 \text{ for any } \lambda , \\ 0, & \text{at } m=0,\ \lambda = -(-1)^J \end{cases}$$

$$T = -\frac{1}{2M}\frac{1}{R^2}\frac{\partial}{\partial R} R^2 \frac{\partial}{\partial R} + \frac{1}{M}\frac{1}{R^2}(\vec{r}_c \cdot \nabla_{\vec{r}})\left(1 + R\frac{\partial}{\partial R}\right) - \frac{2}{R^2}\rho\Delta_{\xi\eta}, \qquad (20a)$$

$$V^J_{mm} = V + \frac{2m^2}{R^2}\frac{\rho}{\zeta^2} + \frac{J(J+1) - 2m^2}{2MR^2} .$$

$$H^{J\lambda}_{m\,m\pm1} = T^{J\lambda}_{m\,m\pm1} + V_{m\,m\pm1} .$$

$$T^{J\lambda}_{m\,m\pm1} = \pm\frac{\gamma^{J\lambda}_{m\,m\pm1}}{2MR^2}\mathfrak{L}_{\xi\eta}, \quad V^{J\lambda}_{m\,m\pm1} = \frac{\gamma^{J\lambda}_{m\,m\pm1}}{2MR^2}(m \pm 1)\frac{z_c}{\zeta} .$$

$$\gamma^{J\lambda}_{m\,m+1} = -(1 + (\sqrt{2}-1)\delta_{m0})[(J+m+1)(J-m)]^{1/2} .$$

$$\gamma^{J\lambda}_{m\,m-1} = -(1 + (\sqrt{2}-1)\delta_{m0})[(J-m+1)(J+m)]^{1/2} , \qquad (20b)$$

$$\gamma^{J\lambda}_{10} = 0 \quad \text{at } \lambda = -(-1)^J .$$

The quantities $M = M_0/m_0$, $(\vec{r}_c \cdot \nabla_{\vec{r}})$, ρ, $\Delta_{\xi\eta}$, V, ζ, $\mathfrak{L}_{\xi\eta}$, z are given by relations (2) and (12b).

The operators T, $T^{J\lambda}_{m\,m\pm1}$ and potentials V^J_{mm}, $V^{J\lambda}_{m\,m\pm1}$ can be written in a more convenient form by introducing the notation:

$$y_1 = \xi \quad y_2 = \eta, \quad y_3 = R, \quad \zeta = [(y_1^2 - 1)(1 - y_2^2)]^{1/2} . \qquad (20c)$$

$$T = -\frac{1}{r}\sum_{i=1}^{3}\sum_{j=1}^{3}\frac{\partial}{\partial y_i} a_{ij}(y)\frac{\partial}{\partial y_j} .$$

$$r = \frac{1}{8} y_3^5 (y_1^2 - y_2^2), \quad a_{ij}(y) = a_{ji}(y), \quad i,j = 1,2,3, \qquad (20d)$$

$$a_{11} = \frac{1}{4} y_3^3 \rho (y_1^2 - 1), \quad a_{22} = \frac{1}{4} y_3^3 \rho (1 - y_2^2), \quad a_{33} = \frac{y_3^5}{16M}(y_1^2 - y_2^2),$$

$$a_{12} = 0, \quad a_{13} = -\frac{y_3^4}{16M}(y_1^2 - 1)(y_1 - \kappa y_2), \quad a_{23} = -\frac{y_3^4}{16M}(1 - y_2^2)(y_2 - \kappa y_1), \qquad (20e)$$

$$T^{J\lambda}_{m\,m\pm1} = \pm\frac{\gamma^{J\lambda}_{m\,m\pm1}}{2r}\left(b_1\frac{\partial}{\partial y_1} + b_2\frac{\partial}{\partial y_2}\right),$$

$$b_1 = \frac{y_3^3}{8M}\zeta(y_2 - \kappa y_1), \quad b_2 = -\frac{y_3^3}{8M}\zeta(y_1 - \kappa y_2),$$

$$V^J_{mm} = V + \frac{2m^2}{y_3^2}\frac{\rho}{\zeta^2} + \frac{J(J+1) - 2m^2}{2My_3^2} .$$

$$V = \frac{Z_a Z_b}{y_3} - \frac{2}{y_3(y_1^2 - y_2^2)}[(Z_a + Z_b) y_1 + (Z_b - Z_a) y_2] . \qquad (20f)$$

$$\rho = 1 + \frac{1}{4M}(y_1^2 + y_2^2 - 1 - 2\kappa y_1 y_2 + \kappa^2), \quad V^{J\lambda}_{m\,m\pm1} = \frac{\gamma^{J\lambda}_{m\,m\pm1}}{2My_3^2}(m \pm 1)\frac{y_1 y_2 - \kappa}{\zeta} .$$

The systen of equations (20) in the region Ω is equivalent to the starting Schrödinger equation (12) in the region $\Omega \times \Omega_{\phi\theta\Phi}$. Note that when no external field is present there is a $2J+1$-tuple degeneration in m_J, the projection J of onto the Z -axis of the space-fixed system.

4. BOUNDARY CONDITIONS FOR WAVE FUNCTIONS OF THE DISCRETE SPECTRUM AND VARIATIONAL FUNCTIONAL

We are interested in bound states of mesic molecules with total moment J = 1 and total parity $\lambda = +(-1)^J = -1$, i.e., we consider the solutions $F \equiv \{F_0, F_1\}$ to the system (20) which are finite

in region Ω (hereafter indices J and λ will be omitted). In this case it is convenient to rewrite the system (20) in the form

$$LF = EF. \tag{21}$$

The operator L is given in the matrix form

$$L = \begin{pmatrix} T & T_{01} \\ T_{01}^* & T \end{pmatrix} + \begin{pmatrix} V_0 & V_1 \\ V_1 & V_2 \end{pmatrix}.$$

$$T_{01} = -\frac{1}{r}\{b_1 \frac{\partial}{\partial y_1} + b_2 \frac{\partial}{\partial y_2}\}, \quad T_{01}^* = \frac{1}{r}\{\frac{\partial}{\partial y_1} b_1 + \frac{\partial}{\partial y_2} b_2\},$$

$$V_0 \equiv V_{00}^1, \quad V_1 \equiv V_{01}^1, \quad V_2 \equiv V_{11}^1.$$

Quantities T , r , b_1, b_2, V_{00}^1, V_{01}^1, V_{11}^1 are defined be relations (20).

Boundary conditions for the functions $\{F_0, F_1\}$ follows from the finiteness of solutions (21) on the boundary $\partial\Omega: \{y_3 = 0\}$, $\{y_1 = 1\}$, $\{y_2 = -1\}$ and $\{y_2 = 1\}$ of region (13). In view of that the coefficients a_{ij} of operator T vanish on $\partial\Omega$, a correct formulation of boundary conditions requires to study the behaviour of functions rV_i, $i = 0,1,2$ (20) near the boundary $\partial\Omega$ [12,13]. Since $\lim_{y_3 \to 0} |rV_i| < \infty, i = 0,1,2$ the requirement for F_0 and F_1 to be finite at $y_3 = 0$ reduces to the boundary conditions

$$\lim_{y_3 \to 0} y_3^5 \frac{\partial F_0}{\partial y_3} = 0, \quad \lim_{y_3 \to 0} y_3^5 \frac{\partial F_1}{\partial y_3} = 0. \tag{22}$$

From relations $\lim_{y_1 \to 1} |rV_0| < \infty$ and $\lim_{y_1 \to 1} |rV_i| = \infty$, $i = 1,2$ we get

$$\lim_{y_1 \to 1} (y_1^2 - 1) \frac{\partial F_0}{\partial y_1} = 0, \quad F_1(1, y_2, y_3) = 0, \tag{23}$$

whereas from $\lim_{y_2 \to \pm 1} |rV_0| < \infty$ and $\lim_{y_2 \to \pm 1} |rV_i| = \infty$, $i = 1,2$ it follows that

$$\lim_{y_2 \to \pm 1} (1 - y_2^2) \frac{\partial F_0}{\partial y_2} = 0, \quad F_1(y_1, \pm 1, y_3) = 0. \tag{24}$$

We set the range of definition D(L) of the operator L as follows:

The functions $u = \{u_0, u_1\} \in D(L)$ provided that:

1. $u_i \in W_2^2(\Omega)$, $i = 0,1$;
2. $Lu \in L_2(\Omega)$;
3. The functions u_0 and u_1 obey the boundary conditions (22)-(24);
4. For any two functions $u = \{u_0, u_1\}$ and $v = \{v_0, v_1\}$ there hold valid the relations

$$\lim_{y_3 \to \infty} a_{i3} W_{y_i}^k = 0, \quad i = 1,2,3; \quad k = 0,1$$

$$\lim_{y_1 \to \infty} a_{11} W_{y_1}^k = 0, \quad \lim_{y_1 \to \infty} a_{13} W_{y_3}^k = 0, \quad k = 0,1, \tag{25}$$

where

$$W_{y_i}^k = u_k \frac{\partial v_k}{\partial y_i} - v_k \frac{\partial u_k}{\partial y_i}, \quad i = 1,2,3, \quad k = 0,1.$$

Here $W_2^2(\Omega)$ is the Hilbert space of the functions whose second-order derivatives belong to the space $L_2(\Omega)$; the latter being the Hilbert space with weight r, i.e., if $u \in L_2(\Omega)$ then $\int_\Omega r(u_0^2 + u_1^2) dy_1 dy_2 dy_3 < \infty$. The scalar product for functions u , $v \in L_2(\Omega)$ is defined by:

$$(u, v) = \int_\Omega r(u_0 v_0 + u_1 v_1) dy_1 dy_2 dy_3.$$

The condition (25) provided a sufficiently rapid decrease of the functions $F \in D(L)$ at infinity. It may be verified that the operator L is self-adjoint, i.e., $L = L^*$ and $D(L) = D(L^*)$. This is the reason to assert that the spectrum of operator L is real.

Now let us present the variational formulation of the problem (21)-(25). Consider a bilinear form $a(u,v) = (Lu, v)$, $u, v \in D(L)$. That the operator L is self-adjoint means that $a(u,v) = a(v,u)$. Then using the conditions (22)-(25) we get

$$a(u,v) = \int_\Omega \{\sum_{k=0}^{1} \sum_{i=1}^{3} \sum_{j=1}^{3} a_{ij} \frac{\partial u_k}{\partial y_i} \frac{\partial v_k}{\partial y_j} -$$

$$- b_1(u_0 \frac{\partial v_1}{\partial y_1} + v_0 \frac{\partial u_1}{\partial y_1}) - b_2(u_0 \frac{\partial v_1}{\partial y_2} + v_0 \frac{\partial u_1}{\partial y_2}) + \tag{26}$$

$$+ r[V_0 u_0 v_0 + V_1(u_0 v_1 + v_0 u_1) + V_2 u_1 v_1]\} dy_1 dy_2 dy_3.$$

The variational functional of the problem (21)-(25) is given by the relation

$$R(v) = a(v,v)/(v,v). \tag{27}$$

Stationary points F of this functional are eigenfunctions of the problem (21)-(25) and then the eigenvalues may be calculated by the formulae $E = R(F)$.

When $J = 0$, the system of eqs.(21) is simplified to (see (20)):

$$(T+V)F_0 = E F_0. \tag{28}$$

The range of definition of the operator in the l.h.s. of (28) may be given by means of the same conditions for D(L) if put $F = \{F_0, 0\}$, $F \in D(L)$. Then the variational functional of problem (28) results from (27) if the potential V_0 is replaced by V defined by relation (20).

5. CANONICAL FORM OF THE SCHRÖDINGER EQUATION

Equations (21) contain cross serivatives. This makes difficult to discretize these equations and to apply effective numerical methods.

Cross derivatives may be eliminated by the introducing of new-variables [7]

$$x_1 = y_1, \quad x_2 = y_2, \quad x_3 = y_3\sqrt{\rho}, \tag{29}$$

where $x_3 \equiv \mathcal{R}$ defines the hyper-radius of a three-particle system: $\mathcal{R}_G = \sqrt{M_0}\,\mathcal{R}$. Partial derivatives are expressed in terms of new coordinates

$$\frac{\partial}{\partial y_1} = \frac{\partial}{\partial x_1} + \frac{x_3}{\rho}\frac{x_1 - \kappa x_2}{4M}\frac{\partial}{\partial x_3}$$

$$\frac{\partial}{\partial y_2} = \frac{\partial}{\partial x_2} + \frac{x_3}{\rho}\frac{x_2 - \kappa x_1}{4M}\frac{\partial}{\partial x_3}, \quad \frac{\partial}{\partial y_3} = \sqrt{\rho}\,\frac{\partial}{\partial x_3}. \tag{30}$$

Upon inserting (30) into (26) and performing some computations we arrive at a new variational functional without cross derivatives

$$\bar{a}(u,v) = \int_{\Omega_H} \{ \sum_{k=0}^{1}\sum_{i=1}^{3} a_i \frac{\partial u_k}{\partial x_i}\frac{\partial v_k}{\partial x_i} -$$

$$-\bar{b}_1\left(u_0\frac{\partial v_1}{\partial x_1} + v_0\frac{\partial u_1}{\partial x_1}\right) - \bar{b}_2\left(u_0\frac{\partial v_1}{\partial x_2} + v_0\frac{\partial u_1}{\partial x_2}\right) +$$

$$+\bar{\tau}\left(\bar{V}_0 u_0 v_0 + \bar{V}_1(u_0 v_1 + v_0 u_1) + \bar{V}_2 u_1 v_1\right)\} dx_1 dx_2 dx_3. \tag{31}$$

Here we have adopted the notation

$$a_1 = \frac{1}{4}\frac{x_3^3}{\rho}(x_1^2 - 1), \quad a_2 = \frac{1}{4}\frac{x_3^3}{\rho}(1 - x_2^2), \quad a_3 = \frac{1}{16M}\frac{x_3^5}{\rho}(x_1^2 - x_2^2),$$

$$\bar{b}_1 = \frac{x_3^3}{8M}\frac{\zeta}{\rho^2}(x_2 - \kappa x_1), \quad \bar{b}_2 = -\frac{x_3^3}{8M}\frac{\zeta}{\rho^2}(x_1 - \kappa x_2),$$

$$\bar{\tau} = \frac{1}{8}\frac{x_3^5}{\rho^3}(x_1^2 - x_2^2), \quad \bar{V}_0 = \tilde{V} + \frac{1}{2M}\frac{\rho}{x_3^2},$$

$$\bar{V}_2 = \tilde{V} + \frac{2\rho^2}{x_3^2\zeta^2}, \quad \bar{V}_1 = -\frac{1}{M}\frac{\rho}{x_3^2}\frac{x_1 x_2 - \kappa}{\zeta},$$

$$\tilde{V} = \frac{\sqrt{\rho}}{x_3}\{Z_a Z_b - \frac{2}{(x_1^2 - x_2^2)}[(Z_a + Z_b)x_1 + (Z_b - Z_a)x_2]\}.$$

Equating the variation of the functional (31) to zero we obtain the system of eqs.(21) in the canonical form

$$\left(-\frac{1}{\tau}\bar{L} + \bar{V}\right)u = E u, \tag{32}$$

where

$$\bar{L} = \begin{pmatrix} \bar{T} & \bar{T}_{01} \\ \bar{T}_{10} & \bar{T} \end{pmatrix}, \quad \bar{V} = \begin{pmatrix} \bar{V}_0 & \bar{V}_1 \\ \bar{V}_1 & \bar{V}_2 \end{pmatrix},$$

$$\bar{T} = \sum_{i=1}^{3}\frac{\partial}{\partial x_i}a_i\frac{\partial}{\partial x_i}, \quad \bar{T}_{01} = \bar{b}_1\frac{\partial}{\partial x_1} + \bar{b}_2\frac{\partial}{\partial x_2}, \quad \bar{T}_{10} = \bar{T}_{01}^{*}.$$

The scalar product is given by

$$(u,v) = \int_{\Omega_H} \bar{\tau}\,(u_0 v_0 + u_1 v_1)\,dx_1 dx_2 dx_3,$$

$$\Omega_H = \{1 \le x_1 \le \infty, \ -1 \le x_2 \le 1, \ 0 \le x_3 < \infty\}.$$

It is not difficult to verify that the wave functions of discrete spectrum (32) satisfy the boundary conditions (22)-(25). Equation (32) in the well-known hyperspherical coordinates is presented in ref[7].

CONCLUSION

Using the variational functional (27) one may construct effective difference scheme for the numerical solution of a three-body problem with the Coulomb interaction. In new coordinates $\{\xi\eta\Re\}$[7] this functional takes a convenient form. So, to minimize it the finite-element method[13,14] seems to be worth-while. The accuracy of calculations in this case may be estimated on the basis of general finite-element theory. Equation (32) can be used for describing collision processes in a three-body system since the asymptotics of its solutions is put in accord with the physical boundary conditions in Jacoby variables[7].

The necessity to solve, with a high accuracy, the three-body problem in the total-momentum representation arises not only in the problem of muon calatylis, but also in describing experiments on the weak μ-capture[20] in the hydrogen, which occurs in the mesic molecule $pp\mu$ in states $J = 0,1$[21,22]. The energy and wave functions of these states may be found by minimizing functional (27) at $\kappa = 0$. Besides, functional (27), for a corresponding change of the potential energy, can be utilized for solving the three-body problem in which interaction between particles possesses only axial symmetry (see, e.g., ref.[16]). Note that Hamiltonian (10) may be useful for introducing of various coordinates in the three-body problem, which have dimensional parameter, e.g., elliptic-cylindrical, toroidal, etc. Moreover one gives possibility to determine easily some asymptotics in the same problem.

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Касчиев М.С., Виницкий С.И. Е4-85-467

Уравнение Шредингера системы трех частиц в представлении полного момента

Уравнение Шредингера системы трех частиц в представлении полного момента J сведено к системе J+1 трехмерных дифференциальных уравнений в вытянутой сфероидальной системе координат. Для соответствующей трехмерной спектральной задачи с неразделяющимися переменными построен вариационный функционал Рэлея-Ритца и получены граничные условия для волновых функций дискретного спектра. Предложенная формулировка ориентирована на применение вариационных и вариационно-разностных методов численного решения задачи трех тел.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Kaschiev M., Vinitsky S.I. E4-85-467

Schrödinger Equation for a Three-Particle System in Spheroidal Coordinates

The Schrödinger equation for a three-particle system in the total-angular-momentum J representation is reduced to a system of J+1 three-dimensional equations in prolate spheroidal coordinates. For the corresponding three-dimensional nonseparate spectral problem the Rayleigh-Ritz variational functional is constructed and boundary conditions are found for the wave functions of discrete spectrum. Final formulation of the problem is adapted for applying variational and variational-difference methods for numerical solving of the three-body problem.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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