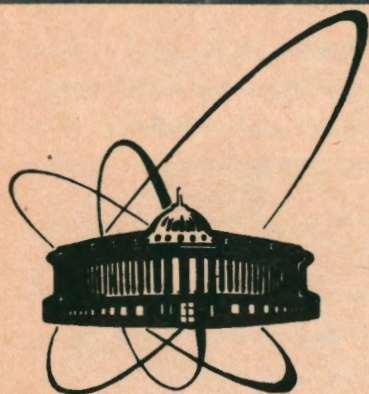


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СООБЩЕНИЯ  
ОБЪЕДИНЕННОГО  
ИНСТИТУТА  
ЯДЕРНЫХ  
ИССЛЕДОВАНИЙ  
ДУБНА

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BOUND STATES OF HYDROGEN MESIC  
MOLECULAR IONS: VARIATIONAL APPROACH

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Связанные состояния мезомолекулярных ионов водорода:  
вариационный подход

Предложен вариационный метод для расчета связанных состояний трехчастичных систем с произвольным орбитальным моментом  $J$  и пространственной четностью  $\lambda$ . Метод применяется для расчета полного набора связанных (32 состояний) мезомолекулярных ионов изотопов водорода с  $J = 0, 1, 2, 3$  и четностью  $\lambda = (-1)^J$  и  $\lambda = -(-1)^J$ .

Работа выполнена в Лаборатории теоретической физики ОИЯИ и Лаборатории вычислительной техники и автоматизации ОИЯИ.

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Bound States of Hydrogen Mesic Molecular Ions:  
Variational Approach

A variational method is proposed for computation of bound states of three-particle systems with an arbitrary total angular momentum  $J$  and spatial parity  $\lambda$ . It is applied to compute the complete set of bound states (32 states) of mesic molecular ions of hydrogen isotopes with  $J = 0, 1, 2, 3$  and parity  $\lambda = (-1)^J$  and  $\lambda = -(-1)^J$ .

The investigation has been performed at the Laboratory of Theoretical Physics, JINR and Laboratory of Computing Techniques and Automation, JINR.

During the last decade, the energy levels of the bound states of mesomolecular ions of hydrogen isotopes were subject of intensive study of the phenomenon of muon catalyzed fusion [1-6]. Characteristics of the bound states with the spatial parity  $\lambda = (-1)^J$  are computed there, and especially ones of weakly bound states of mesic molecular ions  $dd\mu$  and  $dt\mu$  defining mainly the kinetics of physical processes. Last year papers studying mesomolecular states with the so-called anomalous parity  $\lambda = -(-1)^J$  were appeared [7-9]. These states differ essentially from the usual ones in their physical properties. They are assumed to play a role as hindering factors in the process of muonic catalysis. Having captured a muon they withdraw it from a normal catalytic cycle.

However, with the growth of the total angular momentum the amount of energy level calculations provided with different methods decreases significantly and already for the  $F$ -state of mesomolecular ion  $tt\mu$  there is not any variational calculation and the only one was carried out with the use of adiabatic approach [1]. In this paper we present the results of calculation for the energy levels of 32 states of mesomolecular ions of hydrogen isotopes.

It turns out that these states, 22 states of normal parity and 10 states of anomalous parity, represent the whole list of bound states of mesic molecular ions.

The variational approach to be expounded below was used in our previous papers [2,7]. We extended the method to states of an arbitrary spatial parity and a total angular momentum  $J \geq 2$ . The form proposed for the trial functions allow us to take into account

peculiarities of a behaviour of the wave function components connected with the use of rotational and spatial symmetries and to compute effectively matrix elements. As computation shows, the instability doesn't increase dramatically with the number of trial functions and it allows to carry out calculations with more than 2600 basis functions.

## 1. Theory

As it is well known, a hydrogen mesic molecular ion is a system of three particles: a negatively charged muon  $\mu^-$ , and two nuclei  $a$  and  $b$  of hydrogen isotopes ( $a, b = p, d$  or  $t$ ). The nonrelativistic Hamiltonian of the system in the Jacobi coordinates ( $e = \hbar = m_e = 1$ ) is

$$H = -\frac{1}{2\mu_{12}}\Delta_{\mathbf{R}} - \frac{1}{2\mu_3}\Delta_{\mathbf{r}} - \frac{1}{r_a} - \frac{1}{r_b} + \frac{1}{R},$$

$$\mu_{12}^{-1} = m_1^{-1} + m_2^{-1} = M_a^{-1} + M_b^{-1},$$

$$\mu_3^{-1} = m_3^{-1} + (m_1 + m_2)^{-1} = m_\mu^{-1} + (M_a + M_b)^{-1}. \quad (1)$$

Here  $\mathbf{R}$  is the position vector of nucleus  $a$  relative to nucleus  $b$  with the masses  $M_a \geq M_b$ ,  $\mathbf{r}$  is the position vector of the muon with the mass  $m_\mu$  relative to the center of mass of the nuclei. We will connect a moving frame with this system with respect to which the Euler angles will be determined. To do that we will direct the  $z'$  axis along the nuclei of the molecule, and the  $x'$  axis will be placed in the plane of three particles in the direction of the muon.

Since equation (1) is invariant under three dimensional rotations, we may separate the states with a certain quantum number of the total angular momentum  $J$  and its projection  $M$  onto the  $z$  axis. The wave function may be expressed in terms of the Wigner  $D$ -functions,  $D(\alpha, \beta, \gamma)$ , dependent on the Euler angles of the moving frame:

$$\Psi_M^J(\mathbf{R}, \mathbf{r}) = \sum_{m=-J}^J D_{Mm}^J(\alpha, \beta, \gamma) F_m^J(R, r, \theta), \quad (2)$$

where  $\theta$  is the angle between vectors  $\mathbf{R}$  and  $\mathbf{r}$ . The Hamiltonian also commutes with the operator of spatial parity  $P_\lambda : (\mathbf{R}, \mathbf{r}) \rightarrow (-\mathbf{R}, -\mathbf{r})$ , having eigenvalues  $\lambda = 1$  and  $\lambda = -1$ . This operator acts on the Wigner  $D$ -functions as follows:

$$P_\lambda D_{Mm}^J(\alpha, \beta, \gamma) = D_{Mm}^J(\pi + \alpha, \pi - \beta, \pi - \gamma) = (-1)^{J-m} D_{M, -m}^J(\alpha, \beta, \gamma).$$

To determine the wave function of a given spatial parity  $\lambda$ , we introduce the symmetrized Wigner  $D$ -functions

$$D_{Mm}^{J\lambda}(\alpha, \beta, \gamma) = \left[ \frac{2J+1}{16\pi^2(1+\delta_{m0})} \right]^{\frac{1}{2}} \left[ D_{Mm}^J(\alpha, \beta, \gamma) + \lambda(-1)^{J-m} D_{M, -m}^J(\alpha, \beta, \gamma) \right],$$

which are eigenfunctions of the operators  $\mathbf{J}^2$ ,  $J_z$  and  $P_\lambda$ :

$$\mathbf{J}^2 D_{Mm}^{J\lambda} = J(J+1) D_{Mm}^{J\lambda}; \quad J_z D_{Mm}^{J\lambda} = -M D_{Mm}^{J\lambda};$$

$$P_\lambda D_{Mm}^{J\lambda} = \lambda D_{Mm}^{J\lambda}, \quad \lambda = 1, -1;$$

and are normalized so that

$$\int d\alpha \int \sin\beta d\beta \int d\gamma \left[ D_{Mm}^{J\lambda}(\alpha, \beta, \gamma) D_{M'm'}^{J'\lambda'}(\alpha, \beta, \gamma) \right] = \delta_{JJ'} \delta_{MM'} \delta_{mm'}.$$

The wave function in the representation of the total angular momentum and spatial parity has the form

$$\Psi_M^{J\lambda}(\mathbf{R}, \mathbf{r}) = \sum_{m=\mu(\lambda)}^J D_{Mm}^{J\lambda}(\alpha, \beta, \gamma) F_m^{J\lambda}(R, \tau, \theta); \quad (3)$$

$$\mu(\lambda) = \begin{cases} 0, & \text{for } \lambda = (-1)^J; \\ 1, & \text{for } \lambda = -(-1)^J; \end{cases}$$

This expression is a starting point for further construction of a variational trial function. The states of parity  $\lambda = (-1)^J$  and  $\lambda = -(-1)^J$  are called, respectively, the states with normal and anomalous parity.

Another form of the wave function expansion follows from the Schwartz representation [10] based on bipolar harmonics. We will present it because it explicitly describes the behaviour of the wave function of a state in the vicinity of coalescence points of particles with a given spatial parity and a total angular momentum:

$$\Psi_M^{J\lambda}(\mathbf{R}, \mathbf{r}) = \sum_{\substack{l_1+l_2=J \\ |l_1-l_2|\leq J}} Y_{JM}^{l_1 l_2}(\hat{\mathbf{R}}, \hat{\mathbf{r}}) R^{l_1} r^{l_2} G_{l_1 l_2}^{J\lambda}(R, \tau, \theta), \quad (4a)$$

for  $\lambda = (-1)^J$ ;

$$\Psi_M^{J\lambda}(\mathbf{R}, \mathbf{r}) = \sum_{\substack{l_1+l_2=J+1 \\ |l_1-l_2|\leq J}} Y_{JM}^{l_1 l_2}(\hat{\mathbf{R}}, \hat{\mathbf{r}}) R^{l_1} r^{l_2} G_{l_1 l_2}^{J\lambda}(R, \tau, \theta), \quad (4b)$$

for  $\lambda = -(-1)^J$ ;

where

$$Y_{JM}^{l_1 l_2}(\hat{\mathbf{R}}, \hat{\mathbf{r}}) = \sum_{m_1 m_2} Y_{l_1 m_1}(\hat{\mathbf{R}}) Y_{l_2 m_2}(\hat{\mathbf{r}}) (l_1 m_1 l_2 m_2 | JM).$$

and

$$G_{l_1 l_2}^{J\lambda}(R, \tau, \theta) = G_{l_1 l_2}^{J\lambda}(0, \tau, \theta) \left[ 1 + \frac{1}{\mu_{12}(l_1+1)} R + \mathbf{R} \cdot \mathbf{u} + O(R^2) \right].$$

The last expression is the so-called Kato coalescence condition [11,12]. Note that the number of components in the expansion (4a) is equal to  $J$ , whereas in (4b) to  $J-1$ , which coincides with the number of components in the expansion of the state with the corresponding parity in (3).

In the expansion (4b)  $l_1$  and  $l_2$  differ from zero, therefore the asymptotic scattering states of parity  $\lambda = -(-1)^J$ , for  $R \rightarrow \infty$ , consist of an isolated nucleus and an atom with nonzero angular momentum. Thus, the energy of dissociation for the molecule with anomalous parity is equal to the energy of the isolated atom with principal quantum number  $n = 2$ :  $E_a = -R y m_a / 4$ , where  $m_a$  is the reduced mass of the atom with the heavier nucleus.

Applications of the Wigner's  $D$ -functions to three-body calculation were developed by many authors [13]. They differ in positioning of the moving frame of references and, thus, they have different partition of the wave function to the components depending on intrinsic coordinates of the problem. Our choice is convenient to the adiabatic calculations involving two heavy particles and one light particle of an opposite charge.

## 2. The wave function

To obtain an accurate variational solution for the Schrödinger equation with the Hamiltonian (1) it is necessary to take into account the peculiarities of the behaviour of the wave function.

Symmetry allows to reduce the equation onto a subspace of states with certain quantum numbers of the total angular momentum and spatial parity. The wave function of the state as well as separate components of the wave function representation obeys certain

requirements imposed on the behaviour at the vicinity of points of collisions or in the case of axial singularity when a position of a moving frame isn't determined. In particular, a three-particle system is properly described by the wave function (4) with well-behaved components  $G_{l_1 l_2}^{J\lambda}(R, r, \theta)$ . Unfortunately, this expansion leads to significant difficulties in matrix element calculations for high numbers of total angular momentum. We would like to investigate the behaviour of the components of the expansion (3) to provide necessary conditions for constructing of a suitable trial function for this approach.

To determine the asymptotics of the components of (3) when  $R \rightarrow 0$  we make use of the Chang-Fano relation [14] between the bipolar harmonics and Wigner  $D$ -functions:

$$Y_{JM}^{l_1 l_2}(\hat{\mathbf{R}}, \hat{\mathbf{r}}) = \sqrt{2\pi} \sum_{m=\mu(\lambda)} T_{l_1 l_2}^{Jm\lambda} D_{Mm}^{J\lambda}(\alpha, \beta, \gamma) Y_{l_2 m}(\theta, 0), \quad (5)$$

where the coefficients  $T_{l_1 l_2}^{Jm\lambda}$  are expressed through the Clebsch-Gordan coefficients:

$$T_{l_1 l_2}^{Jm\lambda} = \left[ \left( \frac{1 + \lambda(-1)^{l_1 + l_2}}{1 + \delta_{0m}} \right) \frac{2l_1 + 1}{2J + 1} \right]^{\frac{1}{2}} \langle l_1 0 l_2 m | Jm \rangle.$$

The relation (5) allows us to express the components of the wave function expansion (3) in terms of the components of expansion (4):

$$F_m^{J\lambda}(R, r, \theta) = \sqrt{2\pi} \sum_{l_2=m}^J T_{l_1 l_2}^{Jm\lambda} Y_{l_2 m}(\theta, 0) R^{l_1} r^{l_2} G_{l_1 l_2}^{J\lambda}(R, r, \theta), \quad (6)$$

where  $\begin{cases} l_1 = J - l_2, & \text{for } \lambda = (-1)^J, \\ l_1 = J + 1 - l_2, & \text{for } \lambda = -(-1)^J. \end{cases}$

From this representation it is seen that the functions  $F_m^{J\lambda}$  have the asymptotics  $O(1)$  when  $R \rightarrow 0$  for the states of normal parity and  $O(R)$  for the states of anomalous parity. It is to be noted that, when  $R = 0$ , the components  $F_m^{J\lambda}$  with different  $m$  are dependent on each other and may be expressed through one component, for example  $F_J^{J\lambda}$ .

The behaviour of the components in the neighborhood of the nuclei coalescence point restricts to the choose of intrinsic variables describing the trial function. The functions  $G_{l_1 l_2}^{J\lambda}(R, r, \theta)$  of the expansion (4) do not depend on the angle  $\theta$  at  $R = 0$  [12]. Hence, the components of (3) have the angular dependence, when  $R \rightarrow 0$ , and this dependence is to be taken into account. It is hardly reasonable to use the distances between particles:  $r_{ab}$ ,

$r_{a\mu}$  and  $r_{b\mu}$  (the so-called Hylleraas variables), as intrinsic coordinates with expansion (3) because, for  $r_{ab} = 0$ ,  $r_{a\mu}$  and  $r_{b\mu}$  are equal to each other, and it is impossible to determine the angle variable  $\theta$  in terms of them. On the contrary, the spheroidal coordinates,  $\xi = (r_{a\mu} + r_{b\mu})/R$  and  $\eta = (r_{a\mu} - r_{b\mu})/R$ , at  $R = 0$  give, respectively, the radial and angular dependence of the function  $F_m^{J\lambda}$ . It is quite surprising result because the Hylleraas coordinates are very useful with the Schwartz expansion (4) [3-5].

Now consider the behaviour of the components of (3) when three particles lie on the same line (axial singularity). To do this let us express the wave function in terms of the coordinates:  $\alpha, \beta, R, x_*, y_*, z_*$ , where the first three coordinates are spherical coordinates of the vector  $\mathbf{R}$ , and the last three are coordinates of the vector  $\mathbf{r}$  with respect to the frame of the spherical coordinates of the vector  $\mathbf{R}$ . The singularity occurs when the coordinates  $x_*$  and  $y_*$  become equal to zero. In this case the position of the moving frame is indefinite.

It is known that the wave function is infinitely differentiable beyond the coalescence points [15]. Therefore it may be expanded in a Taylor series around a regular point placed on the axis:

$$\Psi_M^{J\lambda}(\mathbf{R}, \mathbf{r}) = \sum_{i+j \leq J} x_*^i y_*^j f_{ij}(\alpha, \beta, R, z) + \rho^{J+1} \Phi_M^{J\lambda}(\alpha, \beta, R, x_*, y_*, z_*), \quad (7)$$

where  $\rho = (x_*^2 + y_*^2)^{1/2}$ .

Multiplying the function  $\Psi_M^{J\lambda}$  by  $D_{Mm}^{J\lambda}(\alpha, \beta, \gamma)$  and integrating over the angular variables, we obtain the component of expansion (3),  $F_m^{J\lambda}$ . On the other hand, integrating first over the angular variable  $\gamma$  and considering that

$$\int_0^{2\pi} x_*^i y_*^j D_{Mm}^{J\lambda}(\alpha, \beta, \gamma) d\gamma \equiv 0, \quad \text{for } i + j < m.$$

we find that  $F_m^{J\lambda}(R, \rho, \gamma) = \rho^m H_m^{J\lambda}(R, \rho, \gamma)$  and the functions  $H_m^{J\lambda}$  are bounded in the neighborhood of the axis.

We now can construct the expansion for the wave function that defines the Rayleigh-Ritz variational procedure for the stationary Schrödinger equation. Using the spheroidal

coordinates we introduce the expansion for the components  $F_m^{J\lambda}$  of (3):

$$F_m^{J\lambda}(R, \xi, \eta) = R^m [(\xi^2 - 1)(1 - \eta^2)]^{m/2} \times \\ \times \sum_n C_n R^{in} \xi^{jn} \eta^{kn} \exp(-(\alpha_n + \beta_n \xi)R), \quad (8)$$

and  $\begin{cases} i_n \geq j_n, & \text{if } \lambda = (-1)^J, \\ i_n > j_n, & \text{if } \lambda = -(-1)^J; \end{cases}$

that takes into account the asymptotics of the axial singularity since

$$\rho = \frac{R}{2} [(\xi^2 - 1)(1 - \eta^2)]^{\frac{1}{2}}.$$

The inequality establishing admissible values for powers of the variables  $R$  and  $\xi$  provides the behaviour:  $F_m^{J\lambda} \rightarrow \text{const}$  for normal parity and  $F_m^{J\lambda} \sim R$  for anomalous parity, when  $R \rightarrow 0$ . Note that the condition connecting the components at the coalescence point of nuclei complicates the computation of the matrix elements and it will be omitted.

For identical nuclei the Hamiltonian commutes with the permutation operator of particles  $P_{ab}$ :  $(\mathbf{R}, \mathbf{r}) \rightarrow (-\mathbf{R}, \mathbf{r})$ , and the wave function can be decomposed on parts symmetric and antisymmetric under permutation:

$$\Psi_M^{J\lambda s}(\mathbf{R}, \mathbf{r}) = (1 + P_{ab}) \Psi_M^{J\lambda}(\mathbf{R}, \mathbf{r}), \quad (9)$$

$$\Psi_M^{J\lambda a}(\mathbf{R}, \mathbf{r}) = (1 - P_{ab}) \Psi_M^{J\lambda}(\mathbf{R}, \mathbf{r}),$$

The operator  $P_{ab}$  acts on the Wigner functions:  $P_{ab} D_{Mm}^J = (-1)^J D_{M, -m}^J$ , which determines a symmetric and antisymmetric parts of the components of expansion (3):

$$F_m^{J\lambda s}(R, \xi, \eta) = \left[ F_m^{J\lambda}(R, \xi, \eta) + \lambda (-1)^m F_m^{J\lambda}(R, \xi, -\eta) \right], \quad (10)$$

$$F_m^{J\lambda a}(R, \xi, \eta) = \left[ F_m^{J\lambda}(R, \xi, \eta) - \lambda (-1)^m F_m^{J\lambda}(R, \xi, -\eta) \right].$$

The components  $F_m^{J\lambda}$  are here either even or odd with respect to the variable  $\eta$ . Therefore it is necessary to retain either even or odd powers of this variable under the sum sign in (8).

To describe the behaviour of the wave function, when  $R \rightarrow 0$ , we make use of the representation (4). Symmetric and antisymmetric terms of the components of the wave function expansion (4) are of the form

$$G_{i_1 i_2}^{J\lambda s}(R, \tau, \theta) = \left[ G_{i_1 i_2}^{J\lambda}(R, \tau, \theta) + (-1)^{i_1} G_{i_1 i_2}^{J\lambda}(R, \tau, \pi - \theta) \right],$$

$$G_{i_1 i_2}^{J\lambda a}(R, \tau, \theta) = \left[ G_{i_1 i_2}^{J\lambda}(R, \tau, \theta) - (-1)^{i_1} G_{i_1 i_2}^{J\lambda}(R, \tau, \pi - \theta) \right], \quad (11)$$

$0 \leq \theta < \pi.$

When  $G_{i_1 i_2}^{J\lambda t}(R, \tau, \eta)$  ( $t = s$  or  $a$ ) is odd with respect to the variable  $\eta = \cos \theta$  then it vanishes at the coalescence point of the nuclei (we recall that component  $G_{i_1 i_2}^{J\lambda}$  does not depend on angular variable for  $R = 0$ ). Thus the necessary corrections to the behaviour of the function  $F_m^{J\lambda t}(R, \xi, \eta)$  can be done by using the formula (6) for symmetric and antisymmetric terms respectively.

The representation (8) for the symmetric wave function was for the first time used in [16] for calculating of the energy level of the mesic molecular ion  $pp\mu$  in a state with total angular momentum  $J = 1$  and normal spatial parity.

### 3. Calculation of matrix elements

Substitution of the basis sets of (3), (8) into the functional

$$(\Psi, H\Psi) / (\Psi, \Psi)$$

reduces the initial equation (1) to the generalized algebraic eigenvalue problem

$$Ax = \lambda Bx, \quad (12)$$

where the matrix  $A$  is composed of the Hamiltonian matrix elements  $(\Psi_i, H\Psi_j)$ , and  $B$  is the overlap matrix of basis functions  $(\Psi_i, \Psi_j)$ , both are symmetric.

To compute the matrix elements in (12), we carry out at first integration over angular variables, it allows us to obtain the system of differential equations in a three-dimensional domain of intrinsic coordinates describing internal position of particles. As a next step, we rewrite that system in spheroidal coordinates of the two-center problem:  $R, \xi, \eta$ . Then, inserting the basis functions of the expansion (8), we reduce the problem to the calculation of certain integrals that can be found analytically.

Before computing the integrals over angles, we rewrite the kinetic energy operator in a convenient form:

$$T = \frac{1}{2\mu_{12}} \left[ -\frac{1}{R^2} \frac{\partial}{\partial R} R^2 \frac{\partial}{\partial R} + \frac{(\mathbf{J} - \mathbf{l})^2}{R^2} \right] - \frac{1}{2\mu_3} \Delta_{\mathbf{r}}. \quad (13)$$

Here  $\mathbf{J}$  is the operator of total angular momentum,  $\mathbf{l}$  is the operator of the muon orbital momentum with respect to the center of mass of nuclei, and the last term is the operator

of the muon kinetic energy, where the vector  $\mathbf{r}_*$  is expressed in terms of the cylindrical coordinates,  $\gamma, \rho, z_*$ , with respect to the frame of reference of spherical coordinates of the vector  $\mathbf{R}$ . We recall that the position of the reference frame of spherical coordinates is defined by the Euler angles  $\alpha, \beta, 0$  ( $\alpha$  and  $\beta$  are spherical angles of the vector  $\mathbf{R}$ ).

The first term in (13) acts only on the functions dependent on the intrinsic variables of the system, whereas the operator of the total angular momentum is expressed in terms of the Euler angles and its action on the Wigner functions is defined by

$$J_x \mathcal{D}_{Mm}^{J\lambda} = -m \mathcal{D}_{Mm}^{J\lambda},$$

$$J_{\pm} \mathcal{D}_{Mm}^{J\lambda} = -(\pm J_x - i J_y) \mathcal{D}_{Mm}^{J\lambda} = \pm \sqrt{J(J+1) - m(m \pm 1)} \mathcal{D}_{M, m \pm 1}^{J\lambda},$$

where  $J_x, J_y$  and  $J_z$  are components of the vector  $\mathbf{J}$  with respect to the moving reference frame. The position of the moving frame is determined by rotation of the reference frame of the spherical coordinates of the vector  $\mathbf{R}$  on an angle  $\gamma$ . The operator  $\mathbf{l}$  in the moving frame is given by expressions:

$$l_x = -i \frac{\partial}{\partial \gamma},$$

$$l_{\pm} = -(\pm l_x - i l_y) = \pm \frac{z}{\rho} \frac{\partial}{\partial \gamma} - \left[ z \frac{\partial}{\partial \rho} - \rho \frac{\partial}{\partial z} \right].$$

Since the components of  $\mathbf{J}$  and  $\mathbf{l}$  commute ( $[J_i, l_i] = 0, i = x, y, z$ ), we may transform the second term of (13) as follows:

$$\frac{(\mathbf{J} - \mathbf{l})^2}{2\mu_{12}R^2} = \frac{\mathbf{J}^2 + \mathbf{l}^2 - 2(\mathbf{J}, \mathbf{l})}{2\mu_{12}R^2} = \frac{\mathbf{J}^2 + \mathbf{l}^2 - 2J_x l_x}{2\mu_{12}R^2} + \frac{J_y l_y + J_z l_z}{2\mu_{12}R^2}.$$

The kinetic energy operator of the muon in the cylindrical coordinates may be written

$$-\frac{1}{2\mu_3} \left\{ \frac{1}{\rho^2} \frac{\partial^2}{\partial \gamma^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial z^2} \right\}.$$

Next we insert the expansion (3) into the kinetic energy operator (13) and integrate over the angular variables. Upon simple calculations, using the expressions obtained for the operator components and the orthogonality relations for the Wigner functions, we get the system of equations for the components of the expansion (3):

$$\sum_{m'=\mu(\lambda)}^J (H_{mm'} - \delta_{mm'} \epsilon) F_m^{J\lambda} = 0, \quad (14)$$

$$m = \mu(\lambda), \dots, J;$$

$$H_{mm} = \frac{1}{\mu_{12}} \left\{ -\frac{1}{R^2} \frac{\partial}{\partial R} R^2 \frac{\partial}{\partial R} - \frac{1}{R^2} \left[ \mathcal{L}^2 + \frac{z}{\rho} \mathcal{L} \right] + \frac{J(J+1) - m^2 + z^2 m^2 / \rho^2}{R^2} \right\} + \frac{P_m^2}{2\mu_3} + V(R, \rho, z); \quad (14')$$

$$H_{m, m \pm 1} = \frac{\gamma_{m, m \pm 1}^{J\lambda}}{2\mu R^2} \left[ \frac{z}{\rho} (m \pm 1) \pm \mathcal{L} \right].$$

Here

$$\mathcal{L} = z \frac{\partial}{\partial \rho} - \rho \frac{\partial}{\partial z}, \quad P_m^2 = \frac{m^2}{\rho^2} - \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{\partial^2}{\partial z^2},$$

$$\gamma_{m, m \pm 1}^{J\lambda} = \left\{ \left[ 1 + \delta_{m0} \lambda (-1)^J \right] [J(J+1) - m(m+1)] \right\}^{1/2},$$

$$\gamma_{m+1, m}^{J\lambda} = \gamma_{m, m+1}^{J\lambda},$$

and  $V(R, \rho, z)$  is the potential energy of the Coulomb interaction. So, the problem of separation of angular variables is completed.

Now the Hamiltonian may be finally written in the spheroidal coordinates of the two-center problem:

$$H_{mm} = \frac{1}{2\mu_{12}} \left\{ -\frac{1}{R^2} \frac{\partial}{\partial R} R^2 \frac{\partial}{\partial R} + \frac{2}{R^2 (\xi^2 - \eta^2)} \left[ (\xi^2 - 1) \xi \left( R \frac{\partial^2}{\partial R \partial \xi} + \frac{\partial}{\partial \xi} \right) + (1 - \eta^2) \eta \left( R \frac{\partial^2}{\partial R \partial \eta} + \frac{\partial}{\partial \eta} \right) \right] + \frac{2\kappa}{R^2 (\xi^2 - \eta^2)} \left[ (\xi^2 - 1) \eta \left( R \frac{\partial^2}{\partial R \partial \xi} + \frac{\partial}{\partial \xi} \right) + (1 - \eta^2) \xi \left( R \frac{\partial^2}{\partial R \partial \eta} + \frac{\partial}{\partial \eta} \right) \right] + \frac{r^2}{R^2} P_m^2 + \frac{J(J+1) - 2m^2}{R^2} \right\} + \frac{1}{2\mu_3} P_m^2 + V(R, \xi, \eta); \quad (15a)$$

where  $\frac{r^2}{R^2} = (\xi^2 + \eta^2 - 1 + 2\kappa\xi\eta + \kappa^2)$ ;

$$H_{m, m \pm 1} = \frac{\gamma_{m, m \pm 1}^{J\lambda}}{2\mu_{12}R^2} \left[ \frac{\xi\eta}{\rho} (m \pm 1) \pm \frac{\rho}{\xi^2 - \eta^2} \left( \eta \frac{\partial}{\partial \xi} - \xi \frac{\partial}{\partial \eta} \right) \right] + \frac{\kappa \gamma_{m, m \pm 1}^{J\lambda}}{2\mu_{12}R^2} \left[ \frac{m \pm 1}{\rho} \pm \frac{\rho}{\xi^2 - \eta^2} \left( \xi \frac{\partial}{\partial \xi} - \eta \frac{\partial}{\partial \eta} \right) \right]; \quad (15b)$$

$$H_{mm'} = 0; \quad \text{when } |m - m'| \geq 2; \quad (15c)$$

$$P_m^2 = \frac{4}{R^2 (\xi^2 - \eta^2)} \left[ \frac{m^2 (\xi^2 - \eta^2)}{\rho^2} - \frac{\partial}{\partial \xi} (\xi^2 - 1) \frac{\partial}{\partial \xi} - \frac{\partial}{\partial \eta} (1 - \eta^2) \frac{\partial}{\partial \eta} \right];$$

$$V(R, \xi, \eta) = \frac{1}{R} + \frac{4\xi}{R^2 (\xi^2 - \eta^2)}; \quad \rho = \frac{R}{2} \sqrt{(\xi^2 - 1)(1 - \eta^2)};$$

and the parameter  $\kappa = (M_b - M_a)/(M_a + M_b)$  determines the shift of the origin of the vector  $\mathbf{r}$  from the center of mass of nuclei to their geometric center.

To determine the matrix elements  $(\Psi_i, H\Psi_j)$  it is necessary to insert the basis functions (8) into (15a-c). Considering that the element of volume in the spheroidal coordinates is equal to  $R^5 (\xi^2 - \eta^2)/8$ , we find that fractional powers and rational parts of expression are cancelled out and only a polynomial of variables  $R, \xi$  and  $\eta$  multiplied by exponential remains. In this way the problem reduces to the computation of integrals of the form:

$$\Gamma_{lm}(\alpha, \beta) = \int_0^\infty dR \int_1^\infty R^l \xi^m \exp[-(\alpha + \beta\xi)R] d\xi, \quad \text{and} \quad \Gamma_n = \int_{-1}^1 \eta^n d\eta.$$

The first integral after integrating by parts is reduced to

$$\Gamma_{lm}(\alpha, \beta) = \frac{m!(l-m-1)!}{\beta^{m+1}(\alpha+\beta)^{l-m}} \sum_{i=0}^m \frac{(l-m+i-1)!}{(l-m-1)!i!} \left(\frac{\beta}{\alpha+\beta}\right)^i.$$

The basis functions (8) are either even or odd with respect to the permutation of heavy particles. To simplify the computation of matrix elements we separate the part linearly dependent on the asymmetry coefficient  $\kappa$  from the Hamiltonian (15). Then the remaining part connects basis functions of the same permutational parity, whereas the separated part connects functions of the different parity.

One can see from the formulas (15a-c) of the Hamiltonian, it is well fitted to the calculation of the adiabatic systems. Indeed, the reduced mass of the heavy particles  $\mu_{12}$  in this case is much greater than the reduced mass of the light particle  $\mu_3$ , and a ratio  $\mu = \mu_3/\mu_{12}$  can be used as the adiabatic parameter of the system. Off-diagonal terms of equations (14) - (15) and the part connecting symmetric and asymmetric components of the wave function are proportional to the small parameter  $\mu$ , and, thus, the quantum numbers  $m$  and the eigenvalues of the permutation operator are approximate quantum numbers of the adiabatic systems.

#### 4. Results

Here we shall analyse the results of computation of the binding energy levels of mesomolecular ions of hydrogen isotopes. Partially they were published earlier in [2,7,19] and they were obtained with the use of some slight modifications of the method we have expounded in this paper. Without going into details we explain only the strategy of choice of the sets of the basis functions:

The basis functions (8) depend on the nonlinear parameters  $\alpha$  and  $\beta$ . Search for optimal nonlinear parameters for every basis function is a cumbersome task. Therefore, in practice, a set of nonlinear parameters  $\alpha_{mt}, \beta_{mt}$  is used which depends on a component number  $m$  and on a permutation parity of two heavy particles  $t$  of a given basis function. The wave function is a complicate function of the variable  $R$ , and it is convenient to introduce two groups of nonlinear parameters that provide good convergence of the expansion at the vicinity of zero and at long distances. In particular, this trick was successfully applied to study weakly bound states when a molecule is extended in the coordinate space. Here we use two sets of nonlinear parameters in all calculations.

The eigenvalue for the certain state of the mesomolecular ion is computed as follows. For fixed values of nonlinear parameters the problem (12) is solved for a given state, either ground or excited. Then the eigenvalue is minimized by varying nonlinear parameters. Since the estimation for the energy derived from (12) provides the upper bound estimate, the minimization retains this property and only increases the accuracy of the solution. The nonlinear parameters we have used here are cited in [2,7,19].

The algebraic problem for eigenvalues (12) was solved by inverse iteration method (it can be found, e.g. in Ref. 17) for the following reasons. First, a particular bound state is calculated for some values of nonlinear parameters optimal for the given state. Therefore, it is sufficient to look for only one eigenvalue and the remaining part of the spectrum is not necessary. Second, this method provides less computational time. We make use of the symmetric structure of the problem and the number of operations is about  $n^3/6$  multiplications which is significantly lower comparing to other direct methods of the eigenvalue computation. This is especially important for calculations with a large number



of basis functions when the computational time of the problem (12) rapidly grows with the number of functions and very soon becomes dominant.

As the number of basis functions increases, the algebraic eigenvalue problem (12) becomes more and more singular. The inverse iteration method is the most stable one for the solution of that problem. However, it also cannot ensure the stability of eigenvalues for large matrices. The stability is achieved when we solve the following regularized eigenvalue problem [18]:

$$A_*x = \lambda B_*x, \quad \text{where } A_* = A + \delta D, \quad B_* = B;$$

where  $\delta$  is a small parameter, and a diagonal matrix  $D$  is composed of elements  $|a_{ii} - \lambda b_{ii}|$ . That removes from the spectrum infinite eigenvalues defining the singularity of the problem and causing instability of the true eigenvalues. To be successful this procedure requires the following condition:

$$\varepsilon (\|A\|^2 + \|B\|^2)^{1/2} \frac{\|x\|}{[(x, Ax)^2 + (x, Bx)^2]^{1/2}} \ll 1;$$

where  $x$  is an examined eigenvector, and  $\varepsilon$  is a round-off error [18]. When an exponential expansion [3-5] is used, the latter condition is not satisfied, therefore the only way is to increase the precision of calculations to quadruple precision. In our calculations this condition was checked and it was fulfilled even when 2600 basis functions were used. The parameter  $\delta$  was taken in the interval  $10^{-14} - 10^{-15}$  and its variation allowed approximately estimate the accuracy of a calculated eigenvalue.

The energy levels of mesomolecular ions are reported in Table 1 (normal parity) and Table 2 (anomalous parity). The values for  $S$ - and  $P$ -states presented in Table 1 have been computed in Ref. 2. The only exception is the calculation of the weakly bound state of  $dt\mu$  with  $J = 1$  for which a more accurate series of computations was performed and listed in Table 3 below, here  $n_i$  is the number of basis functions employed. The values of  $D$ - and  $F$ -states obtained with the use of this variational method are published for the first time. The corresponding series of computations with a growing number of basis functions are reported in Table 4 (the number of basis functions was pointed out in parentheses). The energy levels of mesomolecular ions with anomalous parity have been studied in [7,19], here we present only the results (Table 2). In the calculations we made use of the following values

**Table 1:** Binding energies  $-\varepsilon_{Jv}$  (in eV) of mesomolecular ions of hydrogen isotopes with spatial parity  $\lambda = (-1)^J$ .

$J v$	$pp\mu$	$dd\mu$	$tt\mu$	$pd\mu$	$pt\mu$	$dt\mu$
0 0	253.1523	325.0735	362.9097	221.5494	213.8402	319.1396
0 1	-	35.8436	83.7711	-	-	34.8340
1 0	107.2658	226.6815	289.1419	97.4980	99.1262	232.4714
1 1	-	1.97475	45.2057	-	-	0.6600
2 0	-	86.4936	172.7022	-	-	102.6486
3 0	-	-	48.8376	-	-	-

**Table 2:** Binding energies  $-\varepsilon_{Jv}$  (in eV) of mesomolecular ions of hydrogen isotopes with spatial parity  $\lambda = -(-1)^J$ .

$J v$	$pp\mu$	$dd\mu$	$tt\mu$	$pd\mu$	$pt\mu$	$dt\mu$
1 0	13.5400	22.5942	27.4122	3.6849	1.5788	19.1247
2 0	-	9.8203	17.7713	-	-	7.8990
3 0	-	-	5.4187	-	-	-

of physical constants:  $M_p = 1836.1515m_e$ ,  $M_d = 3670.481m_e$ ,  $M_t = 5496.918m_e$ ,  $m_\mu = 206.7686m_e$ ,  $Ry = 13.6058041eV$ . The energy levels have been obtained in Ref. 2 with the use of muonic mass  $m_\mu = 206.769m_e$  here we convert these values to the given mass set adding the energy shifts computed in Ref. 20.

Tables 6–8 contains a comparison of muonic molecular calculations with the best literature results. One can easily see that  $S$ - and  $P$ -state energy levels are in a good agreement with the highly accurate exponential Slater-type basis set [4] results. As far as the states of higher rotational numbers is concerned the situation changes. The only one result that is lower than ours was obtained with the use of the same Slater-type basis set method for the mesomolecular ion  $dt\mu$  ( $J = 2$ ) [5]. The reason is that the evaluation of angular integrals with bipolar harmonics of high angular momentum and/or anomalous spatial parity (Eq.(4)) becomes very laborious. In any case our results seems to have the errors of computation comparable with the error dependent on the uncertainty in the measurement of the mass values.

An important characteristic of a molecule is its mean size. In Table 5 we present mean sizes of mesomolecular ions of hydrogen isotopes for states with the total angular momentum  $J \geq 2$  with normal parity in units  $e = \hbar = m_\mu = 1$ . The accurate values of mean sizes of mesomolecular ions with  $J \leq 1$  of normal parity were calculated in Ref. 21 (in our approach we reproduce usually four figures of their results). Mean sizes of mesomolecular ions of anomalous parity have been calculated in Ref. 19.

We have also studied the possibility of the existence of other bound states. The operator  $H - \epsilon_e E$ , where  $\epsilon_e$  is the energy of the molecule dissociation, has as many negative eigenvalues as there are bound states of the molecule. Therefore, if we insert a trial function of high dimension we have the right to expect that a finite-dimensional matrix  $A - \epsilon_e B$  exactly reproduces the number of negative eigenvalues of the initial operator and thus determines the number of bound states of a molecular system. This estimation has been performed for all the systems presented in Tables 1 and 2 and for the mesic molecular ion  $tt\mu$  with the total angular momentum  $J = 4$  with the use of about 700–800 basis functions and this investigation has shown that there are no other bound states for mesomolecular ions of hydrogen isotopes.

**Table 3:** Series of calculations of the energy level of a weakly bound state of mesic molecular ion  $dt\mu$ .

$i$	$n_i$	$-\epsilon_{11}(n_i)$
1	1513	0.65923
2	2084	0.65968
3	2174	0.65985
4	2313	0.65990
5	2660	0.65999

**Table 4:** Series of calculations of binding energies  $-\epsilon_{Jv}$  (in eV) of mesomolecular ions of normal spatial parity with the total angular momentum  $J \geq 2$ .

$dd\mu$ ( $J = 2$ )	$tt\mu$ ( $J = 2$ )	$dt\mu$ ( $J = 2$ )	$tt\mu$ ( $J = 3$ )
86.48790 (160)	172.69753 (160)	102.64146 (212)	48.83234 (160)
86.49237 (222)	172.70066 (222)	102.64422 (274)	48.83570 (222)
86.49361 (426)	172.70215 (426)	102.64861 (550)	48.83764 (442)

**Table 5:** Mean sizes of mesic molecular ions of normal spatial parity with the total angular momentum  $J \geq 2$ .

	$J$	$-\epsilon_J$	$R$	$r_b$	$r_a$	$R^2$	$r_b^2$	$r_a^2$
$dd\mu$	2	86.494	3.910	2.688	2.688	16.86	10.03	10.03
$tt\mu$	2	172.702	3.298	2.359	2.359	11.76	7.423	7.423
$dt\mu$	2	102.649	3.599	2.634	2.408	14.15	9.376	7.923
$tt\mu$	3	48.838	4.040	2.750	2.750	17.77	10.49	10.49

**Table 6:** Comparison of muonic molecular calculations (normal parity,  $J = 0, 1$ ).

	$J$	$v$	This work	Ref. 4	Ref. 1
$pp\mu$	0	0	253.1523	253.152332	253.0
$dd\mu$	0	0	325.0735	325.073540	325.0
$dd\mu$	0	1	35.8436	35.844360	35.8
$tt\mu$	0	0	362.9097	362.909770	363.0
$tt\mu$	0	1	83.7711	83.771216	83.9
$pd\mu$	0	0	221.5494	221.549410	221.5
$pt\mu$	0	0	213.8402	213.840179	214.0
$dt\mu$	0	0	319.1396	319.139722	319.2
$dt\mu$	0	1	34.8340	34.834491	34.9
$pp\mu$	1	0	107.2658	107.265971	107.0
$dd\mu$	1	0	226.6815	226.681678	226.6
$dd\mu$	1	1	1.97475	1.974817	1.956
$tt\mu$	1	0	289.1419	289.141783	289.2
$tt\mu$	1	1	45.2057	45.205856	45.2
$pd\mu$	1	0	97.4980	97.498160	97.4
$pt\mu$	1	0	99.1262	99.126501	99.0
$dt\mu$	1	0	232.4714	232.471594	232.4
$dt\mu$	1	1	0.6600	0.660178	0.656

**Table 7:** Comparison of muonic molecular calculations (normal parity,  $J \geq 2$ ).

	$J$	$v$	This work	Ref. 5	Ref. 3	Ref. 1
$dd\mu$	2	0	86.4936	-	86.4341	86.3
$tt\mu$	2	0	172.7022	-	172.5264	172.7
$dt\mu$	2	0	102.6486	102.64891	102.6318	102.5
$tt\mu$	3	0	48.8376	-	-	48.7

**Table 8:** Comparison of muonic molecular calculations (anomalous parity).

	$J$	$v$	This work	Ref. 8
$pp\mu$	1	0	13.5400	13.542
$dd\mu$	1	0	22.5942	22.595
$tt\mu$	1	0	27.4122	27.413
$pd\mu$	1	0	3.6849	3.684
$pt\mu$	1	0	1.5788	1.566
$dt\mu$	1	0	19.1247	19.124
$dd\mu$	2	0	9.8203	-
$tt\mu$	2	0	17.7713	-
$dt\mu$	2	0	7.8990	-
$tt\mu$	3	0	5.4187	-

There exists a less complicated but also less rigorous proof of the statement. The shift of energy levels due to the rotational motion of a molecule is proportional to  $m_\mu/\mu_{12}$  [22]. According to this rule we may extrapolate the energy levels given in Tables 1 and 2 to higher values of  $J$ . All the extrapolated values belong to the continuous spectrum which means that the corresponding bound states of mesomolecular ions do not exist.

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### Appendix A. Variational form in spheroidal coordinates

Matrix elements of the Hamiltonian  $(\Psi_i, H\Psi_j)$  can be determined from the variational functional:

$$(\Psi, H\Psi) = \int \sum_{m=\mu(\lambda)}^J \left\{ T_{mm}^\sigma + T_{mm}^\kappa + \gamma_{m,m-1}^{J\lambda} T_{m,m-1} + \gamma_{m,m+1}^{J\lambda} T_{m,m+1} + V(R, \xi, \eta) |F_m^{J\lambda}|^2 \right\} \frac{R^5}{8} (\xi^2 - \eta^2) \cdot dR d\xi d\eta;$$

where elements  $T$  compose the operator of kinetic energy and are of the form:

$$T_{mm}^\sigma = \frac{1}{2\mu_{12}} \left\{ \left| \frac{\partial F_m}{\partial R} \right|^2 - \frac{1}{R(\xi^2 - \eta^2)} \left[ \frac{\partial F_m^*}{\partial R} \left( (\xi^2 - 1)\xi \frac{\partial F_m}{\partial \xi} + (1 - \eta^2)\eta \frac{\partial F_m}{\partial \eta} \right) + \left( (\xi^2 - 1)\xi \frac{\partial F_m^*}{\partial \xi} + (1 - \eta^2)\eta \frac{\partial F_m^*}{\partial \eta} \right) \frac{\partial F_m}{\partial R} \right] + \frac{J(J+1) - 2m^2}{R^2} |F_m|^2 + \frac{\xi^2 + \eta^2 - 1 + \kappa^2}{4} P_m^2 \right\} + \frac{1}{2\mu_3} P_m^2;$$

$$T_{mm}^\kappa = \frac{\kappa}{2\mu_{12}} \left\{ -\frac{1}{R(\xi^2 - \eta^2)} \left[ \frac{\partial F_m^*}{\partial R} \left( (\xi^2 - 1)\eta \frac{\partial F_m}{\partial \xi} + (1 - \eta^2)\xi \frac{\partial F_m}{\partial \eta} \right) + \left( (\xi^2 - 1)\eta \frac{\partial F_m^*}{\partial \xi} + (1 - \eta^2)\xi \frac{\partial F_m^*}{\partial \eta} \right) \frac{\partial F_m}{\partial R} \right] + \frac{\xi\eta}{2} P_m^2 \right\};$$

$$P_m^2 = \frac{4}{R^2(\xi^2 - \eta^2)} \left[ \frac{m^2(\xi^2 - \eta^2)}{\rho^2} |F_m|^2 - \frac{\partial F_m^*}{\partial \xi} (\xi^2 - 1) \frac{\partial F_m}{\partial \xi} - \frac{\partial F_m^*}{\partial \eta} (1 - \eta^2) \frac{\partial F_m}{\partial \eta} \right];$$

$$T_{m,m\pm 1} = T_{m,m\pm 1}^\sigma + T_{m,m\pm 1}^\kappa;$$

$$T_{m,m\pm 1}^\sigma = \frac{1}{2\mu_{12}R^2} F_m^* \left[ \frac{\xi\eta}{\rho} (m \pm 1) F_{m\pm 1} \pm \frac{\rho}{\xi^2 - \eta^2} \left( \eta \frac{\partial}{\partial \xi} - \xi \frac{\partial}{\partial \eta} \right) F_{m\pm 1} \right];$$

$$T_{m,m\pm 1}^\kappa = \frac{\kappa}{2\mu_{12}R^2} F_m^* \left[ \frac{m \pm 1}{\rho} F_{m\pm 1} \pm \frac{\rho}{\xi^2 - \eta^2} \left( \xi \frac{\partial}{\partial \xi} - \eta \frac{\partial}{\partial \eta} \right) F_{m\pm 1} \right];$$

$$\rho = \sqrt{(\xi^2 - 1)(1 - \eta^2)}; \quad \kappa = (M_b - M_a)/(M_a + M_b);$$

$$\gamma_{m,m+1}^{J\lambda} = \left\{ \left[ 1 + \delta_{m0}\lambda(-1)^J \right] [J(J+1) - m(m+1)] \right\}^{1/2}, \quad \gamma_{m+1,m}^{J\lambda} = \gamma_{m,m+1}^{J\lambda}.$$

Matrix elements  $T^\sigma$  connect basis functions  $\Psi_i$  and  $\Psi_j$  of the same permutation parity and are equal to zero for functions with opposite parity, whereas matrix elements  $T^\kappa$  connect functions with opposite parity and vanish otherwise.

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