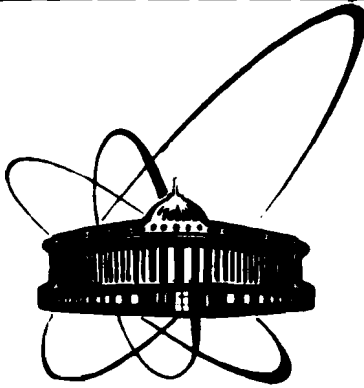


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VARIATIONAL CALCULATION OF MESIC
MOLECULE BOUND STATES WITH ORBITAL
MOMENTUM $J = 1$ AND SPATIAL PARITY $\lambda = +1$

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1. The energy levels of the bound states of the mesic molecules of hydrogen isotopes with spatial parity $\lambda = (-1)^J$ are calculated with high accuracy in different approaches [1,2] at present time. Beside the above states there are some metastable P-states with the positive parity ($\lambda = -(-1)^J$, $J = 1$). Some adiabatic estimations of these states have been presented in ref [3].

This paper is devoted to variational calculation of mesic molecule metastable P-states with the usage of the approach developed in refs [4,5].

2. Hamiltonian of the mesic molecule consisting of the nuclei a and b of the hydrogen isotopes ($a, b = p, d$ or t) and a negative charged muon $c = \mu$ in Jacobi coordinates have the form ($c = b = m_p = 1$):

$$H = -\frac{1}{2M} \Delta_{\mathbf{R}} - \frac{1}{2m} \Delta_{\mathbf{r}} - \frac{1}{r_a} - \frac{1}{r_b} + \frac{1}{R}, \quad (1)$$

$$M^{-1} = M_a^{-1} + M_b^{-1}, \quad m^{-1} = m_\mu^{-1} + (M_a + M_b)^{-1}.$$

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 muon c with the mass m_μ relative to the center mass of the nuclei. The operators of total orbital momentum \mathbf{J}^2 , its projection J_z onto the space-fixed axis Z and the operator of the total spatial inverse P_{tot} are commuted with Hamiltonian (1). The existence of these integrals of motion allows us to separate bound states with the different spatial parity $\lambda = (-1)^J$ and $\lambda = -(-1)^J$ for the fixed values of the total orbital momentum J .

The binding energy $\varepsilon_{J\lambda}$ of a mesic molecule is defined by the difference $-\varepsilon_{J\lambda} = (E - E_{na})$ (a.u.) of the total energy E and the dissociation threshold $E_{na} = -\left(m_\mu/2n^2\right)$ a.u. where m_μ is the reduced muon mass of atom (ac). For the calculations of the bound states with the spatial parity $\lambda = (-1)^J$ this threshold has to be equal to the energy of the ground state of the mesic atom (ac). For the calculations of the metastable P-states with the parity $\lambda = -(-1)^J$ the binding energy has to be set to the energy of the excited mesoatom state with the principal quantum number $n=2$. At that the mesic molecule wave function of these states has the form [6]:

$$\Psi^{1+}(\mathbf{R}, \mathbf{r}) = [\mathbf{r} \times \mathbf{R}] G(R, r, \theta_{12}), \quad (2)$$

where θ_{12} is the angle between the position vectors \mathbf{R} and \mathbf{r} .

3. For the solution of the eigenvalue problem with Hamiltonian (1) we make the use of basis functions of the following form [5]:

$$\begin{aligned} \Psi^{1+}(\mathbf{R}, \mathbf{r}) &= [\mathbf{r} \times \mathbf{R}] \times \\ & \sum_{s=1}^2 \sum_{i,j,k} \alpha_{ij,k}^s R^i \xi^j \eta^k \exp[-(\alpha_s + \beta_s \xi) R], \end{aligned} \quad (3)$$

$$j \geq 0, \quad i \geq j, \quad k \geq 0.$$

Here $\xi = (r_a + r_b)/R$ and $\eta = (r_b - r_a)/R$ are spheroidal coordinates. The following constants were used in our calculations: $M_p = 1836.1515m_e$, $M_d = 3670.481m_e$, $M_t = 5496.918m_e$, $m_\mu = 206.7686m_e$, $Ry = 13.605804eV$.

The values of the nonlinear parameters used in our calculations are listed in Table 1 in units ($e = \hbar = m_a = 1$). Table 2 performs the calculations of the binding energies $-\varepsilon_{1+} = 2Ry \cdot (E + m_a/8)$ for metastable P-states of mesic molecules. These values were obtained as the result of solving the algebraic generalized eigenvalue problem $Ax = \lambda Bx$, where x corresponds to the coefficients a_{ijk}^s in the expansion (3). The number in parentheses under each value of $-\varepsilon_{1+}$ is the number of the basis functions used in that calculation. It gives the possibility for one to see the convergence of the calculated values of the energy levels with the growth of the number of basis functions. The adiabatic estimations of ref.[3] are also given for convenience in Table 2.

Table 1. Nonlinear parameters for the wave functions of mesic molecule metastable bound states.

	tt μ	dt μ	dd μ	pp μ	dp μ	tp μ
α_1	1.0	1.0	1.0	1.0	1.0	1.0
β_1	0.28	0.28	0.28	0.28	0.28	0.28
α_2	0.4	0.4	0.4	0.4	0.3	0.0
β_2	0.32	0.32	0.32	0.32	0.32	0.32

Table 2. Binding energies $\varepsilon_{J\lambda}$ (in eV) of mesic molecules with total orbital momentum $J=1$ and spatial parity $\lambda=+1$.

	tt μ	dt μ	dd μ	pp μ	pd μ	pt μ
<i>Ref.[3]</i>	24	16	20	12	2	0.5
<i>present work</i>	27.4084 (198)	19.1201 (348)	22.5901 (198)	13.5336 (198)	3.6718 (348)	1.5662 (348)
	27.4115 (384)	19.1238 (534)	22.5935 (384)	13.5382 (384)	3.6814 (534)	1.5759 (534)
	27.4122 (630)	19.1247 (896)	22.5942 (630)	13.5400 (630)	3.6849 (896)	1.5788 (896)

4. Performed variational calculation of the metastable P-states gives us some additional information about the spectrum of the energy levels of the mesic molecules. The wave function of these states is equal to zero at the coalescence point of the nuclei, that's provided the rather small probability of the nuclear fusion. The usual dipole transitions to the S-states of the mesic molecules are also forbidden. Therefore a capture of a muon into the states with abnormal parity would lead to dropping one from MCF cycle. Up to now a mechanism of the formation of the metastable P-states were not discussed. The role of these states in MCF can be entirely understood after some estimations of the corresponding formation rates will be given.

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