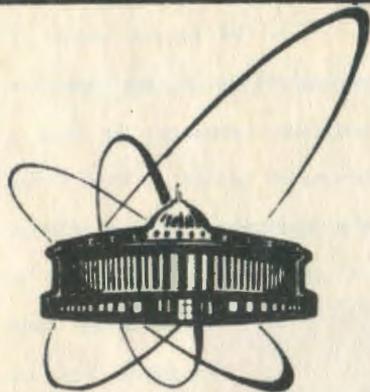


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ABNORMAL PARITY STATES OF MESIC MOLECULES
OF HYDROGEN ISOTOPES
WITH TOTAL ORBITAL MOMENTUM $J \geq 2$

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Bound states of mesic molecules of hydrogen isotopes with abnormal spatial parity and total angular momentum $J = 1$ have been a goal of intensive studying in the last few years [1-3]. This works were initiated by an earlier work by Carter [4], in which he pointed out the existence of states of that kind but made a number of methodological mistakes. A more thorough investigation has shown that the phenomenology of bound states with abnormal spatial parity is not exhausted with P-states. In this paper, we present calculations of the binding energy levels of mesic molecules of hydrogen isotopes with a total orbital momentum $J \geq 2$. A detailed analysis of the computations shows that the obtained 10 bound states of the mesic molecules completely describe the discrete spectrum of the states with abnormal spatial parity of this considered three-particle systems.

1. A hydrogen mesic molecule consists of two heavy nuclei (a, b = p, d or t) and a negative-charged muon μ . We shall describe their interaction with the nonrelativistic Schrödinger equation for a three-particle system with Coulomb interaction which is in the Jacoby coordinates ($R = R_b - R_a$, $r = r_\mu - (M_a R_a + M_b R_b) / (M_a + M_b)$) of the following form ($e = \hbar = m_\mu = 1$):

$$H\psi = \epsilon\psi, \quad (1)$$

$$H = -\frac{1}{2\mu_{12}} \Delta_R - \frac{1}{2\mu_3} \Delta_r - \frac{1}{r_a} - \frac{1}{r_b} + \frac{1}{R},$$

where μ_{12} and μ_3 are reduced masses of particles: $\mu_{12}^{-1} = M_a^{-1} + M_b^{-1}$, $\mu_{12}^{-1} = m_\mu^{-1} + (M_a + M_b)^{-1}$.

The Hamiltonian operator in (1) commutes with the operator of the total orbital momentum J^2 , its projection on the Z axis of the fixed frame J_z and with the operator of spatial parity P_λ : (R, r)

$\rightarrow (-R, -r)$. These operators define quantum numbers of the state of the system J, M and λ respectively.

The state wave function can be represented in the form:

$$\psi_M^{J\lambda}(R, r) = \sum_{m=\mu(\lambda)}^J D_{Mm}^{J\lambda}(\alpha, \beta, \gamma) F_m^{J\lambda}(R, r, \theta_{12}) ; \quad (2)$$

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

where α, β, γ are Euler angles of a moving frame connected with the three-particle system so that nuclei of the molecule form the Z axis and the X axis lies in the plane of the three particles in the direction of the muon. The functions $D_{Mm}^{J\lambda}(\alpha, \beta, \gamma)$ are symmetrized Wigner D-functions,

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

with given quantum numbers J, M and spatial parity λ .

States with parities $\lambda = (-1)^J$ and $\lambda = -(-1)^J$ differ to each other in their properties to a great extent. We will call these states the states with normal and abnormal parity, respectively. The dissociation energy of the molecule in a state with normal parity is determined by the ground-state energy of an atom with a heavier nucleus, whereas the molecule in a state with parity $\lambda = -(-1)^J$ decays into a system of an atom and a particle with the atom having a nonzero orbital momentum, therefore the dissociation limit of the molecule is defined by the energy level of a heavy atom with the principal quantum number $n=2$: $E_a = -Ry m_a / 8$, where m_a is the reduced mass of the atom. Thus, the bound states of the molecule with abnormal parity are sunk into the continuous spectrum of the states with normal spatial parity.

Another peculiarity is the behaviour of the wave function of the

solution when $R \rightarrow 0$. For the states with abnormal parity the wave function has the asymptotics $O(1)$ in the vicinity of the coalescence point, whereas the wave function of parity $\lambda = (-1)^J$ in the vicinity of that point becomes constant [5].

2. We make numerical study of equation (1) by the variational method based on a trial function of a molecular type. We used that method successfully in studies of the energy levels of hydrogen - isotope molecules in the states with normal parity [6] and in precision computations of weakly bound states of mesic molecules $dd\mu$ and $dt\mu$ [7], accurate analysis of which is a quite complicated computational problem. To determine components of the wave function (2) of a state with abnormal parity, we employ the following expansion of the test function¹

$$F_m^{J\lambda}(R, \xi, \eta) = R^{m+1} [(\xi^2-1)(1-\eta^2)]^{m/2} \times \quad (3)$$

$$\times \sum_n C_n R^{i_n} \xi^{j_n} \eta^{k_n} \exp(-(\alpha_n + \beta_n \xi)R),$$

and $i_n \geq j_n$.

The factor in front of the sum describes the asymptotic behaviour of the wave function $F_m^{J\lambda} \sim \rho^m$, when $\rho \rightarrow 0$, where $\rho = \frac{R}{2} \times [(\xi^2-1)(1-\eta^2)]^{1/2}$ is the distance between a third particle and the axis formed by nuclei.

Substitution of the finite sums of expansions (2) - (3) into the functional $(\Psi, H\Psi)/(\Psi, \Psi)$ reduces solution of the initial equation (1) to a generalized algebraic eigenvalue problem

$$Ax = \lambda Bx, \quad (4)$$

where the matrix A is composed of elements of the Hamiltonian $(\Psi_1, H\Psi_j)$, and B is the overlap matrix (Ψ_1, Ψ_j) . Matrices A and B are symmetric.

¹The coordinates $\xi = (r_a + r_b)/R$ and $\eta = (r_b - r_a)/R$ are spheroidal coordinates of a light particle.

The problem (4) will be solved by the inverse iteration method. As is known, the sensitivity of eigenvalues to roundoff errors rapidly grows with increasing number of the basis functions. The inverse iteration method is the most stable procedure in solving that problem. Besides, it allows us to take into account quite easily the symmetric structure of the problem and to construct on this way an effective procedure of the computation of energy levels.

3. Calculated energy levels of the hydrogen-isotope mesic molecules are presented in Table 1. The number in parentheses under each value is the number of basis functions used in that calculation. Accurate solutions have been obtained with the use of two groups of nonlinear parameters (α_1, β_1) and (α_2, β_2) that adequately describe the wave function behaviour at small and large distances of R , respectively. The values of the parameters are collected in Table 2. The following physical constants were used in our calculations: $M_d = 3670.481m_e$, $M_t = 5496.918m_e$, $m_\mu = 206.7686m_e$, $Ry = 13.6058041eV$.

A complete set of the abnormal parity bound states and mean sizes of mesic molecules in units $e\hbar/m_\mu = 1$ are presented in Tables 3 and 4. The results show that the mean distances between particles in the molecule are about 3-4 times as large as those in molecules with normal parity. For comparison, the mean distances of the ground state of the mesic molecule $d_{t\mu}$ equal: $r_{dt} = 2.648$, $r_{d\mu} = 2.041$, $r_{t\mu} = 1.951$ [8].

The existence of other bound states was also investigated. The operator $H - \epsilon_d E$, where ϵ_d is the dissociation energy level of a molecule, has as many negative eigenvalues as bound states of the mesic

molecule have. Therefore, inserting a trial function of a quite large dimension into the operator we have a right to expect that a finite-dimensional matrix $(A - \epsilon B)$ reproduces exactly the number of negative eigenvalues of the initial operator and, thus, determines the amount of bound states of a molecular system. Such estimates were made for all the systems indicated in Table 3 and for the mesic molecule $t\mu$ with total orbital momentum $J = 4$. This analysis shows that there are no other bound states with abnormal parity for hydrogen-isotope mesic molecules.

There exists another more visual (but less rigorous) foundation of that statement. The shift of energy level due to the rotational motion of a molecule depends on the masses of particles approximately as m_{μ}/M [9] where M is the reduced mass of heavy particles. This approximate rule is confirmed by the analysis of the Table of the energy levels of hydrogen-isotope mesic molecules in the normal parity states given in [10]. Using this rule, we may easily extrapolate the energy levels to higher values of J in the given Table. All the extrapolated values lie in the continuous spectrum what signifies the absence of the corresponding bound states of mesic molecules.

Table 1. Binding energies of hydrogen-isotope mesic molecules
with abnormal spatial parity ($J \geq 2$).

$dd\mu(20)$	$tt\mu(20)$	$dt\mu(20)$	$tt\mu(30)$
9.81342 (100)	17.75434 (100)	7.88333 (144)	5.39083 (100)
9.81934 (144)	17.77000 (144)	7.89812 (196)	5.41454 (152)
9.82027 (206)	17.77125 (206)	7.89904 (258)	5.41872 (214)

Table 2. Nonlinear parameters for the wave functions ($J \geq 2$).

	$dd\mu(20)$	$tt\mu(20)$	$dt\mu(20)$	$tt\mu(30)$
α_1	0.6	1.2	1.0	1.0
β_1	0.32	0.32	0.32	0.32
α_2	0.2	0.4	0.4	0.3
β_2	0.32	0.32	0.32	0.32

Table 3. Binding energies of mesic molecules $\epsilon_{J\nu}$ (in eV).

J	ν	$pp\mu$	$dd\mu$	$tt\mu$	$pd\mu$	$pt\mu$	$dt\mu$
1	0	13.540	22.594	27.412	3.685	1.579	19.125
2	0	--	9.820	17.771	--	--	7.899
3	0	--	--	5.419	--	--	--

Table 4. Mean sizes of mesic molecules (in units $e=h=m_{\mu}=1$).

	J	energy	R	r_b	r_a	R^2	r_b^2	r_a^2
pp μ	1	13.540	12.33	8.755	8.755	167.3	99.80	99.80
dd μ	1	22.595	10.55	7.749	7.749	119.2	74.93	74.93
tt μ	1	27.413	9.908	7.380	7.380	103.8	66.91	66.91
pd μ	1	3.685	12.54	10.82	6.814	177.2	151.0	59.32
pt μ	1	1.579	13.05	11.75	6.372	195.7	178.2	51.53
dt μ	1	19.125	10.27	7.969	7.203	112.5	78.37	64.50
dd μ	2	9.820	11.69	8.353	8.353	147.4	89.44	89.44
tt μ	2	17.771	10.54	7.720	7.720	117.8	74.11	74.11
dt μ	2	7.899	11.19	8.651	7.499	134.2	94.00	71.25
tt μ	3	5.419	11.75	8.345	8.345	146.5	88.96	88.96

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