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A NEW SERIES IN SPECTRA OF MUONIC MOLECULES

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The first adiabatic calculation of bound states of muonic molecules was done in 1959 [1]. It was followed by the first variational calculation of symmetric molecules in 1964 [2]. Interest in the problem was resumed after 1973 when a loosely bound state of the $dd\mu$-ion was found in the adiabatic approach [3]. Further adiabatic calculation of the $dt\mu$ loosely bound state (1978) was a sort of sensation [4]. After that several groups contributed to the problem and finally the results of two independent variational calculations were published in the same volume of Physical Review [5,6]. Table 1 demonstrates some energy values from the already mentioned papers. One can definitely say that the problem is solved.

Up to our knowledge only states with normal parity, i.e., for $p = (-1)^J$, where p is the parity quantum number and J is that of the total angular momentum, were considered until now. In this paper we present the results of the adiabatic calculation of $(J = 1,\ p = 1)$ states of muonic molecules $xy\mu$, where $x,y = p, d, t$. Our adiabatic approach is definitely different from that used by the Dubna group during a rather long period of time [7]. The basic equation of our method was produced by two subsequent transformations of the usual adiabatic (Born-Oppenheimer) Schrödinger equation [8,9]. Actually, these transformations lead to a sort of hyperspherical adiabatic approach [10], which is now widely used by many authors for a large class of problems. Recently, we have demonstrated that it is quite effective for the calculation of $(J = 0,\ p = 1)$ states of the $dt\mu$-ion [11]. The way of solving the adiabatic problem in this paper is different from that in [11]. We use here a proper variant of the semianalytic approach described in [12].

The hyper-radius R for a system of two nuclei x and y and a negative muon μ is defined by

$$MR^2 = MX^2 + mx^2\ , \qquad (1)$$

where M and m are the reduced masses of the systems (x,y) and $(x+y,\ \mu)$, respectively,

$$1/M = 1/m_x + 1/m_y , \quad (2)$$

$$1/m = 1/m_\mu + 1/(m_x + m_y) , \quad (3)$$

$\vec{X}$ is the position vector of y relative to x and $\vec{x}$ is that of μ with respect to the centre of mass of (x + y).

Table 1

Normal parity bound states. Only selective references are given in order to illustrate the increasing accuracy of calculations (in eV)

	ddμ (J=1, ground)	ddμ(J=1, excited)	dtμ(J=1, excited)
1959,[1], adiab.	226	-	-
1964,[2], var.	226.55	-	-
1973,[3], adiab.	224	0.7	-
1978,[4], adiab.	226.25	1.96	0.85
1985,[7], adiab.		1.956	0.656
1988,[5], var.	226.6816786	1.9748717	0.6601721
1988,[6], var.			0.660030 ± 0.00002

The Hamiltonian for our system is given using the hyperradius by [8-10]

$$H = -\frac{1}{2M}\frac{1}{R^5}\frac{\partial}{\partial R}R^5\frac{\partial}{\partial R} + h(\hat{o};R), \quad (4)$$

where h is the adiabatic Hamiltonian operator which includes R as a parameter, and $\hat{o}$ represents five dimensionless variables. Following [8,9] we use the set $\hat{o} = (\alpha, \beta, \gamma, \xi, \eta)$, where (α, β, γ) define the Euler rotation specifying the body-fixed frame with its unit vectors to coincide with the principal axes of the inertia tensor of a three-body system. The hyperspheroidal coordinates ξ and η are given by

$$\xi = (r_{\mu x} + r_{\mu y})/R , \quad \eta = (r_{\mu x} - r_{\mu y})/R . \quad (5)$$

A physical solution of the Schödinger equation

$$(H - E)\Psi = 0 \quad (6)$$

with the well-defined total angular momentum J and total parity p is supplied with the partial-wave representation of the wave function Ψ in the form [9]

$$\Psi^{JpM_J}(\vec{X},\vec{x}) = \sum_{m=0}^{J} B_m^{JpM_J}(\alpha,\beta,\gamma)\,\psi_m^{Jp}(R,\xi,\eta). \quad (7)$$

The angular part of the wave function has the form

$$B_m^{JpM_J}(\alpha,\beta,\gamma) = \frac{(-i)^m}{4\pi}\sqrt{\frac{2J+1}{1+\delta_{0m}}}\{D^J_{-m-M_J}(\gamma,\beta,\alpha) + p(-1)^J D^J_{m-M_J}(\gamma,\beta,\alpha)\}. \quad (8)$$

It contains the Wigner D-functions with $|M_J| \le J$ and $0 \le m \le J$ being the projections of $\vec{J}$ onto the space and body-fixed z-axis, respectively. The projection of the Schrödinger equation (6) onto the states (7) leads to the system of J + 1 (for normal parity states when $p = (-1)^J$) or J (for abnormal parity states when $p = -(-1)^J$) Schödinger equations. In our particular case of abnormal parity states with $J = 1$ and $p = 1$ this system degenerates into one equation as it follows directly from the analytic expression (8). As a result, the total wave function can be searched for in the form

$$\Psi(\vec{X},\vec{x}) = -\frac{i\sqrt{3}}{4\pi}B_1(\alpha,\beta,\gamma)\,\psi_1(R,\xi,\eta). \quad (9)$$

The adiabatic part $h(\hat{o};R)$ of the Hamiltonian operator (5) [9]

$$h(\hat{o};R) = h_0 + T_R + T_{Coriolis} , \quad (10)$$

where

$$T_R = \frac{1}{2}\left(\frac{J_1^2}{I_1} + \frac{J_2^2}{I_2} + \frac{J_3^2}{I_3}\right) \quad (11)$$

is the Hamiltonian of an asymmetric top with the classical expressions for the principal inertia moments

$$I_1 = I_2 + I_3 = MR^2, \quad I_2 = \frac{1}{2} MR^2 \, (1 + \sqrt{1-\Delta}) \tag{12}$$

and J_i are projections of the total angular momentum $\vec{J}$ in the body-fixed frame. The operator

$$h_0 = -\frac{2}{m} \rho^2 \frac{\hat{a}_{\xi\eta}}{R^2} + V - \frac{3}{2MR^2} \tag{13}$$

includes the nonrotational part of $h(\hat{o}; R)$. In the last expression the differential part is

$$\hat{a}_{\xi\eta} = \frac{1}{\xi^2 - \eta^2} \left[\frac{\partial}{\partial\xi} (\xi^2 - 1) \frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta} (1 - \eta^2) \frac{\partial}{\partial\eta} \right] \tag{14}$$

and all other quantities we need are functions of the coordinates and Jacobi masses

$$\kappa = (m_x - m_y)/(m_x + m_y), \quad \tilde{a} = m/4M,$$

$$\rho = 1 + \tilde{a}(\xi^2 + \eta^2 - 2\kappa\xi\eta + \kappa^2 - 1), \tag{15}$$

$$s = [(\xi^2 - 1)(1 - \eta^2)]^{1/2},$$

$$\Delta = 4\tilde{a}s^2/\rho^2.$$

The total volume element is

$$dv = R^5 \, dR \, \frac{\xi^2 - \eta^2}{\rho^2} \, d\xi \, d\eta \, \sin\beta \, d\alpha \, d\beta \, d\gamma, \tag{16}$$

and V is the potential energy operator. Using the results of [9] we have

$$J_1 B_1 = 0, \quad J_2^2 B_1 = B_1, \quad J_3^2 B_1 = B_1,$$

$$T_{\text{Coriolis}} \, B_1 = 0, \tag{17}$$

$$\langle B_1 | T_R | B_1 \rangle = \frac{2}{mR^2} \rho^2/s^2.$$

Thus, the projected Hamiltonian operator for $(J = 1, p = 1)$ states reads

$$\boldsymbol{H} = -\frac{1}{2M} \frac{1}{R^5} \frac{\partial}{\partial R} R^5 \frac{\partial}{\partial R} + \boldsymbol{h} \tag{18}$$

with the dynamic two-center Hamiltonian operator

$$\boldsymbol{h} = -\frac{1}{2m} \frac{\rho^2}{R^2} \left[\hat{a}_{\xi\eta} - \frac{1}{s^2} \right] + V - \frac{3}{2MR^2}. \tag{19}$$

Next, we use the adiabatic idea and search for the solution of the exact Schrödinger equation

$$(\boldsymbol{H} - E)\, \psi_1(R, \xi, \eta) = 0 \tag{20}$$

in the form

$$\psi_1(R, \xi, \eta) = R^{-5/2} \chi_1(R)\, \phi_1(\xi, \eta; R), \tag{21}$$

where $\phi_1(\xi, \eta; R)$ is the ground state eigenfunction of the eigenproblem

$$[\boldsymbol{h} - \epsilon(R)]\, \phi(\xi, \eta; R) = 0. \tag{22}$$

Six lowest potential curves $\epsilon_i(R)$ defined by this eigenproblem are given in Fig.1. Their particular behaviour justifies

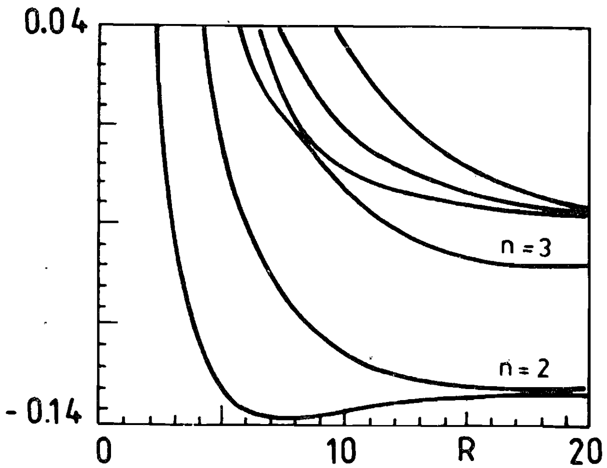

Fig.1. Six lowest hyperspherical adiabatic potentials for abnormal parity states with J = 1, p = 1.

the one-state ansatz (21). Actually, the ground state, which produces minimum at $R \approx 8$, is well separated from the other eigenvalues in that region. The important property of the ground potential curve is that its dissociating limit is $n = 2$ hydrogenic-like state (n stands for the principal quantum number).

Now with the known $\epsilon_1(R)$ and $\phi_1(\xi, \eta; R)$ we get the Schrödinger equation for $\chi_1(R)$

$$[-\frac{d^2}{dR^2} + 2MV_1(R) - 2ME]\chi_1 = 0; \tag{23}$$

where $V_1(R)$ is the effective potential containing the diagonal nonadiabatic correction

$$V_1(R) = \epsilon_1(R) + \frac{1}{2M} < \frac{\partial \phi_1}{\partial R} | \frac{\partial \phi_1}{\partial R} > + \frac{15}{8MR^2}. \tag{24}$$

The diagonal matrix element from (24) is given in Fig.2. The bound state energies (in eV) of the $xy\mu$ molecules are presented in Table 2.

We have obtained for the first time the (J=1,p=1) bound state in all muonic molecules $xy\mu$ where $x,y = p,t$ or d. One-state adiabatic approximation with the asymptotically correct hyperradial adiabatic potential has been used[9]. The nonadiabatic diagonal matrix element was also included into the analysis.

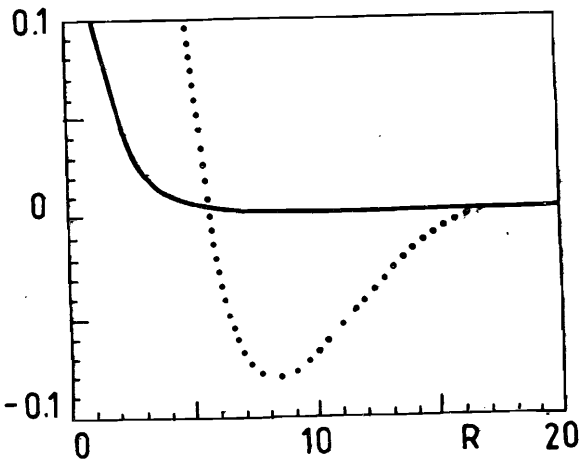

Fig.2. The effective ground (J = 1, p = 1) hyperspherical adiabatic potential (24) and the diagonal matrix element given separately.

Table 2

Abnormal parity bound states (J = 1, p = 1) of $xy\mu$ muonic molecules (in eV)

$tt\mu$	$dt\mu$	$dd\mu$	$pp\mu$	$pd\mu$	$pt\mu$
24	16	20	12	2	0.5

The energies from Table 2 are really the upper bounds of the eigenvalues of the exact Schrödinger equation (20) for (J=1, p = 1) states of the muonic molecules. Now when the question of the existence of the bound states is positively solved, the direct variational solution of the three-dimensional problem (20) should be more adequate in order to get more accurate values of the state energies. Two systems, namely $pd\mu$ and $pt\mu$, have a loosely bound state. One can believe them to play an important role in μCF. This problem will be discussed in the subsequent paper.

Note added in proof:

As we have found, B.P.Carter (Phys.Rev., 1968, 173,p.55) made lower estimates for bound state energies of $xy\mu$ muonic molecules. He used the Born - Oppenheimer $2p\pi$-term without a matrix element. Those estimates are uncertain as he added an arbitrary 1/8 term to simulate approximately the n=2 atomic dissociation limit of the $xy\mu$ system which should depend on the reduced masses. His partial wave analysis is also not exact and misleading. As a result, he used the same $2p\pi$-term to calculate (J = 1, p = 1) and (J = 0, p = 1) states of muonic molecules which was wrong [9]. One should, of course, remember that his paper was published 20 years ago.

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Исихара Т. и др. E4-88-849

Новая серия в спектрах мюонных молекул

Для мюонных молекул впервые рассчитаны связанные состояния с аномальной четностью. Две системы, $pd\mu$ и $pt\mu$, имеют слабосвязанное состояние.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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A New Series in Spectra of Muonic Molecules

Abnormal parity bound states of muonic molecules are calculated for the first time. Two molecules $pd\mu$ and $pt\mu$ have a loosely bound state.

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

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