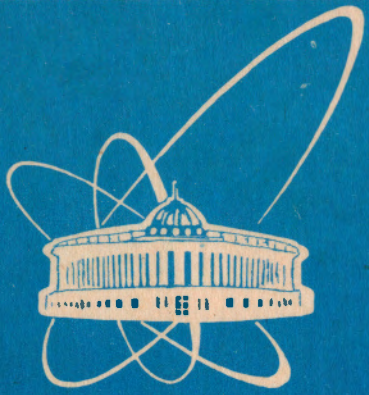

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BINDING ENERGIES AND NONRADIATIVE DECAY RATES OF *Hedμ*-MOLECULAR IONS

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Расчет энергии связи и скорости безызлучательного перехода мезомолекулярных ионов $Hed\mu$

Метод «поверхностных» гиперсферических функций применен к расчету собственных значений и собственных функций мезомолекулярных ионов $^{3,4}Hed\mu$. Получены энергии связи и скорости безызлучательного распада для состояний с полным угловым моментом $L = 0,1,2$.

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

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Binding Energies and Nonradiative Decay Rates of $Hed\mu$-Molecular Ions

The method of hyperspherical «surface» functions has been applied to the calculation of eigenvalues and eigenfunctions of muonic molecular ions $^{3,4}Hed\mu$. Binding energies and nonradiative decay rates for the states of the total angular momentum $L = 0,1,2$ have been obtained.

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

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I. INTRODUCTION

The reasons for investigation of the charge-nonsymmetric muonic molecules like $HeH\mu$ are as follows. First, a direct charge-exchange reaction from the ground-state muonic hydrogen atom to helium nuclei is suppressed, the transfer proceeds through the formation of the molecule in the intermediate state. Hence, the kinetics of muons in media is defined to a large extent by the probability of this process. Indeed, the role of the formation of a muonic molecule in a charge-exchange reaction was confirmed in a number of experiments [1], [2], [3], [4].

The measurement of the yield of γ-rays due to the decay of the $Hed\mu$ molecules [5], [6] revives interest in the investigation of this system. The experiment gives evidence of an additional nonradiative decay channel. This possibility was discussed in papers [7], [8], [9].

Next, eigenenergies of both usual molecules of media and muonic molecules, as it follows from the results of [10], [11], are comparable. For this reason one can expect an active interaction of muonic molecules with media.

As soon as the charge-nonsymmetric molecules are produced, the possibility of nuclear transitions arises. The investigation of a nuclear reaction at typical mesomolecular energies has a fundamental importance due to absence of any experimental data on the strong interaction of charged particles in this energy range.

Qualitatively properties of the $HeH\mu$ system are defined as follows. Coulomb interaction is not able to bind the systems under consideration due to the repulsion in the $He\mu + H$ channel. Only a 3−body resonant state can be formed. States like that are supported by the attractive polarization potential in the $H\mu + He$ channel and therefore are clustered.

The goal of this paper is to perform systematical calculations of energy levels and nonradiative decay rates of the $^{3,4}Hed\mu$ systems for all possible values of the

total angular momentum. Only the transition to the channel with the $He\mu$ atom in the ground state has been considered. Transitions from the molecular states with $L = 1, 2$ to the channels with the $He\mu$ atom in the $2s, 2p$ states will be suppressed due to exponentially small overlapping of the initial and final state wave-functions.

The treatment of this problem met essential difficulties due to necessity to describe the Coulomb three-body system above the two-body threshold. Some approaches to describing these systems have been applied in [11], [7], [8], [9].

The approach, using the hyperspherical "surface" functions method [12], [13] has been applied in this paper. The following advantages of this method in treating the posed problems can be mentioned. The method operates with a discrete set of coupled one-dimensional differential equations. Physical boundary conditions for their solution can be easily formulated. Moreover, coupling of channels turns out to be rather small in our case and allows one to use the decoupled one-level approximation. It is worthwhile to mention the analogous calculation of the $LiH\mu$ and $BeH\mu$ molecules [14].

The article is organized in the following way. The description of the method will be given in the next section, section 3 contains numerical results, section 4 - discussion and conclusion.

II. METHOD

The Hamiltonian of three charged particles in the Jacobi variables is:

$$H = -\Delta_{\mathbf{x}_i} - \Delta_{\mathbf{y}_i} + \sum_{s=1}^{3} \frac{q_s}{x_s}, \tag{1}$$

where

$$\mathbf{x}_i = \sqrt{\frac{m_k m_j}{m(m_k + m_j)}}(\mathbf{r}_k - \mathbf{r}_j),$$
$$\mathbf{y}_i = \sqrt{\frac{m_i(m_k + m_j)}{m(m_i + m_k + m_j)}}(\mathbf{r}_i - \frac{m_j \mathbf{r}_j + m_k \mathbf{r}_k}{m_j + m_k}), \tag{2}$$

$$q_i = 2Z_j Z_k \sqrt{\frac{m_k m_j}{m(m_k + m_j)}}. \tag{3}$$

$\mathbf{r}_i, m_i, Z_i$ - coordinate, mass and charge of the i-th particle. $\hbar^2/(me^2)$, $me^4/(2\hbar^2)$ have been used as length and energy units. Here m is arbitrary mass and was taken equal to the muonic mass. For definiteness muon, hydrogen nucleus and nucleus of the charge Z have been enumerated as particles with number 1, 2 and 3.

Coordinates ρ, α_i, θ_i have been introduced by the relations

$$x_i = \rho cos\frac{\alpha_i}{2},$$
$$y_i = \rho sin\frac{\alpha_i}{2},$$
$$cos\theta_i = \frac{(\mathbf{x}_i \cdot \mathbf{y}_i)}{x_i y_i}, \tag{4}$$
$$0 \leq \alpha_i, \theta_i \leq \pi.$$

Below the notation Ω will be used for an arbitrary pair α_i, θ_i.

Since the systems have two heavy and one light particles, it is reasonable to assume that the main part of the total angular momentum is carried by the pair of heavy particles. This is reason why the following form of the solution of the Schrödinger equation has been used:

$$\Psi_{LM}(\mathbf{x}, \mathbf{y}) = Y_{LM}(\hat{\mathbf{x}}_1)\Phi_L(\rho, \Omega). \tag{5}$$

Obviously, this form of the wave function is exact for $L = 0$.

Under the representation (5) the Schrödinger equation for the states with total angular momentum L takes the form:

$$[-\frac{1}{\rho^5}\frac{\partial}{\partial\rho}(\rho^5\frac{\partial}{\partial\rho})-\frac{4}{\rho^2}\Delta_\Omega+\sum_{s=1}^{3}\frac{q_s}{x_s}-E]\Phi_L(\rho,\Omega)=0, \tag{6}$$

where

$$\Delta_\Omega=\frac{1}{sin^2\alpha_i}[\frac{\partial}{\partial\alpha_i}(sin^2\alpha_i\frac{\partial}{\partial\alpha_i})+\frac{1}{sin\theta_i}\frac{\partial}{\partial\theta_i}(sin\theta_i\frac{\partial}{\partial\theta_i})]-\frac{L(L+1)}{4cos^2\alpha_1}. \tag{7}$$

Following [12] and [13] "surface" functions $\varphi_n(\Omega;\rho)$ can be introduced as finite solutions of the equation:

$$[\Delta_\Omega-\frac{\rho^2}{4}\sum_{s=1}^{3}\frac{q_s}{x_s}+\lambda_n(\rho)]\varphi_n(\Omega;\rho)=0. \tag{8}$$

Expanding the solution of the equation (6) onto the set of the hyperspherical "surface" functions:

$$\Phi_L(\rho,\Omega)=\rho^{-5/2}\sum_n u_n(\rho)\varphi_n(\Omega;\rho), \tag{9}$$

one immediately comes to the system of one-dimensional equations

$$[\frac{d^2}{d\rho^2}-\frac{15}{4\rho^2}-\varepsilon_n(\rho)+E]u_n(\rho)+$$
$$\sum_i[Q_{ni}(\rho)\frac{d}{d\rho}+\frac{d}{d\rho}Q_{ni}(\rho)-P_{ni}(\rho)]u_i(\rho)=0, \tag{10}$$

where

$$Q_{ni}(\rho)=\langle\varphi_n|\frac{\partial}{\partial\rho}\varphi_i\rangle, \tag{11}$$

$$P_{ni}(\rho)=\langle\frac{\partial}{\partial\rho}\varphi_n|\frac{\partial}{\partial\rho}\varphi_i\rangle, \tag{12}$$

$$\varepsilon_n(\rho)=\frac{4}{\rho^2}\lambda_n(\rho). \tag{13}$$

$\langle\cdot|\cdot\rangle$ means the integration on the hypersphere over $d\Omega=sin^2\alpha_i d\alpha_i dcos\theta_i$.

One of the most complicated problems of this approach is the computation of $Q_{ni}(\rho)$ and $P_{ni}(\rho)$, defined in (11) and (12). By this reason, the following exact expressions have been used:

$$Q_{ni}=-\frac{\rho}{4}(\lambda_i-\lambda_n)^{-1}\langle\varphi_n|\sum_{s=1}^{3}\frac{q_s}{x_s}|\varphi_i\rangle, \tag{14}$$

$$P_{ni}=-(Q^2)_{ni}. \tag{15}$$

The form (14), (15) allow one to avoid the calculation of the derivatives of the "surface" functions on the parameter ρ and use only already known matrix elements $V_{ni}(\rho)$ and eigenvalues $\lambda_i(\rho)$ of equation (8).

The variational approach has been applied to solve equation (8). The "surface" functions have been chosen as a linear combination of trial functions from the following set:

$$\begin{aligned}&\phi_{nl}^{(\sigma)}(\alpha_\sigma)P_l(cos\theta_\sigma),\quad \sigma=2,3,\\&sin^l\alpha_3 C_{n-l-1}^{l+1}(cos\alpha_3)P_l(cos\theta_3),\\&n>0,\ n>l\geq 0,\end{aligned} \tag{16}$$

where

$$\begin{aligned}&\phi_{nl}^{(\sigma)}(\alpha)=R_{nl}(\frac{|q_\sigma|}{n}\rho cos\frac{\alpha}{2}),\\&R_{nl}(t)=exp(-t/2)t^l L_{n-l-1}^{2l+1}(t)\end{aligned} \tag{17}$$

In equations (16) and (17) $P_l(x)$; $L_m^k(x)$, $C_n^m(x)$ are the Legendre, Laguerre and Gegenbauer polynomials. The set of trial functions has been chosen in the form (16) in order to describe properly the three-body wave-function at both large and small interparticle distances. The first line of (16) will describe the system separated into two clusters. In this case, one of the clusters is a hydrogen-like atom and hydrogen-like functions (17) will be proper trial functions. The second line of (16) will describe the configuration with all three particles close to each other. In this case, the centrifugal term in (6) dominates and eigenfunctions of the operator (7) are used. The set of trial functions (16)can be easily adjusted to the different values of the parameter ρ. For this purpose numbers of channel-type functions and hyperspherical harmonics have

been changed with changing ρ. It is necessary to emphasize that the dependence of the numbers of the trial functions on the parameter ρ has not been exploited in analogous calculations. This dependence gives rise to more flexibility of the basis and allows one to avoid numerical instabilities when solving equation (8).

As a result of the solution of equation (8) eigenpotentials $\varepsilon_n(\rho)$, $Q_{12}(\rho)$, $P_{12}(\rho)$ have been obtained. The properties of mesomolecules and transition rates are mostly defined by the specific form of the effective potentials $\varepsilon_n(\rho)$. The lowest effective potential $\varepsilon_1(\rho)$ describes asymptotically the decay channel $H + He\mu$ and is repulsive at all ρ values. The next effective potential $\varepsilon_2(\rho)$ describes asymptotically the channel $He + H\mu$. As it was already mentioned this potential has an attractive part and supports the resonant state we are interested. $Q_{12}(\rho)$ and $P_{12}(\rho)$ give rise coupling of channels. In case of small coupling energy levels of $^4Hed\mu$ and $^3Hed\mu$ will be found as eigenvalues of the equation:

$$[\frac{d^2}{d\rho^2} - \frac{15}{4\rho^2} - \varepsilon_2(\rho) - P_{22}(\rho) + E]u_2(\rho) = 0 \tag{18}$$

for zero boundary conditions

$$u_2(0) = u_2(\infty) = 0. \tag{19}$$

Analogously the continuum wave-function has been found in the one-level approximation as a solution of the equation:

$$[\frac{d^2}{d\rho^2} - \frac{15}{4\rho^2} - \varepsilon_1(\rho) - P_{11}(\rho) + E]u_{1k}(\rho) = 0 \tag{20}$$

for the following boundary and asymptotic conditions:

$$\begin{aligned} u_{1k}(0) &= 0, \\ u_{1k}(\rho) &\underset{\rho\to\infty}{\longrightarrow} sin(k\rho + \delta), \end{aligned} \tag{21}$$

where $k = (E - \varepsilon_1(\infty))^{1/2}$ and phase δ is of no interest for our purposes. The radiationless decay rate is given by

$$\lambda = \frac{1}{k}|M_k|^2 \cdot \frac{me^4}{\hbar^3}s^{-1}, \tag{22}$$

where the matrix element of the channel coupling operator is

$$M_k = \int_0^\infty d\rho u_{1k}(\rho)[Q_{12}(\rho)\frac{d}{d\rho} + \frac{d}{d\rho}Q_{12}(\rho) - P_{12}(\rho)]u_2(\rho). \tag{23}$$

III. NUMERICAL RESULTS

The following values of the masses were used in calculations: $m_\mu = 206.769m_e$, $m_d = 3670.481m_e$, $m_{^4He} = 7294.295m_e$, $m_{^3He} = 5495.881m_e$. Equation (8) has been solved for a number of ρ values in the interval $0 \le \rho \le 45$. Variations of the upper bound of this interval do not change final results. Expressions (13)-(15) have been used to calculate $\varepsilon_n(\rho), Q_{ni}(\rho), P_{ni}(\rho)$ for these ρ values. The set of trial functions (16) has been adjusted in the following way: numbers of channel-type functions N_1 and hyperspherical harmonics N_2 were chosen as:

$$\begin{aligned} &N_1 = 2,\ N_2 = 105, && \rho \le 5; \\ &N_1 = 6,\ N_2 = 91, && 5 < \rho < 7; \\ &N_1 = 6,\ N_2 = 105, && 7 < \rho \le 15; \\ &N_1 = 12,\ N_2 = 78, && 15 < \rho. \end{aligned} \tag{24}$$

The relative accuracy of two lowest eigenpotentials $\varepsilon_1(\rho), \varepsilon_2(\rho)$ calculated in the above mentioned interval of ρ can be estimated as 10^{-4}. For the $Q_{12}(\rho), P_{11}(\rho), P_{12}(\rho), P_{22}(\rho)$ the estimate of the relative accuracy is 10^{-2}. Mesomolecular binding energies E_L and radiationless decay rates λ_L for angular momentum values $L = 0, 1, 2$ have been calculated as described in the previous section.

The integrand in (23) contains the rapidly oscillating function $u_{1k}(\rho)$, the sharp functions $u_2(\rho), Q_{12}(\rho), P_{12}(\rho)$ and their derivatives. In consequence of these facts, special care has been taken of the evaluation of this integral. For this purpose,

$u_2(\rho), Q_{12}(\rho)$ and $P_{12}(\rho)$ were expressed as a product of sharp functions given in the analytical form and of smooth functions given numerically. A few per cent variation of decay rates was found when using different ways for analytical representation of sharp functions.

The calculated values of the binding energies $E_{BL} = E_{d\mu} - E_L$ and decay rates for the $^{3,4}Hed\mu$ systems are presented in Table 1 in comparison with the results of other authors.

Table 1

system		[7]	[11]	[8]	[9]	present
$^4Hed\mu$	E_{B0}			77.96	78.7	77.49
	E_{B1}	58.22	57.84	56.10	57.6	55.74
	E_{B2}				20.3	17.47
	λ_0			2.3	1.85	0.73
	λ_1	1.67		2.4	1.38	1.20
	λ_2				0.9	1.04
$^3Hed\mu$	E_{B0}		70.74	69.96	70.6	69.37
	E_{B1}	48.42	47.90	46.75	48.2	46.31
	E_{B2}				9.6	7.11
	λ_0			8.0	3.58	2.87
	λ_1	5.06		7.0	2.77	3.22
	λ_2				1.54	1.74

Table 1. Binding energies E_{BL} (eV) and decay rates λ_L $(10^{11}s^{-1})$ of the systems $^{3,4}Hed\mu$ calculated in Ref. [7], [8], [9], [11] and in the present paper.

IV. DISCUSSION

From Table 1 it is clear that binding energies for a given L are close to each other in all calculations. One can see that energies of the present paper are higher in comparison with calculations [7] and [11]. The method of this work gives an upper bound of eigenenergy if the coupling of channels is omitted. One can conclude that this fact supports the validity of the one-level approximation in our approach.

The comparison with the results obtained in the framework of the Born-Oppenheimer approximation ([8], [9]) cannot be done straightforwardly due to the following reasons. First, mass values and thresholds are introduced in these calculations *ad hoc* and do not coincide with the physical ones. The importance of these procedures for the calculation of the decay rate is not clear. Unlike the eigenenergy problem, the calculation of the decay rate is very sensitive to the fine details of wave-functions, as is clear from expression (23). The quasiclassical approximation used in the calculation of the decay rate in the paper ([9]) can be an origin of an additional uncertainty.

Qualitatively, all calculations support the strong isotopic dependence of the decay rates observed in experiment ([5], [6]) Nevertheless, the calculated values are quite different and consistency of theoretical results should be reached.

It is accepted that the formation of $Hed\mu$ molecules takes place in the state with $L = 1$. In this connection, for comparison with experiment, the most important is the ratio $\lambda_\gamma/(\lambda_\gamma + \lambda_1)$, where λ_γ is the radiative decay rate from the molecular state $L = 1$. Using λ_γ from the paper [11] and the present values of λ_1, one comes to the ratio $\lambda_\gamma/(\lambda_\gamma + \lambda_1) = 0.585$ for $^4Hed\mu$ and $\lambda_\gamma/(\lambda_\gamma + \lambda_1) = 0.325$ for the $^3Hed\mu$ systems. Other processes, which may be important in the experiment, are collisional transitions to the muonic molecular states with angular momentum $L \neq 1$.

Finally, one would like to emphasize the necessity of the systematic study in the framework of the same approach of the processes involved in the formation, rear-

rangement and decay of systems under consideration.

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