Calculation of the energy levels of hydrogen mesic molecules by taking into account adiabatic corrections for nuclear motion

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The binding energy of all known vibrational levels of the hydrogen mesic molecules $pp\mu$, $dd\mu$, $tt\mu$, $pd\mu$, $pt\mu$, and $dt\mu$ are calculated. A new vibrational level $v = 1$ with a low binding energy $\epsilon = 0.7$ eV is found for the $dd\mu$-mesic molecule in the state with an angular momentum $L = 1$. First-order adiabatic corrections to the nuclear motion are taken into account in the calculations.

INTRODUCTION

The calculation of the binding energies of the mesic molecules has been the subject of quite a large number of papers, which can be divided into two groups: variational[1] and adiabatic[2] computations. Variational calculations are apparently preferable when computing the binding energies of the ground state of mesic molecules, but they become unduly complicated when we go over to the excited states. The advantages of the adiabatic calculations lie in their clearness and in the uniformity of the computations both in the case of the ground state and in the case of the excited states.

The most recent adiabatic calculations of the binding energies of mesic molecules were performed in the period 1960–1962 and the adiabatic corrections for the motion of the nuclei were in these calculations either not taken into consideration at all, or they were only approximately allowed for. The necessary corrections have been accurately computed in a number of papers[3,4] in the past years, and this allows us to return to the formulated problem at a new level. In the present paper we find the energies of all the known vibrational states of the mesic molecules of the hydrogen isotopes: ppμ, ddμ, ttμ, pdμ, ptμ, and dtμ, with exact allowance for the first-order adiabatic corrections. In the course of these calculations we discover in the system ddμ a new state with a very low binding energy ($\epsilon \approx 0.7$ eV). These results are obtained with the aid of the new algorithm of solving eigenvalue problems that has been described in a previous paper by the authors[5].

FORMULATION OF THE PROBLEM

The energy levels E of the mesic molecules can be found with allowance for the first-order adiabatic corrections from the system of equations[2,6]

$$\begin{gathered}-\frac{1}{2M}\frac{d^2\chi_g}{dR^2}+\left[\frac{1}{R}+\frac{L(L+1)}{2MR^2}+E_g(R)+\frac{1}{2M}K_{gg}(R)\right]\chi_g\\+\frac{1}{2M}\left[K_{gu}(R)-\frac{2Q_{gu}(R)}{R}\right]\chi_u+\frac{1}{M}Q_{gu}(R)\frac{d\chi_u}{dR}=E\chi_g,\\-\frac{1}{2M}\frac{d^2\chi_u}{dR^2}+\left[\frac{1}{R}+\frac{L(L+1)}{2MR^2}+E_u(R)+\frac{1}{2M}K_{uu}(R)\right]\chi_u\\+\frac{1}{2M}\left[K_{ug}(R)-\frac{2}{R}Q_{ug}(R)\right]\chi_g+\frac{1}{M}Q_{ug}(R)\frac{d\chi_g}{dR}=E\chi_u.\end{gathered}\tag{1}$$

The matrix elements of the operators of the nuclear motion

$$\begin{gathered}K_{gu}(R)=\int d\mathbf{r}\,\varphi_g(\mathbf{r};R)\,(-\Delta_{\mathbf{R}})\,\varphi_u(\mathbf{r};R),\\Q_{gu}(R)=\frac{\mathbf{R}}{R}\int d\mathbf{r}\,\varphi_g(\mathbf{r};R)\,(-\nabla_{\mathbf{R}})\,\varphi_u(\mathbf{r};R)\end{gathered}\tag{2}$$

are taken between the wave functions of the two-nucleus problem, $\varphi_g(\mathbf{r};R)$ and $\varphi_u(\mathbf{r};R)$ being the symmetric and antisymmetric solutions of the problem, while $E_g(R)$ and $E_u(R)$ are the terms which correspond to these solutions[7] and which go over, as $R \to \infty$, into the level 1sσ of the isolated hydrogen atom. Equations (1) have been written in a system of units in which $e = \hbar = m = 1$, where

$$\begin{gathered}\frac{1}{m}=\frac{1}{M_3}+\frac{1}{M_1+M_2};\\\frac{1}{M}=m\left(\frac{1}{M_1}+\frac{1}{M_2}\right)=\frac{M_3(M_1+M_2)^2}{M_1M_2(M_1+M_2+M_3)};\end{gathered}\tag{3}$$

M_3 is the mass of the μ^- meson; M is the reduced mass of the nuclei in units of m; M_1 and M_2 are the nuclear masses of the hydrogen isotopes. We shall assume, without loss of generality, that $M_1 \leq M_2$.

For $R \to \infty$, when the three-particle system breaks up into a mesic atom and a nucleus, the internal states of the mesic atoms with the nuclei M_1 and M_2 are respectively described by the wave functions[2]

$$\varphi_1=(\varphi_g-\varphi_u)/\sqrt{2},\quad \varphi_2=(\varphi_g+\varphi_u)/\sqrt{2}.\tag{4}$$

The transformation (4) generates a similar transformation of the functions χ_g and χ_u, which describe the relative motion of the nuclei, and the corresponding transformation of the matrix elements (2)[6]. Taking into account the equalities[4]

$$\begin{gathered}K_{gu}(R)=H_{gu}(R)+\frac{2Q_{gu}(R)}{R}+\frac{dQ_{gu}(R)}{dR};\\H_{gu}(R)=H_{ug}(\mathrm{R})=\int d\mathbf{r}\,\nabla_{\mathbf{R}}\varphi_g(\mathbf{r};R)\,\nabla_{\mathbf{R}}\varphi_u(\mathbf{r};R),\\Q_{gu}(R)=-Q_{ug}(R),\quad Q_{gg}(R)=Q_{uu}(R)\equiv 0\end{gathered}\tag{5}$$

we can reduce the transformation (4) to the following system of equations for the functions χ_1 and χ_2:

$$\chi_i''-2M[\varepsilon_i+V_i(R)-V_i(\infty)]\chi_i=V_{ij}(R)\chi_j+2Q_{ij}(R)\chi_j',\tag{6}$$

where $\epsilon_i = V_i(\infty) - E$ is the mesic-molecule binding energy reckoned from the value $V_i(\infty)$, while the effective potentials are determined by the following relations (the upper and lower signs correspond to the values i = 1 and i = 2):

$$\begin{gathered}V_i(R)=\frac{1}{R}+\frac{L(L+1)}{2MR^2}+\frac{1}{2}[\tilde{E}_g(R)+\tilde{E}_u(R)]\mp\frac{1}{2M}H_{gu}(R),\\V_{ij}(R)=M[\tilde{E}_g(R)-\tilde{E}_u(R)]+\frac{dQ_{ij}(R)}{dR},\\\tilde{E}_g(R)=E_g(R)+\frac{1}{2M}H_{gg}(R),\ \tilde{E}_u(R)=E_u(R)+\frac{1}{2M}H_{uu}(R),\\Q_{12}(R)=Q_{gu}(R)=-Q_{21}(R).\end{gathered}\tag{7}$$

The structure of the matrix elements have the following form:

$$H_{\alpha\beta}(R)=H_{\alpha\beta}^{(+)}(R)+\varkappa H_{\alpha\beta}^{(-)}(R)+\varkappa^2 H_{\alpha\beta}^{(\bullet)}(R),\qquad \varkappa=(M_2-M_1)/(M_2+M_1). \tag{8}$$

In the symmetric case of equal nuclear charges

$$H_{gg}^{(-)}(R)=H_{uu}^{(-)}(R)=H_{gu}^{(+)}(R)=H_{gu}^{(\bullet)}(R)=Q_{gu}^{(+)}(R)\equiv 0, \tag{9}$$

while for the remaining matrix elements the asymptotic relations

$$\begin{gathered}H_{gg}^{(+)}(\infty)=H_{gg}^{(\bullet)}(\infty)=H_{uu}^{(+)}(\infty)=H_{uu}^{(\bullet)}(\infty)=-{}^1/_2E_g(\infty)=-{}^1/_2E_u(\infty),\\ H_{gu}^{(-)}(\infty)=H_{ug}^{(-)}(\infty)=E_g(\infty)=E_u(\infty)=-{}^1/_2\end{gathered} \tag{10}$$

are valid (the last equality is valid only for the ground state).

The quantities (7) and (8), which were computed earlier[3,4], are shown in Fig. 1. The values of $V_i(\infty)$ are equal to the energies of the corresponding mesic atoms in the adiabatic approximation. Using the results of the investigations[4,6,8], we can verify that

$$V_i(\infty)=-{}^1/_2[1-(\varkappa\pm 1)^2/4M] \tag{11}$$

and that it coincides with the true energy of the isolated mesic atoms up to terms of order M_3/M_i inclusively. Indeed, by taking into account the equalities (7)—(10) and going over to the mesoatomic units $e = \hbar = M_3 = 1$, we obtain

$$V_i(\infty)=-\frac{m}{2}\left[1-\frac{m}{4M}(\varkappa\pm 1)^2\right]=-\frac{1}{2}\left[1-\frac{1}{M_i}+O(M_i^{-2})\right]. \tag{12}$$

RESULTS OF THE COMPUTATIONS

In Tables I and II we present the results of the computations of the binding energies ϵ_{Lv} of the mesic hydrogen molecules for all their possible vibrational quantum states v associated with a given orbital angular momentum L. The values ϵ_{Lv} are given in eV1). The binding energies of the mesic molecules with different nuclei (pdμ, ptμ, and dtμ) are reckoned from the ground-state energy level of the heavier mesic atom (dμ and tμ), i.e., from the value of $V_2(\infty)$. Accordingly, in Eqs. (6), we should set $\epsilon_2 = \epsilon_{Lv}$ and $\epsilon_1 = \epsilon_{Lv} + V_1(\infty) - V_2(\infty) = \epsilon_{Lv} + \kappa/2M$. The results of other investigations have also been recalculated in accordance with these conditions and presented in the Tables. For the recalculation, we used the latest data on the fundamental constants and the values of the particle masses[11] (see Table III).

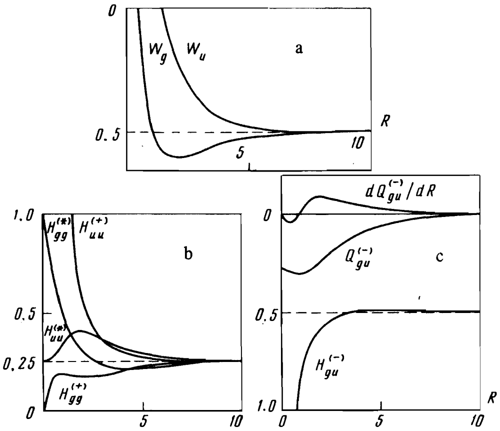

FIG. 1. a—Terms of the two-nucleus problem with allowance for the Coulomb repulsion between the nuclei: $W_g = 1/R + E_g(R)$ is the symmetric case and $W_u = 1/R + E_u(R)$ the antisymmetric case. b,c—Matrix elements of the nuclear-motion operators taken between the two-nucleus problem wave functions and given by the relations (2) and (8).

Mesic molecule	L = 0		L = 1		L = 2 v = 0	L = 3 v = 0	Method of computation
	v = 0	v = 1	v = 0	v = 1			
ppμ	253 [9]	—	107,23 [10]	—	—	—	Variational
	248	—	102	—	—	—	Present work
ddμ	324.2 [9]	32.7 [9]	226.55 [10]	—	—	—	Variational
	323	32.9	224	0.7	83.6	—	Present work
ttμ	361.2 [9]	75 [9]	288.72 [10]	—	—	—	Variational
	361	81.4	288	43.1	171	46.7	Present work

TABLE II. The binding energies ϵ_{Lv}(eV) of mesic hydrogen molecules with different nuclei

Mesic molecule	L = 0		L = 1, v = 0	L = 2, v = 0	Method of computation
	v = 0	v = 1			
pdμ	221.2 [9]	—	—	—	Variational
	214	—	89.7	—	Present work
ptμ	212.8 [9]	—	—	—	Variational
	206	—	91.1	—	Present work
dtμ	318.1 [9]	32.9 [9]	—	—	Variational
	317	31.7	230	99.3	Present work

Note. The binding energies ϵ_{Lv} are given in eV and are reckoned from the ground-state energy level of the heavier hydrogen isotope, i.e., from the $E_{d\mu}$ level for the molecule pdμ and from the $E_{t\mu}$ level for the molecules ptμ and dtμ (see Table III).

For the molecule ppμ, there are two possible bound states: L = 0, v = 0 and L = 1, v = 0, while for the molecule ddμ there are five: two (v = 0 and v = 1) in the state with L = 0, two (v = 0 and v = 1) in the state with L = 1, and one state with the quantum numbers L = 2, v = 0.

For the molecule ttμ there are six possible quantum states: two vibrational levels (v = 0 and v = 1) in each of the states with the orbital angular momenta L = 0 and L = 1 and one level with v = 0 in each of the states with L = 2 and L = 32).

In Table II we present the binding energies of the molecules with different nuclei: of two pdμ and ptμ states with the quantum numbers (L = 0, v = 0) and (L = 1, v = 0) and of four dtμ states: two vibrational levels (v = 0 and v = 1) in the state with the orbital angular momentum L = 0 and one level (v = 0) in each of the states with L = 1 and L = 2. Some of them have been computed for the first time in the present work.

The computation of the binding energy of the mesic molecule ddμ in the state (L = 1, v = 1) requires special mention. The existence of this level was assumed by Belyaev et al. and by Zel'dovich and Gershteĭn in their investigations[2] and was recently demonstrated in[12]. The computed value $\epsilon_{11} = 0.7$ eV is in good agreement with the value that is necessary for the explanation of the experiments designed to measure the rate of production of ddμ molecules at different temperatures[13]. The potentials

$$V_g(R)=\frac{1}{R}+\frac{L(L+1)}{2MR^2}+E_g(R)$$

and the energy-level diagram for this case are shown in Fig. 2 and the plots of the wave functions χ_{Lv} for the states (L = 1, v = 0) and (L = 1, v = 1) are shown in Fig. 3.

In computing ϵ_{Lv} from (6), we used the terms $E_g(R)$ and $E_u(R)$, as well as the corresponding matrix elements $H_{gg}(R)$, $H_{gu}(R)$, etc., obtained with the aid of the algorithm expounded in[3,4]. Other details and distinctive features of the calculations can be found in our papers[5,14].

TABLE III. The principal characteristics of the mesic hydrogen atoms.

	Nuclear mass in units of the electron mass	Ground-state energy of mesic atom		Nuclear mass in units of the electron mass	Ground-state energy of mesic atom
μ	206,769		d	3670.398	2663.23
p	1836,109	2528.52	t	5496.753	2711,27

Notes. The mesoatomic unit of energy ϵ_μ = 5626.53 eV. The mesoatomic unit of length $a_\mu = 2.55927 \times 10^{-11}$ cm. The cited quantities were computed on the basis of Taylor, Parker, and Landenberg's and Selinov's data [11].

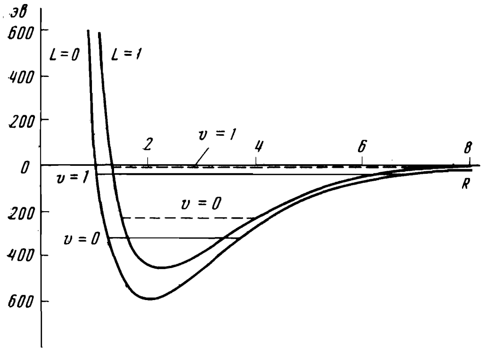

FIG. 2. Effective potentials $V_i(R)$ of the nuclear motion of the mesic molecule ddμ in the states with the orbital angular momenta L = 1 and L = 0. The positive maximum of the potential $V_i(R)$ in the state with L = 1 is located at the distance R = 11.4. In the units of the problem, e = ħ = m = 1, the depth of the well D = 0.0824 and the binding-energy values $\epsilon_{10} = 0.4099$ and $\epsilon_{11} = 1.3 \times 10^{-4}$.

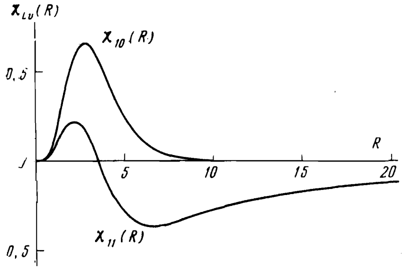

FIG. 3. Wave functions of the vibrational levels v = 0 and v = 1 of the mesic molecule ddμ in the state with the orbital angular momentum L = 1.

ESTIMATE OF THE ACCURACY OF THE RESULTS

The error in the adiabatic calculations that take into account the corrections $\sim M_3/M_i$ for the nuclear motion is usually assumed to be equal to the ratio $(M_3/M_i)^2$. It is, in order of magnitude, equal to the error in the determination of the energy reference point $V_i(\infty)$ and, for the mesic hydrogen molecules, it constitutes 10^{-3}—10^{-2} of the depth D ≈ 500 eV of the effective potentials $V_i(R)$. Comparison with the latest variational calculations confirms this conclusion (Tables I and II). In some cases the accuracy of the computations is slightly higher than the above-cited upper bound and improves as the ratio M_3/M_i decreases. On the whole, the comparison carried out attests to the correctness of the adiabatic calculations both in the case of the ground state and in the case of the excited states of the mesic molecules, for which latter case the corresponding variational calculations have not yet, for the most part, been carried out.

In conclusion, we note that to raise the accuracy of the adiabatic calculations, we can use the existing regular method[6], which allows us to more accurately determine the potentials $V_i(R)$ up to terms of order $(M_3/M_i)^2$ inclusively. This method requires, however, long preliminary computations of the higher terms of the two-nucleus problem and the corresponding matrix elements, and we do not intend to discuss here the details of its realization. One of the methods by which the corrections $\sim (M_3/M_i)^2$ can be partially taken into account is investigated in[14].

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1) The scaling factor β for the conversion of the values of ϵ_{Lv} in the units e = ħ = m = 1 of the problem to its values in eV ($\epsilon_{Lv}(\text{eV}) = \beta\epsilon_{Lv}$) is equal to $\beta = \frac{m}{m_e} 2\text{Ry} = \frac{M_3(M_1 + M_2)}{m_e(M_1 + M_2 + M_3)} \times 27.211652$ eV, where m_e is the electron mass.

2) In the case of equal masses $M_1 = M_2$, the quantities $K_{gu}(R) = Q_{gu}(R) \equiv 0$, and the system (1) breaks up into two independent equations. The binding energy $\epsilon_{Lv} = \tilde{E}_g(\infty) - E$ is then determined from the equation for the function χ_g. Of course, the values of ϵ_{Lv} can equally well be found in this case from the system (6).

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