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Continuous Analog of Newton's Method as Applied to the Calculation of the Binding Energy of Mesic Molecules

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On the basis of the continuous analog of Newton's method, a method of numerical solving of Sturm–Liouville's problem is suggested, which has some advantages compared with the hitherto known ones. This method is used for calculating the binding energies of all the vibrational states of the mesic molecules $pp\mu$, $dd\mu$ and $tt\mu$. In particular, one has first succeeded in calculating the binding energy of the highly excited level with $L = 1$, $v = 1$ of the mesic molecule $dd\mu$ which is important for interpreting experimental data.

1. INTRODUCTION

The calculation of the binding energy of mesic molecules has been performed in many papers which may be divided into two groups: variational calculations [1] and adiabatic calculations [2]. The variational methods appear to be more preferable for the calculation of the ground state energies. The adiabatic calculations are more usual and, thus, are uniform for both the ground and excited states. In the present paper all the vibrational states of the mesic molecules $pp\mu$, $dd\mu$, and $tt\mu$ are calculated taking into account adiabatic corrections to nuclear motion.

In the adiabatic approximation the problem of the calculation of the binding energy of the mesic molecules with equal nuclei reduces to finding the eigenvalues ϵ_{Lv} for the Schroedinger equation describing the molecule in a vibrational stat v with orbital momentum L [2]

$$\frac{d^2\chi_{Lv}(R)}{dR^2} + 2M\left[\epsilon_{Lv} - (\tilde{E}_g(R) - \tilde{E}_g(\infty)) - \frac{1}{R} - \frac{L(L+1)}{2MR^2}\right]\chi_{Lv}(R) = 0, \tag{1}$$

where

$$2M = \frac{2M_1 + \mu}{2\mu}, \qquad \tilde{E}_g(R) = E_g(R) + \frac{1}{2M}K_{gg}(R)$$

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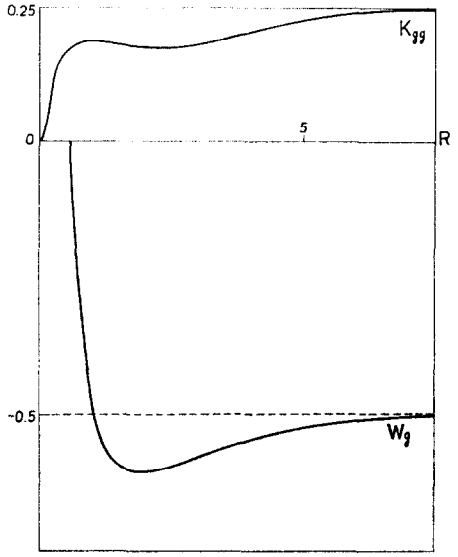

FIG. 1. Diagrams of the symmetric term for the two-center problem $W_g = E_g(R) + 1/R$ and the diagonal element $K_{gg}(R)$ by means of which the effective potential $q(R)$ of the boundary value problem (3a) is formed.

M_1, μ are the masses of the nuclei and the μ meson, respectively, $E_g(R)$ is the symmetric term of the two-center problem [3, 4], $K_{gg}(R)$ is the diagonal matrix element of the nuclear motion operator over the wave functions of the symmetric state of the two-center problem [5]. The diagrams of the functions $W_g(R) = E_g(R) + 1/R$ and $K_{gg}(R)$ are given in Fig. 1.

After introducing the notations

$$y(R) = \chi_{Lv}(R),$$
$$V^L(R) = \tilde{E}_g(R) - \tilde{E}_g(\infty) + \frac{1}{R} + \frac{L(L+1)}{2MR^2}, \tag{2}$$
$$\lambda = -2M\epsilon_{Lv}, \qquad R = x, \qquad \text{and} \qquad q(x) = -2MV^L(x),$$

Eq. (1) assumes the standard form of the Sturm–Liouville problem

$$\frac{d^2y(x)}{dx^2} + (q(x) - \lambda)\, y(x) = 0 \tag{3a}$$

on the interval $0 \leqslant x < \infty$ with boundary conditions

$$y(0) = y(\infty) = 0. \tag{3b}$$

The potentials $V^L(R) = -q(R)/2M$ for the $dd\mu$ molecule are given in Fig. 2.

There is no unified method for solving the Sturm–Liouville problem (3). The latter becomes more complicated when the potential $q(x)$ is given numerically. As a rule, when solving the problem (3), we first calculate the eigenvalues of λ and only afterwards do we find the corresponding eigenfunctions [6]. Such a procedure leads, in a number of cases, to large errors. Therefore, it is more reasonable to use the algorithms in which the eigenvalue λ and the corresponding eigenfunction

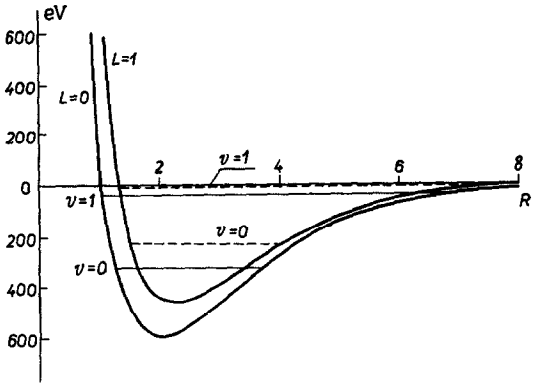

FIG. 2. Diagrams of the functions $V^L(R) = -(1/2M)q(R)$ which correspond to the physical potentials of the molecules $dd\mu$ in the states with angular momenta $L = 0$ and $L = 1$.

$y(x)$ of the problem are calculated simultaneously, as a single unknown $z = [\lambda, y(x)]$ of a certain nonlinear functional equation $\varphi(z) = 0$. Such a method is especially effective for many physical problems when there is much a priori information on the qualitative and, in part, quantitative behaviour of the solution.

2. THE IDEA OF THE METHOD

In the present paper we have developed and realized an algorithm for solving the Sturm–Liouville problem on the basis of the continuous analog of the Newton method.

The method suggested is based on the ideas of papers [7, 8] and is, to a large extent, validated in papers [9, 10]. Such an approach makes it possible to increase the number of computational schemes and is close to the idea of "invariant imbedding" [11]. The main idea of the method is as follows. The differential equation

$$\varphi^{(1)}(\lambda, y) \equiv y''(x) + [q(x) - \lambda]\, y(x) = 0 \tag{4a}$$

together with the boundary conditions on the interval $a \leqslant x \leqslant b$

$$\varphi^{(2)}(\lambda, y) \equiv y'(a) + f(\lambda, a)\, y(a) = 0, \tag{4b}$$

$$\varphi^{(3)}(\lambda, y) \equiv y'(b) + g(\lambda, b)\, y(b) = 0 \tag{4c}$$

is supplementarily defined by the normalization condition

$$\varphi^{(4)}(\lambda, y) \equiv \int_a^b y^2(x)\, dx - 1 = 0. \tag{4d}$$

Then the problem (3) for the eigenvalues is a nonlinear equation of the form

$$\varphi(z) = 0, \tag{5}$$

where the operator φ means the set of the operators $\varphi^{(i)}$ defined by the relations (4) and the argument $z = [\lambda, y(x)]$ belongs to the direct product of the space of real numbers R and the space of the functions doubly differentiable on the interval $[a, b]$: $z \in R \times C^2[a, b]$. The operator φ transforms the elements of the space Z to the elements of the space $W = R^3 \times C[a, b]$ under certain restrictions on $q(x)$.

We suppose that Eq. (5) has at least one solution z^*. Let us introduce a continuous parameter $0 \leqslant t < \infty$ in such a manner that the relation

$$\frac{d}{dt}\, \varphi(z(t)) = -\varphi(z(t)), \qquad z(0) = z_0 \tag{6}$$

is valid. This equation has the integral $\varphi(z(t)) = \varphi(z_0)\, e^{-t}$ from which it is seen that $\varphi(z(t)) \to 0$, as $t \to \infty$.

Equation (6) is linear in z' and can be presented in the form

$$z' = -[\varphi'(z)]^{-1}\, \varphi(z), \qquad z(0) = z_0\,, \tag{7}$$

which is the continuous analog of Newton's method [7]. With certain restrictions on the form of the operator φ and the choice of the initial approximation z_0, the solution $z(t)$ for Eq. (7) exists for all t and the solution $z(t)$ converges to the desired solution of the eigenvalue problem $z^* = [\lambda^*, y^*(x)]$.

The appropriate theorem has been proved in paper [9].

THEOREM. *Let Eq.* (6) *have a unique solution* z^* *in the open region* D *of space* Z. *We suppose that in* D *there exist continuous Fréchet derivatives* $\varphi'(z)$, $\varphi''(z)$ *and also the inverse operator* $[\varphi'(z)]^{-1}$, *which satisfies the inequality*

$$\|[\varphi'(z)]^{-1}\| \leqslant B$$

Then there exists the sphere S: $\| z - z^* \| \leqslant \epsilon$ *belonging to the region* D, *such that*

for arbitrary $z_0 \in S$ *the differential equation* (7) *has a unique solution* $z(t)$ *for* $0 \leqslant t < \infty$ *and*

$$\lim_{t\to\infty} \| z^* - z(t)\| = 0.$$

The fact that the solutions for Eq. (7) are asymptotically stable allows to expect that the difference methods and, in particular, Euler's method for differential equations should be numerically stable. We notice that the similar method developed in paper [12] and based on the method of continuous parameter suggested by Davidenko [13] does not poses such an asymptotic stability. We consider the detailed comparative analysis of the problems of stability of various calculation schemes to be the subject of particular interest, therefore in what follows we restrict ourselves to describing the calculation algorithm which realizes the suggested principle.

3. Realization of the Method

We introduce the parameter t on which the solutions $z(t) = [\lambda(t), y(x, t)]$ for Eq. (7) depend continuously. We define the functions $\mu(t)$ and $v(x, t)$ by the relations

$$\begin{aligned} \mu(t) &= \lambda(t) + (d/dt)\,\lambda(t), \\ v(x, t) &= (\partial/\partial t)\, y(x, t). \end{aligned} \tag{8}$$

By assuming $\varphi^{(i)}(\lambda(t), y(x, t)) \equiv \varphi^{(i)}(t)$ the equations of the system (6) can be rewritten in the developed form

$$\begin{aligned} v''(x, t) + [q(x) - \lambda(t)]\, v(x, t) &= -\varphi^{(1)}(t) - [\lambda(t) - \mu(t)]\, y(x, t), \\ v'(a, t) + f(\lambda(t), a)\, v(a, t) &= -\varphi^{(2)}(t) + [\lambda(t) - \mu(t)](\partial/\partial\lambda) f(\lambda(t), a), \\ v'(b, t) + g(\lambda(t), b)\, v(b, t) &= -\varphi^{(3)}(t) + [\lambda(t) - \mu(t)](\partial/\partial\lambda)\, g(\lambda(t), b) \end{aligned} \tag{9}$$

(the prime denotes everywhere the derivative $(\partial/\partial x)$),

$$2\int_a^b y(x, t)\, v(x, t)\, dx = -\varphi^{(4)}(t) \tag{10}$$

with the initial conditions

$$z_0 = [\lambda_0\,, y_0(x)], \qquad \lambda(0) = \lambda_0\,, \qquad y(x, 0) = y_0(x) \tag{11}$$

from a certain vicinity of the desired solution $z^* = [\lambda^*, y^*(x)]$.

Following Euler's method of the solution for the system (9–11) we divide the

semiaxis $0 \leqslant t < \infty$ by nodal points t_k ($k = 0, 1, 2,...$) with step τ_k. In this case

$$t_{k+1} = t_k + \tau_k . \tag{12}$$

By introducing the notations

$$\begin{gathered} \lambda_k = \lambda(t_k), \qquad \mu_k = \mu(t_k), \qquad v_k(x) = v(x, t_k), \qquad \varphi_k^{(i)} = \varphi^{(i)}(t_k), \\ y_k(x) = y(x, t_k), \qquad f_k = f(\lambda(t_k), a), \qquad g_k = g(\lambda(t_k), b) \end{gathered} \tag{12a}$$

and replacing the relations (8) by their difference analogs

$$\begin{aligned} \lambda_{k+1} &= \lambda_k + \tau_k(\mu_k - \lambda_k), \\ y_{k+1}(x) &= y_k(x) + \tau_k v_k(x), \end{aligned} \tag{8a}$$

we are led to a boundary value problem for the functions $v_k(x)$ on the interval $[a, b]$:

$$v_k''(x) + [q(x) - \lambda_k]\, v_k(x) = -\varphi_k^{(1)} - (\lambda_k - \mu_k)\, y_k(x),$$

$$\begin{aligned} v_k'(a) + f_k v_k(a) &= -\varphi_k^{(2)} + (\lambda_k - \mu_k)(\partial f_k/\partial\lambda), \\ v_k'(b) + g_k v_k(b) &= -\varphi_k^{(3)} + (\lambda_k - \mu_k)(\partial g_k/\partial\lambda), \end{aligned} \tag{9a}$$

$$2\int_a^b y_k(x)\, v_k(x)\, dx = -\varphi_k^{(4)}. \tag{10a}$$

For known λ_k and $y_k(x)$ the solution for the problem (9a) is a single-parameter (with respect to the parameter μ_k) family of functions and can be presented in the form

$$v_k(x) = v_{1k}(x) + \mu_k v_{2k}(x). \tag{13}$$

The functions $v_{\alpha k}(x)$ ($\alpha = 1, 2$; $k = 1, 2, 3...$) are the solutions for the boundary value problem

$$\begin{aligned} v_{\alpha k}''(x) + [q(x) - \lambda_k]\, v_{\alpha k}(x) &= P_{\alpha k}(x), \\ v_{\alpha k}'(a) + f_k v_{\alpha k}(a) &= \psi_{\alpha k}, \\ v_{\alpha k}'(b) + g_k v_{\alpha k}(b) &= \theta_{\alpha k}, \end{aligned} \tag{14}$$

where

$$\begin{aligned} P_{1k}(x) &= -[y_k''(x) + q(x)\, y_k(x)], \\ P_{2k}(x) &= y_k(x), \\ \psi_{1k} &= -[y_k'(a) + f_k y_k(a)] + \lambda_k(\partial f_k/\partial\lambda), \\ \psi_{2k} &= -(\partial f_k/\partial\lambda), \\ \theta_{1k} &= -[y_k'(b) + g_k y_k(b)] + \lambda_k(\partial g_k/\partial\lambda), \\ \theta_{2k} &= -(\partial g_k/\partial\lambda). \end{aligned} \tag{15}$$

After the functions $v_{\alpha k}(x)$ have been calculated from these equations, we determine the parameter μ_k from the relation

$$\mu_k = \left[\frac{1}{2} - \frac{1}{2}\int_a^b y_k^2(x)\, dx - \int_a^b y_k(x)\, v_{1k}(x)\, dx\right]\left[\int_a^b y_k(x)\, v_{2k}(x)\, dx\right]^{-1}, \tag{16}$$

which follows from the normalization condition (10a) and the definition (13). Then the values of t_{k+1}, $\lambda_{k+1}(x)$ and $y_{k+1}(x)$ are found by Eqs. (12) and (8a). For given initial values of λ_0 and $y_0(x)$ the process of calculation of λ_k and $y_k(x)$ for $k = 1, 2, 3...$ has, thus, been defined completely.

The scheme considered is discrete only with respect to the variable t. In order to construct the complete discrete scheme it is necessary to approximate the boundary value problems (14) by their finite-difference analogues for each $t = t_k$. If for each t_k we conserve the same network of nodes with respect to variable x then the scheme in question may be interpreted as a result of application of the continuous analog of Newton's method to the difference equation, which approximates the problem (3) in questions, with subsequent replacement of the continuous parameter t by a discrete one. In the case considered this scheme is a generalization of the algorithm proposed by Kalitkin [8] and may be validated with the aid of the results of his paper. The grounds for the method of finite differences of solving the Sturm–Liouville problem are also given in Refs. [6, 14]. The alternating direction implicit method [15] is very effective for the realization of these schemes.

We note that this approach allows a direct generalization to the case of the coupled systems of differential equations.

4. Account of Physical Peculiarities of the Problem

The given algorithm may be realized only on the finite interval $[a, b]$ of the change of the independent variable x, while the initial physical problem is defined on a

semiinfinite interval $[0, \infty)$. However, knowing the particular features of the problem in question, it is possible to take into account this difference.

For $R \gg 1$ the following asymptotic expansion [16]

$$E_g(R) - E_g(\infty) + \frac{1}{R} \cong -\frac{9}{4} R^{-4} - \frac{15}{2} R^{-6} - \frac{213}{4} R^{-7} - \frac{7755}{64} R^{-8} - 2Re^{-(R+1)} \left(1 + \frac{1}{2} R^{-1} - \frac{25}{8} R^{-2} - \frac{131}{48} R^{-3}\right) \quad (17)$$

holds. For sufficiently large R it is possible to neglect the exponentially small term and then the expressions for the potential $q(x)$ and the solutions $y(x)$ in the asymptotic domain take the form

$$q(x) = 2M \sum_{s=2}^{N} c_s x^{-s}, \qquad \tilde{y}(x) = ce^{-\sqrt{\lambda}\, x} \sum_{n=0}^{N} a_n x^{-n}, \quad (18)$$

where

$$a_0 = 1, \qquad a_{n+1} = \frac{1}{2\sqrt{\lambda}} \left(\frac{\alpha_n}{n+1} - n a_n\right), \qquad \alpha_n = 2M \sum_{s=0}^{n} a_s c_{n+2-s},$$
$$c_2 = -\frac{L(L+1)}{2M}, \qquad c_3 = 0, \qquad c_4 = \frac{9}{4}, \qquad c_5 = 0, \quad (19)$$
$$c_6 = \frac{15}{2}, \qquad c_7 = \frac{213}{4}, \qquad c_8 = \frac{7755}{64}.$$

The constant c is determined from the condition of sewing the asymptotic solution $\tilde{y}(x)$ and the solution $y_k(x)$ at the point $x = b$.

The boundary conditions (4b) and (4c) and the normalization condition (4d) are modified as follows

$$\varphi^{(2)}(\lambda, y) \equiv y(0) = 0, \quad (20b)$$

$$\varphi^{(3)}(\lambda, y) \equiv y'(b) + \left[\sqrt{\lambda} + \frac{\sum_{n=0} n a_n b^{-(n+1)}}{\sum_{n=0} a_n b^{-n}}\right] y(b) = 0, \quad (20c)$$

$$\varphi^{(4)}(\lambda, y) \equiv \int_0^b y^2(x)\, dx - 1 + \Delta I = 0, \qquad \Delta I = \int_b^\infty \tilde{y}^2(x)\, dx. \quad (20d)$$

The correction ΔI can be found by numerical integration using the analytic representation (18) for the function $\tilde{y}(x)$ in the asymptotic domain. Other necessary

changes in Eqs. (10) and (16) are quite obvious and can be realized by taking into account the equality

$$\tilde{v}_k(x) = (\mu_k - \lambda_k)\frac{\partial \tilde{y}_k}{\partial \lambda}. \tag{21}$$

When integrating the system (14) numerically, it is convenient to take as the initial approximation $z_0 = [\lambda_0, y_0(x)]$ the solution for the problem (3) which approximates the true solution by a certain analytic function. The potentials given in Fig. 2 are well approximated by Morse's potential [17] with the aid of the three parameters R_0, D, and α:

$$V(R) = D[e^{-2\alpha(R-R_0)} - 2e^{-\alpha(R-R_0)}], \tag{22}$$

where R_0 is the R-value for which the potential $V(R)$ reaches its minimum $V(R_0) = \min V(R) = -D$. The parameter α is determined from the condition

$$\alpha = \left[\frac{V''(R_0)}{2D}\right]^{1/2}. \tag{23}$$

The eigenvalue λ_v and the corresponding eigenfunction $y_v(x)$ with the number of zeros v are expressed as [17]

$$\lambda_v = 2M\epsilon_v = 2MD\left(1 - \frac{\alpha}{\sqrt{2MD}}(v + \tfrac{1}{2})\right)^2, \tag{24}$$

for $v = 0$

$$y_v(x) = [\alpha/\Gamma(2s)]^{1/2} e^{-\xi/2}\xi^s,$$

for $v = 1$

$$y_v(x) = [\alpha(2s+1)/\Gamma(2s)]^{1/2} e^{-\xi/2}\xi^s\left(1 - \frac{\xi}{2s+1}\right).$$

The following notion is introduced

$$s = \frac{\sqrt{\lambda_v}}{\alpha}, \qquad \xi = \frac{2\sqrt{2MD}}{\alpha} e^{-\alpha(x-R_0)}. \tag{25}$$

5. Some Details of the Calculation Procedure

The suggested algorithm of solving the Sturm–Liouville problem can be easily realized on computers. A program for calculating the mesic molecule energy levels is written in FORTRAN and is realized on the CDC-1604 A computer. The linear

boundary value problems (14) for the functions $v_{\alpha k}(x)$ for each value of the parameter t_k which corresponds to a kth iteration of the solution z_k in the initial approximation z_0 are solved with the aid of the alternating direction implicit method [15] on a uniform network of nodes $x_n \in [0, b]$ with step h.

The transition to the next iteration $z_{k+1} = [\lambda_{k+1}, y_{k+1}(x)]$ is realized by formulas (8a). The convergence of the process is seen from the decrease of the quantity:

$$\delta_k = \max_n | \varphi_h^{(1)}(\lambda_k, y_k(x_n))| \tag{26}$$

where $\varphi_h^{(1)}$ is the difference operator

$$\varphi_h^{(1)}(\lambda, y(x_n)) \equiv h^{-2}[y(x_n + h) - 2y(x_n) + y(x_n - h)] + [q(x_n) - \lambda]\, y(x_n) \tag{27}$$

which approximates Eq. (4a) with the accuracy of the order $0(h^2)$. The process finishes if $\delta_k < \epsilon$, where ϵ is small enough. In choosing the ϵ value one should bear in mind the estimates of Ref. [14].

The convergence of the calculation procedure depends considerably on the choice of the dynamic parameter τ_k (the integration step in Euler's method). Satisfactory results were obtained when τ_k was chosen to be proportional to the ratio δ_{k-1}/δ_k. For $\epsilon = 10^{-4}$, $h = 0.0125$ and $b = 20$ to find the solution $z^* \approx z_k$ of the initial problem about ten iterations are needed ($k \approx 10$). The convergence depends weakly on the choice of the initial approximation $y_0(x)$ which can be taken in the form of a sinusoid for $0 \leqslant x \leqslant 2R_0$ (see (22)) and a decreasing exponential for $x > 2R_0$.

Some calculation aspects for the case of the $dd\mu$ molecule in states with orbital moment $L = 1$ and quantum numbers $v = 0$ and $v = 1$ are presented in more detail in Table I.

With the given values of ϵ, h and b, for $N = 6$ in expansions (17) the computation time on CDC-1604 A is about 2 min. By varying N, decreasing h and increasing b in the limits allowed by the memory of the computer we see that with the above values of h, b, and N the relative accuracy is about 10^{-3}.

To verify additionally the accuracy of the method the Sturm–Liouville problem (3) has been solved for the same ϵ, h, and b for the case of Morse's potential (22) the shape of which for $\alpha = 0.67$; $R_0 = 2.15$; $D = 0.106$ is rather close to that of the potential $V(R)$ for the case of the $pp\mu$ mesic molecule in the state with orbital momentum $L = 0$. The value $\lambda_v = 0.4353$ obtained by the formula (24) for the ground state ($v = 0$) is found to be in good agreement with the value $\lambda = 0.4348$ obtained from Eqs. (4) for $\delta_k = 5.10^{-4}$. Thus, δ_k, in the order of magnitude, is equal to the absolute error of calculation of the eigenvalue λ and may serve as a measure of calculation accuracy.

TABLE I[a]

Levels of $dd\mu$ molecule	$L = 1 \quad v = 0$	$L = 1 \quad v = 1$
k	8	9
δ_0	60.5	39.7
δ_k	5.6×10^{-5}	9.0×10^{-6}
λ_0	0.7703	3.26×10^{-2}
λ_k	0.7474	2.24×10^{-3}

[a] The given characteristics of the calculation process correspond to the following choice of the values $\epsilon = 10^{-4}, h = 0.0125, b = 20, N = 6, \tau_k = (\delta_{k-1}/\delta_k)\,\tau_{k-1}, \tau_0 = 0.1$. The initial approximation $z_0 = [\lambda_0, y_0(x)]$ and the corresponding value of δ_0 are calculated by Eqs. (22), (24), and (26) for the following values of the parameters of the Morse potential for the molecule $dd\mu$ in the state with orbital moment $L = 1$: $R_0 = 2.25$, $D = 8.24 \times 10^{-2}$, $\alpha = 0.697$.

The main restriction on the calculation accuracy is defined by the magnitude of of the step h of the difference scheme since the order of approximation of the difference operator (27) is $O(h^2)$. Difference schemes of higher accuracy are discussed in Refs. [8, 14].

6. The Results of Calculations

In Table II we give the results of calculations of the binding energy ϵ_{Lv} of the mesic molecules $pp\mu$, $dd\mu$ and $tt\mu$ in all vibrational quantum states.

With a given orbital momentum L the energy levels for the mesic molecules are labeled by the vibrational quantum number v which is equal to the number of zeros of the eigenfunction $y_v(x)$.

For the molecule $pp\mu$ two levels with quantum numbers $L = 0$, $v = 0$ and $L = 1$, $v = 0$ are possible. For the $dd\mu$ molecule five levels: 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 level with quantum numbers $L = 2$, $v = 0$. For the $tt\mu$ molecule six quantum levels are possible: two levels ($v = 0$ and $v = 1$) in each of the states with orbital momenta $L = 0$ and $L = 1$ and one ($v = 0$) level in each of the states with $L = 2$ and $L = 3$.

It follows from Table II that our calculations are in satisfactory agreement with all recent variational calculations. A special attention should be paid to the calculation of the binding energy of the mesic molecule $dd\mu$ in the state with $L = 1$,

TABLE II

Binding Energy ϵ_{Lv}(eV) of the Mesic Molecules[a]

Mesic molecule	$L = 0$		$L = 1$		$L = 2$	$L = 3$	Method of calculation
	$v = 0$	$v = 1$	$v = 0$	$v = 1$	$v = 0$	$v = 0$	
$pp\mu$	253[b]	—	107.23[c]	—	—	—	Variational
$M_1 = 1836.109$	248	—	101	—	—	—	Present article
$dd\mu$	324.2[b]	32.7[b]	226.55[c]	—	—	—	Variational
$M_1 = 3670.398$	323	32.9	224	0.7	83.5	—	Present article
$tt\mu$	361.2[b]	75[b]	288.72[c]	—	—	—	Variational
$M_1 = 5496.753$	361	81.4	288	43.1	171	46.7	Present article

[a] The values M_1 and $\mu = 206.769$ are given in electronic masses m_e on the basis of the data of Taylor *et al.* [20] and Selinov [20]. The binding energies ϵ_{Lv} are given in electron volt. The transition coefficient β from the eigenvalues of λ (3) to the ϵ_{Lv}(eV) values is ϵ_{Lv}(eV) $= \beta\lambda$, $\beta = 4M_1(\mu/(2M_1 + \mu))^2 \cdot 27.21165$ eV.

[b] B. R. CARTER, *Phys. Rev. 165* (1968), 139.

[c] A. HALPERN, *Phys. Rev. 135*A (1964), 34.

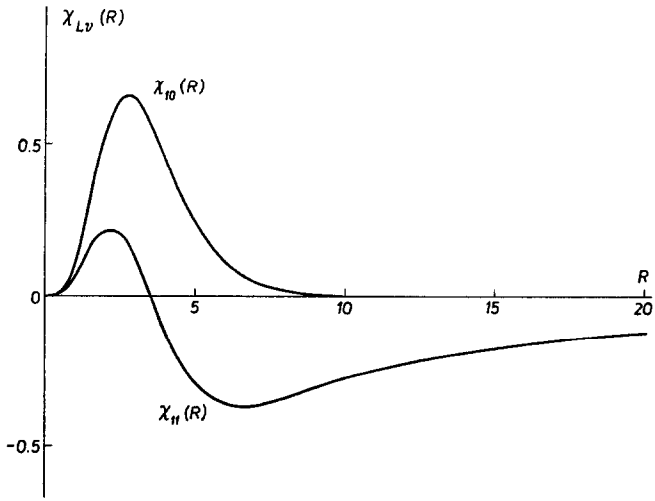

FIG. 3. The wave functions χ_{Lv} of the molecule $dd\mu$ in the state with angular momentum $L = 1$. The function $\chi_{10}(R)$ corresponds to the ground vibrational state ($v = 0$, $\epsilon_{10} = 224$ eV) the function $\chi_{11}(R)$ to the excited state ($v = 1$, $\epsilon_{11} = 0.7$ eV).

$v = 1$. The existence of this level was supposed already by Beliaev et al., Zel'dovich and Gershtein [2] and has recently been proved in Ref. [18]. The calculated value $\epsilon_{11} = 0.7$ eV is in satisfactory agreement with that which is needed for $dd\mu$ formation probability measurements to be explained [19]. The diagrams of the wave functions $\chi_{Lv}(R) \equiv y_v(x)$ for the $L = 1$, $v = 0$ and $L = 1$, $v = 1$ states of the $dd\mu$ mesic molecule are given in Fig. 3.

In the calculations the values of $E_g(R)$ and $K_{gg}(R)$ are used which are found with the accuracy 10^{-11} and 10^{-7}, respectively, by means of the algorithm realized in the papers [4] and [5].

The adiabatic calculations are known to contain an error which is due to an approximate determination of the potential $V(R)$. In the present paper the adiabatic corrections of the first order $(1/2M)\, K_{gg}(R)$ to the term $E_g(R)$ have been taken into account. As Table II shows when these corrections are taken into account the adiabatic calculations coincide with the recent variational calculations within $\sim 10^{-3}$. As it should be expected, the larger the nuclear mass of mesic molecules the better the agreement. A more detailed comparison has been performed in the author's paper [21].

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