

forces, and coupled to the  $o$ -world by "bridges" of massive particles  $x_i$  and with the  $\gamma_j$  worlds by the bridges  $x_{ij}$ . The most stringent bounds on the parameters of such a picture come from cosmology based on the theory of the hot Universe (the big-bang model).

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<sup>1</sup>We shall not discuss here the fantastic version in which there exists a world  $z$ , at present completely isolated from our world and having its own gravitons. The coupling to the  $z$ -world could have disappeared as a result of a peculiar phase transition above the Planck temperature.

<sup>1</sup>L. B. Okun', Pis'ma Zh. Eksp. Teor. Fiz. 31, 156 (1980) [JETP Lett. 31, 144 (1980)].

<sup>2</sup>L. B. Okun', ITEP Preprint 6 (1980).

<sup>3</sup>I. Yu. Kobzarev, L. B. Okun' and I. Ya. Pomeranchuk, Yad. Fiz. 3, 1154 (1966) [Sov. J. Nucl. Phys. 3, 837 (1966)].

<sup>4</sup>Ya. B. Zel'dovich, A. A. Klypin, M. Yu. Khlopov, and V. N. Chechetkin, Yad. Fiz. 31, 1286 (1980) [Sov. J. Nucl. Phys. 31, 664 (1980)].

<sup>5</sup>S. Tremaine and J. E. Gunn, Phys. Rev. Lett. 42, 407 (1979).

<sup>6</sup>D. Walsh, R. F. Caswell, and R. I. Weyman, Nature 279, 381 (1979).

<sup>7</sup>J. L. Brady, Publ. Astron. Soc. Pacif. 84, 314 (1972).

<sup>8</sup>R. L. Duncombe, in: Recent Advances in Dynamical Astronomy, ed. by B. D. Tapley and V. Szebehely, D. Reidel Publishing Co., Dordrecht-Boston (1973), p. 301.

<sup>9</sup>S. Weinberg, Gravitation and Cosmology, Wiley, New York, (1973), Ch. 8, § 6 [Russian Transl. "Mir" (1975)].

<sup>10</sup>Fizicheskiĭ éntsiklopedicheskiĭ slovar' (Physics encyclopedic dictionary), "Sov. Entsiklopediya" (1960), p. 488.

<sup>11</sup>P. Melchior, Fizika i dinamika planet (Physics and dynamics of planets) part I, Russian Transl., "Mir" (1975).

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## Calculation of the energy levels of $\mu$ -mesic molecules of hydrogen isotopes in the adiabatic representation of the three-body problem

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The energy levels  $\epsilon_{Jv}$  of the mesic molecules  $pp\mu$ ,  $pd\mu$ ,  $pt\mu$ ,  $dd\mu$ ,  $dt\mu$ , and  $tt\mu$  in the states ( $Jv$ ) of the rotational and vibrational motion are calculated. The calculations are made in the adiabatic representation of the three-body problem, in which the wave function of the  $\mu$ -mesic molecule is expanded with respect to a complete set of solutions to the quantum-mechanical two-center problem. A numerical investigation was made into the rate of convergence of the expansion. For the weakly bound states ( $J = 1, v = 1$ ) of the mesic molecules  $dd\mu$  and  $dt\mu$  the values  $\epsilon_{11}(dd\mu) = -1.91$  eV and  $\epsilon_{11}(dt\mu) = -0.64$  eV were obtained.

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### 1. INTRODUCTION

At the Laboratory of Nuclear Problems at the Joint Institute for Nuclear Research, Dubna, an experimental measurement was recently made<sup>1</sup> of the rate of formation  $\lambda_{dt\mu}$  of the mesic molecules  $dt\mu$  and the lower bound  $\lambda_{dt\mu} > 10^8$  sec<sup>-1</sup> was obtained. According to the calculations of Ref. 2, the high rate of this process is due to the resonance mechanism of formation of the mesic molecules  $dt\mu$  in the weakly bound rotational-vibrational state with quantum numbers  $J=1, v=1$ . The binding energy of this state,  $\epsilon_{Jv} \approx 1$  eV, was calculated earlier<sup>2</sup> for the first time by perturbation theory realized in the adiabatic representation of the three-body problem.<sup>3-7</sup>

For the detailed study of  $\mu$ -mesic molecular processes in a mixture of hydrogen isotopes and, in particular, to describe the process of resonance formation of the mesic molecules  $dt\mu$ , it is necessary to know their energy levels to an accuracy  $\sim 0.01$  eV, which is  $\sim 10^{-6}$  mesic-atomic energy units  $\epsilon_{\mu} = 2m_{\mu}Ry$

$= 5626.51$  eV.<sup>2</sup>

In the present paper, we present the results of calculations of the energies  $\epsilon_{Jv}$  of various ( $Jv$ ) states of  $\mu$ -mesic molecules of the hydrogen isotopes. The calculations are made in the adiabatic representation of the three-body problem, in which the wave function of the  $\mu$ -mesic molecule is expanded in a complete set of solutions to the quantum-mechanical two-center problem.<sup>3-5</sup> In this approach, the original eigenvalue problem for the nonrelativistic Schrödinger equation in a six-dimensional space reduces to the solution of a Sturm-Liouville problem for a system of ordinary integro-differential equations. The matrices of the coefficients of this system (the effective potentials of the three-body problem in the adiabatic representation) are calculated with the necessary accuracy by means of the algorithms of Refs. 8-13.

The corresponding Sturm-Liouville problem is solved numerically with the required relative accuracy in the framework of the continuous analog of Newton's

method<sup>14,15</sup> by means of algorithms<sup>16-18</sup> realized in the form of a set of programs written in FORTRAN-4. All the calculations were made with a CDC-6500 computer. In our preceding papers, this Sturm-Liouville problem was solved in the two-level approximation,<sup>6</sup> and also by perturbation theory.<sup>7</sup> The results of these calculations, and also the results of the best variational calculations<sup>19,20</sup> are compared with the values of  $\epsilon_{J\nu}$  obtained in the present paper.

## 2. FORMULATION OF THE PROBLEM

The wave functions  $\Psi_{n\tau}(\mathbf{r}, \mathbf{R})$  and the total energies  $E_{n\tau}$  of the states  $|n\tau\rangle$  of  $\mu^-$ -mesic molecules of the hydrogen isotopes are found from the nonrelativistic Schrödinger equation in the six-dimensional  $(\mathbf{r}, \mathbf{R})$  space<sup>4</sup>:

$$(H - E_{n\tau})\Psi_{n\tau}(\mathbf{r}, \mathbf{R}) = 0, \quad (1)$$

where (in units with  $e = \hbar = 1$ )

$$H = \hat{T}_a + \hat{h}_a + 1/R; \quad (2)$$

$$\hat{T}_a = -\frac{1}{2M_0} \left[ \left( \nabla_{\mathbf{r}} + \frac{\kappa}{2} \nabla_{\mathbf{r}'} \right)^2 - \left( \frac{1+\kappa}{2} \right)^2 \Delta_{\mathbf{r}'} \right],$$

$$\hat{h}_a = -\frac{1}{2m_a} \Delta_{\mathbf{r}} - \frac{1}{r_a} - \frac{1}{r_b}, \quad (3)$$

$$\frac{1}{M_0} = \frac{1}{M_a} + \frac{1}{M_b}, \quad \frac{1}{m_a} = \frac{1}{m_\mu} + \frac{1}{M_a}, \quad \kappa = \frac{M_b - M_a}{M_b + M_a}.$$

Here,  $\mathbf{R}$  is the vector joining the nuclei of the mesic molecules  $a$  and  $b$  with masses  $M_a$  and  $M_b$  (in what follows,  $M_a \geq M_b$ );  $\mathbf{r}$  is the vector joining the center of the interval  $R$  and the  $\mu^-$  meson with mass  $m_\mu$ ;  $r_a$  and  $r_b$  are the distances from the nuclei  $a$  and  $b$  to the  $\mu^-$  meson.

The motion of the  $\mu^-$  meson in the mesic molecule is characterized by the three parabolic quantum numbers  $n \equiv [n_1 n_2 m]$ , and the relative motion of the nuclei  $a$  and  $b$  by the set of quantum numbers  $\tau = (J m_J \nu \lambda)$ , where  $J$  and  $m_J$  are the total orbital angular momentum of the three-body system and its projection onto the  $z$  axis of the laboratory coordinate system,  $\nu$  is the vibrational quantum number, and  $\lambda = \pm(-)^J$  is the total parity of the three-body system.

The most interesting energy levels of the mesic molecules correspond to the ground state of the motion of the  $\mu^-$  meson, i.e., the state with quantum numbers  $n = [000]$ . In the absence of a magnetic field, the energy of the  $\mu^-$ -mesic molecules does not depend on the quantum number  $m_J$ , and in what follows we shall therefore omit it. Thus, for states with  $n = [000]$  and given total parity  $\lambda$  the wave function depends only on the quantum numbers  $J$  and  $\nu$ :

$$\Psi_{n\tau}(\mathbf{r}, \mathbf{R}) = \langle \mathbf{r}, \mathbf{R} | n\tau \rangle = \langle \mathbf{r}, \mathbf{R} | J\nu \rangle = \Psi_{J\nu}(\mathbf{r}, \mathbf{R}). \quad (4)$$

These wave functions satisfy the orthogonality relation

$$\langle J\nu | J'\nu' \rangle = \int d\mathbf{r} d\mathbf{R} \Psi_{J\nu}^*(\mathbf{r}, \mathbf{R}) \Psi_{J'\nu'}(\mathbf{r}, \mathbf{R}) = \delta_{JJ'} \delta_{\nu\nu'}. \quad (5)$$

The adiabatic basis with respect to which the wave function  $\langle \mathbf{r}, \mathbf{R} | J\nu \rangle$  of the state  $(J\nu)$  of the mesic molecule is expanded is a complete set of solutions to the quantum-mechanical two-center problem,<sup>5</sup> i.e., the problem of the motion of the  $\mu^-$  meson in the Coulomb field of two fixed nuclei  $a$  and  $b$  separated by the distance  $R$ :

$$\hat{h}\phi_j(\mathbf{r}; R) = E_j(R)\phi_j(\mathbf{r}; R), \quad (6a)$$

$$\phi_j(\mathbf{r}; R) = \langle \mathbf{r}; R | j \rangle = \langle \mathbf{r}; R | n_1 n_2 m p \rangle;$$

$$\hat{h}\phi_c(\mathbf{r}; R) = \frac{1}{2}k^2\phi_c(\mathbf{r}; R), \quad (6b)$$

$$\phi_c(\mathbf{r}; R) = \langle \mathbf{r}; R | c \rangle = \langle \mathbf{r}; R | k n_2 m p \rangle,$$

where

$$\hat{h} = -\frac{1}{2}\Delta_{\mathbf{r}} - \frac{1}{r_a} - \frac{1}{r_b} \quad (6c)$$

is the Hamiltonian of the two-center problem,  $E_j(R)$  is the term corresponding to the state  $|j\rangle$  of the discrete spectrum of this problem, and  $k$  is the momentum of the  $\mu^-$  meson corresponding to the state  $|c\rangle$  of the continuous spectrum of this problem.

The states  $|j\rangle \equiv |j\rangle p$  of the discrete spectrum are labeled by the set  $j = [n_1 n_2 m]$  of parabolic quantum numbers  $n_1$ ,  $n_2$ ,  $m$  and parity  $p = (g, u)$  under inversion  $\mathbf{r} \rightarrow -\mathbf{r}$  about the origin. In the spheroidal coordinates

$$\mathbf{r} = \{\xi, \eta, \varphi\}, \quad \xi = (r_a + r_b)/R, \quad \eta = (r_a - r_b)/R,$$

the solutions  $\phi_j(\mathbf{r}; R)$ , which are bounded in the region  $1 \leq \xi < \infty$ ,  $-1 \leq \eta \leq 1$ ,  $0 \leq \varphi \leq 2\pi$ ,  $0 \leq R < \infty$ , can be represented in the form

$$\phi_j(\mathbf{r}; R) = \phi_{jp}(\mathbf{r}; R) = \phi_{jp}(\xi, \eta, \varphi; R) = \varphi_{jp}(\xi, \eta; R) \frac{1}{(2\pi)^{1/2}} \begin{cases} (-)^m e^{im\varphi} \\ e^{-im\varphi} \end{cases}. \quad (7a)$$

They satisfy the orthogonality relation

$$\langle j'p' | j'p' \rangle = \int d\mathbf{r} \phi_{j'p'}^*(\mathbf{r}; R) \phi_{j'p'}(\mathbf{r}; R) = \delta_{j'p'j''p''} \delta_{n_1 n_1'} \delta_{n_2 n_2'} \delta_{m m'} \delta_{m m'}, \quad (7b)$$

$$d\mathbf{r} = \frac{1}{2}R^2 (\xi^2 - \eta^2) d\xi d\eta d\varphi.$$

The continuum states  $|c\rangle \equiv |ksp\rangle$  of the two-center problem are characterized by the momentum  $k$  of the  $\mu^-$  meson, the set  $s = [n_2 m]$  of parabolic quantum numbers  $n_2$  and  $m$ , and the parity  $p$ . The corresponding solutions, which are bounded in the region  $1 \leq \xi < \infty$ ,  $-1 \leq \eta \leq 1$ ,  $0 \leq \varphi \leq 2\pi$ ,  $0 \leq R < \infty$ ,

$$1 \leq \xi < \infty, \quad -1 \leq \eta \leq 1, \quad 0 \leq \varphi \leq 2\pi, \quad 0 \leq R < \infty,$$

$$\phi_c(\mathbf{r}; R) = \phi_{cp}(\mathbf{r}; k, R) = \phi_{cp}(\xi, \eta, \varphi; k, R) = \varphi_{cp}(\xi, \eta; k, R) \frac{1}{(2\pi)^{1/2}} \begin{cases} (-)^m e^{im\varphi} \\ e^{-im\varphi} \end{cases}. \quad (8a)$$

satisfy the orthogonality relation

$$\langle c | c' \rangle = \int d\mathbf{r} \phi_c^*(\mathbf{r}; R) \phi_{c'}(\mathbf{r}; R) = \delta_{cp'c''p''} \delta_{n_2 n_2'} \delta_{m m'} \delta(k - k'). \quad (8b)$$

The dependence of the wave function  $\Psi_{J\nu}(\mathbf{r}, \mathbf{R})$  on the angular variables  $\Theta$  and  $\Phi$  of the vector  $\mathbf{R} = \{R, \Theta, \Phi\}$  in the laboratory coordinate system, and also on the azimuthal angle  $\varphi$  of the vector  $\mathbf{r} = \{\xi, \eta, \varphi\}$  in the coordinate system which rotates with the vector  $\mathbf{R}$ , is separated by means of a symmetrized combination of normalized Wigner  $D$  functions:

$$\mathcal{D}_{mm'}^J(\Phi, \Theta, \varphi)$$

$$= [4\pi(1 + \delta_{0m})]^{-1/2} [(-)^m e^{im\varphi} \mathcal{D}_{mm'}^J(\Phi, \Theta, 0) + e^{-im\varphi} \mathcal{D}_{-mm'}^J(\Phi, \Theta, 0)], \quad (9)$$

which correspond to total parity  $\lambda = +(-)^J$ .

Using the solutions (7b) and (8b) and the functions (9), we can represent the wave function (4) in the form of the expansion

$$\Psi_{n\tau}(\mathbf{r}, \mathbf{R}) = \sum_{m=0}^J \mathcal{D}_{mm'}^J(\Phi, \Theta, \varphi) R^{-1} F_{m'}^J(\xi, \eta, R), \quad (10a)$$

$$F_m^{j\nu}(\xi, \eta, R) = \sum_{p=g, u} \sum_{n_1=0}^{\infty} \left\{ \sum_{n_2=0}^{\infty} \varphi_{ip}(\xi, \eta; R) \chi_{jp}^{j\nu}(R) + \int_0^{\infty} dk \varphi_{ip}(\xi, \eta; k, R) \chi_{jp}^{j\nu}(k, R) \right\}. \quad (10b)$$

The functions

$$\begin{aligned} \chi_{jp}^{j\nu}(R) &= \langle R; jp | J\nu \rangle = \langle R; n_1 n_2 m p | J\nu \rangle, \\ \chi_{jp}^{j\nu}(k, R) &= \langle R; ksp | J\nu \rangle = \langle R; kn_2 m p | J\nu \rangle, \end{aligned} \quad (11)$$

which are regular at  $R=0$  and bounded on the half-axis  $0 \leq R < \infty$ , describe the relative radial motion of the nuclei  $a$  and  $b$  in the  $\mu$ -mesic molecule and satisfy an orthogonality relation that follows from (5), (7b), and (8b):

$$\sum_{p=g, u} \sum_{m=0}^{\infty} \sum_{n_2=0}^{\infty} \left\{ \sum_{n_1=0}^{\infty} \int_0^{\infty} dR \chi_{jp}^{j\nu}(R) \chi_{jp}^{j\nu'}(R) + \int_0^{\infty} dk \int_0^{\infty} dR \chi_{jp}^{j\nu}(k, R) \chi_{jp}^{j\nu'}(k, R) \right\} = \delta_{\nu\nu'}. \quad (11a)$$

When one imposes on the wave function (10a) boundary conditions corresponding to the correct limit of dissociation of the  $\mu$ -mesic molecule into a mesic atom and a nucleus,<sup>4</sup> the solutions

$$\begin{aligned} \varphi_{ig}(\xi, \eta; R), \quad \varphi_{iu}(\xi, \eta; R), \quad \varphi_{ig}(\xi, \eta; k, R), \quad \varphi_{iu}(\xi, \eta; k, R) \end{aligned}$$

in the expansion (10b) are usually replaced by the linear combinations (in which the arguments are omitted)

$$\varphi_{ja} = 2^{-1/2}(\varphi_{ig} - \varphi_{iu}), \quad \varphi_{jb} = 2^{-1/2}(\varphi_{ig} + \varphi_{iu}) \quad (12a)$$

with similar combinations for  $\varphi_{sa}$  and  $\varphi_{sb}$ .

The transformation (12a) induces a transformation for the functions  $\chi_{jg} \equiv \chi_{jg}^{j\nu}(R)$  and  $\chi_{ju} \equiv \chi_{ju}^{j\nu}(R)$ :

$$\chi_{ja} = 2^{-1/2}(\chi_{ig} - \chi_{iu}), \quad \chi_{jb} = 2^{-1/2}(\chi_{ig} + \chi_{iu}) \quad (12b)$$

and a similar transformation is induced for  $\chi_{sg}^{j\nu}(k, R)$  and  $\chi_{su}^{j\nu}(k, R)$ . Since the relation

$$\varphi_{ig}\chi_{js} + \varphi_{iu}\chi_{ju} = \varphi_{ja}\chi_{sa} + \varphi_{ib}\chi_{sb} \quad (13)$$

is satisfied, the expansion (10b) preserves its form with a changed meaning of the index  $p$ :

$$p=(g, u) \rightarrow p=(a, b).$$

Substituting the expansion constructed in this manner for the wave function  $\Psi_{n\tau}(\mathbf{r}, \mathbf{R})$  in Eq. (1) and averaging it over the variables  $\Phi, \Theta, \varphi, \xi, \eta$ , we arrive at an infinite system of ordinary integro-differential equations on the half-axis  $0 \leq R < \infty$ :

$$\begin{aligned} \hat{I} \left\{ \frac{d^2}{dR^2} - \frac{J(J+1) - 2m^2}{R^2} - \frac{2M}{R} + 2M\epsilon_{j\nu} \right\} \chi_i(R) \\ = \sum_{j=1}^{\infty} \hat{U}_{ij}(R) \chi_j(R) + \sum_{j=1}^{\infty} \int_0^{\infty} dk \hat{U}_{ij}(k, R) \chi_j(k, R), \\ \hat{I} \left\{ \frac{d^2}{dR^2} - \frac{J(J+1) - 2m^2}{R^2} - \frac{2M}{R} + 2M\epsilon_{j\nu} \right\} \chi_s(k, R) \\ = \sum_{i=1}^{\infty} \hat{U}_{si}(k, R) \chi_i(R) + \sum_{i=1}^{\infty} \int_0^{\infty} dk' \hat{U}_{si}(k, k', R) \chi_s(k', R) \end{aligned} \quad (14)$$

with the boundary conditions ( $0 \leq k < \infty$ )

$$\begin{aligned} \chi_i(0) = 0, \quad \lim_{R \rightarrow \infty} \chi_i(R) = 0, \quad i=1, 2, \dots, \\ \chi_s(k, 0) = 0, \quad \lim_{R \rightarrow \infty} \chi_s(k, R) = 0, \quad s=1, 2, \dots; \end{aligned} \quad (15)$$

where  $M = M_0/m_a$ ,  $\epsilon_{j\nu} = E_{n\tau} - E_{1a}$  is the energy of the state ( $J\nu$ ) of the  $\mu$ -mesic molecule measured from the energy  $E_{1a}$  of the ground state of the mesic atom ( $m_\mu, M_a$ ), and all quantities are measured in units of  $e = \hbar = m_a = 1$ .

The system of equations (14) is written in the "two-component form"<sup>3,4</sup>:

$$\begin{aligned} \chi_i(R) = \chi_i^{j\nu}(R) = \begin{pmatrix} \chi_{ia}(R) \\ \chi_{ib}(R) \end{pmatrix}, \quad \chi_s(k, R) = \chi_s^{j\nu}(k, R) = \begin{pmatrix} \chi_{sa}(k, R) \\ \chi_{sb}(k, R) \end{pmatrix}, \\ \hat{U}_{ij}(R) = \begin{pmatrix} U_{ia,ja}(R) & U_{ia,jb}(R) \\ U_{ib,ja}(R) & U_{ib,jb}(R) \end{pmatrix}, \quad \hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \quad (16)$$

with similar expressions for the matrices  $\hat{U}_{is}(k, R)$ ,  $\hat{U}_{st}(k, R)$ , and  $\hat{U}_{ss}(k, k', R)$ .

The potentials  $U_{ip, jp}(R)$  are calculated using expressions that follow from the transformations (12a) and (12b):

$$\begin{aligned} U_{ia, ja}(R) &= 1/2 \{ (V_{ig, jg} + V_{iu, ju}) - (V_{ig, ju} + V_{iu, jg}) \} - 2ME_{1a} \delta_{ij}, \\ U_{ia, jb}(R) &= 1/2 \{ (V_{ig, jg} - V_{iu, ju}) + (V_{ig, ju} - V_{iu, jg}) \}, \\ U_{ib, ja}(R) &= 1/2 \{ (V_{ig, jg} - V_{iu, ju}) - (V_{ig, ju} - V_{iu, jg}) \}, \\ U_{ib, jb}(R) &= 1/2 \{ (V_{ig, jg} + V_{iu, ju}) + (V_{ig, ju} + V_{iu, jg}) \} - 2ME_{1a} \delta_{ij}. \end{aligned} \quad (17)$$

The potentials  $V_{ig, jg} = V_{ig, jg}(R)$ , etc., are expressed in terms of the terms  $E_j(R)$  and the matrix elements  $H_{ij}^{(\pm)}(R)$ ,  $H_{ij}^{(*)}(R)$ ,  $Q_{ij}^{(\pm)}(R)$ , and  $B_{ij}^{(\pm)}(R)$ , which are defined as follows<sup>8-10, 12, 13</sup>:

$$\begin{aligned} V_{ig, jg}(R) &= 2ME_{ig}(R) \delta_{ij} + H_{ig, jg}^{(*)}(R) - (1+2\kappa) H_{ig, jg}^{(\pm)}(R) \\ &+ B_{ig, jg}^{(*)}(R) + \frac{d}{dR} Q_{ig, jg}^{(*)}(R) + 2Q_{ig, jg}^{(*)}(R) \frac{d}{dR}, \end{aligned} \quad (18)$$

$$V_{ig, ju}(R) = \kappa \left\{ H_{ig, ju}^{(-)}(R) + B_{ig, ju}^{(-)}(R) + \frac{d}{dR} Q_{ig, ju}^{(-)}(R) + 2Q_{ig, ju}^{(-)}(R) \frac{d}{dR} \right\}. \quad (19)$$

Similar relations hold for  $V_{iu, ju}(R)$  and  $V_{iu, jg}(R)$  with the obvious substitution  $g \rightarrow u$  on the right-hand side of Eqs. (18) and (19).

For the potentials  $V_{ip, jp}(k, R)$ , which couple the states of the discrete,  $|i\rangle$ , and continuous,  $|c\rangle$ , spectra of the two-center problem, the relations (18) and (19) hold as before.

The potentials  $V_{sp, sp}(k, k', R)$ , which couple the continuum states  $|c\rangle$  and  $|c'\rangle$  of the two-center problem, can be represented in the general case in the form

$$V_{sp, sp}(k, k', R) = V_{sp, sp}(k, R) \delta(k-k') + v_{sp, sp}(k, k', R). \quad (20)$$

The potentials  $V_{sg, sg}(k, R)$ , like those in (18), can be represented as

$$\begin{aligned} V_{sg, sg}(k, R) &= 2M \frac{k^2}{2} \delta_{ss} + H_{sg, sg}^{(*)}(k, R) - (1+2\kappa) H_{sg, sg}^{(\pm)}(k, R) \\ &+ B_{sg, sg}^{(*)}(k, R) + \frac{d}{dR} Q_{sg, sg}^{(*)}(k, R) + 2Q_{sg, sg}^{(*)}(k, R) \frac{d}{dR}. \end{aligned} \quad (21)$$

The expressions for the potentials  $V_{su, su}(k, R)$ ,  $V_{sg, su}(k, R)$ , and  $V_{su, sg}(k, R)$  are constructed as in (18) and (19).

Using the asymptotic behavior of the matrix elements  $H_{ij}^{(\pm)}(R)$ ,  $H_{ij}^{(*)}(R)$ ,  $Q_{ij}^{(\pm)}(R)$ ,  $B_{ij}^{(\pm)}(R)$  in the limit  $R \rightarrow \infty$ ,<sup>21</sup> we find that the origin for the measurement of the energy  $E_{n\tau}$  (in units with  $e = \hbar = m_a = 1$ ) is<sup>4</sup>

$$(2M)^{-1} V_{1a, 1a}(\infty) = E_{1a}(\infty) = E_{1a} = -1/2,$$

i.e., it is equal to the energy of the ground state of the

mesic atom ( $m_\mu, M_a$ ). At the same time,  $U_{1a,1a}(\infty) = 0$ .

Solving the singular Sturm-Liouville problem (14)–(15) with the potentials (17)–(21), we can find the energy levels  $\epsilon_{J\nu}$  and the wave functions  $\chi_j(R)$  and  $\chi_s(k, R)$  of the mesic molecules.

### 3. SOLUTION TO THE STURM-LIOUVILLE PROBLEM FOR A SYSTEM OF ORDINARY DIFFERENTIAL EQUATIONS

To solve the singular Sturm-Liouville problem (14)–(15) for the infinite system of ordinary integro-differential equations on the ray  $0 \leq R < \infty$  we approximate it by the regular Sturm-Liouville problem for a finite system of equations of dimension  $N$  on the finite interval  $0 \leq R \leq R_m$  (Refs. 22 and 23):

$$\hat{I} \left\{ \frac{d^2}{dR^2} - \frac{J(J+1) - 2m^2}{R^2} - \frac{2M}{R} + 2M\epsilon_{J\nu} \right\} \chi_i(R) = \sum_{j=1}^{N_i} \hat{U}_{ij}(R) \chi_j(R) + \sum_{s=1}^{N_s} \int_0^{k_m} dk \hat{U}_{is}(k, R) \chi_s(k, R), \quad (22a)$$

$$\hat{I} \left\{ \frac{d^2}{dR^2} - \frac{J(J+1) - 2m^2}{R^2} - \frac{2M}{R} + 2M\epsilon_{J\nu} \right\} \chi_s(k, R) = \sum_{i=1}^{N_i} \hat{U}_{si}(k, R) \chi_i(R) + \sum_{s'=1}^{N_s} \int_0^{k_m} dk' \hat{U}_{ss'}(k, k', R) \chi_{s'}(k', R)$$

with boundary conditions

$$\begin{aligned} \chi_i(0) = \chi_i(R_m) = 0, \quad 1 \leq i \leq N_i, \\ \chi_s(k, 0) = \chi_s(k, R_m) = 0, \quad 1 \leq s \leq N_s, \quad 0 \leq k \leq k_m. \end{aligned} \quad (22b)$$

The numerical investigation of the convergence of the expansion (10) made in the present work shows that for the calculation of the energy levels of the  $\mu$ -mesic molecules with accuracy  $\sim 0.1$  eV it is sufficient to set  $N_i = 13$ ,  $N_s = 6$ ,  $R_m = 60$ ,  $k_m = 10$ . The interval  $0 \leq k \leq k_m$  for each state  $|ks\rangle$  is divided up by  $N_k^{(s)}$  points  $k_\alpha$  ( $\alpha = 1, 2, \dots, N_k^{(s)}$ ) with step  $\Delta k_\alpha$  and all integrals over  $k$  are replaced by sums of the form

$$\int_0^{k_m} f(k) dk = \sum_{\alpha=1}^{N_k^{(s)}} f(k_\alpha) \varphi(k_\alpha) \Delta k_\alpha, \quad (23)$$

where  $\varphi(k_\alpha) \Delta k_\alpha$  are the weights of Simpson's quadrature formula. When the continuous spectrum is made discrete in this manner, the total number of pairs of equations in the system (22) is

$$N = (N_i + N_c), \quad N_c = \sum_{s=1}^{N_s} N_k^{(s)}.$$

In the present work  $N_c = 119$ , i.e., the total number of equations in the system (22) is  $2N = 264$ .

The potentials  $V_{ij}(R)$ , which couple the states  $|i\rangle = |n_1 n_2 m\rangle$  and  $|j\rangle = |n'_1 n'_2 m'\rangle$  of the discrete spectrum of the two-center problem for all sets of quantum numbers satisfying the condition

$$\begin{aligned} n = n_1 + n_2 + m + 1 \leq 3, \\ n' = n'_1 + n'_2 + m' + 1 \leq 3, \end{aligned}$$

and also the potentials  $V_{ij}(R)$  and  $V_{jj}(R)$ , which couple the  $(g, u)$  pair of states  $|1\rangle = |000\rangle$  to the three pairs of states  $|j\rangle = |300\rangle, |210\rangle, |120\rangle$  in the shell  $n = 4$ , were calculated by means of the algorithms of Refs. 8 and 9

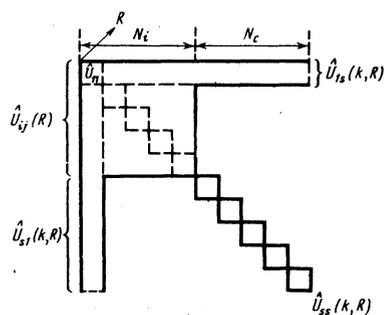


FIG. 1. Schematic form of the matrix of effective potentials  $U_{ij}(R)$  used in the solution of the system of equations (22a). The numbers  $N_i$  and  $N_c$  are the dimensions of the matrices  $U_{ij}(R)$  and  $U_{is}(k, R)$  which couple the states of the discrete spectrum and the states of the discrete and continuous spectra, respectively. The broken lines show the matrix used in the program BAAP.

over the interval  $R = 0.1(0.1)20(1)100$  with relative error  $\sim 10^{-7}$ . The total number of potentials  $V_{ij}(R)$  used was 436.

The potentials  $V_{1s}(k, R)$ , which couple a pair of ground states of the two-center problem,  $|000g\rangle$  and  $|000u\rangle$ , to the pairs  $|ksg\rangle$  and  $|ksu\rangle$  of states of the continuum, were calculated with absolute accuracy  $\sim 10^{-5}$  on the interval  $R = 0.1(0.1)5(0.2)11(0.5)20$ .<sup>11,12</sup> For the states  $s = [n_2 m] = [00]$ , the potentials were calculated for the values  $k = 0.2(0.1)1(1)10$  ( $N_k^{(s)} = 18$ ), for the states  $[10], [20], [01]$ , and  $[11]$  for  $k = 0.2(0.1)1(0.2)2(1)10$  ( $N_k^{(s)} = 22$ ), and for the states  $[30]$  for  $k = 0.2(0.2)2(1)5$  ( $N_k^{(s)} = 13$ ). The total number of potentials  $V_{1s}(k, R)$  and  $V_{s1}(k, R)$  used was 476.

The diagonal matrix elements  $V_{sg,sg}(k, R)$ ,  $V_{su,su}(k, R)$ , etc., which couple the pairs of states  $|c\rangle = |kn_2 mg\rangle$  and  $|c'\rangle = |kn_2 mu\rangle$  of the continuous spectrum of the two-center problem, were calculated in Ref. 13 with absolute accuracy  $\sim 10^{-5}$  for the sets  $n_2 = 0, 1, 2, 3$ , and  $m = 0, 1$  for the values  $k = 0.2(0.1)1(0.2)2(1)10$  in the interval  $R = 0.1(0.1)5(0.2)11(0.5)20$ .

The general form of the matrix of the potentials  $\hat{U}(R)$  calculated at the present time is shown in Fig. 1.

For the numerical solution of the Sturm-Liouville problem (22) we used the algorithms of Refs. 16–18 constructed on the basis of the continuous analog of Newton's method<sup>14</sup> and its modifications.<sup>15</sup> The required values of  $\epsilon_{J\nu}$ ,  $\chi_i(R)$ , and  $\chi_s(k, R)$  were calculated by means of the programs ITER (Ref. 17) and BAAP

TABLE I. Binding energies  $-\epsilon_{J\nu}$  (eV) of the  $(J\nu)$  states of the mesic molecules  $pp\mu$ ,  $pd\mu$ ,  $pt\mu$ .

(Jν)						Method
(00)	(10)	(00)	(10)	(00)	(10)	
$pp\mu$		$pd\mu$		$pt\mu$		Two-level approximation Perturbation theory ITER BAAP Variational calculation
247.31	101.47	215.68	91.35	207.28	92.21	
253.55	107.33	221.49	98.79	213.85	101.30	
252.89	106.95	221.52	97.36	213.96	99.06	
252.95	106.96	221.52	97.40	213.97	99.01	
253.09 [19b]	107.23 [20]	221.28 [19b]	—	213.0 [19a]	—	

TABLE II. Binding energies  $-\epsilon_{Jv}$  (eV) of the  $(Jv)$  states of the mesic molecules  $dd\mu$  and  $dt\mu$ .

$(Jv)$					Method
(00)	(01)	(10)	(11)	(20)	
Mesic molecule $dt\mu$					
322.89	33.14	224.08	0.64	83.56	Two-level approximation
324.99	35.66	226.74	1.83	85.34	Perturbation theory
325.05	35.81	226.61	1.39	86.31	ITER*
325.04	35.80	226.61	1.91**	86.32	BAAP
324.27 [19b]	32.76 [19b]	226.55 [20]	-	-	Variational calculation
Mesic molecule $dd\mu$					
317.04	32.21	230.10	-0.47	99.90	Two-level approximation
319.09	34.70	232.61	0.63	103.16	Perturbation theory
319.15	34.87	232.43	0.17	102.52	ITER*
319.15	34.87	232.44	0.64**	102.54	BAAP
318.07 [19b]	32.95 [19b]	-	-	-	Variational calculation

\*The calculations with the program ITER were made for  $R_m = 20$ .  
 \*\*The values obtained with the program BAAP for  $R_m = 60$ . For  $R_m = 20$ , we have  $-\epsilon_{11}(dd\mu) = 1.39$  eV and  $-\epsilon_{11}(dt\mu) = 0.17$  eV, i.e., these values are just the same as the results obtained by the program ITER.

(Ref. 18). The initial approximations for  $\epsilon_{Jv}$  and  $\chi_i(R)$  were calculated using the program system,<sup>18</sup> which makes it possible to solve a partial Sturm-Liouville problem for a system of ~40 ordinary differential equations. The initial approximations for the functions  $\chi_s(k, R)$  were taken equal to zero.

The program ITER makes it possible to solve the partial Sturm-Liouville problem (22)-(23) for a system of ordinary differential equations of dimension ~300 for the matrix of potentials shown in Fig. 1.

The program BAAP is constructed on the basis of the program ITER to solve the problem (22)-(23) with a matrix of potentials of special form, which contains only the potentials  $U_{1j}(R)$ ,  $U_{j1}(R)$ ,  $U_{1s}(k, R)$ ,  $U_{s1}(k, R)$ ,  $U_{jj}(R)$ , and  $U_{ss}(k, R)$  (in Fig. 1, this matrix is indicated by the broken lines). This makes it possible to shorten the computing time by an order of magnitude compared with the program ITER.

With the chosen method of dividing the interval  $0 \leq R \leq R_m$  by the points  $R_\alpha$ , at which the values of the potentials  $\hat{U}_{1j}(r)$ ,  $\hat{U}_{1s}(k, R)$ , and  $\hat{U}_{s1}(k, R)$  are specified, and also for the chosen values of  $N_i, N_s, N_k^{(s)}, R_m$ , the relative accuracy in the solution of the Sturm-Liouville problem (22) by means of the algorithms ITER and BAAP is  $10^{-4} - 10^{-5}$ .

#### 4. DISCUSSION OF THE RESULTS

The results of the calculations are given in Tables I-V. In the first row of Tables I-III we give the

TABLE III. Binding energies  $-\epsilon_{Jv}$  (eV) of the  $(Jv)$  states of the mesic molecule  $tt\mu$ .

$(Jv)$						Method
(00)	(01)	(10)	(11)	(20)	(30)	
361.56	81.61	287.65	43.23	170.95	46.81	Two-level approximation
362.89	83.68	289.19	45.15	172.79	48.90	Perturbation theory
362.95	83.87	289.15	45.24	172.64	48.69	ITER
362.95	83.88	289.15	45.24	172.65	48.70	BAAP
361.4 [19a]	75.2 [19a]	288.72 [20]	-	-	-	Variational calculation

TABLE IV. Contribution of the various states  $|j\rangle = |n_1 n_2 m\rangle$  of the spectrum of the two-center problem to the binding energy  $-\epsilon_{Jv}$  (eV) of the mesic molecules ( $\epsilon_{discr} = \epsilon_{Jv}^{(0)} + \epsilon_{discr}^{(2)}$ ).

n	$[n_1 n_2 m]$	$(Jv)$					
		(00)	(10)	(00)	(10)	(11)	(11)
		$pp\mu$		$pd\mu$		$dd\mu$	$dt\mu$
1	[000]	246.947	101.236	215.401	91.141	0.558	-0.645
	[100]	1.591	1.114	1.213	0.946	0.310	0.282
2	[010]	1.779	1.639	1.725	1.797	0.409	0.395
	[001]	-	0.465	-	0.321	0.104	0.067
	[200]	0.332	0.229	0.232	0.181	0.059	0.053
	[110]	0.221	0.138	0.284	0.245	0.048	0.051
3	[020]	0.001	0.003	0.000	0.001	0.008	0.003
	[101]	-	0.130	-	0.099	0.021	0.015
	[011]	-	0.000	-	0.000	0.001	0.001
	[300]	0.128	0.088	0.088	0.069	0.022	0.019
4	[210]	0.075	0.041	0.106	0.087	0.017	0.018
	[120]	0.001	0.002	0.000	0.001	0.003	0.002
	$-\epsilon_{discr}^{(2)}$	4.128	3.849	3.648	3.747	1.002	0.906
	$-\epsilon_{discr}$	251.075	105.085	219.049	94.888	1.560	0.261

values of  $\epsilon_{Jv} = \epsilon_{Jv}^{(0)}$  calculated in the two-level approximation ( $N_i = 1, N_s = 0$ ) of the adiabatic method of Refs. 4-7 by means of the algorithm SYSTEM. In this approximation, the matrix of the potentials  $\hat{U}(R)$  consists of only one block  $\hat{U}_{11}(R)$  (see Fig. 1), the accuracy in the calculation of the energy  $\epsilon_{Jv}$  for deep levels in 1-5 eV, and  $\epsilon_{11}^{(0)}(dd\mu) = -0.64$  eV. The  $(J=1, v=1)$  stationary state of the mesic molecule  $dt\mu$  in this approximation is absent, and instead there is a quasistationary state with energy  $\epsilon_{11}^{(0)}(dt\mu) = +0.47$  eV and width ~0.2 eV. With the extension of the system of equations (22), this quasistationary level moves to the boundary of the continuum, and for  $N_i = 4, N_s = 0$  the quasistationary state becomes stationary. In the variational calculations of Refs. 19 and 20, the  $(J=1, v=1)$  stationary state of the molecule  $dt\mu$  was not found.

In the second row of Tables I-III we give the values of  $\epsilon_{Jv} = \bar{\epsilon}_{Jv} + \epsilon_{cont}^{(2)}$  calculated perturbatively in accordance with the algorithm of Ref. 3; the contribution of the discrete spectrum  $\bar{\epsilon}_{Jv} = \epsilon_{Jv}^{(0)} + \epsilon_{discr}^{(2)}$  was calculated by means of the program SYSTEM for  $N_i = 13, N_s = 0$ , and the functions  $\chi_{1a}$  and  $\chi_{1b}$ , found in the solution of this system, were used to calculate the contribution  $\epsilon_{cont}^{(2)}$  [see (25)].

The third row contains the results of calculations of

TABLE V. Contribution of the discrete and continuum states of the two-center problem to the binding energy  $-\epsilon_{Jv}$  (eV) of the mesic molecules.

	$(Jv)$					
	(00)	(10)	(00)	(10)	(11)	(11)
$-E_{1a}$	$pp\mu$ 2528.52		$pd\mu$ 2663.23		$dd\mu$ 2711.27	$dt\mu$
$-\epsilon_{Jv}^{(0)}$	246.947	101.236	215.401	91.141	0.558*	-0.645*
$-\epsilon_{discr}^{(2)}$	4.127	3.849	3.604	3.747	1.002	0.906
$-\epsilon_{cont}^{(2)}$	1.488	1.723	2.199	2.321	0.349	0.374
$-\epsilon_{Jv}^{(2)}$	5.615	5.572	5.803	6.068	1.351	1.280
$-\epsilon_{Jv}^{(0)} - \epsilon_{Jv}^{(2)}$	252.562	106.808	221.204	97.203	1.909	0.635
$-\epsilon_{Jv}$	252.954	106.982	221.543	97.399	1.907	0.636

\*Values obtained in accordance with Eq. (24). In the two-level approximation of the system (14), we obtain  $\epsilon_{11}^{(0)}(dd\mu) = -9.640$  eV and  $\epsilon_{11}^{(0)}(dt\mu) = 0.474$  eV instead of the given values.

$\epsilon_{jv}$  by the program ITER with completely filled matrix of potentials  $\hat{U}(R)$ , the form of the matrix being shown in Fig. 1. The fourth row contains the results of calculations by the program BAAP.

In all the listed cases we used only the diagonal matrix elements (20), which couple the states  $|ks\rangle$  of the continuum, i.e., the potentials in Eqs. (22) have the form  $\hat{U}_{ss}(k, k', R) = \hat{U}_{ss}(k, R) \delta_{ss} \delta(k - k')$ , and in the potentials  $\hat{U}_{ss}(k, R)$  allowance is made for only the leading term

$$U_{ss}(k, R) = iMk^2.$$

In the fifth row, we give the results of the best variational calculations.<sup>19, 20</sup>

In the calculations, we used the following values of the masses of the particles (in units of the electron mass  $m_e$ ) and the value of  $Ry^{24}$ :

$$m_\mu = 206.769, \quad M_p = 1836.152, \quad M_d = 3670.481, \\ M_t = 5496.918, \quad Ry = 13.6058 \text{ eV}.$$

It can be easily seen in Tables I–III that the values of  $\epsilon_{jv}$  calculated by perturbation theory are very close to the values calculated by the programs ITER and BAAP. The values of  $\epsilon_{jv}$  calculated by these two programs are equal to a high accuracy ( $\sim 10^{-2}$  eV). This means that in calculations to this accuracy the contribution of the potentials  $\hat{U}_{ij}(R)$  for  $i \neq j \neq 1$  can be ignored. As a rule, the results of calculations of  $\epsilon_{jv}$  with the boundary conditions (22b) for  $R_m = 60$  and  $R_m = 20$  do not differ to accuracy  $\sim 10^2$  eV, and therefore the calculations by means of the program ITER were made for  $R_m = 20$ . An exception was the weakly bound states ( $J=1, v=1$ ) of the mesic molecules  $dd\mu$  and  $dt\mu$ , for which the values of  $\epsilon_{jv}$  calculated for  $R_m = 20$  and  $R_m = 60$  differ appreciably (see Table II).

Having calculated the functions  $\chi_j(R)$  and  $\chi_s(k, R)$  by, for example, the program BAAP, we can find the contribution made to  $\epsilon_{jv}$  by each pair of states  $|j\rangle = |n_1 n_2 m\rangle$  and  $|c\rangle = |kn_2 m\rangle$  of the two-center problem. In turn, this makes it possible to investigate numerically the rate of convergence of the expansion (10b) and determine the minimal number of terms in this expansion needed to calculate  $\epsilon_{jv}$  with the given accuracy.

To this end, we represent the energy  $\epsilon_{jv}$  of the state ( $Jv$ ) in the form of a sum analogous to the perturbation theory series of Ref. 3:

$$\epsilon_{jv} = \epsilon_{jv}^{(0)} + \epsilon_{jv}^{(2)}, \quad (24)$$

where

$$\epsilon_{jv}^{(0)} = (2M)^{-1} \int_0^{R_m} dR \chi_j(R) \times \left\{ -\hat{I} \left( \frac{d^2}{dR^2} - \frac{J(J+1) - 2m^2}{R^2} - \frac{2M}{R} \right) + \hat{U}_{11}(R) \right\} \chi_j(R), \quad (25)$$

$$\epsilon_{jv}^{(2)} = \epsilon_{discr}^{(2)} + \epsilon_{cont}^{(2)}$$

$$\epsilon_{discr}^{(2)} = \sum_{n_1=0}^{N_1} \sum_{n_2=0}^{N_2} \sum_{m=0}^{N_3} \epsilon_{jv}^{(2)} [n_1 n_2 m] = \sum_{j=1}^{N_1} \epsilon_{jv}^{(2)} [j],$$

$$\epsilon_{cont}^{(2)} = \sum_{n_2=0}^{N_2} \sum_{m=0}^{N_3} \int_0^{h_m} dk \epsilon_{jv}^{(2)} [kn_2 m] = \sum_{s=1}^{N_s} \int_0^{h_m} dk \epsilon_{jv}^{(2)} [ks], \quad (25a)$$

$$\epsilon_{jv}^{(2)} [j] = (2M)^{-1} \int_0^{R_m} dR \chi_j(R) \hat{U}_{11}(R) \chi_j(R),$$

$$\epsilon_{jv}^{(2)} [ks] = (2M)^{-1} \int_0^{R_m} dR \chi_j(R) \hat{U}_{1s}(R) \chi_s(k, R).$$

The functions  $\chi_j(R)$  and  $\chi_s(k, R)$  are normalized by the condition

$$\sum_{j=(a,b)} \left\{ \sum_{j=1}^{N_j} \int_0^{R_m} dR \chi_{jp}^2(R) + \sum_{s=1}^{N_s} \int_0^{h_m} dk \int_0^{R_m} dR \chi_{sp}^2(k, R) \right\} = 1, \quad (26)$$

which approximates the normalization condition (11a) in the same sense in which the system of equations (22) approximates the system (14). The sums on the right-hand sides of Eqs. (25a) are to be understood in accordance with the definitions (16), for example,

$$\chi_i \hat{U}_{ij} \chi_j = \chi_{ia} \hat{U}_{ia} \chi_{ia} + \chi_{ia} \hat{U}_{ia} \chi_{ib} + \chi_{ib} \hat{U}_{ib} \chi_{ia} + \chi_{ib} \hat{U}_{ib} \chi_{ib}, \quad (27)$$

etc.

Note that  $\epsilon_{jv}^{(0)}$  and  $\epsilon_{jv}^{(2)}$  calculated in accordance with Eqs. (24) and (25a) are only approximately equal to the analogous quantities calculated by perturbation theory in Refs. 3 and 7; this is because the employed functions  $\chi_j(R)$  and  $\chi_s(k, R)$  differ from the functions constructed in perturbation theory already in the second order in  $(2M)^{-1}$ .

In Table IV, we give the contributions  $-\epsilon_{jv}^{(2)} [n_1 n_2 m]$  of the different states  $|j\rangle = |n_1 n_2 m\rangle$  of the discrete spectrum of the two-center problem to the binding energy  $-\epsilon_{jv}$ . It can be seen that these values exhaust the contribution of the states  $|j\rangle$  of the discrete spectrum to accuracy  $\sim 0.1$  eV.

In Fig. 2, we have plotted the functions  $\epsilon_{jv}^{(2)} [kn_2 m]$  corresponding to the level ( $J=1, v=1$ ) of the mesic molecule  $dt\mu$ . It is readily seen that a significant contribution to  $\epsilon_{cont}^{(2)}$  is made only by the region of values  $0 \leq k \leq 3$ .

In Fig. 3 we have plotted for the state ( $J=1, v=1$ ) of the mesic molecule the values of  $-\epsilon_{jv}^{(2)} [n_1]$ , and also the functions

$$-\epsilon_{jv}^{(2)}(k) = -\sum_{n_2, m} \epsilon_{jv}^{(2)} [kn_2 m], \quad (28)$$

which shows the contribution of the states  $|j\rangle$  and  $|ks\rangle$  to the binding energy  $-\epsilon_{11}(dt\mu)$ .

In Table V we give the relative contributions of the discrete and continuous spectra of the two-center problem to  $\epsilon_{jv}$ . It is readily seen that for the deep levels the decisive contribution to  $\epsilon_{jv}$  is made by the pair of states  $|j\rangle = |000g\rangle, |000u\rangle$ , whereas for the weakly bound states it is necessary to take into account

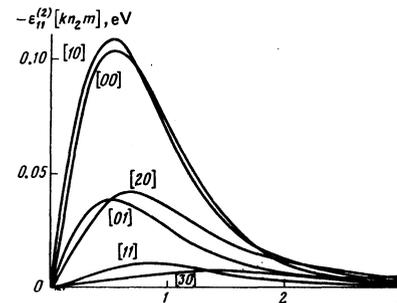


FIG. 2. Contribution of various  $[kn_2 m]$  continuum states of the two-center problem to the binding energy of the ( $J=1, v=1$ ) level of the mesic molecule  $dt\mu$ .

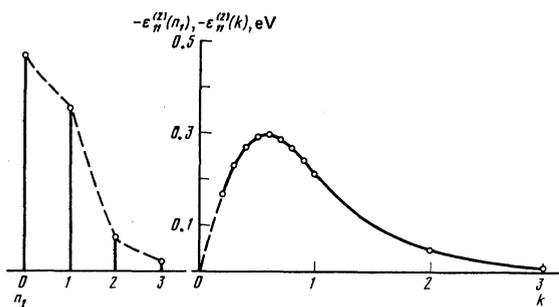


FIG. 3. Comparison of the contributions of the discrete and continuous spectra of the two-center problem to the binding energy of the ( $J=1, v=1$ ) level of the mesic molecule  $dt\mu$ . The contributions summed over the quantum numbers  $[n_2 m]$  are given:

$$\varepsilon_{11}^{(2)}(n_i) = \sum_{n_2, m} \varepsilon_{11}^{(2)}[n_1 n_2 m], \quad \varepsilon_{11}^{(2)}(k) = \sum_{n_2, m} \varepsilon_{11}^{(2)}[k n_2 m].$$

the contributions  $\varepsilon_{jv}^{(2)}[j]$  and  $\varepsilon_{jv}^{(2)}[ks]$  from the excited states  $|j\rangle$  and  $|ks\rangle$ .

Further details of the investigation into the convergence of our method of calculating the energy levels of the mesic molecules can be found in our communication Ref. 25.

## CONCLUSIONS

In this paper, we have shown that the expansion (10b) of the wave function  $\Psi_m(\mathbf{r}, \mathbf{R})$  with respect to the adiabatic basis converges fairly fast and can be successfully used for accurate calculation of the energy levels of  $\mu$ -mesic molecules. In contrast to the earlier studies Refs. 2–3, in which perturbation theory was used to solve the problem (22), the results of the present paper do not depend on the value of the small parameter  $(2M)^{-1}$ , which arises naturally in the adiabatic method.<sup>4–7</sup>

Analysis of the obtained results indicates that the relative accuracy  $\Delta\varepsilon/\varepsilon$  achieved in the present paper in the calculation of the energy levels of  $\mu$ -mesic molecules ( $\sim 10^{-3}$  for deep levels and  $\sim 10^{-2}$  for weakly bound levels) may be improved by extending the system of equations (22), and also by a more rational choice of the values of  $R_m$ ,  $k_m$ ,  $\Delta R$ , and  $\Delta k$ .

The absolute accuracy in the calculation of the energy of the deep levels achieved in the present paper,  $\sim 0.1$  eV, can also be improved by extending the system of equations (22), as follows from the analysis of Table V. The absolute accuracy in the calculation of the energies of the weakly bound states of the mesic molecules is somewhat higher at  $\sim 0.05$  eV.

Weakly bound ( $J=1, v=1$ ) states of the mesic molecules  $dd\mu$  (Ref. 6) and  $dt\mu$  (Ref. 2) were found earlier. The energies  $\varepsilon_{jv}$  of these states calculated in the present paper for the chosen values of  $N_t$ ,  $N_s$ ,  $N_k^{(s)}$ ,  $R_m$ ,  $\Delta R$ , and  $\Delta k$  are

$$\varepsilon_{11}(dd\mu) = -1.91 \text{ eV}, \quad \varepsilon_{11}(dt\mu) = -0.64 \text{ eV}.$$

Because of the importance of the obtained result for describing the process of  $\mu$  catalysis in a mixture of deuterium and tritium,<sup>26</sup> it would be very desirable to

calculate the energies of these states in some different way, using, for example, various variational methods,<sup>19,20,27</sup> expanding the solutions  $\Psi_{jv}(\mathbf{r}, \mathbf{R})$  with respect to two-center functions of Sturm type of a purely discrete spectrum,<sup>28</sup> solving the corresponding Faddeev equations in the coordinate space,<sup>29</sup> or directly solving the eigenvalue problem for the function  $F_m^{jv}(\xi, \eta, R)$  in the three-dimensional space  $(\xi, \eta, R)$ .<sup>30</sup>

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- <sup>1</sup>V. M. Bystritskiĭ, V. P. Dzhelepov, Z. V. Ershova, V. G. Zinov, V. K. Kapyshchev, S. M. Mukhamet-Galeeva, V. S. Nadezhdin, L. A. Rivkis, A. I. Rudenko, V. I. Safarov, N. V. Sergeeva, L. N. Somov, V. A. Stolupin, and V. V. Fil'chenkov, Soobshchenie OIYaI (JINR Communication), D1-12696, Dubna (1979); Pis'ma Zh. Eksp. Teor. Fiz. 31, 249 (1980) [JETP Lett. 31, 228 (1980)].
- <sup>2</sup>S. I. Vinit'skiĭ, L. I. Ponomarev, I. V. Puzynin, T. P. Puzyrina, L. N. Somov, and M. P. Faifman, Zh. Eksp. Teor. Fiz. 74, 849 (1978) [Sov. Phys. JETP 47, 444 (1978)].
- <sup>3</sup>S. I. Vinit'skiĭ and L. I. Ponomarev, Zh. Eksp. Teor. Fiz. 72, 1670 (1977) [Sov. Phys. JETP 45, 876 (1977)].
- <sup>4</sup>M. Born, Gött. Nachrich 1 (1951); S. I. Vinit'skiĭ and L. I. Ponomarev, Yad. Fiz. 20, 576 (1974) [Sov. J. Nucl. Phys. 20, 310 (1975)]; L. I. Ponomarev and S. I. Vinit'skiĭ, J. Phys. B12, 567 (1979); L. I. Ponomarev, S. I. Vinit'skiĭ, and F. Vukajlovic, J. Phys. B13, 847 (1980).
- <sup>5</sup>I. V. Komarov, L. I. Ponomarev, and S. Yu. Slavyanov, Sferoidal'nye i kulonovskie sferoidal'nye funktsii (Spheroidal and Coulomb Spheroidal Functions), Nauka (1976).
- <sup>6</sup>L. I. Ponomarev, I. V. Puzynin, and T. P. Puzyrina, Zh. Eksp. Teor. Fiz. 65, 28 (1973) [Sov. Phys. JETP 38, 14 (1974)]; L. I. Ponomarev, I. V. Puzynin, and T. P. Puzyrina, J. Comput. Phys. 13, 1 (1973).
- <sup>7</sup>S. I. Vinit'skiĭ, L. I. Ponomarev, I. V. Puzynin, T. P. Puzyrina, and L. N. Somov, Soobshchenie OIYaI (JINR Communication), R4-10336, Dubna (1976).
- <sup>8</sup>L. I. Ponomarev and T. P. Puzyrina, Zh. Vychisl. Mat. Mat. Fiz. 8, 1256 (1968); Preprint R4-5040 [in Russian], JINR, Dubna (1970).
- <sup>9</sup>N. F. Truskova, Soobshchenie OIYaI (JINR Communication), R11-11218, Dubna (1978).
- <sup>10</sup>L. I. Ponomarev, T. P. Puzyrina, and N. F. Truskova, J. Phys. B11, 3861 (1978).
- <sup>11</sup>L. I. Ponomarev and L. N. Somov, J. Comput. Phys. 20, 183 (1976).
- <sup>12</sup>L. I. Ponomarev, T. P. Puzyrina, and L. N. Somov, J. Phys. B10, 1335 (1977).
- <sup>13</sup>L. I. Ponomarev, S. Yu. Slavyanov, and L. N. Somov, Preprint R4-13028 [in Russian], JINR, Dubna (1979).
- <sup>14</sup>E. P. Zhidkov, G. I. Makarenko, and I. V. Puzynin, Fiz. Elem. Chastits At. Yadra 4, 127 (1973) [Sov. J. Part. Nucl. 4, 53 (1973)].
- <sup>15</sup>S. I. Vinit'skiĭ, V. S. Melezhik, I. V. Puzynin, T. P. Puzyrina, and L. N. Somov, Soobshchenie OIYaI (JINR Communication), R5-12788, Dubna (1979).
- <sup>16</sup>S. I. Vinit'skiĭ, V. S. Melezhik, I. V. Puzynin, T. P. Puzyrina, and L. N. Somov, Soobshchenie OIYaI (JINR Communication), R5-12787, Dubna (1979).
- <sup>17</sup>V. S. Melezhik, I. V. Puzynin, T. P. Puzyrina, and L. N. Somov, Soobshchenie OIYaI (JINR Communication), R5-12789, Dubna (1979).
- <sup>18</sup>V. S. Melezhik, I. V. Puzynin, T. P. Puzyrina, and L. N. Somov, Soobshchenie OIYaI (JINR Communication), R5-12790, Dubna (1979).

- <sup>19</sup>B. P. Carter, Phys. Rev. a) 141, 863 (1966); b) 165, 139 (1968).
- <sup>20</sup>A. Halpern, Phys. Rev. Lett. 13, 660 (1964).
- <sup>21</sup>M. P. Faifman, L. I. Ponomarev, and S. I. Vinitzky, J. Phys. B9, 2255 (1976); D. I. Abramov, S. Yu. Slavyanov, and L. N. Somov, Soobshchenie OIYaI (JINR Communication), R4-80-82, Dubna (1980).
- <sup>22</sup>A. A. Samarskiĭ, Teoriya raznostnykh skhem (Theory of Difference Schemes), Nauka (1977).
- <sup>23</sup>L. V. Kantorovich and V. I. Krylov, Priblizhennyye metody vysshego analiza (Approximate Methods of Higher Analysis), Gostekhizdat (1952).
- <sup>24</sup>E. R. Cohen and V. N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).
- <sup>25</sup>S. I. Vinitzkiĭ, V. S. Melezhik, L. I. Ponomarev, I. V. Puzyrin, T. P. Puzynina, L. N. Somov, and N. F. Truskova, Soobshchenie OIYaI (JINR Communication), R4-13036, Dubna (1980).
- <sup>26</sup>S. S. Gerstein and L. I. Ponomarev, Phys. Lett. B72, 80 (1977).
- <sup>27</sup>C. L. Pekeris, Phys. Rev. 112, 1649 (1958); 115, 1217 (1959).
- <sup>28</sup>A. I. Sherstyuk, Opt. Spectrosk. 38, 1040 (1975) [Opt. Spectrosc. 38, 601 (1975)].
- <sup>29</sup>S. P. Merkuriev, C. Gignoux, and A. Laverne, Ann. Phys. 99, 30 (1976); S. P. Merkur'ev and S. A. Pozdneevev, Yad. Fiz. 30, 941 (1979) [Sov. J. Nucl. Phys. 30, 489 (1979)].
- <sup>30</sup>I. M. Bassett, B. R. E. Lederer, and G. C. Vorliček, J. Comput. Phys. 22, 74 (1976).

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## Parity nonconservation in bismuth atoms and neutral weak-interaction currents

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Results are presented of measurements of the natural optical activity of atomic bismuth vapor in the region of the  $M1$  transition  $^4S_{3/2}-^2D_{5/2}$  at  $\lambda = 648$  nm. The measured value of the circular polarization  $P = -2R = -2 \operatorname{Im} [A(E1)/(M1)] = (40.4 \pm 5.4) \times 10^{-8}$  agrees with the results of the calculations performed within the framework of the Weinberg-Salam method with  $\sin^2\theta = 0.25$ .

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Following the discovery of neutral currents in weak interactions between neutrinos and nucleons,<sup>1-3</sup> the interest in weak-interaction gauge theories, which had predicted the existence of these interactions, has increased, and the problem of the existence of an analogous interaction between electrons and nucleons has become vital. As early as in 1959, Zel'dovich<sup>4</sup> has indicated that the weak interaction of electrons with nucleons can lead to parity nonconservation in atoms. The parity-nonconserving interaction of electrons with nucleons leads to a mixing of levels of opposite parity in atoms. It can be shown<sup>5</sup> that the spatial distribution of the electron spin in the atom has in this case a spiral structure, which in turn leads to a difference between the interaction of right- and left-polarized photons with the atoms and, as a consequence, to circular polarization of the radiation and to natural optical activity of matter in the atomic state.

An important step towards real experiments aimed at a search for this interaction was made by M. Bouchiat and C. Bouchiat,<sup>6</sup> who called attention to the enhancement of the parity-nonconservation effects in heavy atoms, and proposed an experiment for the measurement of circular polarization in the strongly forbidden magneto-dipole transition in cesium. This was soon followed by a number of suggestions<sup>7-9</sup> of studying the natural optical activity of vapors of heavy metals near the normal magnetodipole transitions.

It is known<sup>10</sup> that the parity-violating weak interaction of electrons with nucleons leads to the appearance of  $P$ -odd correlations of the form  $\sigma \cdot \mathbf{p}$ ,  $\sigma_n \cdot \mathbf{p}$ , and  $\sigma_n \times \sigma \cdot \mathbf{p}$  where  $\sigma$  and  $\mathbf{p}$  are the spin and momentum of the electron, and  $\sigma_n$  is the spin of the neutron or proton. In heavy atoms, the parity-nonconservation effects due to the correlation of the electron spin with its momentum are  $Z$  times larger than the effects due to correlation of the spin of the nucleon with the electron momentum, since the latter are determined only by nucleons with unpaired spins.

We present below the results of an experimental search for a parity-nonconserving weak interaction between electrons and nucleons, initiated by us in 1974 under the influence of discussions with I. B. Khriplovich at our Institute.

We chose for the investigation the red bismuth line  $\lambda = 648$  nm; we started from the fact that this line can be obtained from the dependable tunable cw dye laser with a sufficiently narrow line. A shortcoming of this transition is that it lies in a region overlapped by the rather dense spectrum of molecular bismuth (the partial vapor pressures of atomic and molecular bismuth are approximately equal).

The ground state of the bismuth atom pertains to the configuration  $6p^3$ , i. e., it has three outer  $p$  electrons in excess of the filled shells. Normal  $M1$  transitions are