

Convergence of the adiabatic expansion in the three-body problem with Coulomb interaction

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A method is proposed for calculating the contributions of the higher states of the discrete spectrum and the continuum in the two-center problem to the binding energy of a system of three bodies. The method makes it possible to find the energy levels of mesic molecules with accuracy $\sim 10^{-3}$ eV. The convergence of the expansion of the wave functions of mesic molecules of the hydrogen isotopes with respect to an adiabatic basis is investigated numerically.

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1. INTRODUCTION

The Schrödinger equation for the three-body problem with Coulomb interaction with two positively charged particles (nuclei) a and b with charges and masses $(Z_a M_a)$ and $(Z_b M_b)$, and a negatively charged particle c (electron or μ -meson, $Z_c = -1$, $m_c = m_e$ or m_μ) has the form¹

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

Here, \mathbf{R} is the distance between nuclei a and b , \mathbf{r} is the distance from particle c to the middle of the segment \mathbf{R} , and n and τ are the quantum numbers characterizing the state of the three-body system.

The set of quantum numbers $n = (Nlm)$ of a hydrogen-like atom with charge $Z = Z_a + Z_b$, to which the three-body system goes over in the limit $R \rightarrow 0$,² characterizes the motion of particle c in the field of the nuclei a and b . The set $\tau = (vJm_J\lambda)$ characterizes the relative motion of the nuclei: J is the total angular momentum of the three-body system, m_J is its projection, $\lambda = \pm(-1)^J$ is the total parity of the system, and v is the vibrational quantum number.

The Hamiltonian of the three-body system has the form³ (in units of $e = \hbar = m_e = 1$)

$$\hat{H} = -\frac{1}{2M} \left\{ \left(\nabla_{\mathbf{R}} + \frac{\mathbf{x}}{2} \nabla_{\mathbf{r}} \right)^2 - \frac{(1+x)^2}{4} \Delta_r \right\} - \frac{1}{2} \Delta_r - \frac{Z_a}{r_a} - \frac{Z_b}{r_b} + \frac{Z_a Z_b}{R}, \quad (2)$$

$$\frac{1}{M} = m_a \left(\frac{1}{M_a} + \frac{1}{M_b} \right), \quad \frac{1}{m_a} = \frac{1}{m_c} + \frac{1}{M_a}, \quad x = \frac{M_b - M_a}{M_a + M_b}, \quad (2a)$$

where r_a and r_b are the distances from particle c to nuclei a and b .

In the adiabatic representation of the three-body problem, we seek the wave function $\Psi_{n\tau}(\mathbf{r}, \mathbf{R})$ of the system in the form of the expansion^{1,3}

$$\Psi_{n\tau}(\mathbf{r}, \mathbf{R}) = R^{-1} \sum_{\alpha=1}^{\zeta} \left[\frac{1}{2} (1 + \delta_{0\alpha}) \right]^{1/2} \left\{ \sum_{N=1}^{N_\alpha} \sum_{l=0}^{N-1} \varphi_{Nlm}(\mathbf{r}; R) \chi_{Nlm}^{j\nu}(R) + \sum_{l=0}^{\zeta} \int_{k_0}^{k_m} dk \varphi_{lm}(\mathbf{r}; k, R) \chi_{lm}^{j\nu}(k, R) \right\} D_{mm_J}^J(\Phi, \Theta, 0), \quad (3)$$

where $\zeta = \min(l, J)$, the functions $\varphi_{Nlm}(\mathbf{r}; R)$ and $\varphi_{lm}(\mathbf{r}; k, R)$ are regular and bounded solutions to the two-center problem of quantum mechanics,²

$$(\hat{h} - E_{Nlm}(R)) \varphi_{Nlm}(\mathbf{r}; R) = 0, \quad (4a)$$

$$(\hat{h} - k^2/2) \varphi_{lm}(\mathbf{r}; k, R) = 0, \quad (4b)$$

with Hamiltonian

$$\hat{h} = -\frac{1}{2} \Delta_r - \frac{Z_a}{r_a} - \frac{Z_b}{r_b}, \quad (4c)$$

corresponding to the discrete spectrum and the continuum, Θ and Φ are the angular variables of the vector $\mathbf{R} = \{R, \Theta, \Phi\}$, and the Wigner functions $D_{mm_J}^J(\Phi, \Theta, 0)$ are normalized to unity.

Substituting the expansion (3) in Eq. (1) and averaging over the coordinates \mathbf{r}, Θ, Φ , we arrive at the system of ordinary differential equations¹

$$\left\{ \frac{d^2}{dR^2} + 2M\varepsilon_{j\nu} - U_{ii'}(R) \right\} \chi_i(R) = \sum_{j=1}^{N_i} U_{ij}(R) \chi_j(R) + \sum_{s=1}^{N_s} \int_{k_0}^{k_m} dk U_{is}(k, R) \chi_s(k, R), \quad (5a)$$

$$\left\{ \frac{d^2}{dk^2} + 2M\varepsilon_{j\nu} - U_{ss'}(k, R) \right\} \chi_s(k, R) = \sum_{j=1}^{N_j} U_{sj}(k, R) \chi_j(R) + \sum_{s'=1}^{N_s} \int_{k_0}^{k_m} dk' U_{ss'}(k, k', R) \chi_{s'}(k', R), \quad (5b)$$

where we have introduced the abbreviated notation $j \equiv (Nlm)$, $s \equiv (lm)$,

$$\chi_j(R) = \chi_{Nlm}^{j\nu}(R) = |j\rangle, \quad \chi_s(k, R) = \chi_{lm}^{j\nu}(k, R) = |ks\rangle,$$

$$U_{ii'}(R) = \frac{J(J+1) - 2m^2}{R^2} + \frac{2M}{R} + U_{ii}(R),$$

$$U_{ss'}(k, R) = \frac{J(J+1) - 2m^2}{R^2} + \frac{2M}{R} + U_{ss}(k, R),$$

and the effective potentials $U_{ii}(R)$, $U_{ss}(k, R)$, $U_{ss'}(k, k', R)$, $U_{ij}(k, R)$ are defined in Ref. 1 and calculated in Refs. 4-8; the energy

$$\varepsilon_{j\nu} = E_{n\tau} - E_{1s}$$

of the three-body system is measured from the energy $E_{1s} = -\frac{1}{2}$ of the ground state of the isolated atom (M_a, m_c).

In the limit $N_i \rightarrow \infty$, $N_s \rightarrow \infty$, $k_0 \rightarrow 0$, $k_m \rightarrow \infty$, $R_m \rightarrow \infty$, the system of equations (5) with the boundary conditions

$$\chi_i(0) = \chi_s(k, 0) = \chi_j(R_m) = \chi_s(k, R_m) = 0, \quad (5c)$$

and the normalization condition

$$\sum_{i=1}^{N_i} \int_0^{k_m} dR \chi_i^2(R) + \sum_{i=1}^{N_g} \int_{k_0}^{k_m} dk \int_0^{R_m} dR \chi_i^2(k, R) = 1 \quad (6)$$

is equivalent to the original equation (1), the expansion (3) in this limit being exact since the solutions (4) form a complete set.

In our previous investigations,¹ the system of equations (5) was used to calculate the energies of the states of μ -mesic molecules of the hydrogen isotopes for $N_i = 13$, $N_g = 6$, $k_0 = 0$, $k_m = 10$, $R_m = 60$.

The accuracy achieved in the calculations, ~ 0.1 eV, was insufficient for detailed description of the process of formation of μ -mesic molecules,⁹ and must be improved by at least an order of magnitude. For this, it is above all necessary to calculate the contribution to the energy ϵ_{Jv} of the higher states $|j\rangle$ and $|ks\rangle$ of the two-center problem, i.e., to calculate ϵ_{Jv} in the limit $N_i \rightarrow \infty$, $k_0 \rightarrow 0$. To solve this problem in the present paper, we used the values $N_i = 23$, $N_g = 6$, $k_0 = 0.2$, $k_m = 10$, $R_m = 100$.

2. METHOD OF SOLUTION

The system of equations (5)–(6) was solved by means of the VAAR program,¹⁰ which is based on algorithms which employ the continuous analog of Newton's method.^{11,13} The matrix $\hat{U}(R)$ of the effective potentials of the system of equations (5) has the form given in Ref. 1. It consists of 2×2 blocks $U_{ij}(R)$, $U_{ia}(k, R)$, $U_{aj}(k, R)$, and $U_{aa}(k, k', R)$, for example,

$$U_{ij}(R) = \begin{pmatrix} U_{ig,je} & U_{ig,jv} \\ U_{iu,je} & U_{iu,jv} \end{pmatrix}, \quad \chi_i(R) = \begin{pmatrix} \chi_{ie} \\ \chi_{iv} \end{pmatrix}, \quad (7)$$

etc., where the states $|ig\rangle$ and $|iu\rangle$ in the limit $R \rightarrow \infty$ form pairs with the same set of parabolic quantum numbers $[n, n_2, mp]$, differing only in the parity¹¹: $p = g, u = (-1)^l$.

In the VAAR program, we used a matrix $\hat{U}(R)$ consisting of the "rows" $U_{ij}(R)$ and $U_{ia}(k, R)$, "diagonals" $U_{jj}(R)$ and $U_{aa}(k, R)$, and "columns" $U_{ji}(R)$ and $U_{aj}(k, R)$. The special investigation made in Ref. 1 showed that the inclusion of the potentials $U_{ij}(R)$ for $i \neq j \neq 1$ in the system of equations (5) does not change the results of calculations of the energies ϵ_{Jv} of mesic molecules to relative accuracy $\sim 10^{-4}$.

Solving the system of equations (5) with the normalization condition (6), we find the energies ϵ_{Jv} and the wave functions $\chi_i(R)$ and $\chi_a(k, R)$ with relative accuracy $\sim 10^{-4}$ (Ref. 1), after which we can determine the contribution made to ϵ_{Jv} by each of the states $|j\rangle$ and $|ks\rangle$. For this,

TABLE I. Binding energies $-\epsilon_{Jv}$ (eV) of mesic molecules and the corrections $-\delta\epsilon_{Jv}$ (eV) to them.

	$\frac{pd\mu}{(J=0, v=0)}$	$\frac{dd\mu}{(J=1, v=0)}$	$\frac{dt\mu}{(J=1, v=0)}$	$\frac{dd\mu}{(J=1, v=1)}$	$\frac{dt\mu}{(J=1, v=1)}$
$-\epsilon_{Jv}$	221.691	226.683	232.512	1.9420	0.6845
$-\delta\epsilon_{Jv}$	0.221	0.104	0.095	0.0585	0.0544

*All calculations were made for the masses $m_\mu = 206.769$, $M_p = 1836.152$, $M_d = 3670.481$, $M_t = 5496.918$ of the particles and $2Ry = 27.2107$ eV.

we represent ϵ_{Jv} in the form

$$\epsilon_{Jv} = \epsilon_{Jv}^d + \epsilon_{Jv}^c, \quad (8)$$

$$\epsilon_{Jv}^d = \sum_{N=1}^{N_0} \epsilon_N, \quad \epsilon_N = \sum_{i=0}^{N-1} \sum_{m=0}^i \epsilon_{Nim},$$

$$\epsilon_{100} = (2MC)^{-1} \int_0^{R_m} dR \left\{ \chi_{100}(R) \left[-\frac{d^2}{dR^2} + U'_{100,100}(R) \right] + \chi_{210}(R) U_{210,100}(R) \right\} \chi_{100}(R),$$

$$\epsilon_{210} = (2MC)^{-1} \int_0^{R_m} dR \left\{ \chi_{210}(R) \left[-\frac{d^2}{dR^2} + U'_{210,210}(R) \right] + \chi_{100}(R) U_{100,210}(R) \right\} \chi_{210}(R),$$

$$\epsilon_{Nim} = (2MC)^{-1} \int_0^{R_m} dR \left\{ \chi_{100}(R) U_{100, Nim}(R) + \chi_{210}(R) U_{210, Nim}(R) \right\} \chi_{Nim}(R), \quad (9)$$

$$\epsilon_{Jv}^c = \int_{k_0}^{k_m} e(k) dk, \quad e(k) = \sum_{i=0}^{l_0} \sum_{m=0}^i \epsilon_{im}(k),$$

$$\epsilon_{im}(k) = (2MC)^{-1} \int_0^{R_m} dR \left\{ \chi_{100}(R) U_{100, im}(k, R) + \chi_{210}(R) U_{210, im}(k, R) \right\} \chi_{im}(k, R),$$

$$C = \int_0^{R_m} dR \left[\chi_{100}^2(R) + \chi_{210}^2(R) \right].$$

The relations (8)–(9) are an exact consequence of the system of equations (5). They are obtained after multiplication of the first pair of equations from the left by the function $\chi_1(R) = (\chi_{1g}, \chi_{1u})$ and integration over R . These relations, in contrast to those used earlier in Ref. 1, which were obtained using perturbation theory,¹³ are obtained without any approximations and make possible a numerical investigation of the convergence of the adiabatic expansion (3). This approach replaced the investigation of the convergence of the expansion (3) by the solution of the system of equations (5) with a successively increasing number of these equations.

In Table I, we give the binding energies $-\epsilon_{Jv}$ found by numerical integration of the system (5) using the VAAR program; they are equal to the values calculated in accordance with Eqs. (8) and (9). The value of R_m was taken to be $R_m = 20$ for the states ($J=0, v=0$), ($J=1, v=0$) and $R_m = 100$ for the states ($J=1, v=1$) of the mesic molecules $pd\mu$, $dd\mu$, and $dt\mu$.

In Table II, we give the contributions $-\epsilon_N$ to $-\epsilon_{Jv}^d$ of the various states of the mesic molecules $pd\mu$, $dd\mu$, and $dt\mu$. In calculating the contribution ϵ_N from the

TABLE II. Contributions ϵ_N (eV) of the states $|j\rangle$ of the discrete spectrum of the two-center problem to the binding energies $-\epsilon_{Jv}$ (eV) of mesic molecules.

N	$\frac{pd\mu}{(J=0, v=0)}$	$\frac{dd\mu}{(J=1, v=0)}$	$\frac{dt\mu}{(J=1, v=0)}$	$\frac{dd\mu}{(J=1, v=1)}$	$\frac{dt\mu}{(J=1, v=1)}$
1	213.685	224.098	229.876	0.5509	-0.8497
2	2.998	0.605	0.736	0.3107	0.4652
3	2.087	0.922	0.842	0.5730	0.5291
4	0.402	0.171	0.167	0.0914	0.0928
5	0.162	0.070	0.068	0.0449	0.0396
6	0.083	0.036	0.035	0.0224	0.0205
$-\sum_{N=7}^9 \epsilon_N$	0.038	0.014	0.015	0.0101	0.0099
$-\epsilon_{Jv}^d = -\sum_{N=1}^9 \epsilon_N$	219.455	225.916	231.740	1.6033	0.3073

TABLE III. Contribution $-\varepsilon(k)$ (eV) of the continuum states $|ks\rangle$ of the two-center problem to $-\varepsilon_{J\nu}$.

k	$(J=0, \nu=0)$	$(J=1, \nu=0)$	$(J=1, \nu=0)$	$(J=1, \nu=1)$	$(J=1, \nu=1)$
0.2	0.697	0.325	0.297	0.1846	0.1702
0.4	1.178	0.535	0.494	0.2943	0.2789
0.6	1.375	0.597	0.560	0.3125	0.3086
0.8	1.340	0.554	0.527	0.2652	0.2770
1.0	1.192	0.463	0.448	0.2014	0.2224
2.0	0.439	0.116	0.128	0.0373	0.0500
5.0	0.034	0.002	0.005	0.0006	0.0012
10.0	0.004	0.000	0.000	0.0000	0.0000
$-\varepsilon_{J\nu}^c$	2.236	0.767	0.872	0.3387	0.3773

shells $N = 7, 8, 9$, we took into account only some of the states with different l and m (their total contribution is given in the table).

In Table III, we give the analogous contributions $-\varepsilon(k)$ to $-\varepsilon_{J\nu}^c$ from the continuum states of the two-center problem. In calculating $\varepsilon_{J\nu}^c$, we took into account all contributions $\varepsilon_{l,m}(k)$ with $m=0, l=0, 1, \dots, 7$ and $m=1, l=1, 2, 3, 4$. The ignored contributions

$$\varepsilon_{l,m} = \int_{k_0}^{k_m} \varepsilon_{l,m}(k) dk$$

from the higher l do not exceed 0.01 eV.¹

3. CALCULATION OF $\delta\varepsilon_{J\nu}^d$ AND $\delta\varepsilon_{J\nu}^c$

In calculating the contributions $\delta\varepsilon_{J\nu}^d$ and $\delta\varepsilon_{J\nu}^c$ from the higher states $|j\rangle$ and $|ks\rangle$ of the two-center problem, we take into account in the first place the circumstance that the wave functions $\chi_j(R)$ and $\chi_s(k, R)$ are damped exponentially outside the region $R \approx 3$ (at large $\varepsilon_{J\nu}$) or $R \approx 7$ (for weakly bound states).^{14,13} This means that in the calculation of ε_j and $\varepsilon_s(k)$ it is sufficient to know the matrix elements $U_{1j}(R)$ and $U_{1s}(k, R)$ only in the restricted region $R \leq 7$. In this region, the two-center functions $\varphi_j(\mathbf{r}; R)$ and $\varphi_s(\mathbf{r}; k, R)$ can be approximated with good accuracy by the single-center functions of a hydrogenlike atom with charge $Z = Z_a + Z_b$ of the nucleus provided the conditions²

$$p_j = \frac{R}{2} \{-2E_j(R)\}^{1/2} \approx \frac{RZ}{2N} \ll 1, \quad c = \frac{kR}{2} \ll 1 \quad (10)$$

are satisfied, i.e., for $N \geq 7$ and $k \leq 0.3$. For these values of N and k , the wave functions of the discrete spectrum and the continuum of the hydrogen atom go over into each other when the substitution $Z/N \rightarrow ik$ is made.^{14,15}

The relations (9) for $N \gg 1$ and $k \ll 1$ can be represented in the form

$$\delta\varepsilon_{J\nu}^d = \sum_{N=N_1+1}^{\infty} \varepsilon_N \approx \int_{N_1}^{\infty} \varepsilon_N dN = \int_{N_1}^{\infty} \frac{N^3}{Z^2} \varepsilon_N d\left(-\frac{Z^2}{2N^2}\right) = \int_{E_1}^0 f_d(E) dE, \quad (11)$$

$$\delta\varepsilon_{J\nu}^c = \int_0^{k_0} \varepsilon(k) dk = \int_0^{k_0} \frac{\varepsilon(k)}{k} d\left(\frac{k^2}{2}\right) = \int_0^{E_0} f_c(E) dE,$$

where $E = -Z^2/2N^2$ and $E = k^2/2$, respectively, for the discrete spectrum and the continuum of the hydrogen atom, and the functions

$$f_d(E) = \frac{N^3}{Z^2} \varepsilon_N, \quad f_c(E) = \frac{\varepsilon(k)}{k} \quad (12)$$

are equal in the limit $N \rightarrow \infty$ and $k \rightarrow 0$:

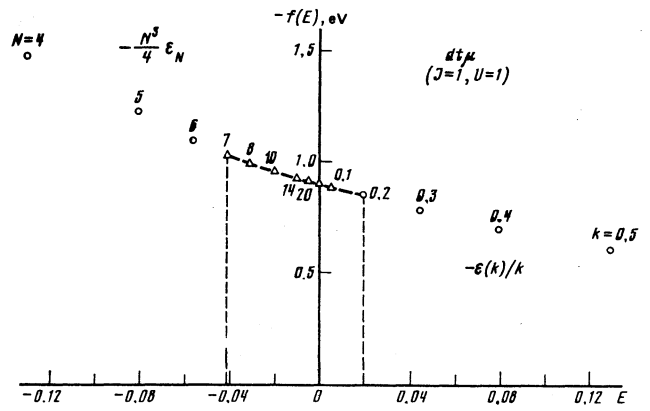


FIG. 1. Calculation of the contributions $-\delta\varepsilon_{J\nu}^d$ and $-\delta\varepsilon_{J\nu}^c$ to the binding energy $-\varepsilon_{J\nu}$ of the state $(J=1, \nu=1)$ of the mesic molecule $d\mu$. The open circles are the values of the functions $-f_d(E)$ and $-f_c(E)$ calculated in accordance with (9) and (12). The open triangles are the values of the function $-f(E)$ (13) with the coefficients given in Table IV. For $E=0$, which corresponds to $k=0$ or $N=\infty$, $f(0)=A$. The contributions $-\delta\varepsilon_{J\nu}^d = 0.036$ and $-\delta\varepsilon_{J\nu}^c = 0.018$ eV are equal to the areas bounded by the dashed line and the segments $E_1 \leq E \leq 0$ and $0 \leq E \leq E_0$ of the abscissa, respectively. They are calculated in accordance with Eqs. (14) for $N_1 = 7$, $E_0 = 0.02$, and $f_d(E) = f_c(E) = f(E)$. The values of E are given in the units $e = \hbar = m_a = 1$.

$$f_d(0) = f_c(0) = A, \quad (12a)$$

i.e., at the boundary of the discrete spectrum and the continuum of the hydrogenlike atom, which agrees with the well-known properties^{14,15} of its wave functions.

In Fig. 1, we give the values of the functions $-f_d(E)$ and $-f_c(E)$ calculated in accordance with the formulas (12) for $N=4, 5, 6$ and $k=0.2, 0.3, 0.4, 0.5$, and also the interpolation function $-f(E)$, which represents them in the region $E_1 \leq E \leq E_0$. The function $f(E)$ is chosen in the form

$$f(E) = A + BE + CE^2, \quad (13)$$

and its coefficients, determined from the values of the functions $f_d(E)$ and $f_c(E)$ at the points $N=5$ and 6 and $k=0.2$ and 0.3 , are given² in Table IV.

The corrections $\delta\varepsilon_{J\nu}^d$ and $\delta\varepsilon_{J\nu}^c$ are calculated in accordance with

$$\delta\varepsilon_{J\nu}^d = \sum_{N=N_1}^{N_2} \frac{4}{N^3} \left(A - B \frac{2}{N^2} + C \frac{4}{N^4} \right) + \frac{2A}{N_1^2} - \sum_{N=N_1}^0 \varepsilon_N, \quad (14)$$

$$\delta\varepsilon_{J\nu}^c = AE_0 + BE_0^2/2 + CE_0^3/3$$

for $E_0 = 0.02$, $N_1 = 7$, $N_2 = 40$, which follow from the de-

TABLE IV. Coefficients of the expansion of the function $-f(E)$ and the values of $-\delta\varepsilon_{J\nu}^d$, $-\delta\varepsilon_{J\nu}^c$, $-\delta\varepsilon_{J\nu}$, and $\Delta(\delta\varepsilon_{J\nu})$ in eV.

	$(J=0, \nu=0)$	$(J=1, \nu=0)$	$(J=1, \nu=0)$	$(J=1, \nu=1)$	$(J=1, \nu=1)$
$-A \pm \Delta A$	3.69±0.06	1.70±0.05	1.57±0.03	0.969±0.039	0.915±0.020
$-B \pm \Delta B$	-11±2	-3.8±1.7	-4.6±0.9	-3±1.3	-2.7±0.6
$-C \pm \Delta C$	63±50	17±4.9	23±26	23±36	13±18
$-\delta\varepsilon_{J\nu}^d$	0.149	0.071	0.064	0.0396	0.0366
$-\delta\varepsilon_{J\nu}^c$	0.072	0.033	0.031	0.0189	0.0178
$-\delta\varepsilon_{J\nu} \pm \Delta(\delta\varepsilon_{J\nu})$	0.221±0.004	0.104±0.003	0.095±0.002	0.0585±0.0026	0.0544±0.0012

finitions (9) and (12) and Fig. 1.

The error $\Delta(\delta\epsilon_{Jv})$ in the calculation of the contribution

$$\delta\epsilon_{Jv} = \delta\epsilon_{Jv}^d + \delta\epsilon_{Jv}^c \quad (15)$$

of the higher states $|j\rangle$ and $|ks\rangle$ to the energy ϵ_{Jv} is determined by the errors in the calculation of the coefficients A , B , and C and the errors of the numerical integration in the calculation of ϵ_N and $\epsilon(k)$ in accordance with Eqs. (9).

The values of $-\delta\epsilon_{Jv}$ for deep levels of the mesic molecules are ~ 0.2 eV, and for the levels ($J=1$, $v=1$) of the mesic molecules $dd\mu$ and $dt\mu$ do not exceed ~ 0.05 eV. The errors $\Delta(\delta\epsilon_{Jv})$ are due mainly to the error $\Delta A/A \leq 10^{-2}$ in the determination of the coefficients of the function $f(E)$. They are given in Table IV and are ≈ 0.004 eV for the deep levels and ≈ 0.001 eV for the levels ($J=1$, $v=1$) of the mesic molecules $dd\mu$ and $dt\mu$.

4. CONCLUSIONS

Our investigation gives a regular method of calculating the contributions $\delta\epsilon_{Jv}$ to the energy ϵ_{Jv} of mesic molecules from the higher states $|Nlm\rangle$ and $|klm\rangle$ of the two-center problem in the limit $N \rightarrow \infty$ and $k \rightarrow 0$. It follows from the investigation that the use of a restricted set of two-center basis functions in the expansion (3) of the three-body wave function in the calculation of the energies ϵ_{Jv} of the states (Jv) of mesic molecules is not an obstacle to the finding of ϵ_{Jv} with high accuracy. The obtained result depends weakly on the smallness of the formal expansion parameter $(2M)^{-1}$, which in the case of mesic molecules is ~ 0.1 , and can be used to calculate the binding energies of systems such as $e^+e^-e^+$ and H^- , for which $(2M)^{-1}$ is $\frac{1}{2}$ and ≈ 1 , respectively.

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1) The correspondence rules are

$$n_1 = N - l - 1, \quad n_2 = [l - m - (1 - (-1)^{l-m})/2]/2.$$

2) The values of $f_d(E)$ for $N = 7, 8$, and 9 are less than the corresponding values of the function $f(E)$ because ϵ_N was calculated using only some of the states $|Nlm\rangle$: for $N = 7$, only seven out of the 13 states, for $N = 8$ only four of the 15, and for $N = 9$ only one of the 17. Therefore, in the construction of $f(E)$ the values of $f_d(E)$ for $N = 7, 8, 9$ were not used.

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