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Schrödinger perturbation theory in the adiabatic representation of the three-body problem

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A perturbation theory for the calculation of the binding energy and the wave functions of a three-body system is developed for the problem of three bodies with Coulomb approximation. The zeroth approximation used was an adiabatic basis, i.e., solutions and terms of the two-center problem of quantum mechanics, and the kinetic energy of the relative motion of like charged particles is regarded as a perturbation. The method is illustrated with the calculation of the binding energy of the $pd\mu$ mesic molecule as an example.

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1. INTRODUCTION

To calculate the binding energy of three particles with charges and masses (Z_a, M_a), (Z_b, M_b) and $(-1, m_\mu)$ several methods have been proposed and realized.[1–3] They were used to calculate the energies of the mesic molecules $pp\mu$, $pd\mu$, etc., and also that of the electron-positron system $e^+e^-e^+$.

In the calculation of the binding energy of the ground state of a three-body system, the most accurate result seems to be obtained by different modifications of variational calculation methods,[1,2] but on going over to the excited states these methods become much more complicated. The advantage of adiabatic calculation is their simplicity and lucidity, both in the case of the ground state and in the case of excited states. A classical example of an adiabatic calculation is the Born–Oppenheimer method in the theory of molecular spectra.[4]

It is known[3,4] that in the adiabatic representation of the three-body problem there appears a small parameter $(2M)^{-1}$, where $M \approx M_a M_b/(M_a + M_b)m_\mu$. The Born-Oppenheimer approximation consists of discarding from the equations for the relative motion of the nuclei all the terms $\sim (2M)^{-1}$. The need for this approximation was dictated by insufficient knowledge of the adiabatic basis, i.e., of the solutions of the two-center problem of quantum mechanics.[5] This was also one of the reasons for the loss of interest in the adiabatic method altogether.[1)] By now these difficulties have been overcome to a considerable degree,[7] so that the scope of the Born-Oppenheimer approximation can be expanded and a consistent scheme can be developed for calculations in the adiabatic basis, using the small parameter $(2M)^{-1}$.

We describe here a simple algorithm for the calculation of the binding energy of a three-body system, accurate to terms $\sim (2M)^{-3}$ inclusive.

We recall that in the adiabatic approximation the wave function $|\Psi\rangle$ of a system of three bodies is expanded in the complete set $|\Phi\rangle$ of the eigenfunctions of the Hamiltonian $\hat{W}$ of the two-center problem:

$$\hat{W}|\Phi\rangle = W|\Phi\rangle, \tag{1}$$

$$|\Psi\rangle = |\Phi\rangle\langle\Phi|\Psi\rangle. \tag{2}$$

The initial Schrödinger equation for the three-body system

$$(\hat{T}+\hat{W})|\Psi\rangle = E|\Psi\rangle \tag{3}$$

then goes over into an equivalent infinite system of homogeneous integro-differential equations for the functions $\langle\Phi|\Psi\rangle$[4]:

$$\langle\Phi|\hat{T}+\hat{W}|\Phi\rangle\langle\Phi|\Psi\rangle = E\langle\Phi|\Psi\rangle. \tag{4}$$

Here $\hat{T} = -(2M)^{-1}\Delta_R$ is the operator of the kinetic ener-

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gy of the relative motion of particles Z_a and Z_b (nuclei) having charges of the same polarity, R is the distance between them, and E is the total energy of the system. The Born-Oppenheimer approximation in this scheme corresponds to discarding all the off-diagonal matrix elements in the left-hand side of (4), which form the perturbation matrix that contains the small parameter $(2M)^{-1}$.

The perturbation-theory method proposed by Schrödinger[8] for the solution of eigenvalue problems of the type (3) consists in replacing the initial homogeneous problem

$$(\hat{H}-E)\,|\Psi\rangle=0 \tag{5}$$

by a system of inhomogeneous equations

$$\begin{aligned}&(\hat{H}^{(0)}-E^{(0)})\,|\Psi^{(0)}\rangle=0,\\&(\hat{H}^{(0)}-E^{(0)})\,|\Psi^{(1)}\rangle=(E^{(1)}-\hat{V})\,|\Psi^{(0)}\rangle,\\&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\&(\hat{H}^{(0)}-E^{(0)})\,|\Psi^{(s)}\rangle=(E^{(1)}-\hat{V})\,|\Psi^{(s-1)}\rangle+\sum_{t=2}^{s}E^{(t)}\,|\Psi^{(s-t)}\rangle.\end{aligned} \tag{6}$$

Here

$$\hat{H}=\hat{H}^{(0)}+\hat{V},\quad |\Psi\rangle=\sum_{s=0}|\Psi^{(s)}\rangle,\quad E=\sum_{s=0}E^{(s)}. \tag{7}$$

The method of separating the Hermitian perturbation operator $\hat{V}$ is determined by considerations of convenience in the computations.[9] If the wave functions $|\Psi^{(s)}\rangle$ are normalized by the intermediate-normalization condition

$$\langle\Psi^{(0)}\,|\,\Psi^{(s)}\rangle=\delta_{0s} \tag{8}$$

and the perturbation operator $\hat{V}$ is Hermitian, then the formulas[10]

$$\begin{aligned}E^{(2s)}&=\langle\Psi^{(s)}|\hat{V}|\Psi^{(s-1)}\rangle-\sum_{u=1}^{s}\sum_{t=1}^{s-1}E^{(2s-u-t)}\langle\Psi^{(u)}\,|\,\Psi^{(t)}\rangle,\\E^{(2s+1)}&=\langle\Psi^{(s)}|\hat{V}|\Psi^{(s)}\rangle-\sum_{u=1}^{s}\sum_{t=1}^{s}E^{(2s+1-u-t)}\langle\Psi^{(u)}\,|\,\Psi^{(t)}\rangle\end{aligned} \tag{9}$$

can be used to calculate the corrections to the energy $E^{(2s+1)}$ in terms of the corrections $\Psi^{(s)}$ of order not higher than s.

Thus, the first-order approximation for the wave function

$$|\Psi\rangle\approx|\Psi^{(0)}\rangle+|\Psi^{(1)}\rangle \tag{10}$$

can be used to determine the binding energy accurate to terms of third-order inclusive:

$$E\approx E^{(0)}+E^{(1)}+E^{(2)}+E^{(3)}. \tag{11}$$

Formulas (6)–(9) are valid for an arbitrary quantum system and in any representation of its solutions. Let us spell them out concretely for the case of the adiabatic representation of the three-body problem.

2. ADIABATIC REPRESENTATION OF THE THREE-BODY PROBLEM

The Schrödinger equation for the three-particle system consisting of two nuclei and an electron (or μ^- meson) with respective charges and masses (eZ_a, M_a), (eZ_b, M_b) and $(-e, m_\mu)$ is given by

$$(\hat{H}-E_{n\tau})\,|n\tau\rangle=0. \tag{12}$$

Here $\hat{H}$ is the complete Hamiltonian of the system in units $e=\hbar=m^*=1$[11,12]:

$$\begin{aligned}&\hat{H}=\hat{T}+\hat{W},\quad \hat{W}=h_0+Z_aZ_b/R,\\&\hat{T}=-\frac{1}{2M}\left[\Delta_R+\frac{\varkappa}{2}(\nabla_R\nabla_r+\nabla_r\nabla_R)\right],\end{aligned} \tag{13}$$

where

$$\begin{aligned}&h_0=-\frac{1}{2}\Delta_r-\frac{Z_a}{r_a}-\frac{Z_b}{r_b},\quad \varkappa=\frac{M_b-M_a}{M_b+M_a},\\&M=\frac{M_0}{m^*}=\frac{M_0}{m_\mu}+\frac{1}{4},\quad \frac{1}{M_0}=\frac{1}{M_a}+\frac{1}{M_b},\\&\frac{1}{m_0}=\frac{1}{m_\mu}+\frac{1}{M_a+M_b},\quad \frac{1}{m^*}=\frac{1}{m_0}+\frac{\varkappa^2}{4M_0}=\frac{1}{m_\mu}+\frac{1}{4M_0}\end{aligned} \tag{14}$$

and we have introduced the following notation: $\mathbf{R}$ is the vector joining the charges Z_a and Z_b; r_a, r_b, and r are the distances from the nuclei Z_a and Z_b and from the center of the segment R to the electron (meson); $E_{n\tau}<0$ is the total energy of the three-particle system the state determined by the sets of quantum numbers n and τ;

$$|n\tau\rangle=\langle\mathbf{r},\,\mathbf{R}|n\tau\rangle=\Psi_{n\tau}(\mathbf{r},\,\mathbf{R}) \tag{15}$$

is the wave function of the system, normalized by the condition

$$\langle n'\tau'|n\tau\rangle=\int d\mathbf{R}d\mathbf{r}\,\Psi^{+}_{n'\tau'}(\mathbf{r},\mathbf{R})\,\Psi_{n\tau}(\mathbf{r},\mathbf{R})=\delta_{nn'}\delta_{\tau\tau'}. \tag{16}$$

The adiabatic basis

$$|j\rangle\equiv|jm\rangle=\langle\mathbf{r};\,R|j\rangle=\Phi_j(\mathbf{r};\,R)\equiv\Phi_{jm}(\mathbf{r};\,R) \tag{17}$$

(the index m will as a rule be omitted) is defined as the complete set of the eigenfunctions of the Hamiltonian h_0 of the two-center problem[5]:

$$\hat{h}_0|j\rangle=E_j(R)\,|j\rangle, \tag{18}$$

where $E_j(R)$ are the terms of the two-center problem, and the wave functions are normalized by the conditions

$$\langle j'|j\rangle=\int d\mathbf{r}\,\Phi_{j'}^{*}(\mathbf{r};R)\,\Phi_j(\mathbf{r};R)=\begin{cases}\delta_{NN'}\delta_{ll'}\delta_{mm'}, & E_j(R)<0\\ \delta(k-k')\,\delta_{ll'}\delta_{mm'}, & E_j(R)>0\end{cases}. \tag{19}$$

For the case $E_j(R)<0$, the index $j\equiv jm=(Nlm)$ of the representation is a set of three quantum numbers, principal (N), orbital (l), and magnetic (m) (in accord with the classification of the unified atom[5]); in the case $E_j(R)=k^2/2>0$, the quantum numbers l and m retain the same meaning, but the discrete number N is replaced as the index of the representation $j\equiv jm=(klm)$ by the momentum k of the two-center problem.

The bound state $|n\tau\rangle$ of the three-body system $E_{n\tau}<0$ is characterized by a set of seven quantum numbers and is expanded in the adiabatic basis $|j\rangle \equiv |jm\rangle$ as follows:

$$|n\tau\rangle = |n\nu JM\lambda\rangle = |jm\rangle\langle jm|n\nu JM\lambda\rangle. \tag{20}$$

The index of the state n, just as the index of the representation j, is determined by three quantum numbers of the two-center problem, while the index of the state $\tau=(\nu JM\lambda)$ characterizes the relative motion of the nuclei (νJM) and the total parity λ of the three-particle system. The quantum numbers J and M are the eigenvalues of the operators of the total angular momentum of the system $\mathbf{J}^2$ and its projection J_z on the Z axis of the immobile coordinate system, while the parity λ is defined as the eigenvalue of the operator of total inversion of the coordinates

$$\hat{P}_{tot}\Psi_{n\tau}(\mathbf{r},\mathbf{R}) = \Psi_{n\tau}(-\mathbf{r},-\mathbf{R}) = \lambda\Psi_{n\tau}(\mathbf{r},\mathbf{R}). \tag{21}$$

Separating the angle variables (θ,ϕ) of the vector $\mathbf{R}$, we change from the expansion (2) to the expansion[12]

$$\begin{aligned}|n\tau\rangle \equiv |n\nu JM\lambda\rangle &= R^{-1}|jmJM\lambda\rangle\langle jm|n\nu J\lambda\rangle \\ &= R^{-1}\sum_{l,m=0}\Big\{\sum_{N=1}^{\infty}|NlmJM\lambda\rangle\langle Nlm|n\nu J\lambda\rangle \\ &\quad + \int_0^{\infty} dk\,|klmJM\lambda\rangle\langle klm|n\nu J\lambda\rangle\Big\},\end{aligned} \tag{22}$$

where the summation over l and m in the case $E_j(R)<0$ extends to $N-1$, and in the case of $E_j(R)=k^2/2>0$ it extends to infinity.

The functions $|jmJM\lambda\rangle = |jmJM(\pm)\rangle$ corresponding to the values $\lambda=\pm(-)^J$ are determined by the relations

$$\begin{aligned}|jmJM(\pm)\rangle &= [2(1+\delta_{0m})]^{-1/2}\{|jmJM\rangle \pm |j(-m)JM\rangle\}, \\ |j(\pm m)JM\rangle &= \Phi_{j(\pm m)}(\mathbf{r};R)D^{J}_{(\pm m)M}(\phi,\theta,0),\end{aligned} \tag{23}$$

where the D-functions are normalized by the condition

$$\int \sin\theta\, d\theta d\phi D^{J'*}_{mM'}(\phi,\theta,0)D^{J}_{mM}(\phi,\theta,0) = \delta_{JJ'}\delta_{MM'}. \tag{23a}$$

The functions $\langle jm|n\nu J\lambda\rangle = \chi^{J\lambda}_{jn\nu}(R)$ depend only on the radial variable R and satisfy the orthogonality conditions

$$\begin{aligned}\langle n'v'J'\lambda'|n\nu J\lambda\rangle = \langle n'v'J'\lambda'|j\rangle\langle j|n\nu J\lambda\rangle &= \sum_{l,m=0}\Big\{\sum_{N=1}^{\infty}\int_0^{\infty} dR\,\chi^{J'\lambda'}_{Nlmn'v'}(R)\chi^{J\lambda}_{Nlmn\nu}(R) \\ &\quad + \int_0^{\infty}dk\int_0^{\infty}dR\,\chi^{J'\lambda'}_{lmn'v'}(k,R)\chi^{J\lambda}_{lmn\nu}(k,R)\Big\} = \delta_{nn'}\delta_{vv'}\delta_{JJ'}\delta_{\lambda\lambda'},\end{aligned} \tag{24}$$

which follow from relations (16), (19) and (23a). The vibrational quantum number v is equal to the number of zeros of the wave function $\chi^{J\lambda}_{jn\nu}(R)$ on the semi-axis $0<R<\infty$.

Substitution of the expansion (22) in Eq. (12) and averaging over the coordinates $\mathbf{r}$, θ, and ϕ with the functions $\langle jmJM\lambda|$ leads to an infinite-dimensional system of homogeneous integro-differential equations for the radial functions $\chi^{J\lambda}_{jn\nu}$ [11,12](R)[11,12] (the index λ will henceforth be omitted)

$$\sum_j\Big[\Big(\frac{d^2}{dR^2}+2ME_{n\nu J}\Big)\delta_{ij}-V_{ij}{}^{J}(R)\Big]\chi^{J}_{jn\nu}(R)=0, \tag{25}$$

where

$$\begin{aligned}\sum_j V_{ij}{}^{J}(R)\chi^{J}_{jn\nu}(R) &= \sum_{jm'}V^{J}_{im,jm'}(R)\chi^{J}_{jm'n\nu}(R) \\ &= \sum_{l',m'=0}\Big[\sum_{N'=1}^{\infty}V^{J}_{im,N'l'm'}(R)\chi^{J}_{N'l'm'n\nu}(R)+\int_0^{\infty}dk'V^{J}_{im,l'm'}(k',R)\chi^{J}_{l'm'n\nu}(k',R)\Big].\end{aligned} \tag{26}$$

The effective potentials $V^{J}_{ij}(R)$ have the following structure[12]:

$$\begin{aligned}V_{ij}{}^{J}(R) &= \delta_{mm'}\Big\{\delta_{ij}\Big[\frac{J(J+1)-2m^2}{R^2}+2MW_{im}(R)\Big] \\ &\quad + H_{ij}(R)+\frac{d}{dR}Q_{ij}(R)+2Q_{ij}(R)\frac{d}{dR}\Big\}+B_{im,jm'}(R),\end{aligned} \tag{27}$$

where

$$W_{im}(R)=E_{im}(R)+\frac{Z_aZ_b}{R},\quad B_{im,jm'}(R)=-\gamma^{J}_{mm'}b_{im,jm'}(R),$$

$$\begin{aligned}\gamma^{J}_{mm'} &= (1+\delta_{m0}\delta_{m'1}+\delta_{m'0}\delta_{m1})^{1/2}\{[(J-m+1)(J+m)]^{1/2}\delta_{m'm-1} \\ &\quad +[(J+m+1)(J-m)]^{1/2}\delta_{m'm+1}\}.\end{aligned}$$

The terms $E_{im}(R)$ and the matrix elements $H_{ij}(R)$, $Q_{ij}(R)$, and $b_{im,jm'}(R)$ are defined and calculated in[7].

The state index n numbers the eigenvalues of the three-body system and determines the character of the motion of the meson in the two nuclei + μ^- meson system. To make its meaning clearer, we consider the wave functions of the system at fixed values of $\tau=(\nu J\lambda)$. The aggregate of such solutions

$$\{\chi^{J}_{jn\nu}(R)\}\equiv\{\chi_{jn}\}=\begin{pmatrix}\chi_{11}\dots\chi_{1n}\dots\\ \vdots\quad\vdots\\ \chi_{j1}\dots\chi_{jn}\dots\\ \vdots\quad\vdots\end{pmatrix} \tag{28}$$

constitutes an infinite-dimensional matrix. In the Born-Oppenheimer approximation, this matrix becomes diagonal:

$$\{\chi^{(0)}_{jn}\}=\{\chi_{jn}\delta_{jn}\},$$

and the system of equations (25) takes the form

$$\Big[\frac{d^2}{dR^2}+2ME^{(0)}_{n\tau}-V_{nn}{}^{J}(R)\Big]\chi^{(0)}_{nn}=0. \tag{29}$$

Figure 1 shows schematically the system of potentials $V^{J}_{jj}(R)$ and the level $\varepsilon^{(0)}_{n\tau}=E^{(0)}_{n\tau}-(2M)^{-1}V^{J}_{nn}(\infty)$ in one of these potentials. It is easily seen that in this approximation the energy of the three-body system $E_{n\tau}\approx E^{(0)}_{n\tau}$ is completely determined if the quantum numbers (j,J) (which determine the form of the potential $V^{J}_{jj}(R)=V^{J}_{nn}(R)$) and the vibrational quantum number v (which determines the number of the level in the chosen potential) are given. Thus, the state index n and the representation index j are equal to each other in the Born-Oppenheimer approximation. When the off-diagonal potentials $V^{J}_{ij}(R)$ are included, this agreement is violated and each state $|n\tau\rangle$ of the three-body system is represented in the form of the expansion (20)

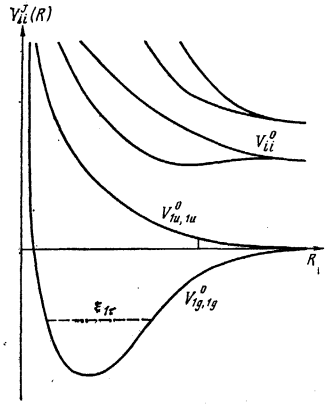

FIG. 1. Schematic behavior of the effective potentials (27) in Eq. (25). The potential $V_{11}^0(R) \equiv V_{1g,1g}$ determines in the Born-Oppenheimer approximation the relative motion of the nuclei of the three-body system in the ground state relative to the electron motion ($n = j = 1g = 1s\sigma_g$). The binding energy in the state $\tau = (v J \lambda) = (v0+)$ is equal to $\varepsilon_{1\tau}$.

$$|n\tau\rangle = |j\rangle\langle j|n\tau\rangle, \tag{20a}$$

but the identification $n \sim j$ remains meaningful as before, since (as will be shown below) the contribution of the states $|j\rangle$ with $j \neq n$ to the sum (20a) amounts to $\sim (2M)^{-1}$, i.e.,

$$\langle j|n\tau\rangle \ll \langle n|n\tau\rangle.$$

3. ADDITIONAL SYMMETRY OF THE SOLUTIONS IN THE CASE $Z_a = Z_b$ AND TWO-LEVEL APPROXIMATION IN THE THREE-BODY PROBLEM

Each three-body-system state $|n\tau\rangle$ with fixed state indices n and τ corresponds in the adiabatic approximation to a vector-column of the functions

$$\langle j|n\tau\rangle = \{\chi_j\} = \begin{pmatrix} \chi_1 \\ \vdots \\ \chi_j \\ \vdots \end{pmatrix}, \tag{30}$$

which satisfy the infinite-dimensional system of equations

$$[d^2/dR^2 + 2ME]\chi_i = \sum_j V_{ij}\chi_j \tag{31}$$

where $E \equiv E_{n\tau}$, $V_{ij} \equiv V_{ij}^J(R)$, $\chi_j \equiv \chi_{jnv}^{J\lambda}(R)$, and the sum over j is understood, for example, in the sense of the definition (26).

The representation index j, defined by the three quantum numbers (19), numbers uniquely the two-center basis $|j\rangle$ and the corresponding components of the solution vector (30). In the symmetric case of equal nuclear charges $Z_a = Z_b$, however, a complete classification of the solutions calls for one more quantum number, the parity $P_{g,u} = (-)^l$, which is defined as the eigenvalue of the electron (μ^--meson) coordinate inversion operator:

$$\hat{P}_\mu \Phi_j^{(g,u)}(\mathbf{r}; R) = \Phi_j^{(g,u)}(-\mathbf{r}; R) = P_{g,u}\Phi_j^{(g,u)}(\mathbf{r}; R). \tag{32}$$

In the limit as $R \to \infty$, the wave functions of the two-center problem

$$\Phi_j^{(g)}(\mathbf{r}; R) = \Phi_{jg} = |jg\rangle, \quad \Phi_j^{(u)}(\mathbf{r}; R) = \Phi_{ju} = |ju\rangle,$$

which differ only in parity, correspond to the same value of the energy $E_{jg}(\infty) = E_{ju}(\infty)$ and to the identical sets $j = [n_1 n_2 m]$ of the parabolic quantum numbers.[5] At $m = 0$, the even states (g) correspond to the value $l = 2n_2$ and $P_g = +1$, while odd states (u) correspond to values $l = 2n_2 + 1$ and $P_u = -1$.

It will be convenient in what follows to choose as the representation index j a set of three parabolic quantum numbers $j = [n_1 n_2 m]$ and the value of the parity $P_{g,u}$. Accordingly, the vector column (30) will be represented in the form of a pair of states

$$\bar{\chi}_j = \begin{pmatrix} \chi_{jg} \\ \chi_{ju} \end{pmatrix}, \tag{33}$$

which satisfy the system of equations

$$\hat{I}\left(\frac{d^2}{dR^2} + 2ME\right)\bar{\chi}_i = \sum_j \hat{V}_{ij}\bar{\chi}_j, \tag{34}$$

where

$$\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \hat{V}_{ij} = \begin{pmatrix} V_{ig,jg} & V_{ig,ju} \\ V_{iu,jg} & V_{iu,ju} \end{pmatrix}. \tag{35}$$

As $R \to \infty$, when the system $Z_a \mu Z_b$ with equal charges $Z_a = Z_b$ breaks up into two subsystems $\mu Z_a + Z_b$ and $Z_a + \mu Z_b$, the motion of the electron in the state j of atoms μZ_a and μZ_b respectively is represented respectively by the functions Φ_{ja} and Φ_{jb}, which are connected with the functions Φ_{jg} and Φ_{ju} by the transformation

$$(\Phi_{ja}, \Phi_{jb}) = (\Phi_{jg}, \Phi_{ju})A^{-1}, \tag{36}$$

which induces the transformation A on the functions χ_{jg} and χ_{ju}

$$\tilde{\chi}_j = \begin{pmatrix} \chi_{ja} \\ \chi_{jb} \end{pmatrix} = A\bar{\chi}_j = A\begin{pmatrix} \chi_{jg} \\ \chi_{ju} \end{pmatrix} \tag{37}$$

with the matrix

$$A = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \tag{38}$$

The functions $\tilde{\chi}_j$ satisfy the system of equations

$$\hat{I}\left(\frac{d^2}{dR^2} + 2M\varepsilon\right)\tilde{\chi}_i = \sum_j \tilde{U}_{ij}\tilde{\chi}_j, \tag{39}$$

where

$$\tilde{U}_{ij} = U_{ij} - \hat{I}U_{na,na}(\infty)\delta_{ij}, \quad U_{ij} = A\hat{V}_{ij}A^{-1},$$
$$\varepsilon \equiv \varepsilon_{na\tau} = E_{n\tau} - (2M)^{-1}U_{na,na}(\infty). \tag{40}$$

If this definition is used, the binding energy of a system

of three particles is reckoned from the value $E_0=(2M)^{-1}U_{j_a,j_a}(\infty)$, which is equal to the binding energy of the insulated atom μZ_a in the state $j=n$ and with nuclear mass $M_a \geqslant M_b$ in the adiabatic approximation and coincides with the true energy E_a of the atom μZ_a, accurate to terms $\sim (2M)^{-1}$ inclusive.[13]

The explicit expressions for the matrix elements of the effective potentials

$$\hat{U}_{ij}=\begin{pmatrix} U_{ia,ja} & U_{ia,jb} \\ U_{ib,ja} & U_{ib,jb} \end{pmatrix} \tag{41}$$

in terms of the elements of the matrix $\hat{V}_{ij}$ take the form

$$\begin{aligned} U_{ia,ja}&=1/2[(V_{ig,jg}+V_{iu,ju})-(V_{ig,ju}+V_{iu,jg})],\\ U_{ia,jb}&=1/2[(V_{ig,jg}-V_{iu,ju})+(V_{ig,ju}-V_{iu,jg})],\\ U_{ib,ja}&=1/2[(V_{ig,jg}-V_{iu,ju})-(V_{ig,ju}-V_{iu,jg})],\\ U_{ib,jb}&=1/2[(V_{ig,jg}+V_{iu,ju})+(V_{ig,ju}+V_{iu,jg})]. \end{aligned} \tag{42}$$

In practically all the calculations performed to date, a two-level approximation was used, i.e., the only terms retained in the system (39) were those with $i=j=1$, which correspond to the pair of states $i=[000]_g$ and $i=[000]_u$ of the two-center problem. Accordingly, only the two upper components were retained in the column vector $\{\chi_j\}$ of the solution:

$$\{\tilde{\chi}_j\}=\begin{pmatrix} \tilde{\chi}_1 \\ 0 \\ \vdots \end{pmatrix}=\begin{pmatrix} \chi_{1a} \\ \chi_{1b} \\ 0 \\ \vdots \end{pmatrix}. \tag{43}$$

In the next section we shall construct a calculation scheme that makes it possible to determine more precisely the energy $E_{n\tau}$ and the wave functions $|n\tau\rangle$ of a system of three bodies with a consistent account of the discarded terms $i,\ j\neq 1$. The calculated formulas are particularly simple in form for the state index $n=1$.

4. PERTURBATION THEORY SCHEME IN THE ADIABATIC BASIS

We represent the matrix (40) of the potentials $\tilde{U}$ in the form of a sum

$$\tilde{U}\equiv\{U_{ij}\}=\{U_{ij}^{(0)}\}+\{U_{ij}^{(1)}\}, \tag{44}$$

where the block matrix of the quasidiagonal approximation is

$$U_{ij}^{(0)}=U_{ij}\delta_{ij}=[U_{ii}-IU_{na,na}(\infty)]\delta_{ij},\quad E_i(R)<0, \tag{44a}$$

$$U_{ij}^{(0)}=I\left[2M\frac{k^2}{2}-U_{na,na}(\infty)+2M\frac{Z_aZ_b}{R}+\frac{J(J+1)-2m^2}{R^2}\right]\delta_{ij},\quad E_i(R)>0, \tag{44b}$$

and the matrix of the perturbation potentials is

$$\hat{U}^{(1)}\equiv\{U_{ij}^{(1)}\}=\{U_{ij}\}-\{U_{ij}^{(0)}\}. \tag{45}$$

When the matrix of the potentials $\tilde{U}$ is so subdivided, the following relation is satisfied:

$$\hat{U}^{(1)}\sim(2M)^{-1}\hat{U}^{(0)}.$$

Naturally, other methods of separating the matrix $U^{(1)}$ are possible, equivalent to rearrangement of the perturbation-theory series.[9] The system (39) now takes the final form (we shall henceforth omit the tilde over the function $\tilde{\chi}$)

$$(\hat{\mathscr{L}}_i+2M\varepsilon\hat{I})\chi_i=\sum_j\hat{U}_{ij}^{(1)}\chi_j, \tag{46}$$

where

$$\hat{\mathscr{L}}_i=\hat{I}\frac{d^2}{dR^2}-\hat{U}_{ii}^{(0)}, \tag{46a}$$

and the summation sign is understood in the sense of the definition (26). The vector function $\{\chi_j\}$ and the system binding energy ε are constructed in the adiabatic approximation in the form of the expansions

$$\{\chi_j\}=\{\chi_j^{(0)}\}+\{\chi_j^{(1)}\}+\ldots,\quad \varepsilon=\varepsilon^{(0)}+\varepsilon^{(1)}+\varepsilon^{(2)}+\varepsilon^{(3)}+\ldots, \tag{47}$$

the successive approximations of $\{\chi_j^{(s)}\}$ being obtained as the solutions of the system of inhomogeneous equations

$$\begin{aligned} &(\hat{\mathscr{L}}_i+2M\varepsilon^{(0)}\hat{I})\chi_i^{(0)}=0,\\ &(\hat{\mathscr{L}}_i+2M\varepsilon^{(0)}\hat{I})\chi_i^{(1)}=\sum_j(\hat{U}_{ij}^{(1)}-2M\varepsilon^{(1)}\hat{I}\delta_{ij})\chi_j^{(0)},\\ &\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\ &(\hat{\mathscr{L}}_i+2M\varepsilon^{(0)}\hat{I})\chi_i^{(s)}=\sum_j(\hat{U}_{ij}^{(1)}-2M\varepsilon^{(1)}\hat{I}\delta_{ij})\chi_j^{(s-1)}-2M\sum_{t=2}^{s}\varepsilon^{(t)}\hat{I}\chi_i^{(s-t)}, \end{aligned} \tag{48}$$

where the corrections to the energy $\varepsilon^{(s)}$ are calculated in accordance with the formulas ($s=1, 2, \ldots$)

$$\begin{aligned} \varepsilon^{(1)}&=(2M)^{-1}\langle\chi^{(0)}|\hat{U}^{(1)}|\chi^{(0)}\rangle,\\ \varepsilon^{(2s)}&=(2M)^{-1}\langle\chi^{(s)}|\hat{U}^{(1)}|\chi^{(s-1)}\rangle-\sum_{u=1}^{s}\sum_{t=1}^{s-1}\varepsilon^{(2s-u-t)}\langle\chi^{(u)}|\chi^{(t)}\rangle,\\ \varepsilon^{(2s+1)}&=(2M)^{-1}\langle\chi^{(s)}|\hat{U}^{(1)}|\chi^{(s)}\rangle-\sum_{u=1}^{s}\sum_{t=1}^{s}\varepsilon^{(2s+1-u-t)}\langle\chi^{(u)}|\chi^{(t)}\rangle. \end{aligned} \tag{49}$$

In the derivation of formulas (49) we used the fact that the perturbation operator is Hermitian, $\hat{U}^{(1)}=\hat{U}^{(1)+}$, a property that follows from the definition (27) and the symmetry relations[12]

$$H_{ij}(R)=H_{ji}(R)\quad Q_{ij}(R)=-Q_{ji}(R),\quad B_{ij}(R)=B_{ji}(R). \tag{50}$$

In addition, formulas (49) are valid only under the assumption that the solutions χ_j are normalized by the intermediate-normalization condition

$$\begin{aligned} \langle\chi^{(0)}|\chi^{(s)}\rangle&=\sum_j\int dR\,\chi_j^{(0)+}\chi_j^{(s)}\\ &=\sum_{\substack{n_1,\,m=0\\ n_1+n_2+m\geqslant 1}}\left(\sum_{n_1=1}^{\infty}+\int_0^{\infty}dk\right)\int_0^{\infty}dR\,[\chi_{ja}^{(0)}\chi_{ja}^{(s)}+\chi_{jb}^{(0)}\chi_{jb}^{(s)}]=\delta_{0s}, \end{aligned} \tag{51}$$

$$j=\begin{cases} n_1n_2m\ -\ \text{discrete spectrum}\\ kn_2m\ -\ \text{continuous spectrum.}\end{cases}$$

On the other hand, if the condition (51) is not satisfied for the functions $\{\chi_j^{(s)}\}$, then it is necessary to substitute in (49) functions constructed from the solutions of the system (48) by means of the formulas

$$\tilde{\chi}^{(s)}=\chi^{(s)}-\chi^{(0)}\langle\chi^{(0)}|\chi^{(s)}\rangle. \tag{52}$$

The system of inhomogeneous equations (48) together with relations (49), (51), and (52) constitute the scheme of the Schrödinger nondegenerate perturbation theory.

Let us examine this scheme in greater detail for the important particular case $n=1$, i.e., for the calculation of the adiabatic corrections to the energy $E_{n\tau}$ of a three-body system in the ground state with respect to the quantum numbers of the electron motion. We confine ourselves here to a calculation of the energy corrections up to third order inclusive; it suffices for this purpose to find only the functions $\chi_j^{(1)}$.

In the Born-Oppenheimer approximation (see Fig. 1) the case $n=1$ corresponds to levels $\varepsilon_{1\tau}$ in the potential $V_{jj}^J(R)$ with quantum numbers $j=1g=1s\sigma_g$ ($N=1$, $l=0$, $m=0$), i.e., in the potential $W_g(R)$ which is well known in the theory of the molecular hydrogen ion H_2^+.[5] Our problem is to find the adiabatic corrections to the energy $\varepsilon_{1av J\lambda}$, i.e., to go outside the framework of the two-level approximation (43) and take successive account of the contributions of all higher discrete levels ($j\geq 2$), and also the contribution of the continuous spectrum of the two-center problem.

For the states of a three-body system with index $n=1$, the series (47) for the column vector of the solutions $\{\chi_j\}$ is of the form

$$\{\chi_j\}=\begin{pmatrix}\chi_1^{(0)}\\0\\\vdots\end{pmatrix}+\begin{pmatrix}0\\\chi_2^{(1)}\\\vdots\end{pmatrix}+\dots \tag{53}$$

It follows hence immediately that the condition (51) is satisfied, and in correspondence with the definitions (44) and (49), that $\varepsilon^{(1)}=0$.[2] The system (48) simplifies in this case and its expanded form becomes

$$\begin{aligned}&[d^2/dR^2+2M\varepsilon^{(0)}-U_{1a,1a}^{(0)}]\chi_{1a}^{(0)}-U_{1a,1b}^{(0)}\chi_{1b}^{(0)}=0,\\&[d^2/dR^2+2M\varepsilon^{(0)}-U_{1b,1b}^{(0)}]\chi_{1b}^{(0)}-U_{1b,1a}^{(0)}\chi_{1a}^{(0)}=0,\\&\varepsilon^{(0)}\equiv\varepsilon_{1a\nu J\lambda}^{(0)}=\varepsilon_{1av J\lambda}^{(0)}=E_{1\tau}-(2M)^{-1}U_{1a,1a}(\infty).\end{aligned} \tag{54}$$

The functions $\chi_1^{(0)}$ are normalized by the condition (51):

$$\langle\chi^{(0)}|\chi^{(0)}\rangle=\int_0^\infty dR[(\chi_{1a}^{(0)})^2+(\chi_{1b}^{(0)})^2]=1. \tag{55}$$

The functions $\chi_j^{(1)}$ for $j\geq 2$ are obtained from the system of inhomogeneous equations

$$\begin{aligned}&[d^2/dR^2+2M\varepsilon^{(0)}-U_{ja,ja}^{(0)}]\chi_{ja}^{(1)}-U_{ja,jb}^{(0)}\chi_{jb}^{(1)}=F_{ja}^{(0)},\\&[d^2/dR^2+2M\varepsilon^{(0)}-U_{jb,jb}^{(0)}]\chi_{jb}^{(1)}-U_{jb,ja}^{(0)}\chi_{ja}^{(1)}=F_{jb}^{(0)},\end{aligned} \tag{56}$$

where

$$\begin{aligned}F_{ja}^{(0)}&=U_{ja,1a}^{(1)}\chi_{1a}^{(0)}+U_{ja,1b}^{(1)}\chi_{1b}^{(0)},\\F_{jb}^{(0)}&=U_{jb,1a}^{(1)}\chi_{1a}^{(0)}+U_{jb,1b}^{(1)}\chi_{1b}^{(0)},\end{aligned} \tag{57}$$

and the representation index j runs through the values $j=2,3,\dots$, including the states of the continuous spectrum of the two-center problem.

The corrections to the energy

$$\varepsilon=\varepsilon_{1av J\lambda}\approx\varepsilon^{(0)}+\varepsilon^{(2)}+\varepsilon^{(3)}$$

are obtained from the formulas

$$\begin{aligned}\varepsilon^{(2)}&=\frac{1}{2M}\langle\chi^{(1)}|F^{(0)}\rangle=\frac{1}{2M}\sum_j\int_0^\infty dR\,\chi_j^{(1)}F_j^{(0)}=\varepsilon_{\text{discr}}^{(2)}+\varepsilon_{\text{cont}}^{(2)}\\&=\frac{1}{2M}\sum_{n_2,m=0}^{\infty}\Big\{\sum_{n_1=0}^{\infty}\int_0^\infty dR[\chi_{n_1n_2ma}^{(1)}(R)F_{n_1n_2ma}^{(0)}(R)+\chi_{n_1n_2mb}^{(1)}(R)F_{n_1n_2mb}^{(0)}(R)]\\&\quad+\int_0^\infty dk\int_0^\infty dR[\chi_{n_2ma}^{(1)}(k,R)F_{n_2ma}^{(0)}(k,R)+\chi_{n_2mb}^{(1)}(k,R)F_{n_2mb}^{(0)}(k,R)]\Big\},\\\varepsilon^{(3)}&=\frac{1}{2M}\langle\chi^{(1)}|\hat U^{(1)}|\chi^{(1)}\rangle=\frac{1}{2M}\sum_{i,j}\int dR\,\chi_i^{(1)}\,U_{ij}^{(1)}\,\chi_j^{(1)},\end{aligned} \tag{58}$$

where the double sum must be understood in analogy with the preceding one:

$$\sum_{ij}=\sum_{\substack{n_2,m=0\\n_2',m'=0}}^{\infty}\Big\{\sum_{n_1,n_1'=0}^{\infty}+\sum_{n_1=0}^{\infty}\int_0^\infty dk'+\int_0^\infty dk\sum_{n_1'=0}^{\infty}+\int_0^\infty dk\int_0^\infty dk'\Big\}, \tag{58a}$$
$$n_1+n_2+m\geq 1,\qquad n_1'+n_2'+m'\geq 1.$$

The total energy $E_{1\tau}$ of the three-body system is calculated in the adiabatic representation from the formula (it is assumed throughout that $M_a\geq M_b$)

$$E_{1\tau}=\varepsilon_{1av J\lambda}+(2M)^{-1}U_{1a,1a}(\infty)=\varepsilon+E_0. \tag{59}$$

We shall demonstrate the effectiveness of the described scheme by using as an example the calculation of the binding energy of the mesic molecule $pd\mu$.

5. CALCULATION OF THE SYSTEM pd

The calculation of the binding energy of the mesic molecule $pd\mu$ has been the subject of many papers, and a complete bibliography is contained in the reviews.[3] Carter's[2] most accurate variational calculations of the ground state ($J=0$, $v=0$) of the mesic molecule $pd\mu$ make use of a function with 84 variational parameters and yield for the total energy of the three-body system and for the binding energy of the $pd\mu$ molecule the respective values

$$E=-2884.42\text{ eV},\qquad \varepsilon_a=-221.28\text{ eV}.$$

The binding energy ε_a of the mesic molecule $pd\mu$ is reckoned from the energy E_a of the ground state of an isolated mesic atom (μZ_a)

$$E_a=-\frac{m_\mu}{2}\left(1+\frac{m_\mu}{M_a}\right)^{-1}\text{ [at. un]}=-2663.14\text{ eV}. \tag{60}$$

TABLE I. Components of the total energy of the ground state ($J=0$, $v=0$) of the mesic molecule $pd\mu$.

Quantity	Value		Quantity	Value	
	m. at. un.	eV		m. at. un	eV
E_0	−0.473250	−2662.66	ε	−0.039451	−221.96
$\varepsilon^{(0)}$	−0.038114	−214.44	$E_{1\tau}$	−0.512700	−2884.62
$\varepsilon^{(2)}_{\text{discr}}$	−0.000788	−4.43	E_a	−0.473335	−2663.14
$\varepsilon^{(2)}_{\text{cont}}$	−0.000549	−3.09	ε_a	−0.039366	−221.48

Note. Carter's variational calculation (1968) yields for the total energy a value $E=-2884.42$ eV (−0.512665 m. at. un.), and accordingly for the binding energy $\varepsilon=-221.28$ eV (−0.039329 m. at. un.).

TABLE II. Contributions $\varepsilon_j^{(2)}$ of different states $j=[n_1n_2m]$ of the discrete spectrum of the two-center problem to the energy of the ground ($J=0$, $v=0$) state of the mesic molecule* $pd\mu$.

j	$[n_1n_2m]$	$\varepsilon_j^{(2)}$, 10^{-4} m. at. un.	$\varepsilon_j^{(2)}$ eV	j	$[n_1n_2m]$	$\varepsilon_j^{(2)}$, 10^{-4} m. at. un.	$\varepsilon_j^{(2)}$ eV
2	100	−2.44	−1.37	11	300	−0.16	−0.09
3	010	−3.89	−2.19	12	210	−0.27	−0.15
5	200	−0.44	−0.25	13	120	−0.00	0.00
6	110	−0.68	−0.38	14	030	0.00	0.00
7	020	−0.00	−0.00	$\varepsilon_{\text{discr}}^{(2)}$		−7.87	−4.43

*The numbering of j corresponds to that used in[7]. The states $j=[n_1n_2m]$ with $m\neq 0$ make no contribution to the energy of the levels with $J=0$. The following particle-mass values were used in the calculations: $m_\mu=206.769$, $M_p=1836.109$, $M_d=3670.398$. The mesic atom energy unit ($e=\hbar=m_\mu=1$) is $\varepsilon_\mu=5626.33$ eV.

The total energy E of the three-body system is an invariant and should not depend on the manner in which it is broken up into a sum of subsystem energies; this yields the equation

$$E=E_a+\varepsilon_a=E_0+\varepsilon=E_{1\tau}. \tag{61}$$

The energy E_0 of an isolated atom (μZ_a) is equal in the adiabatic representation to[13]

$$E_0=-\frac{m^*}{2}\left(1-\frac{1+2\varkappa}{4M}\right)\ [\text{at. un.}]=-2662.66\ \text{eV}. \tag{62}$$

Thus, by calculating the binding energy ε in the adiabatic representation, we can obtain from the relation (61) the true binding energy ε_a. Table I lists the components of the total energy $E_{1\tau}$ of the ground state $\tau(J=0, v=0)$ of the mesic molecule $pd\mu$, obtained in this paper by the described method.

In the calculation of the contribution from the higher states of the discrete spectrum of the two-center problem, we took into account in the sum

$$\varepsilon_{\text{discr}}^{(2)}=\sum_{j=2}^{14}\varepsilon_j^{(2)} \tag{63}$$

all the states $j=[n_1n_2m]$ with $m=0$ to $n=n_1+n_2+1=4$ inclusive. The relative contribution of each of these states is given in Table II. It is easily seen that the decisive contribution to $\varepsilon_{\text{discr}}^{(2)}$ is made by the states $j=[n_110]$, which correspond as $R\to 0$ to the pairs of terms $Nd\sigma_g-Nf\sigma_u$ (see Figs. 2–4). This is apparently

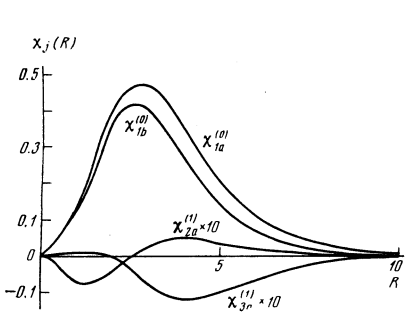

FIG. 2. The wave functions $\chi_{1a}^{(0)}(R)$ and $\chi_{1b}^{(0)}(R)$ and the corrections $\chi_j^{(1)}(R)$ to them for the ground state ($J=0$, $v=0$) of the mesic molecule $pd\mu$; it is seen that $\chi_j^{(1)}\leq(2M)^{-1}\chi_1^{(0)}$, in accord with the statement made in Sec. 2.

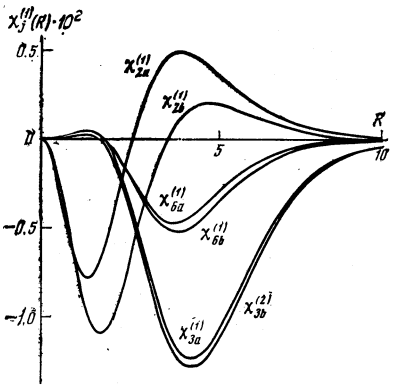

FIG. 3. First-approxxmation corrections $\chi_{ja}^{(1)}(R)$ and $\chi_{jb}^{(1)}(R)$, which determine the contribution of the higher states j of the discrete spectrum of the two-center problem to the total energy $E_{1\tau}$ of the three-body system $pd\mu$, $J=0$, $v=0$).

due to the presence of a weak minimum of the terms $W_j(R)$ corresponding to the states $Nd\sigma_g$.[5]

In the calculation of the contribution from the continuous spectrum of the two-center problem

$$\varepsilon_{\text{cont}}^{(2)}=\sum_{n_2=0}^{3}\int_0^\infty\varepsilon_{n_20}^{(2)}(k)\,dk=\sum_{n_2=0}^{3}\varepsilon_{n_20}^{(2)} \tag{64}$$

we took into account in the sum (64) the states $j=[kn_2m]$ corresponding to the values $m=0$, $n_2=0$, 1, 2, 3, while the functions $\varepsilon_{n_20}^{(2)}$ and the wave functions $\chi_{n_20}^{(1)}(k,R)$ corresponding to them were calculated at $k=0, 2(0,1)1(0,2)2(1)10$. Plots of these functions are shown in Figs. 5 and 6, while the contributions to the binding energy are given in Table III.

In the employed calculation scheme, when the diagonal terms $U_{ii}(R)$ of the matrix $U_{ij}(R)$ are included in the operator $\mathcal{L}_i$ in accordance with formulas (44), (44a), and (46), the greater part of the contribution from third-order perturbation theory is effectively taken into account already in the calculation of $\varepsilon^{(2)}$, and in this connection the contribution $\varepsilon^{(3)}$ turns out to be small. In this case $\varepsilon^{(3)}\approx 3\cdot 10^{-3}$ eV ($\approx 6\times 10^{-7}$ m.at.un.) when account is taken of the potentials $U_{ij}(R)$ for the state pairs $(i,j)=(3,2)$, $(5,2)$, $(5,3)$, $(6,2)$, $(6,3)$, $(6,5)$, $(12,3)$, $(12,6)$, which make the decisive contribution to the sum (58).

To solve the systems of equations we used a continuous analog of Newton's method,[15] which ensures an absolute calculation accuracy to within $\sim 10^{-4}$–10^{-5} in

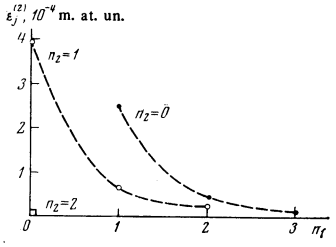

FIG. 4. Values of $\varepsilon_j^{(2)}=\varepsilon_{n_1n_2m}^{(2)}$, which determine the contribution of the discrete spectrum from the shells with principal quantum number $n=2, 3$, and 4 at $m=0$ ($pd\mu$, $J=0$, $v=0$).

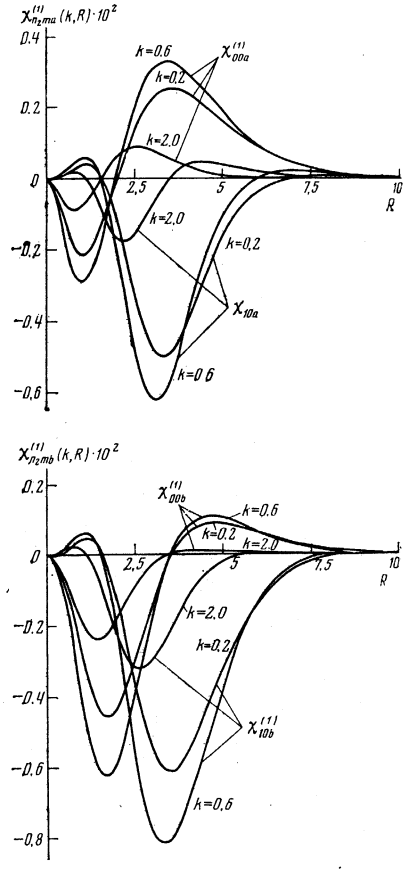

FIG. 5. First-order approximations $\chi^{(1)}_{n_2ma}(k,R)$ and $\chi^{(1)}_{n_2mb}(k,R)$, which determine the contribution of the continuous spectrum of the two-center problem to the total energy of the three-body system ($pd\mu$, $J=0$, $v=0$).

TABLE III. Contribution $\varepsilon^{(2)}_{n_20}$ of various states $j=[kn_2m]$ of the continuous spectrum of the two-center problem to the binding energy of the state ($J=0$, $v=0$) of the mesic molecule $pd\mu$.

n_2	$\varepsilon^{(2)}_{n_20}$, 10^{-4} m. at. un.	$\epsilon^{(2)}_{n_20}$,
0	−1.67	−0.94
1	−3.03	−1.70
2	−0.71	−0.40
3	−0.08	−0.05
$\varepsilon^{(2)}_{\text{cont}}$	−5.49	−3.09

the case of integration intervals $\Delta R=0.025$ on the segment $0\leq R\leq 20$.

CONCLUSION

The described scheme of perturbation theory in the adiabatic representation of the three-body problem is simple enough and convenient in use. In the case of μ-mesic molecules of hydrogens, for which $(2M)^{-1}\sim 0.1$, the described schemes makes it possible to calculate their binding energies with high accuracy both in the ground state ($J=0$, $v=0$), and in the excited vibrational ($v=1$) and rotational ($J=1,2,3$) states.

For example, our calculated value $E_{pd\mu}=-0.51270$

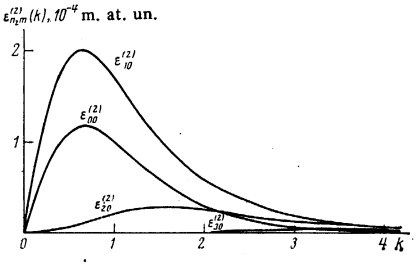

FIG. 6. The functions $\varepsilon^{(2)}_{n_2m}(k)$, which determine the contribution of the continuous spectrum from states with different values of n_2 (pd, $J=0$, $v=0$).

m. at. un. is in good agreement with the variational value $E_{pd\mu}=-0.51267$ m. at. un.[2] of the total energy of the ground state of the mesic molecule $pd\mu$ and meets the specified calculation accuracy requirements ($\sim 10^{-5}$) in the realized scheme.

As a rule, in cases of physical interest it suffices to consider states with index $n=1$, i.e., in the ground state relative to the meson motion, for which all the higher states ($j\geq 2$) of the two-center problem play the role of closed channels in the system of equations (46). This means that for states with $n=1$ we do not encounter the difficulties[16] connected with the long-range character of the matrix elements $B_{jm,jm'}(R)$ of the Coriolis-interaction operator (they are altogether nonexistent for states with $J=0$). We hope, however, that the described scheme can be extended successively also to the case of states with index $n\neq 1$, i.e., for excited states relative to the meson motion.

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[1)]It is of interest in this connection to compare the sections devoted to the adiabatic method (or to the method of perturbed stationary states) in three successive editions of the book by Mott and Massey[6].

[2)]The relation $\chi^{(0)}_j\equiv 0$ at $j\geq 2$ follows from the first equation of the system (48), since the difference $2M\varepsilon_{1\sigma\tau}-U^{(0)}_{jj}(R)<0$ and does not reverse sign over the entire interval of variation of R (see, e.g., [14]). By virtue of the relations $\hat{U}^{(1)}_{11}=0$ and $\varepsilon^{(1)}=0$, the right-hand side of the second equation of the system (48) vanishes at $i=1$, and the resultant equation has only one solution that does not coincide with $\chi^{(0)}_1$, namely $\chi^{(1)}_1\equiv 0$.

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Two-photon absorption of light emitted in a two-photon process

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Two-photon absorption of light emitted in two-photon spontaneous emission in the decay of metastable levels of atoms or ions is considered. It is shown by a quantum-mechanical calculation that the simultaneity of the emission of the two photons in such spontaneous emission leads to a sharp increase of the probability of two-photon absorption as compared with the case of light from ordinary sources. The probability of two-photon absorption is determined by the large instantaneous intensity of the two-photon spontaneous emission and does not depend on the mean intensity of the light beam.

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1. INTRODUCTION

As is well known, two-photon absorption of light is a nonlinear process and depends essentially on the fluctuations of the intensity of the light. In the present paper it is shown that two-photon spontaneous emission from metastable atoms or ions is a source of light whose fluctuations change the character of the two-photon absorption as compared with that of light from ordinary sources.

According to existing ideas, the photons emitted in a single act of spontaneous emission come out almost simultaneously, in a time interval of the order of the optical period; this interval can be estimated by applying the uncertainty principle to the intermediate state of the radiating system. Experimental studies[1–5] of two-photon spontaneous emission from atoms and ions by means of photon-coincidences confirm the simultaneity of the emissions to within the limits of experimental error. A quantum-mechanical calculation made in the present paper shows that owing to the grouping of the photons in time in two-photon simultaneous emission, such radiation is perceived by a two-photon absorber as radiation of large instantaneous intensity. This instantaneous intensity determines the effectiveness of two-photon absorption.

The probability of two-photon excitation of an absorbing atom, calculated per two-photon decay in the source, is independent of the mean luminous flux.

In order to increase the probability of two-photon absorption it is necessary to eliminate the divergence in space of the simultaneously emitted photons, say by focusing the spontaneous radiation with a concave mirror. In this case the coefficient of two-photon absorption of the light emitted in two-photon processes [see Eq. (4) of the present paper] is mainly governed by the same physical factors as the coefficient of ordinary one-photon absorption—the concentration n_0 of absorbing atoms and the ratio of the radiation width Γ of the metastable level to the Doppler width ω_d of the absorbing transition.

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