

Effect of $dt\mu$ quasinucleus structure on energy levels of the $(dt\mu)Xee$ exotic molecule

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Precise energies of rovibrational states of the exotic hydrogen-like molecule $(dt\mu)Xee$ are of importance for $dt\mu$ resonant formation, which is a key process in the muon-catalyzed fusion cycle. The effect of the internal structure and rotation of the $dt\mu$ quasi-nucleus on energy levels is studied using the three-body description of the $(dt\mu)Xee$ molecule based on the hierarchy of scales and corresponding energies of its constituent subsystems. For a number of rovibrational states of $(dt\mu)dee$ and $(dt\mu)tee$, the shifts and splittings of energy levels are calculated in the second order of the perturbation theory.

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I. INTRODUCTION

It is known that one stopped muon in a deuterium-tritium mixture yields more than 100 nuclear fusion reactions. The process of muon-catalyzed fusion has been intensively studied and a detailed description exists in the literature, e.g., in review articles [1–4]. One of the key processes in the muon-catalyzed fusion cycle is the formation of the hydrogen-like exotic molecule $(dt\mu)Xee$ (for the sake of generality X stands for either isotope d , t , or p), in which a $dt\mu$ mesic molecule substitutes for one of the nuclei in the hydrogen molecule. It is widely accepted that the resonance mechanism proposed by Vesman [5] is responsible for the high rate of the $dt\mu$ formation. Due to this mechanism, a $dt\mu$ mesic molecule in a loosely bound excited state to be produced by low-energy collisions of $t\mu$ mesic atoms and DX molecules in a resonance process,



followed by $dt\mu$ transition to the ground state. The rate of the resonance process is sensitive to the precise resonance position and an accuracy better a 1 meV is necessary to obtain reasonable theoretical estimates of the formation rate [1–4].

Resonance formation can take place if the energy released in $dt\mu$ binding is transferred to the rovibrational excitation of the exotic molecule $(dt\mu)Xee$. This is actually the case as $dt\mu$ has a loosely bound excited state with an angular momentum $\lambda=1$ and binding energy which is comparable to vibrational quantum of the $(dt\mu)Xee$ molecule. In a nonrelativistic approximation, different calculations determine with a good accuracy the binding energy of the isolated $dt\mu$ mesic molecule [1–4]. To obtain the precise value of the binding energy one has to correct the nonrelativistic energy for relativistic effects, hyperfine effects, finite nuclear size, vacuum polarization, and others. The resonance position is determined, besides the binding energy of isolated $dt\mu$, by the energy of the rovibrational excitation of the hydrogen-like molecule $(dt\mu)Xee$ with one nucleus being the particle X and the other the excited $dt\mu$ mesic molecule. As the “size” of the excited $dt\mu$ mesic molecule with $\lambda=1$ is of the order of 0.05 a.u. [6], which is much smaller than the internuclear

distance in the whole molecule, the rovibrational spectrum of $(dt\mu)Xee$ can be calculated to a good approximation by treating $dt\mu$ as a point-like charged particle [7,8]. Nevertheless, to reach an accuracy of the order of a tenth of a meV one should take into account the energy shift which arises due to the internal structure and rotation of a $dt\mu$ mesic molecule.

The effect of the $dt\mu$ finite size was previously investigated in a simple approach [9,10] where the energy shifts for the $(dt\mu)dee$ were obtained by multiplying by 1.45 the shift calculated for the atom-like system $(dt\mu)e$ in the second order perturbation theory (PT). Within the framework of this simple approach it is not possible to take account of the molecular structure; in particular, the calculated energy shift is independent of the rovibrational quantum numbers. The effect of the molecular structure, i.e., the dependence on angular momentum, was explicitly demonstrated in the elaborate six-body calculation [6] of the $(dt\mu)dee$ energy shifts in the first order of the perturbation theory. Note, however, that the first- and second-order PT contributions to the energy shift are comparable. Recently, resonance positions in the low-energy $t\mu+D_2$ scattering have been obtained in the elaborate three-body calculation [11,12]. Only a few resonance states with the zero total angular momentum have been considered in these papers.

The main aim of the present paper is to calculate the energy shifts which arise due to the internal structure and rotation of the $dt\mu$ mesic molecule embedded in the hydrogen-like $(dt\mu)Xee$ molecule. The calculation is reduced to solution of a three-body problem for heavy particles $t\mu$, d and X . This approach is based on the hierarchy of scales and corresponding energies of constituent subsystems of the $(dt\mu)Xee$ thus reliably taking into account the specific features of this molecule. As a result, the energy shifts are obtained for a number of vibrational and rotational states of $(dt\mu)dee$ and $(dt\mu)tee$ in the second-order PT.

II. METHOD

The structure of the exotic molecule $(dt\mu)Xee$ is characterized by a hierarchy of scales and corresponding energies

of its constituent subsystems. In this respect, a $t\mu$ mesic atom is small in comparison with its mean separation from a deuteron in the loosely bound $dt\mu$ mesic molecule, which allows $t\mu$ to be treated as a point-like neutral particle interacting with a deuteron by the short-range effective potential. Note that the closed two-body $d\mu+t$ channel is well separated in energy by about 50 eV and can be safely neglected in the present calculation. There is also interaction of $t\mu$ with the second nucleus X ; however, this might be neglected due to large separation between these particles. In turn, the size of a $dt\mu$ mesic molecule is small in comparison with the amplitude of vibrations in $(dt\mu)Xee$; therefore, it moves as a point-like quasi-nucleus near the equilibrium position. For this reason, the effect of the $dt\mu$ structure is considered within the framework of the perturbation theory.

Furthermore, two electrons in the hydrogen-like molecule $(dt\mu)Xee$ move much faster than the heavy particles d , X , and $t\mu$, which makes it possible to use the familiar Born–Oppenheimer (BO) approximation, i.e., to solve an electronic problem with the fixed charged particles d and X , thus obtaining the BO energy which plays a role of the effective potential between d and X . The electronic excitations, which require a considerable amount of energy [13], are not taken into account for the low-energy processes under consideration.

As a result, the description of $(dt\mu)Xee$ is reduced to solution of a three-body problem for three particles $t\mu$, d and X . The interaction between charged d and X is described by the well-known BO potential for the hydrogen molecule. In accord with the treatment of the $t\mu$ mesic atom as a point-like neutral particle, the present calculation does not explicitly use the $t\mu+d$ effective potential; rather the result is expressed via the low-energy $t\mu+d$ scattering phase shifts and characteristics of the $dt\mu$ mesic molecule in the loosely bound excited state.

The $(dt\mu)Xee$ states are either true bound states or narrow resonances if their energy is below or above the $t\mu+DX$ threshold. As the energy shifts are mainly determined by the coupling with closed channels, in the present calculation both resonances and bound states are treated on an equal footing thus neglecting a small contribution to the energy shifts which comes from the coupling with the open $t\mu+DX$ channel.

A. Three-body description

Under the above approximations, the Schrödinger equation for the hydrogen-like molecule $(dt\mu)Xee$ reads as

$$\left[-\frac{1}{2\mu_1}\Delta_r - \frac{1}{2\mu_2}\Delta_\rho + V_1(r) + V_2(|\boldsymbol{\rho} - \boldsymbol{\beta}\mathbf{r}|) + V(|\boldsymbol{\rho} + \boldsymbol{\alpha}\mathbf{r}|) - E \right] \Psi = 0, \quad (1)$$

where the Jacobi coordinates \mathbf{r} and $\boldsymbol{\rho}$ are the vectors from d to the point-like mesic atom $t\mu$ and from the second nucleus X to the $dt\mu$ center of mass, respectively. The reduced masses and parameters α and β are $\mu_1 = m_1 m_2 / (m_1 + m_2)$, $\mu_2 = (m_1 + m_2) m_3 / (m_1 + m_2 + m_3)$, $\alpha = m_1 / (m_1 + m_2)$, and β

$= m_2 / (m_1 + m_2)$, where m_1 , m_2 , and m_3 are the masses of $t\mu$, d , and X , respectively. The atomic units are used throughout the paper unless other is specified. In Eq. (1), $V(|\boldsymbol{\rho} + \boldsymbol{\alpha}\mathbf{r}|)$ denotes the well-known BO potential describing the interaction between charged d and X while the short-range potentials $V_1(r)$ and $V_2(|\boldsymbol{\rho} - \boldsymbol{\beta}\mathbf{r}|)$ describe the interaction of a $t\mu$ mesic atom with a deuteron and X , respectively. In the following, due to large internuclear separation ($\rho \gg r$) in $(dt\mu)Xee$, the short-range interaction $V_2(|\boldsymbol{\rho} - \boldsymbol{\beta}\mathbf{r}|)$ of the $t\mu$ mesic atom with the second nucleus X is negligible and will be omitted.

A natural zeroth-order approximation for the calculation of the $(dt\mu)Xee$ energy levels is to treat the $dt\mu$ mesic molecule as a point quasi-nucleus with the $dt\mu$ mass and the unit charge. The calculations of the energy levels in this approximation are presented in [7,8] for different isotopes X of the hydrogen-like molecule $(dt\mu)Xee$. Clearly, the treatment of $dt\mu$ as a point-like particle is equivalent to the replacement of the exact potential $V(|\boldsymbol{\rho} + \boldsymbol{\alpha}\mathbf{r}|)$ in the Schrödinger equation (1) by the potential $V(\rho)$ which describes the BO interaction between X and the point particle located at the $dt\mu$ center of mass. Thus, the effect of the $dt\mu$ structure, which leads to the shift of the zeroth-order energy levels, originates from the perturbation potential

$$V_p = V(|\boldsymbol{\rho} + \boldsymbol{\alpha}\mathbf{r}|) - V(\rho). \quad (2)$$

In the zeroth-order approximation $V_p=0$, the solutions of Eq. (1) with the total angular momentum L and its projection M are written as a product of the bispherical harmonics $\mathcal{Y}_{l\lambda}^{LM}(\hat{\boldsymbol{\rho}}, \hat{\mathbf{r}})$ describing the angular dependence, the radial function of ρ describing the motion of nuclei in $(dt\mu)Xee$ with the angular momentum l , and the radial function of r describing the internal motion in a mesic molecule with the angular momentum λ . The unperturbed energies E_{nl} and the corresponding square integrable radial functions $\Phi_{nl}(\rho)$ of the $(dt\mu)Xee$ vibrational and rotational states satisfy the equation

$$\left\{ \frac{1}{2\mu_2} \left[-\frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial}{\partial \rho} \right) + \frac{l(l+1)}{\rho^2} \right] + V(\rho) - E_{nl} \right\} \Phi_{nl}(\rho) = 0, \quad (3)$$

where n is the vibrational quantum number. For the problem under consideration, one should consider both the bound and continuum states of the $t+d\mu$ subsystem whose energies and wave functions satisfy the equation

$$\left\{ \frac{1}{2\mu_1} \left[-\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\lambda(\lambda+1)}{r^2} \right] + V_1(r) - E \right\} \phi(r) = 0. \quad (4)$$

Here $E = -\varepsilon_{v\lambda}$ and $\phi(r) = \phi_{v\lambda}(r)$ for the bound states and $E = k^2/2\mu_1$ and $\phi(r) = \phi_{k\lambda}(r)$ for the continuum states with the wave number k . The functions $\phi_{v\lambda}(r)$ are square integrable and the functions $\phi_{k\lambda}(r)$ are normalized by the condition

$$\int_0^\infty r^2 dr \phi_{k\lambda}^*(r) \phi_{q\lambda}(r) = \delta(k - q). \quad (5)$$

In correspondence with the Vesman mechanism, $(dt\mu)Xee$ contains a $dt\mu$ mesic molecule in the weakly bound state with the binding energy $\varepsilon_{11}(v=1, \lambda=1)$. Other $dt\mu$ states, whose binding energies significantly exceed all the characteristic energies of the problem under consideration, will not be taken into account in the calculation of the energy shifts.

B. Perturbation theory

The effect of the $dt\mu$ structure is small due to smallness of $dt\mu$ mesic molecule in comparison with a characteristic length of $dt\mu$ motion in the molecular potential $V(\rho)$. In other words, the perturbation V_p is small in comparison with $V(\rho)$ and can be expanded in powers of the small parameter ar . Correspondingly, the dimensionless parameter of the perturbation theory is the ratio of the average distance between the deuteron and the $dt\mu$ center of mass $\langle r \rangle$ to the average amplitude of vibrations $\langle \rho - a \rangle$ in the molecular potential near the equilibrium internuclear distance a .

One should note that the lowest-order term of the expansion V_p , which is proportional to ar , does not contribute to the energy shifts in the first-order PT; therefore, the energy shift of order $(ar)^2$ must be obtained up to the second-order PT. Besides, V_p couples the rotational states with $l=L\pm 1$ while the state with $l=L$ remains uncoupled. As the separation of the rotational levels is comparatively small, the level coupling cannot be *a priori* neglected and requires explicit treatment. Thus, the energy shifts will be determined in the second-order degenerate PT by solving a secular equation,

$$\det[V^n + W^n + \mathcal{E}_n - E] = 0, \quad (6)$$

where V^n and W^n are the matrices with the matrix elements of the first- and second-order PT $V_{ll_1}^n$ and $W_{ll_1}^n$, respectively, the matrix elements of \mathcal{E}_n are $(E_{nl} + \varepsilon_{11})\delta_{ll_1}$, and E is the level energy.

The first-order PT matrix elements are

$$V_{ll_1}^n = \int d^3r d^3\rho V_p |\phi_{11}(r)|^2 \Phi_{nl}(\rho) \Phi_{n_1 l_1}(\rho) \mathcal{Y}_{l_1}^{LM*}(\hat{\rho}, \hat{r}) \mathcal{Y}_{l_1}^{LM}(\hat{\rho}, \hat{r}), \quad (7)$$

and the second-order PT matrix elements include a sum and an integral over intermediate states describing simultaneous excitations of the hydrogen-like molecule with the quantum numbers ν and l and the embedded $dt\mu$ mesic molecule with the continuum-state wave number k and the angular momentum λ ,

$$W_{ll_1}^n = - \sum_{\nu \ell \lambda} \int \frac{dk Z_{nl, \nu \ell}^\lambda(k) Z_{\nu \ell, n_1 l_1}^\lambda(k)}{k^2/2\mu_1 + E_{\nu \ell} - E}, \quad (8)$$

where

$$Z_{nl, n_1 l_1}^\lambda(k) = \int d^3r d^3\rho V_p \phi_{11}(r) \phi_{k\lambda}(r) \Phi_{nl}(\rho) \times \Phi_{n_1 l_1}(\rho) \mathcal{Y}_{l_1}^{LM*}(\hat{\rho}, \hat{r}) \mathcal{Y}_{l_1}^{LM}(\hat{\rho}, \hat{r}). \quad (9)$$

Bearing in mind that the second-order PT calculation are of order $a^2 \langle r \rangle^2$, we expand V_p up to the second order in ar ,

which corresponds to the multipole expansion

$$V_p = ar \frac{\partial V}{\partial \rho} P_1(\cos \theta) + \frac{1}{6} \alpha^2 r^2 \left[\frac{\partial^2 V}{\partial \rho^2} + \frac{2}{\rho} \frac{\partial V}{\partial \rho} + 2 \left(\frac{\partial^2 V}{\partial \rho^2} - \frac{1}{\rho} \frac{\partial V}{\partial \rho} \right) P_2(\cos \theta) \right], \quad (10)$$

where θ is the angle between the vectors \mathbf{r} and $\boldsymbol{\rho}$. The monopole and quadrupole terms in (10) contribute only in the first-order PT while the dipole one in the second-order PT.

A calculation of the matrix elements $V_{ll_1}^n$ and $W_{ll_1}^n$ with the perturbation V_p in the form (10) results in

$$V_{ll_1}^n = \frac{1}{6} \alpha^2 Q [U_{nl, n_1 l_1}^M \delta_{ll_1} + U_{nl, n_1 l_1}^Q A_2^L(1111)], \quad (11)$$

$$W_{ll_1}^n = - \alpha^2 \sum_{\nu} \sum_{\lambda \ell} U_{n_1 \nu l}^D U_{\nu n_1 l_1}^D A_1^L(11 \ell \lambda) A_1^L(1_1 1 \ell \lambda) I_\lambda(E_{\nu \ell} - E + \varepsilon_{11}), \quad (12)$$

where

$$I_\lambda(\Delta) = \int_0^\infty \frac{[u_\lambda(k)]^2 dk}{k^2/2\mu_1 + \Delta}, \quad (13)$$

$$Q = \int dr r^4 |\phi_{11}(r)|^2, \quad (14)$$

$$u_\lambda(k) = \int dr r^3 \phi_{k\lambda}(r) \phi_{11}(r), \quad (15)$$

$$U_{nl, n_1 l_1}^M = \int \rho^2 d\rho \Phi_{nl}(\rho) \Phi_{n_1 l_1}(\rho) \left(\frac{\partial^2 V}{\partial \rho^2} + \frac{2}{\rho} \frac{\partial V}{\partial \rho} \right), \quad (16)$$

$$U_{nl, n_1 l_1}^Q = 2 \int \rho^2 d\rho \Phi_{nl}(\rho) \Phi_{n_1 l_1}(\rho) \left(\frac{\partial^2 V}{\partial \rho^2} - \frac{1}{\rho} \frac{\partial V}{\partial \rho} \right), \quad (17)$$

$$U_{nl, n_1 l_1}^D = \int \rho^2 d\rho \Phi_{nl}(\rho) \Phi_{n_1 l_1}(\rho) \frac{\partial V}{\partial \rho}, \quad (18)$$

and the angular integrals $A_k^L(l\lambda l_1 \lambda_1)$ are given in the Appendix.

III. RESULTS OF CALCULATION

A. Matrix elements

The simple, though providing the required accuracy, expressions for the multipole matrix elements (16)–(18), are obtained using the following reliable approximations. First, the matrix elements are completely determined by the BO potential for the hydrogen molecule $V(\rho)$ which is fairly well known from the calculations [7,8,14,15]. As $(dt\mu)Xee$ is produced in low-energy $t\mu + \text{DX}$ collisions, only the lowest vibrational states should be taken into account. Because these states are localized near the minimum of $V(\rho)$ at the equilibrium internuclear distance $a \approx 1.4$ a.u., it is natural to use the harmonic approximation

$$V_h(\rho) = \frac{1}{2}\mu_2\omega^2(\rho - a)^2 + V_0, \quad (19)$$

where only the frequency of vibrations ω is of importance for the calculation. Besides, an accuracy of the approximation (19) is estimated using the unharmonic approximation of the BO potential,

$$V_u(\rho) = \frac{1}{2}\mu_2\omega^2(\rho - a)^2[1 - \alpha_M(\rho - a)] + V_0, \quad (20)$$

which takes into account the next term of the expansion in $\rho - a$. The approximation (20) accurately reproduces the exact energies of the lowest vibrational states calculated in [7,8].

Second, the rotational energy in (3) for the hydrogen-like molecule $l(l+1)/2\mu_2\rho^2 \approx l(l+1)/2\mu_2a^2 \approx 10^{-4}$ is two orders of magnitude smaller than the vibrational energy $\omega \approx 10^{-2}$. Therefore, under a usual approximation, the centrifugal term is treated perturbatively, i.e., the eigenenergies are given by

$$E_{nl} = E_{n0} + v_r l(l+1), \quad (21)$$

and the wave functions $\Phi_{nl}(\rho)$ will be taken independent of l in the same approximation. Indeed, the rotational spectrum calculated in [7,8] is in good agreement with the above expression (21) with $v_r \approx 1/2\mu_2a^2 \approx 10^{-4}$. Thus, under the above approximations, the radial wave function $\Phi_{nl}(\rho)$ in the potential (19) coincides with the harmonic-oscillator wave function and the multipole matrix elements (16)–(18) are reduced to l -independent expressions,

$$U_{nv}^D = \sqrt{\frac{\mu_2\omega^3}{2}}(\sqrt{n}\delta_{n-1,v} + \sqrt{n+1}\delta_{n+1,v}),$$

$$U_{nm}^M = \mu_2\omega^2, \quad U_{nm}^Q = 2\mu_2\omega^2. \quad (22)$$

The unharmonic term of the potential $V_u(\rho)$ leads only to modification of the dipole matrix element

$$U_{nv}^D = \sqrt{\frac{\mu_2\omega^3}{2}}\{[\sqrt{n}\delta_{n-1,v} + \sqrt{n+1}\delta_{n+1,v}] - \eta[\sqrt{n(n-1)}\delta_{n,v+2} + \sqrt{(n+1)(n+2)}\delta_{n,v-2} + (2n+1)\delta_{n,v}]\}, \quad (23)$$

where the unharmonic correction is proportional to the dimensionless parameter $\eta = \frac{3}{2}\alpha_M/\sqrt{2\mu_2\omega} \approx 0.14$.

The calculation of the quasi-nucleus matrix elements (14) and (15) is based on the smallness of the $t\mu$ size in comparison with the size of the loosely bound $dt\mu$ state ($v=1, \lambda=1$). Thus, almost in all the configuration space $t\mu$ and d move as free particles and the bound-state wave function is approximated by

$$\varphi_{11}(r) = C_a \frac{1 + \kappa r}{\sqrt{\kappa r^2}} e^{-\kappa r}, \quad (24)$$

where $\kappa = \sqrt{2\mu_1\varepsilon_{11}}$. The asymptotic expression (24) has been widely used in description of the loosely bound states of mesic molecules and the asymptotic normalization constant C_a was determined by a comparison with the exact three-body calculations [9,16,17]. For the same reasons, the

asymptotic expressions are used for the continuum wave functions $\phi_{k\lambda}(r)$, viz.,

$$\phi_{k0}(r) = \sqrt{\frac{2}{\pi}} \frac{\sin(kr + \delta_0(k))}{r}, \quad (25)$$

$$\phi_{k2}(r) = \sqrt{\frac{2}{\pi}} k [\cos \delta_2(k) j_2(kr) + \sin \delta_2(k) y_2(kr)], \quad (26)$$

where $\delta_\lambda(k)$ are the $t\mu+d$ scattering phase shifts and $j_2(kr)$ and $y_2(kr)$ are the spherical Bessel functions. The d -wave phase shift $\delta_2(k)$ is actually very small, which allows either replacing $y_2(kr)$ by the leading term $\cos kr/kr$ of its asymptotic expansion or simply putting $\delta_2(k)=0$ in Eq. (26). Using the wave functions (24)–(26) with $y_2(kr) \rightarrow \cos kr/kr$ one obtains the quadrupole momentum

$$Q = \frac{5}{8} \frac{C_a^2}{\mu_1\varepsilon_{11}} \quad (27)$$

and the expression

$$I_\lambda(\Delta) = \frac{4C_a^2}{\pi\mu_1\varepsilon_{11}^2} J_\lambda(\Delta/\varepsilon_{11}), \quad (28)$$

via the dimensionless integrals

$$J_0(z) = \int_0^\infty \frac{[\sin \delta_0(k) - (k^2+3)(k/2)\cos \delta_0(k)]^2 dk}{(k^2+1)^4(k^2+z)}, \quad (29)$$

$$J_2(z) = \int_0^\infty \frac{[\sin \delta_2(k) + k^3 \cos \delta_2(k)]^2 dk}{(k^2+1)^4(k^2+z)}. \quad (30)$$

B. Shift and splitting of energy levels

Energy shifts are obtained by solving the secular equation (6) which is reduced, due to the selection rules for angular momenta l and l_1 , to a 2×2 matrix equation for $l, l_1 = L \pm 1$ ($L \neq 0$) and a scalar equation for $l = l_1 = L \neq 0$. The energy shifts with respect to the unperturbed rovibrational energies $E_{nl} + \varepsilon_{11}$ are denoted as $\Delta_0(n)$ and $\Delta_\pm(nl)$ for $l=L$ and $l=L \pm 1$, respectively. Note that the state with $L=0$ and $l=l_1=1$ is uncoupled; however, its energy shift $\Delta_+(n1)$ will be determined in the same manner as for the other $L \neq 0$ states.

The first-order PT matrix elements $V_{ll_1}^n$ in Eq. (6) are calculated by substituting the radial integrals $U_{nm}^{M,Q}$ (22), the quadrupole momentum Q (27), and the angular integrals $A_2^L(l_1 l_1 1)$ (A4) in Eq. (11). Note that $V_{ll_1}^n$ appears to be independent of the vibrational quantum number n and this index will be omitted in what follows. The matrix elements are scaled by a single dimensional parameter,

$$v_0 = \frac{m_1 m_3 \omega^2 C_a^2}{16 m_2 (m_1 + m_2 + m_3) \varepsilon_{11}}, \quad (31)$$

which is a characteristic energy for the problem. It should be mentioned that although Eq. (31) does not contain a specific

small parameter, v_0 turns out to be sufficiently small ($v_0/\omega \sim 0.006$) thus making the energy shifts small. As a result, one finds

$$V_{ll_1} = v_0 \begin{cases} 1, & l, l_1 = L(L \neq 0), \\ 2\delta_{ll_1} - B_{ll_1}, & l, l_1 = L \mp 1, \end{cases} \quad (32)$$

where the matrix elements B_{ll_1} form the matrix

$$B = \frac{1}{2L+1} \begin{pmatrix} 1 & 2\sqrt{L(L+1)} \\ 2\sqrt{L(L+1)} & -1 \end{pmatrix}, \quad (33)$$

in which the first row and column correspond to $l, l_1 = L-1$ and the second ones to $l, l_1 = L+1$.

The second-order PT matrix elements $W_{ll_1}^n$ in Eq. (6) are calculated by substituting U_{nv}^D (22) and $I_\lambda(\Delta)$ (28) in Eq. (12), which gives the expression

$$W_{ll_1}^n = -v_0 \frac{32\omega}{\pi \varepsilon_{11}} \sum_{\nu=n\pm 1} \sum_{\ell\lambda} \max(n, \nu) A_1^L(l1\ell\lambda) \times A_1^L(l_1 1 \ell \lambda) J_\lambda \left(1 + \frac{E_{\nu\ell} - E}{\varepsilon_{11}} \right), \quad (34)$$

via the energy scale v_0 and the dimensionless factors. Solving the secular equation (6), one can safely replace, up to an accuracy of the second-order PT, the eigenvalue E in the argument of J_λ by the unperturbed value E_{nl} . Thus, the calculation of the energy shifts is basically accomplished by the derivation of Eqs. (32)–(34).

However, it is reasonable to make a further simplification of (34) by neglecting the difference of the rotational energies in the argument of J_λ , which allows obtaining an explicit and sufficiently accurate dependence of the energy shifts on the quantum numbers n and l . As the rotational energy is much smaller than the vibrational quantum ω , one replaces the energy differences $E_{n\pm 1l} - E$ in the argument of J_λ by the l -independent values $E_{n\pm 10} - E_{n0} = \pm\omega$. Using the angular integrals $A_1^L(l1l_1\lambda)$ (A5) and (A6) and introducing the notation $J_\lambda^\pm = J_\lambda(1 \pm \omega/\varepsilon_{11})$ for integrals independent of n and l one obtains

$$W_{ll_1}^n = v_0 \begin{cases} 1 + \alpha_n - \beta_n, & l, l_1 = L(L \neq 0), \\ (2 - \beta_n)\delta_{ll_1} + (\alpha_n - 1)B_{ll_1}, & l, l_1 = L \mp 1, \end{cases} \quad (35)$$

where

$$\alpha_n = 1 - \frac{16\omega}{3\pi\varepsilon_{11}} \left[(n+1) \left(J_0^+ + \frac{1}{5}J_2^+ \right) + n \left(J_0^- + \frac{1}{5}J_2^- \right) \right], \quad (36)$$

$$\beta_n = 2 - \frac{16\omega}{3\pi\varepsilon_{11}} \left[(n+1) \left(J_0^+ + \frac{7}{5}J_2^+ \right) + n \left(J_0^- + \frac{7}{5}J_2^- \right) \right] \quad (37)$$

determine the explicit dependence on the vibrational quantum number n . As a result, the sum of V_{ll_1} (32) and $W_{ll_1}^n$ (35) takes a simple form

$$V_{ll_1} + W_{ll_1}^n = v_0 \begin{cases} \beta_n - \alpha_n, & l = l_1 = L(L \neq 0), \\ \beta_n \delta_{ll_1} - \alpha_n B_{ll_1}, & l, l_1 = L \mp 1, \end{cases} \quad (38)$$

i.e., the parameter β_n determines the constant shift $v_0\beta_n$ of all level energies E_{nl} whereas α_n determines the level splitting. Using (38) and (21) in the secular equation (6) one obtains

$$\Delta_0(n) = v_0(\beta_n - \alpha_n), \quad (39)$$

$$\Delta_\pm(nl) = v_0\beta_n \mp v_r [2(l \mp 1) + 1] \pm \sqrt{v_0^2\alpha_n^2 + 2v_0\alpha_n v_r + [2(l \mp 1) + 1]^2 v_r^2}. \quad (40)$$

The effect of coupling of the rotational states with $l=L\pm 1$ is explicitly taken into account in expression (40). Generally, the effect decreases with decreasing ratio of the level splitting to the energy difference between the rotational states $v_0\alpha_n/v_r(2L+1)$, i.e., with increasing total angular momentum L . As follows from the numerical values of v_0 , v_r , and α_n for all the considered states $n=2,3$ (Sec. III C), even in the worst case $L=1$ the energy shifts calculated with and without allowance for the coupling of the rotational states differ at the most by 0.01 meV for $(dt\mu)dee$ and 0.03 meV for $(dt\mu)tee$. As these values are beyond the accuracy of the present calculation, it is quite reasonable to neglect coupling, i.e., to use the diagonal approximation for the secular equation (6), which allows obtaining a simple expression,

$$\Delta_\pm(nl) = v_0 \left[\beta_n \pm \frac{\alpha_n}{2(l \mp 1) + 1} \right] = v_0 \left[\beta_n \pm \frac{\alpha_n}{2L+1} \right]. \quad (41)$$

Note that Eqs. (40) and (41) are valid both for $L=0$ and $l=1$ when $\Delta_+(n1) = v_0(\beta_n + \alpha_n)$ and for $L=1$ and $l=0$ when $\Delta_-(n0) = v_0(\beta_n - \alpha_n/3)$. The sign of α_n determines the relative position of the levels so that the energies satisfy the inequalities $E_{nL+1} > E_{nL-1} > E_{nL}$ for $\alpha_n > 0$ and the inverse inequalities for $\alpha_n < 0$. The largest energy splitting is predicted for $l=1$ between the states with $L=0$ and $L=1$, viz., $\Delta_+(n1) - \Delta_0(n) = 2v_0\alpha_n$.

C. Numerical results

The energy shifts and level splittings will be calculated by solving the eigenvalue equation (6) using formulas (31)–(34). In addition to the particle masses $m_\mu = 206.768$ a.u., $m_d = 3670.484$ a.u., and $m_t = 5497.922$ a.u., the calculation of the matrix elements V_{ll_1} and $W_{ll_1}^n$ requires the vibrational ω and rotational v_r energies of the exotic molecule $(dt\mu)Xee$, the binding energy ε_{11} and the asymptotic constant C_a of the $dt\mu$ loosely bound state, and the low-energy $t\mu+d$ scattering phase shifts $\delta_\lambda(k)$ which determine the integrals $J_\lambda(1 + (E_{\nu\ell} - E)/\varepsilon_{11})$.

The vibrational quantum ω and the rotational-energy constant v_r are determined by the BO internuclear potential of the hydrogen molecule near its minimum or, equivalently, by the low-lying part of the $(dt\mu)Xee$ vibrational-rotational spectra calculated in [7,8]. Fitting the BO potential near the equilibrium distance $a=1.401$ to the harmonic, unharmonic,

and Morse potentials provides a consistent determination of both ω and the parameter α_M . As the BO potential is independent of the isotopic composition, both $\mu_2\omega^2$ and α_M are independent of the masses of heavy particles due to Eq. (20). The result of the fit gives $\omega=321.8$ meV for $(dt\mu)dee$ [correspondingly, $\omega=273.1$ meV for $(dt\mu)tee$] with a few per cent accuracy and the parameter $\alpha_M=0.7$. For these parameters, the energies of the lowest vibrational states in the approximate potential are in reasonable agreement with the results of [7,8].

The rotational spectra calculated in [7,8] are fitted to Eq. (21) for $1 \leq l \leq 10$ and each $1 \leq n \leq 4$. For the lowest vibrational state $n=1$, one obtains $v_r=2.43$ meV for $(dt\mu)dee$ and $v_r=1.85$ meV for $(dt\mu)tee$. These values agree with the simple estimate $2\mu_2v_r \approx 1/a^2$ that determines the isotopic dependence of v_r . Although v_r slightly decreases for the higher vibrational states, the above values will be used for $n > 1$, which leads to a few per cent error.

The determination of the binding energy ε_{11} of a $dt\mu$ loosely bound state was a subject of numerous elaborated calculations. As a result, the value $\varepsilon_{11}=596$ meV [1,2,4] is obtained for the lowest hyperfine state by taking into account relativistic effects, hyperfine effects, finite nuclear size, and vacuum polarization. The asymptotic constant C_a was determined in a number of papers [9,16,17] by a comparison of the asymptotic expression (24) with the three-body wave function. In the following, the value $C_a=0.874/\sqrt{2}$ obtained in the latest elaborated calculation [17] of the wave function in a wide asymptotic region of large distances between d and $t\mu$ is accepted. Using C_a , ε_{11} , and ω one can calculate the energy scale v_0 (31). As $\omega^2 \sim 1/\mu_2=(m_1+m_2+m_3)/(m_1+m_2)m_3$, the parameter v_0 (31) is independent of m_3 , i.e., it is the same for any isotope X . Given the above numerical values one obtains $v_0=1.81$ meV.

For the sake of completeness, it is interesting to estimate the energy scale for the molecule $(dd\mu)Xee$ too by using the values $\varepsilon_{11}=1975$ meV, $C_a=1.006/\sqrt{2}$, and $\omega=257$ meV, which gives $v_0=0.4$ meV. Although the present approach requires some modifications to describe $(dd\mu)Xee$, viz., taking into account the identity of nuclei in $dd\mu$ and the essential role of the unharmonic corrections to the BO potential, one can qualitatively conclude that the energy shifts in $(dd\mu)Xee$ are 4–5 times smaller than in $(dt\mu)Xee$.

In the present approach the energy shifts in the first-order PT are given by simple dependence on the angular momentum l (32) and (33) containing a single parameter v_0 . It is worthwhile to compare this result with the first ever elaborate six-body calculation of the $(dt\mu)dee$ energy shifts in the first-order PT [6]. In this paper, the molecular structure, i.e., the dependence on l , was explicitly taken into account in contrast with previous calculations [9,10,18] where the l -independent energy shift was obtained by scaling the result for the atom-like four-body system $(dt\mu)e$. As pointed out in this paper, the monopole contribution calculated in Ref. [6] depends on the choice of the coordinate system that does not allow a comparison. For this reason, only the quadrupole contribution to the first-order PT energy shifts of Ref. [6] will be compared with the present results. The quadrupole contribution of Ref. [6] is given in Table II of that paper,

TABLE I. Quadrupole contributions $\Delta E_Q^{(1)}$ (in meV) to the first-order PT energy shifts of the present calculation and those from Ref. [6] for different l and L . Also presented are the angular integrals $A_2^L(l1l1)$ and the parameter \tilde{v}_0 corresponding to the energy shifts of Ref. [6].

l	L	$A_2^L(l1l1)$	$\Delta E_Q^{(1)}$	$\Delta E_Q^{(1)}$ [6]	\tilde{v}_0
1	0	2/5	2.42	2.35	1.77
1	1	-1/5	-1.21	-1.17	1.76
2	1	1/5	1.21	1.17	1.76
1	2	1/25	0.24	0.23	1.73
2	2	-1/5	-1.21	-1.17	1.76
3	2	4/25	0.96	0.94	1.77

while in the present approach $\Delta E_Q^{(1)}=(10/3)v_0A_2^L(l1l1)$, as follows from Eqs. (11), (22), and (27). The both results are in excellent agreement with each other, as shown in Table I. Note that in the present approach the dependence on angular momenta is completely determined by the factor $A_2^L(l1l1)$ which is also presented in Table I. To a good accuracy, the results of Ref. [6] reveal the same dependence on angular momenta which approves the description of energy shifts by a single parameter v_0 . To emphasize this fact, the quadrupole correction calculated in Ref. [6] is expressed in the form $\Delta E_Q^{(1)}=(10/3)\tilde{v}_0A_2^L(l1l1)$ with the variable \tilde{v}_0 presented in Table I. Indeed, \tilde{v}_0 is practically independent of l and L and agrees with $v_0=1.81$ meV. Agreement between the present one-parameter result for the quadrupole correction and the elaborate six-body calculation [6] is a good argument for the validity of the present approach.

At last, one should obtain $W_{ll_1}^n$ (34), which requires the evaluation of $J_\lambda(1+(E_{\nu\ell}-E)/\varepsilon_{11})$ by using the $t\mu+d$ scattering phase shifts $\delta_\lambda(k)$ in the integrands of Eqs. (29) and (30). The low-energy scattering phase shifts were determined in a number of three-body calculations [19–24], whose results are in good agreement with each other. Using $\delta_\lambda(k)$ from these calculations and integrating (29) and (30) in the energy interval $0 \leq k^2/2\mu_1 \leq 10$ eV, one obtains $J_\lambda(1+(E_{\nu\ell}-E)/\varepsilon_{11})$ with a relative accuracy about 0.01. A good convergence of the integral over the intermediate states in the energy interval up to about 10 eV justifies a possibility to neglect the $d\mu+t$ closed channel whose threshold is approximately 50 eV higher.

Calculating the matrix elements V_{ll_1} (32) and $W_{ll_1}^n$ (34) and solving the eigenvalue equation (6) one obtains energy shifts presented in Table II for $(dt\mu)dee$ and $(dt\mu)tee$. Note that applicability of the harmonic approximation for the BO potential was checked by using the modified dipole matrix element (23) in the calculation, which gives an estimate of the unharmonic correction of the order of 5% in the energy shifts. Calculations reveal that the energy shifts are essentially dependent on the isotopic composition and the molecular quantum numbers n and l , which is basically connected with the cancellation of the first- and second-order PT contributions. In particular, the energy shifts decrease with increasing n so that Δ_\pm become very small or even negative for $n=4$. The reason for this dependence is an increasing in the

TABLE II. Energy shifts (meV) for a few states of $(dt\mu)dee$ and $(dt\mu)tee$ with the vibrational quantum number n , the total angular momentum L , and angular momentum l of the hydrogen-like molecule with the point-like $dt\mu$ quasi-nucleus.

l	L	$(dt\mu)dee$		$(dt\mu)tee$	
		$n=2$	$n=3$	$n=2$	$n=3$
0	1	1.48	0.84	1.70	1.15
1	0	1.99	0.55	2.48	1.25
1	1	1.22	0.98	1.30	1.09
1	2	1.54	0.82	1.78	1.16
2	1	1.73	0.66	2.07	1.19
2	2	1.22	0.98	1.30	1.09
2	3	1.57	0.82	1.82	1.17
3	2	1.65	0.68	1.99	1.16
3	3	1.22	0.98	1.30	1.09
3	4	1.59	0.82	1.84	1.18
4	3	1.62	0.68	1.95	1.15
4	4	1.22	0.98	1.30	1.09
4	5	1.60	0.82	1.86	1.18

dipole matrix element (22) with increasing n , which, in turn, leads to an increase in the second-order PT contribution. The cancellation effect was widely discussed, e. g., in [9,10,18]; nevertheless, the dependence on the molecular quantum state was beyond the scope of those papers where only the atom-like system $(dt\mu)e$ was calculated. On the other hand, the calculation [6] determined the l -dependence only in the first-order PT.

The dependence of the energy shifts on quantum numbers is illustrated in Fig. 1 for the $(dt\mu)dee$ states with $n=2,3$ and $l=0-4$. In addition to a decreasing in the energy shifts for higher n , notice the inverse ordering of levels, i.e., the highest level with $L=l-1$ for $n=2$ becomes the lowest for $n=3$. Except for Δ_+ , whose values at small $l=1,2$ are quite different, the results reveal weak dependence on l with splitting of levels of the order of 0.2 meV.

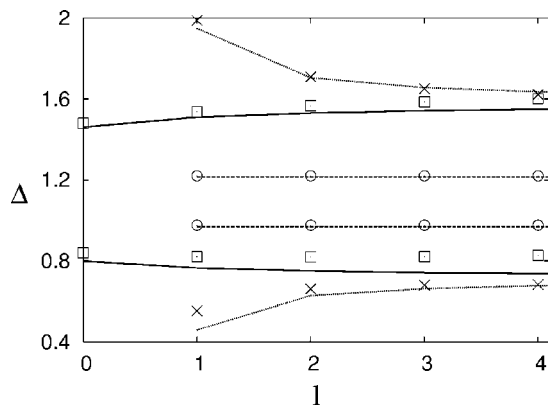


FIG. 1. Energy shifts (meV) of $(dt\mu)dee$. Crosses, squares, and circles denote, respectively, Δ_+ , Δ_- , and Δ_0 . The results obtained by simplified formulas (39) and (41) are denoted by the dotted, solid, and dashed lines, respectively. Three upper curves correspond to the vibrational quantum number $n=2$ and the lower ones to $n=3$.

TABLE III. Dimensionless parameters entering into the simplified expressions (39) and (41) for the energy shifts of $(dt\mu)Xee$.

X	$16\omega/3\pi\epsilon_{11}$	J_0^+	J_0^-	J_2^+	J_2^-
d	0.917	0.113	0.236	0.051	0.073
t	0.778	0.117	0.216	0.052	0.069

As discussed at the end of Sec. III B, the dependence of energy shifts and level splitting on quantum numbers are expressed to a good accuracy by simple formulas (39) and (41) via few parameters. Numerical values of $16\omega/3\pi\epsilon_{11}$ and $J_{0,2}^\pm$ are given in Table III for $(dt\mu)dee$ and $(dt\mu)tee$. As is clearly seen in Fig. 1, the simplified expressions (39) and (41) provide a reliable description of energy shifts.

IV. DISCUSSION AND CONCLUSIONS

The hydrogen-like molecule $(dt\mu)Xee$ is treated within the framework of the three-body model for heavy particles d , $t\mu$, and X . The model is based on the fact that a $t\mu$ mesic atom is small in comparison with its mean separation from a deuteron and that the size of a $dt\mu$ mesic molecule is small in comparison with the amplitude of vibrations in $(dt\mu)Xee$. In this approach, the interaction of the charged particles d and X is described by the well-known BO potential of the hydrogen molecule, while the description of a $dt\mu$ mesic molecule is given in terms of the binding energy ϵ_{11} , the asymptotic constant C_a , and the low-energy s - and d -wave scattering phase shifts $\delta_\lambda(k)$ regardless of the explicit form of the $d+t\mu$ effective potential.

In the present approach, the shift and splitting of the $(dt\mu)Xee$ energy levels which result from the internal structure and rotation of the $dt\mu$ quasi-nucleus are calculated in the second-order PT. This allows one to find the energy levels, i.e., the positions of the $t\mu+DX$ scattering resonances with an accuracy about a tenth of a meV, which is of key importance for determination of the $dt\mu$ formation rate. Calculations are performed for different vibrational ($n=2,3$) and rotational ($0 \leq l \leq 4$) states for the molecules of the different isotope composition $X=d,t$. In this respect, note that different vibrational states of $(dt\mu)Xee$ can be currently observed in the atomic beam experiments [25]. It should be emphasized that the effect of the $dt\mu$ structure removes the degeneracy of unperturbed states with the same l and different L , which produces a triple-resonance structure in place of every unperturbed level except the one with $l=0$. As the splitting value is of the order of the shift itself, the effect of splitting should be taken into account in the energy dependence of the resonance formation rate.

The following aspects of the present calculation are worth mentioning. The first-order PT quadrupole contribution to the energy shifts is in agreement with the elaborate six-body calculation [6], which is a good argument for the validity of the present approach. Furthermore, it is shown that for all the considered states the effect of coupling of the rotational states with $l=L-1$ and $l=L+1$ is beyond the accuracy of the present calculation. In addition, the energy shift and splitting

is conveniently expressed by simple analytical dependence (39) and (41) on the rotational-vibrational quantum numbers n and l .

It is of interest to compare the present result with the direct nonperturbative three-body calculation of $t\mu + D_2$ scattering [11,12] in which the effect of the $dt\mu$ structure is explicitly taken into account. The positions of narrow resonances calculated in these papers correspond to energy levels of $(dt\mu)dee$ for $L=0$ ($l=1$) and $n=3,4$. For two approximations of the effective potential between $t\mu$ and d used in [11,12], energy shifts are, respectively, 1 meV and 4 meV for $n=3$ and 2 meV and 5 meV for $n=4$. The cause of the noticeable difference (about 3 meV) is not clear since both potentials allow a good description of the low-energy properties of the $t\mu + d$ system. The dependence on the choice of the effective potential and a limitation only by $L=0$ hinders a quantitative comparison of the present results and those of [11,12]. Qualitatively, the energy shifts obtained in Ref. [11,12] exceed the present ones and, contrary to PT considerations, the value for $n=4$ is higher than for $n=3$. This n -dependence clearly deserves further investigation.

Finally, it should be mentioned that the present approach, which reliably takes into account the structure of the exotic molecule, is promising for wider applications, in particular, for a determination of the resonance positions and formation rates beyond PT by solving the scattering problem. Until now, except Refs. [11,12], the formation rates have been calculated only in the first-order PT. In this respect, the result of Ref. [26] shows that the first-order PT dipole approximation is questionable and one should do more refined calculations. In addition, it is of interest to apply the present approach to the problem of the resonance formation of metastable $dt\mu$ mesic molecules [27,28] in collisions of excited $t\mu$ mesic atoms with D_2 molecules.

APPENDIX: ANGULAR INTEGRALS

The following angular integrals are necessary to calculate the matrix elements:

$$A_K^L(l\lambda l_1\lambda_1) = \int d\hat{\rho} d\hat{r} P_K(\cos \theta) \mathcal{Y}_{l\lambda}^{LM*}(\hat{\rho}, \hat{r}) \mathcal{Y}_{l_1\lambda_1}^{LM}(\hat{\rho}, \hat{r}), \quad (\text{A1})$$

where θ is the angle between two unit vectors $\hat{r} = \mathbf{r}/r$ and $\hat{\rho} = \boldsymbol{\rho}/\rho$, $P_K(x)$ is the Legendre polynomial, and the bispherical harmonics are defined as

$$\mathcal{Y}_{l\lambda}^{LM}(\hat{\rho}, \hat{r}) = \sum_{m\mu} (lm\lambda\mu|LM) Y_{lm}(\hat{\rho}) Y_{\lambda\mu}(\hat{r}). \quad (\text{A2})$$

Evaluating the integral (A1) one comes to the expression in terms of the Clebsh-Gordon coefficients and $6j$ -symbols,

$$A_K^L(l\lambda l_1\lambda_1) = (-)^{l_1+L} \sqrt{(2l+1)(2\lambda+1)(l_0K0|l_10)(\lambda_0K0|\lambda_10)} \times \left\{ \begin{matrix} l_1 & l & K \\ \lambda & \lambda_1 & L \end{matrix} \right\}. \quad (\text{A3})$$

The matrix elements $V_{ll_1}^n$ (11) are expressed in terms of the integrals (A3) with $K=2$ and $\lambda=\lambda_1=1$ which are explicitly written as

$$A_2^L(l1l_11) = -\frac{1}{5} \delta_{lL} \delta_{l_1L} + \frac{(L+2)}{5(2L+1)} \delta_{lL+1} \delta_{l_1L+1} + \frac{(L-1)}{5(2L+1)} \delta_{lL-1} \delta_{l_1L-1} - \frac{3\sqrt{L(L+1)}}{5(2L+1)} (\delta_{lL-1} \delta_{l_1L+1} + \delta_{lL+1} \delta_{l_1L-1}). \quad (\text{A4})$$

The matrix elements $W_{ll_1}^n$ (12) are expressed in terms of the integrals (A3) with $K=1$, $\lambda=1$, and either $\lambda_1=0$ and $l_1=L$ or $\lambda_1=2$ and $l=L\pm 1$. The explicit expressions read as

$$A_1^L(l1L0) = \frac{1}{\sqrt{3(2L+1)}} (\sqrt{L} \delta_{lL-1} - \sqrt{L+1} \delta_{lL+1}), \quad (\text{A5})$$

$$A_1^L(l1l_12) = \begin{cases} -\frac{1}{2} \sqrt{\frac{(L+l+3)(L+l+4)(L-l-2)(L-l-3)}{15(2l+1)(2l+3)}}, & l_1=l+1, \\ \frac{1}{2} \sqrt{\frac{(L-l+2)(L-l+3)(L+l-2)(L+l-1)}{15(4l^2-1)}}, & l_1=l-1. \end{cases} \quad (\text{A6})$$

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