

# Fine and quadrupole structure of the weakly bound systems $(dt\mu)_{11}dee$ and $(dd\mu)_{11}dee$

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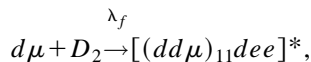
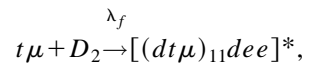
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The interaction of the quadrupole electric moment of the muonic molecules with the Coulomb field of the embedding  $D_2$  molecule gives rise to corrections to the energy levels that depend on the spin and significantly modify the muonic molecule fine structure. We present the first-order calculation of the fine and hyperfine structure of the energy levels of the weakly bound states  $(dt\mu)_{11}$  and  $(dd\mu)_{11}$  that accounts for the quadrupole finite-size corrections as well. The reported results are of interest for the upcoming high-precision measurement of the energy levels and the formation rate of the muonic molecules  $dt\mu$  and  $dd\mu$ . [S1050-2947(98)08304-8]

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## I. INTRODUCTION

The study of the muonic molecules  $dt\mu$  and  $dd\mu$  is not only a central problem for the physics of muon catalyzed fusion, but also a challenge to few-body theory since it allows for the very precise experimental verification of the theoretical predictions [1–3]. The points of particular interest are the anomalously weakly excited bound states of the muonic molecules  $dt\mu$  and  $dd\mu$  with orbital angular momentum  $J_\mu=1$  and vibrational excitation quantum number  $v_\mu=1$  that are formed in the resonant reactions



in which the energy released is transferred to a rovibrational excitation of the six-body bound system:

$$E_{t\mu} + E_{D_2} + \varepsilon_T = E_{[(dt\mu)_{11}dee]^*},$$

$$E_{d\mu} + E_{D_2} + \varepsilon_T = E_{[(dd\mu)_{11}dee]^*}.$$

Here the  $E$ 's denote the energy levels of the corresponding bound states, while  $\varepsilon_T$  is the kinetic energy of the incoming muonic atom. Because of energy conservation, the resonant formation rate  $\lambda_f$  should be expected to be sensitive to both the temperature (through  $\varepsilon_T$ ) and the energy levels of the initial and final bound states; this is why the accurate calculation of the energy levels of the muonic molecule has been considered for years to be of highest priority for the theory of

muon catalyzed fusion. In reality, the strong temperature dependence of  $\lambda_f$  is obscured by the broad thermal energy distribution of the incoming muonic atoms and by the complex structure of the energy levels of the six-body molecular complex that consists of closely lying sublevels, separated by less than the width of the thermal distribution of the muonic atoms. However, the theoretical prediction for the temperature dependence of the resonant formation rate  $\lambda_f = \lambda_f(T)$  remains very sensitive to our detailed knowledge of the structure of these levels.

The above equations exhibit the close similarity between the  $dd\mu$  and  $dt\mu$  muonic ions. To avoid further duplication of formulas, we shall restrict ourselves in what follows to the specific case of the  $dd\mu$  ion; the corresponding expressions for  $dt\mu$  could be easily derived from them.

The six-body system  $E_{[(dd\mu)_{11}dee]^*}$  can be thought of as an excited state of the diatomic molecule  $DM$ , similar to  $DT$ , in which the hypothetic pointlike heavy nucleus  $M$  of mass  $m_M = m_d + m_d + m_\mu$  has been substituted by a  $(dd\mu)_{11}^+$  ion. Accordingly, the six-body system energy levels  $E_{[(dd\mu)_{11}dee]^*}$  can be represented in the form

$$E_{[(dd\mu)_{11}dee]^*} = E_{(dd\mu)_{11}} + E_{(DM)_{J,v_r}} + \Delta E. \quad (1)$$

Here  $E_{(dd\mu)_{11}}$  is the energy level of the isolated three-body system  $dd\mu$ ,  $E_{(DM)_{J,v_r}}$  is the energy of the corresponding excited state of the  $DM$  hydrogenlike molecule, and  $\Delta E$  is a ‘‘finite-size’’ correction term due to the interaction of the constituents of  $M = dd\mu$  with the other particles in the diatomic molecule  $DM$ . The complex structure of the energy levels of  $E_{[(dd\mu)_{11}dee]^*}$  is commonly thought to be due to the

fine and hyperfine splitting of the Coulomb level  $E_{(dd\mu)_{11}}$  [4,5] and the rovibrational excitation spectrum of the  $DM$  molecule. With the exceptions of [6–8], the calculations performed until now ignored the quadrupole splitting of the third term in Eq. (1)—the finite-size correction  $\Delta E$ —and put the main emphasis on estimating the contribution of higher-order perturbation theory [9–11].

The purpose of the present paper is the calculation of the splitting of the finite-size correction  $\Delta E$  that is due to the asymmetry of the electrical field at the site of the composite nucleus  $M$  of the  $DM$  molecule. We are basically following the approach developed earlier in [6], but also make profit of the recent, very precise numerical results of [7,8] for the matrix elements of the perturbation Hamiltonian. We find that the ‘‘quadrupole splitting’’ of the energy levels of the six-body complexes  $E_{[(dd\mu)_{11}dee]_{J_r v_r}}$  and  $E_{[(dt\mu)_{11}dee]_{J_r v_r}}$  has the same order of magnitude as the fine splitting of  $E_{(dd\mu)_{11}}$  and  $E_{(dt\mu)_{11}}$  and should certainly be taken into account in an appropriate way when interpreting the experimental data on the resonant formation of muonic molecules.

## II. QUADRUPOLE VERSUS HYPERFINE SPLITTING OF THE ENERGY LEVELS OF THE MOLECULAR COMPLEX $[(dd\mu)_{11}dee]$

The nonrelativistic Hamiltonian of the six-body molecular complex  $(dd\mu)_{11}dee$ ,  $H_6$ , can be represented in the form

$$H_6 = H_{dd\mu} + H_{DM} + \Delta U \quad (2)$$

where  $H_{dd\mu}$  and  $H_{DM}$  are the nonrelativistic Hamiltonians of the isolated  $dd\mu$  ion and  $DM$  molecule. Denote by  $\vec{R}_c, c=d_1, d_2, \mu$ , the position vectors of the constituents of  $dd\mu$  in a coordinate frame with its origin at the center of mass of the muonic molecule, and by  $\vec{\rho}_i, i=e_1, e_2, d'$ —the position vectors of the  $DM$  molecule constituents; also let  $z_c$  and  $z_i$  denote the corresponding electric charges. In terms of the latter, the explicit form of the finite-size perturbation,  $\Delta U$ , is

$$\Delta U = \sum_{i=e_1, e_2, d'} z_i \left( \sum_{c=d_1, d_2, \mu} \frac{z_c}{|\vec{R}_c - \vec{\rho}_i|} - \frac{\sum_c z_c}{\rho_i} \right). \quad (3)$$

Next, expand  $\Delta U$  in multipoles:  $\Delta U = \sum_{l=0,1,\dots} U^{(l)}$ . The contribution  $\Delta E^{(0,1)}$  from the monopole and dipole terms  $U^{(0,1)}$  to the finite-size correction  $\Delta E$  in Eq. (1) had been evaluated earlier in [7–11]; it is known to cause a *shift* of the unperturbed levels. Consider now the quadrupole terms

$$\begin{aligned} U^{(2)} &= \sum_{i,c} z_i z_c P_2(\cos \theta_{ic}) \left( \Theta(\rho_i - R_c) \frac{R_c^2}{\rho_i^3} + \Theta(R_c - \rho_i) \frac{\rho_i^2}{R_c^3} \right) \\ &= \sum_{i,c} \sum_{m=-2}^2 Y_{2m}^*(\hat{\rho}_i) Y_{2m}(\hat{R}_c) u_{ic}^{(2)}(\rho_i, R_c), \end{aligned} \quad (4)$$

where

$$u_{ic}^{(2)}(\rho_i, R_c) = \frac{4\pi}{5} z_i z_c \left( \Theta(\rho_i - R_c) \frac{R_c^2}{\rho_i^3} + \Theta(R_c - \rho_i) \frac{\rho_i^2}{R_c^3} \right). \quad (5)$$

In first-order of perturbation theory, the quadrupole contribution  $\Delta E^{(2)}$  to  $\Delta E$  in the state  $|\psi\rangle$  of the unperturbed six-body system  $(dd\mu)_{11}dee$  is

$$\Delta E^{(2)} = \langle \psi | U^{(2)} | \psi \rangle. \quad (6)$$

In Ref. [8] the unperturbed wave function of the six-body system,  $\psi$ , is taken to be the direct product of the wave functions of the isolated muonic molecule  $dd\mu$  and the hydrogenlike molecule  $DM$ . The muonic molecule is considered as a bound state of three spinless particles, labeled with the quantum numbers  $J_\mu$  (total angular momentum),  $M_\mu$  (projection of  $\vec{J}_\mu$  on the  $z$  axis), and  $v_\mu$  (vibrational quantum number), while the  $DM$ -molecule states—provided that the electrons are in the ground state—are labeled with the quantum numbers  $J_r$  (total orbital angular momentum),  $M_r$  (projection of  $\vec{J}_r$  on the  $z$  axis), and  $v_r$  (vibrational excitation of  $DM$ ):

$$\begin{aligned} \psi_{J_o M_o}^{(dd\mu)dee}(\vec{R}_c, \vec{\rho}_i) &= \sum_{M_\mu, M_r} C_{J_\mu M_\mu, J_r M_r}^{J_o M_o} \psi_{v_\mu J_\mu M_\mu}^{(dd\mu)} \\ &\times (\vec{R}_c) \psi_{v_r J_r M_r}^{(DM)}(\vec{\rho}_i). \end{aligned} \quad (7)$$

Here  $J_o, M_o$  are the total orbital angular momentum of the six-body molecular complex and its  $z$  axis projection, and  $C_{J_\mu M_\mu, J_r M_r}^{J_o M_o}$  is a Clebsch-Gordan coefficient. Substituting Eq. (7) into Eq. (6) leads to

$$\Delta E_{J_r J_o}^{(2)} = (-1)^{J_\mu + J_o + J_r} \begin{Bmatrix} J_r & 2 & J_r \\ J_\mu & J_o & J_\mu \end{Bmatrix} \bar{u}_{J_r J_\mu, J_r J_\mu}, \quad (8)$$

where  $\bar{u}$  stands for the following combination of the reduced matrix elements of  $Y_{2m}(\hat{\rho}_i)$  and  $Y_{2m}(\hat{R}_c)$ :

$$\begin{aligned} \bar{u}_{J_r J_\mu, J_r J_\mu} &= \sum_{ic} \langle J_r' \| Y_2(\hat{\rho}_i) \| J_r \rangle \\ &\times \langle J_\mu' \| Y_2(\hat{R}_c) \| J_\mu \rangle u_{ic}(J_r', J_\mu'; J_r, J_\mu), \end{aligned} \quad (9)$$

TABLE I. Values of  $\bar{u}_{J_r J_\mu, J_r J_\mu}$  (in meV) for the  $dd\mu$  and  $dt\mu$  muonic molecules (from Table III of Ref. [8]).

$J_r$	0	1	2	3
$dd\mu$	0	3.7	4.1	4.7
$dt\mu$	0	6.2	6.8	7.7

TABLE II. Hyperfine levels of the  $(dt\mu)_{11}$  muonic molecule, in meV (from Ref. [4]).

$J_a$	$F=0$		$F=1$	
	$S=1$	$S=0$	$S=1$	$S=2$
$S-1$	-142.19		44.48	49.95
$S$	-142.02		43.88	50.88
$S+1$	-142.12	40.85	44.36	50.60

$\bar{u}_{ic}(J'_r, J'_\mu; J_r, J_\mu)$  being the integral of  $u_{ic}^{(2)}$  [see Eq. (5)] over all of the arguments of  $\psi_{J_o M_o}^{(dd\mu)dee}$  but the unit vectors  $\hat{R}_c, \hat{\rho}_i$ . Note that Eq. (8) holds for *any* particular choice of the wave functions of  $dd\mu$  and  $DM$  in Eq. (7). According to Eq. (8), the quadrupole correction  $\Delta E^{(2)}$  depends explicitly on the  $DM$  molecule and six-body total orbital angular momenta  $J_r, J_o$ , and implicitly, through  $\bar{u}$ , on the value of the vibrational quantum number  $v_r$  ( $J_\mu, v_\mu$  having the fixed values  $J_\mu = v_\mu = 1$ ). Thus the quadrupole interaction  $U^{(2)}$  splits any of the unperturbed levels  $E_{[(dd\mu)_{11}dee]^*}^{(0)} = E_{(dd\mu)_{11}} + E_{(DM)_{J_r v_r}}$  of the system  $(dd\mu)dee$  to sublevels, labeled with the quantum number  $J_o, |J_r - J_\mu| \leq J_o \leq J_r + J_\mu$ . In slightly different notations the above results were presented in [7,8]; the values of  $\bar{u}$  from [8] are listed in Table I.

The situation changes if taking into account the spin of the muonic molecule constituents. Since the spin interactions  $U^{\text{hfs}}$  couple spin and orbital angular momenta, the classification of the energy levels of the isolated  $dd\mu$  requires additional quantum numbers: the total nuclear spin  $I$ , the total spin of the three-particle system,  $S$ , and the total angular momentum of the muonic molecule,  $J_a$ , obtained according to the coupling scheme  $\vec{I} = \vec{S}_{d_1} + \vec{S}_{d_2}$ ;  $\vec{S} = \vec{I} + \vec{S}_\mu$ ;  $\vec{J}_a = \vec{S} + \vec{J}_\mu$ . (The set of quantum numbers that is best suited for labeling the hyperfine structure levels of  $dt\mu$  involves the total spin  $F$

TABLE III. Hyperfine levels of the  $(dd\mu)_{11}$  muonic molecule, in meV (from Ref. [4]).

$J_a$	$S=1/2$	$S=3/2$
$S-1$		7.64
$S$	-15.90	7.93
$S+1$	-16.13	8.22

of the  $t\mu$  pair rather than  $I$ :  $\vec{F} = \vec{S}_t + \vec{S}_\mu$  [4].) Further on, the quadrupole interactions  $U^{(2)}$  of Eq. (4) couple the above momenta to  $\vec{J}_r$ , so that labeling the energy levels of the molecular complex requires two more quantum numbers:  $J_r$  and the total angular momentum of the six-body system  $J_t, \vec{J}_t = \vec{J}_a + \vec{J}_r$ . The lowest-order perturbative wave function of the molecular complex  $(dd\mu)dee$  therefore has the form

$$\psi^{ISJ_\mu J_a J_r J_t, M_t} = \sum_{I', S', J'_a} \beta_{I' S' J'_a}^{ISJ_\mu J_a J_r J_t} |I' S' J_\mu J'_a J_r J_t, M_t\rangle. \quad (10)$$

Here  $|ISJ_\mu J_a J_r J_t, M_t\rangle$  denote the basis vectors

$$|ISJ_\mu J_a J_r J_t, M_t\rangle = \sum_{M_\mu, \zeta, M_a, M_r} C_{J_a M_a, J_r M_r}^{J_t M_t} C_{J_\mu M_\mu, S \zeta}^{J_a M_a} |IS, \zeta\rangle \times \psi_{v_\mu J_\mu M_\mu}^{(dd\mu)} \psi_{v_r J_r M_r}^{(DM)}, \quad (11)$$

where  $|IS, \zeta\rangle$  is a constant spinor that satisfies  $(\vec{I}^2 - I(I+1))|IS, \zeta\rangle = [\vec{S}^2 - S(S+1)]|IS, \zeta\rangle = (S_z - \zeta)|IS, \zeta\rangle = 0$ . The constant amplitudes  $\beta_{I' S' J'_a}^{ISJ_\mu J_a J_r J_t}$  are to be calculated by diagonalizing the matrix of the perturbation Hamiltonian  $U^{\text{eff}} = U^{(2)} + U^{\text{hfs}}$ . The matrix elements of the spin interaction operator  $U^{\text{hfs}}$  in this basis are nothing but the three-body matrix elements of  $U^{\text{hfs}}$ , calculated in [4,5] and repeated here in Tables II and III:

$$\langle I' S' J'_\mu J'_a J'_r J'_t, M'_t | U^{\text{hfs}} | ISJ_\mu J_a J_r J_t, M_t \rangle = \delta_{J'_t J_t} \delta_{M'_t M_t} \delta_{J'_r J_r} \delta_{J'_a J_a} \langle I' S' J'_\mu J'_a, M'_a | U^{\text{hfs}} | ISJ_\mu J_a, M_a \rangle. \quad (12)$$

The matrix elements of  $U^{(2)}$  in the basis (11) have the form

$$\langle I' S' J'_\mu J'_a J'_r J'_t, M'_t | U^{(2)} | ISJ_\mu J_a J_r J_t, M_t \rangle = \delta_{S' S} \delta_{I' I} \delta_{J'_t J_t} \delta_{M'_t M_t} (-1)^{J_\mu + S - J_t - J'_r + J_a - J'_a} \times \sqrt{(2J'_a + 1)(2J_a + 1)} \begin{Bmatrix} J_\mu & 2 & J'_\mu \\ J'_a & S & J_a \end{Bmatrix} \begin{Bmatrix} J_r & 2 & J'_r \\ J'_a & J_t & J_a \end{Bmatrix} \bar{u}_{J'_r J'_\mu, J_r J_\mu}, \quad (13)$$

where  $\bar{u}_{J'_r J'_\mu, J_r J_\mu}$  was defined in Eqs. (8) and (9). [Remember that in the case of  $(dt\mu)dee$  the quantum number  $I$  should be replaced everywhere by  $F$ .] Similar to the spinless case, the nontrivial computational problem is the evaluation of  $\bar{u}$ ; fortunately this work has already been performed in [7,8]. The matrix elements of the perturbation potential  $U^{\text{eff}} = U^{(2)} + U^{\text{hfs}}$  in the basis (11) are now completely deter-

mined; what remains to be done is to calculate the eigenvalues and eigenvectors of  $\langle U^{\text{eff}} \rangle$ .

### III. NUMERICAL RESULTS AND DISCUSSION

The numerical values of the corrections  $\Delta E$  to the energy levels of the molecular complexes  $(dt\mu)_{11}dee$  and

$(dd\mu)_{11}dee$ , that result from both the spin interactions and the quadrupole terms in the expansion of the finite-size perturbation of Eq. (3), are presented—together with the state vectors  $\beta$ —in Tables IV–VI and VII–VIII, respectively. The abundant numerical data therein need the following comments.

The values of the state vectors  $\beta$  are needed for the calculation of the population of the numerous quantum states of the molecular complexes; the latter, in turn, becomes important when modeling the dependence of the muonic molecule resonant formation rate on the temperature. However, not all of the  $\beta$ 's are really needed: the quantum number  $F$  in the case of  $dt\mu$ , and  $S$  in the case of  $dd\mu$  are “pretty good” in the sense that the admixture of the other states in the representation of Eq. (11) does not exceed 0.1%. Omitting the unnecessary coefficients  $\beta$  significantly reduced their size. The levels with different values of the DM molecule orbital angular momentum  $J_r$  have been kept separate, since the population of the rotational excitations of DM depends on the experimental conditions (temperature and pressure).

The quadrupole corrections preserve the general form of the hyperfine structure of  $(dt\mu)_{11}$  and  $(dd\mu)_{11}$  but increase very significantly the “width” of its components. For instance, the three hyperfine states with  $F=0$ ,  $S=1$ , and

TABLE IV. Quadrupole and hyperfine corrections  $\Delta E_{FSJ_a J_r J_t}$  to the energy values of the  $(dt\mu)_{11}dee$ , in meV, and state vectors in the representation (11). Eigenstates with  $F=0$ .

$J_r$	$\Delta E$ (meV)	$FSJ_a J_t$	$\beta_{F'S'J'_a}$ for $(F'S'J'_a)=$		
			(010)	(011)	(012)
1	-143.2	0121	-0.612	0.465	0.639
	-143.1	0122	0.0	0.471	-0.882
	-143.1	0110	0.0	1.000	0.0
	-141.9	0123	0.0	0.0	1.000
	-141.9	0101	0.725	0.652	0.220
	-141.8	0112	0.0	0.882	0.471
	-140.0	0111	-0.315	0.599	-0.736
	-143.2	0122	0.601	-0.265	-0.754
	-143.1	0123	0.0	0.549	-0.836
	-143.1	0111	0.0	0.855	0.518
2	-141.8	0124	0.0	0.0	1.000
	-141.8	0113	0.0	-0.836	-0.549
	-141.8	0102	0.699	0.631	0.336
	-141.1	0121	0.0	0.518	-0.855
	-141.1	0120	0.0	0.0	1.000
	-141.1	0112	0.387	-0.729	0.564
	-143.2	0123	0.598	-0.187	-0.779
	-143.1	0124	0.0	-0.585	0.811
	-143.1	0112	0.0	0.801	0.598
	-141.8	0125	0.0	0.0	1.000
3	-141.8	0103	0.698	0.598	0.392
	-141.7	0114	0.0	-0.811	-0.585
	-141.3	0122	0.0	0.598	-0.801
	-141.3	0121	0.0	0.0	1.000
	-141.3	0113	-0.393	0.779	-0.488

TABLE V. Quadrupole and hyperfine corrections  $\Delta E_{FSJ_a J_r J_t}$  to the energy values of the  $(dt\mu)_{11}dee$ , in meV, and state vectors in the representation (11). Eigenstates with  $F=1, S\leq 1$ .

$J_r$	$\Delta E$	$FSJ_a J_t$	$\beta_{F'S'J'_a}$ for $(F'S'J'_a)=$				
			(101)	(110)	(111)	(112)	(121)
1	39.8	1011	0.997	-0.003	0.056	0.013	0.047
	41.1	1012	-0.994	0.0	-0.093	0.019	-0.056
	42.6	1110	-0.634	0.0	-0.767	0.0	-0.095
	43.1	1010	0.771	0.0	-0.637	0.0	-0.003
	43.2	1122	-0.078	0.0	0.652	-0.752	0.051
	43.2	1111	0.047	0.454	-0.630	-0.626	-0.052
	44.2	1112	0.061	0.0	-0.746	-0.659	-0.072
	44.4	1101	0.034	-0.798	-0.598	0.031	-0.061
	44.6	1123	0.0	0.0	0.0	1.000	0.0
	46.3	1121	0.021	0.396	-0.480	0.778	-0.075
	39.8	1012	-0.997	0.001	-0.053	-0.007	-0.047
	41.1	1013	-0.993	0.0	-0.099	0.024	-0.056
	41.9	1011	-0.977	0.0	-0.193	-0.057	-0.066
	43.0	1111	-0.205	0.0	0.883	0.417	0.059
	43.1	1113	-0.091	0.0	0.709	-0.697	0.054
	2	43.3	1122	0.030	0.505	-0.408	-0.759
44.4		1112	-0.046	0.586	0.803	-0.047	0.082
44.4		1123	0.056	0.0	-0.692	-0.716	-0.068
44.7		1124	0.0	0.0	0.0	1.000	0.0
45.3		1121	-0.033	0.0	0.418	-0.906	0.047
45.3		1102	-0.021	-0.634	0.417	-0.648	0.051
45.4		1120	0.0	0.0	0.0	1.000	0.0
39.8		1013	-0.997	0.001	-0.053	-0.005	-0.047
41.2		1014	-0.993	0.0	-0.103	0.026	-0.057
41.7		1012	0.985	0.0	0.156	0.047	0.063
3	43.0	1112	-0.164	0.0	0.858	0.482	0.060
	43.1	1114	0.097	0.0	-0.733	0.671	-0.056
	43.3	1123	-0.022	-0.524	0.300	0.796	0.025
	44.4	1113	-0.051	0.446	0.888	-0.045	0.091
	44.4	1124	0.054	0.0	-0.666	-0.741	-0.066
	44.7	1125	0.0	0.0	0.0	1.000	0.0
	45.0	1122	0.038	0.0	-0.481	0.874	-0.052
	45.1	1103	-0.017	-0.725	0.328	-0.603	0.039
	45.2	1121	0.0	0.0	0.0	1.000	0.0

$J_a=0,1,2$  lie within less than 0.2 meV while the quadrupole interactions disperse them to nearly 3.5 meV; similar dispersions occur for the other hyperfine levels too. As a result, formation rates will be much smoother functions of the temperature with much less pronounced resonant peaks than originally predicted.

It is essential to underline that the above results were obtained in first-order of perturbation theory, and there may be doubts about the reliability of some of the quantitative predictions. One source of inaccuracy is the uncertainty of the wave function of the DM molecule in the neighborhood of the nucleus  $M$ ; through Eqs. (8) and (9) it affects the predicted values of  $\Delta E$  linearly. However, more importantly, as demonstrated in a very general form in [9], in the limit of

TABLE VI. Quadrupole and hyperfine corrections  $\Delta E_{FSJ_a J_r J_t}$  to the energy values of the  $(dt\mu)_{11}dee$ , in meV, and state vectors in the representation (11). Eigenstates with  $F=1, S=2$ .

$J_r$	$\Delta E$	$FSJ_a J_t$	$\beta_{F'S'J'_a}$ for $(F'S'J'_a)=$				
			(111)	(112)	(121)	(122)	(123)
	49.2	1212	0.083	0.009	-0.804	0.152	0.567
	49.5	1211	0.092	-0.019	-0.791	0.603	0.0
	49.6	1233	0.0	-0.005	0.0	-0.495	0.869
	50.2	1210	-0.076	0.0	0.995	0.0	0.0
1	50.6	1221	0.059	-0.021	-0.599	-0.798	0.0
	50.8	1222	0.038	-0.002	-0.481	-0.722	-0.495
	50.8	1234	0.0	0.0	0.0	0.0	1.000
	51.0	1223	0.0	-0.007	0.0	-0.869	-0.495
	52.7	1223	0.021	0.005	-0.334	0.675	-0.658
	49.3	1212	0.090	-0.007	-0.781	0.331	0.520
	49.3	1213	-0.078	-0.009	0.763	0.031	-0.639
	49.5	1221	-0.062	0.005	0.682	-0.635	-0.356
	49.7	1234	0.0	-0.006	0.0	-0.588	0.809
	49.8	1220	0.0	-0.012	0.0	-1.000	0.0
	50.5	1211	0.059	-0.015	-0.724	-0.620	-0.294
2	50.7	1222	-0.054	0.010	0.599	0.592	0.535
	50.8	1233	0.043	0.001	-0.550	-0.473	-0.686
	50.9	1235	0.0	0.0	0.0	0.0	1.000
	51.1	1224	0.0	0.007	0.0	0.809	0.588
	51.7	1232	-0.010	-0.004	0.131	-0.735	0.666
	51.7	1223	-0.023	-0.008	0.322	-0.880	0.347
	51.7	1231	-0.002	-0.003	0.034	-0.460	0.887
	49.3	1213	0.090	-0.005	-0.778	0.231	0.576
	49.3	1214	0.076	0.008	-0.750	-0.105	0.647
	49.5	1212	-0.066	0.006	0.698	-0.524	-0.482
	49.7	1235	0.0	-0.007	0.0	-0.633	0.774
	49.8	1221	0.0	0.011	0.0	0.924	0.383
	50.6	1222	-0.057	0.013	0.708	0.548	0.439
	50.7	1233	0.054	-0.007	-0.606	-0.468	-0.640
3	50.8	1234	-0.047	-0.002	0.592	0.305	0.744
	50.9	1236	0.0	0.0	0.0	0.0	1.000
	51.1	1225	0.0	-0.006	0.0	-0.774	-0.633
	51.4	1230	0.0	0.0	0.0	0.0	1.000
	51.5	1224	0.020	0.008	-0.275	0.946	-0.168
	51.5	1231	0.0	0.003	0.0	0.383	-0.924
	51.5	1232	-0.002	-0.005	0.034	-0.651	0.758
	51.6	1223	-0.009	-0.006	0.122	-0.853	0.507

zero binding energy the monopole and quadrupole effects, calculated in first-order of perturbation theory, are exactly canceled by the second-order dipole corrections. This mainly affects the weakly bound state  $(dt\mu)_{11}$  with binding energy of only 0.000 24 (in a.u.). Indeed, the precise numerical results of [11] showed for the simplified model of the atom  $(dt\mu)_{11}e$  that the monopole and dipole corrections cancel each other to about 90%; unfortunately the quadrupole effects are lost in this model. As a result, the size of the broadening of the hyperfine structure levels may be smaller than

TABLE VII. Quadrupole and hyperfine corrections  $\Delta E_{ISJ_a J_r J_t}$  to the energy values of the  $(dd\mu)_{11}dee$ , in meV, and state vectors in the representation of Eq. (11). States with  $S=1/2$ .

$J_r$	$\Delta E$ (meV)	$S$	$J_a$	$J_t$	$\beta_{1S'J'_a}$ for $(S'J'_a)=$	
					(1/2,1/2)	(1/2,3/2)
	-16.7	1/2	3/2	3/2	-0.320	0.947
	-16.6	1/2	1/2	1/2	0.780	0.626
1	-16.0	1/2	3/2	5/2	0.0	1.000
	-15.8	1/2	1/2	3/2	-0.947	-0.320
	-14.8	1/2	3/2	1/2	-0.626	0.780
	-16.7	1/2	3/2	5/2	0.379	-0.925
	-16.6	1/2	3/2	3/2	0.639	0.769
	-16.0	1/2	3/2	7/2	0.0	1.000
2	-15.8	1/2	1/2	5/2	0.925	0.379
	-15.5	1/2	3/2	1/2	0.0	1.000
	-15.4	1/2	1/2	3/2	-0.769	0.639
	-16.7	1/2	3/2	5/2	0.590	0.807
	-16.7	1/2	3/2	7/2	0.408	-0.913
	-15.9	1/2	3/2	9/2	0.0	1.000
3	-15.7	1/2	1/2	7/2	0.913	0.408
	-15.6	1/2	3/2	3/2	0.0	1.000
	-15.5	1/2	1/2	5/2	-0.807	0.590

TABLE VIII. Quadrupole and hyperfine corrections  $\Delta E_{ISJ_a J_r J_t}$  to the energy values of the  $(dd\mu)_{11}dee$ , in meV, and state vectors in the representation of Eq. (11). States with  $S=3/2$ .

$J_r$	$\Delta E$ (meV)	$S$	$J_a$	$J_t$	$\beta_{1S'J'_a}$ for $(S'J'_a)=$		
					(3/2,1/2)	(3/2,3/2)	(3/2,5/2)
	7.2	3/2	3/2	1/2	-0.571	0.821	0.0
	7.3	3/2	1/2	3/2	0.818	-0.243	-0.520
	7.5	3/2	5/2	5/2	0.0	-0.703	0.711
1	7.8	3/2	1/2	1/2	0.821	0.571	0.0
	8.0	3/2	3/2	3/2	0.0	-0.711	-0.703
	8.3	3/2	5/2	7/2	0.0	0.0	1.000
	9.3	3/2	5/2	3/2	0.330	-0.542	0.773
	7.3	3/2	3/2	1/2	0.0	0.966	0.260
	7.3	3/2	1/2	3/2	-0.701	0.556	0.446
	7.3	3/2	1/2	5/2	0.821	-0.038	-0.570
	7.5	3/2	3/2	7/2	0.0	0.763	-0.646
	7.9	3/2	3/2	3/2	0.695	0.672	0.255
2	8.1	3/2	3/2	5/2	0.380	0.780	0.496
	8.2	3/2	5/2	7/2	0.0	-0.646	-0.763
	8.4	3/2	5/2	9/2	0.0	0.0	1.000
	8.6	3/2	5/2	5/2	-0.426	0.624	-0.655
	8.7	3/2	5/2	3/2	0.158	-0.489	0.858
	8.8	3/2	5/2	1/2	0.0	0.260	-0.966
	7.3	3/2	1/2	5/2	-0.734	0.461	0.498
	7.3	3/2	1/2	7/2	0.816	0.043	-0.577
	7.4	3/2	3/2	3/2	0.0	0.930	0.366
	7.4	3/2	3/2	9/2	0.0	0.788	-0.616
	8.0	3/2	3/2	5/2	0.649	0.691	0.317
	8.2	3/2	3/2	7/2	0.342	0.768	0.541
3	8.3	3/2	5/2	9/2	0.0	-0.616	-0.788
	8.4	3/2	5/2	7/2	-0.466	0.639	-0.612
	8.4	3/2	5/2	11/2	0.0	0.0	1.000
	8.6	3/2	5/2	5/2	-0.198	0.556	-0.807
	8.7	3/2	5/2	1/2	0.0	0.0	1.000
	8.7	3/2	5/2	3/2	0.0	0.366	-0.930

the estimates obtained here in first-order of perturbation theory, although qualitatively they should remain unchanged. As for  $dd\mu$ , we expect that the values of the quadrupole splitting of the hyperfine structure levels, reported here, will not be significantly changed by the second-order contributions, since the binding energy of  $(dd\mu)_{11}$  is quite larger [1].

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- [1] L. I. Ponomarev, *Contemp. Phys.* **31**, 219 (1991).  
[2] L. Bracci and G. Fiorentini, *Phys. Rep.* **86**, 175 (1982).  
[3] A. Scrinzi, P. Kammel, J. Zmeskal, W. H. Breunlich, J. Marton, M. P. Faifman, L. I. Ponomarev, and T. A. Strizh, *Phys. Rev. A* **47**, 4691 (1993).  
[4] G. Aissing, D. Bakalov, and H. J. Monkhorst, *Phys. Rev. A* **42**, 116 (1990).  
[5] D. Bakalov and V. I. Korobov, *JINR Rapid Communications* **2**, 15 (1989).  
[6] D. Bakalov and V. S. Melezhik, *JINR Report No. P4-81-835*, Dubna, 1981 (unpublished).  
[7] M. R. Harston, I. Shimamura, and M. Kamimura, *Phys. Rev. A* **45**, 94 (1992).  
[8] M. R. Harston, S. Hara, Y. Kino, I. Shimamura, H. Sato, and M. Kamimura, *Phys. Rev. A* **56**, 2685 (1997).  
[9] L. I. Men'shikov, *Yad. Fiz.* **42**, 1449 (1985) [*Sov. J. Nucl. Phys.* **42**, 918 (1985)].  
[10] D. Bakalov and V. S. Melezhik, *JINR Report No. P4-85-952*, Dubna, 1985 (unpublished).  
[11] A. Scrinzi and K. Szalewicz, *Phys. Rev. A* **39**, 4983 (1989).