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Enhancement of the electric dipole moment of the electron in the YbF molecule

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A semiempirical calculation of the P-odd and P,T-odd interactions in the YbF molecule is made. As a result, the corresponding constants of the effective spin-rotational Hamiltonian of the molecule are obtained. In comparison with atoms, both P-odd and P,T-odd interactions are enhanced approximately 10^3 times. For example, the electric dipole moment of the valence electron feels an internal molecular electric field of 3×10^{10} V/cm. This field is directed along the molecular axis and can be oriented by an external field $\sim 10^4$ V/cm.

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I. INTRODUCTION

In past years impressive results were achieved in the experimental investigation of the violation of inversion symmetry (P) and time-reversal invariance (T) in atoms and molecules. Experimental upper limits on the permanent electric dipole moments (EDM's) of atoms and molecules caused very stringent bounds on fundamental P,T-odd interactions [1]. Experiments with the paramagnetic atoms Cs [2] and Tl [3] gave best upper limit on the EDM of the electron which is now close to the important for the theory of supersymmetry region of $10^{-28}e$ cm. In the same time, experiments with the diamagnetic mercury atom [4] and TlF molecule [5] gave important information on the P,T-odd nuclear forces.

Further progress is possible either by improving the accuracy of measurements, which is already extremely high, or by making experiments with new objects where enhancement of the P,T-odd interactions is larger. As was pointed out in a number of papers [6–11], enhancement factors for P-odd and P,T-odd interactions are several orders of magnitude larger in diatomic paramagnetic molecules, than in atoms. This is true for interactions which depend on the spin of the electron. For example, additional enhancement of the EDM of the electron can be explained by the strong molecular electric field which effects the unpaired electron. This internal field can be oriented along much smaller external electric field. Largest internal fields can be expected for the polar MX molecules, where M is a heavy metal and X is a halogen. Some of these molecules were examined theoretically and largest enhancement was found to be for the HgF molecule [12,13].

At present, in Yale University there is significant progress in formation of the beam of the YbF molecule for the EDM experiment [14]. In this paper we are reporting results of semiempirical calculation for this molecule. For the given EDM of the electron, observable frequency shift for the YbF molecule appears to be only three times smaller than for the HgF molecule and roughly 600 times larger than for Tl. In this paper we use the method developed in [12]. It is based on the close connection between matrix elements of the P,T-odd interactions with matrix elements of magnetic hyperfine interaction. The latter can be measured by means of the electron spin resonance. Results obtained by this method for the HgF molecule are in good agreement with numerical calculations [13].

In the next two sections we give a brief description of the method and determine parameters of the wave function (WF) which are necessary for calculations of the P,T-odd matrix elements. Then, in Secs. IV and V our main results are given in a form of parameters of the spin-rotational Hamiltonian. Discussion follows in Sec. VI.

II. METHOD

In the YbF molecule there is a single unpaired electron out of the strongly polarized core with positive ytterbium and negative fluorine. This unpaired electron is of primary importance for our consideration. Indeed, coupled electrons do not contribute to the hyperfine constants as well as to the P-odd and P,T-odd constants discussed in this paper.

The WF of the unpaired electron for diatomic molecules is the eigenfunction of the projection of the electron angular momentum $\mathbf{j}$ on the molecular axis. This quantum number is called ω. As far as the sum of ω_i for the coupled electrons is zero, then $\omega = \Omega$, where Ω is projection of the total angular momentum of all electrons $\mathbf{J_e}$. In the nonrelativistic approximation quantum number λ (Λ) for the projection of the orbital angular momentum can be defined as well. According to this classification, an unpaired electron of the YbF molecule is in the state with $\lambda = 0, |\omega| = 1/2$ [15]. In this section we assume that λ is a good quantum number. The accuracy of this assumption is discussed in the following section.

In the vicinity of the nucleus of the ytterbium atom WF can be expanded in spherical waves

$$|\lambda, \omega\rangle = \sum_{l,j(=l\pm1/2)} C_{l,j} |l, j, \omega\rangle \quad . \tag{1}$$

Here $|l, j, \omega\rangle$ are normalized four-component spherical waves:

$$|l,j,\omega\rangle = \begin{pmatrix} f_{l,j}Y^{l}_{j,\omega} \\ ig_{l,j}Y^{l'}_{j,\omega} \end{pmatrix} \quad , \tag{2}$$

where f and g are radial functions, $Y^{l}_{j,\omega}$ is the spherical spinor, and $l' = 2j - l$.

Though in general functions f and g can be found only by solving the molecular Schrödinger equation, for the small distances they are defined from much simpler equations up to the normalization constant [16]. It follows from the fact that at small distances potential of the nucleus Z/r (atomic units are used throughout) dominates and is large in comparison with the energy of the electron. The solutions of the Dirac equation with this potential are expressed in terms of Bessel functions:

$$\begin{pmatrix} f_{l,j} \\ g_{l,j} \end{pmatrix} = \frac{k}{|k|}\frac{a_l}{Z^{1/2}r}\begin{pmatrix} (\gamma+k)J_{2\gamma}(x) - \frac{x}{2}J_{2\gamma-1}(x) \\ \alpha Z J_{2\gamma}(x) \end{pmatrix} \quad , \tag{3}$$

where

$$x = \sqrt{8Zr} \quad , \tag{4}$$

$$\gamma = \sqrt{(j+1/2)^2 - \alpha^2 Z^2} \quad , \tag{5}$$

$$k = (l-j)(2j+1) \quad . \tag{6}$$

Normalization coefficients a_l are of the order of unity and are determined by matching with the solution of the nonrelativistic Schrödinger equation in the outer region. With good accuracy they are independent on j.

Not all coefficients $C_{l,j}$ in Eq. (1) are independent. Indeed, for each $l \neq 0$ a pair of functions with $j = l - 1/2$ and $j = l + 1/2$ on the large distances have to form nonrelativistic function $|l, m_l = \lambda, \omega\rangle$. This means that, for $\lambda = 0$ and $\omega = 1/2$, the following relations hold true:

$$C_{1,3/2} = -\sqrt{2}C_{1,1/2}, \; C_{2,5/2} = -\sqrt{3/2}C_{2,3/2}, \text{ etc.} \tag{7}$$

One can see from Eq. (3) that for $r \to 0$

$$\begin{pmatrix} f_{l,j} \\ g_{l,j} \end{pmatrix} = r^{\gamma-1}\begin{pmatrix} f_{l,j,0} \\ g_{l,j,0} \end{pmatrix} \quad . \tag{8}$$

Thus, for small r only several first terms of the series (1) are important. It follows from Eqs. (1)–(3) and (7) that in this region molecular WF is defined by the products

$$\sigma_s = C_{0,1/2}a_0, \; \sigma_p = C_{1,1/2}a_1, \; \sigma_d = C_{2,3/2}a_2, \text{ etc.}, \tag{9}$$

where coefficients a_l are from Eq. (3).

Using Eq. (3) we now can express matrix elements of all operators which depend mainly on the WF of the unpaired electron in the vicinity of the heavy nucleus in terms of few first constants σ_i. Such operators must be (a) singular at the origin and (b) depend on electron spin (second feature is necessary to eliminate contributions of the coupled electrons). Magnetic hyperfine interaction and interaction of the EDM of the electron with the molecular field are the examples of the operators of this type. P,T-odd electron-nucleus interactions caused by the exchange of some heavy particles, such as Z bosons, are even more singular. They can be treated as contact interactions in atomic scale. It means that formula (3) must be improved to take into account the finite size of the nucleus. It is known that, within 15% accuracy, this can be done by cutting WF (3) at the nuclear surface [16].

The hyperfine structure of the diatomic molecule is defined by the axial tensor **A** with two independent parameters:

$$\begin{aligned} A &= \frac{A_{\parallel} + 2A_{\perp}}{3} \\ &= \frac{4}{3}C^2_{-1}h_{-1,-1} + \frac{4}{9}C^2_1 h_{1,1} - \frac{8\sqrt{2}}{9}C_1C_{-2}h_{1,-2} \\ &\quad + \frac{8}{9}C^2_{-2}h_{-2,-2} + \frac{8}{15}C^2_2 h_{2,2} \\ &\quad - \frac{8\sqrt{6}}{15}C_2C_{-3}h_{2,-3} + \frac{4}{5}C^2_{-3}h_{-3,-3} \quad , \end{aligned} \tag{10}$$

$$\begin{aligned} A_d &= \frac{A_{\parallel} - A_{\perp}}{3} \\ &= -\frac{8}{9}C^2_1 h_{1,1} - \frac{2\sqrt{2}}{9}C_1C_{-2}h_{1,-2} - \frac{8}{45}C^2_{-2}h_{-2,-2} \\ &\quad - \frac{8}{15}C^2_2 h_{2,2} - \frac{2\sqrt{6}}{15}C_2C_{-3}h_{2,-3} \\ &\quad - \frac{8}{35}C^2_{-3}h_{-3,-3} \quad , \end{aligned} \tag{11}$$

where we used single index k from Eq. (6) instead of l, j in (1) and

$$h_{i,j} = -\frac{g_n\alpha}{2m_p}\int_0^\infty (f_i g_j + g_i f_j)dr \quad . \tag{12}$$

Here g_n is G factor of the nucleus and m_p is the proton mass. For functions (3) these integrals are calculated analytically, and using (7) and (9) we obtain

$$\begin{gathered} 31170\sigma_s^2 - 1330\sigma_p^2 - 50\sigma_d^2 = 7617, \\ 5510\sigma_p^2 + 370\sigma_d^2 = 102\,. \end{gathered} \tag{13}$$

In the right-hand side of these equations we put experimental values for A and A_d in MHz measured in Ref. [17] by the electron-spin-resonance method.

It is seen from Eqs. (13) that contributions of the spherical waves rapidly decrease as the orbital angular momentum increases. On this ground we can neglect contributions of waves with $l > 2$. But the role of the d wave is questionable, especially in the second Eq. (13). To be sure that contribution of d wave is negligible as well, we have to discuss the possible range of parameters σ_i.

As a rough estimate, we can associate spherical waves of the expansion (1) with the valence atomic orbitals of ytterbium. Then, the semiclassical values can be used for the normalization coefficients a_l in Eqs. (3) and (9),

$$a_l^2 \approx \frac{2\epsilon_l^{3/2}}{Z_c} \quad , \tag{14}$$

where ϵ_l is the bonding energy and Z_c is the core charge. Taking into account that Yb is positively charged ($Z_c =$

2) and using Hartree-Fock-Dirac values for ϵ_l, we obtain

$$a_0^2 \approx 0.38; \quad a_1^2 \approx 0.23; \quad a_2^2 \approx 0.24 \quad . \tag{15}$$

Coefficients $C_{l,j}$ are normalized to unity. From Eq. (15) we see that $a_l^2 \approx 0.3$ and together with (7) it results in approximate normalization condition

$$\sigma_s^2 + 3\sigma_p^2 + \frac{5}{2}\sigma_d^2 \leq 0.3 \sum_{l,j} C_{l,j}^2 = 0.3 \quad . \tag{16}$$

We have to find the solution of Eqs. (13) which meets this condition. For such solution $\sigma_d^2 < 0.02$ and d wave can be neglected in both Eqs. (13). Then

$$\sigma_s^2 = 0.24, \quad \sigma_p^2 = 0.019 \quad . \tag{17}$$

A bit more detailed analysis shows that the error from neglecting d wave must be less then 5% for σ_p^2 and even smaller for σ_s^2.

To calculate matrix elements of the P,T-odd operators we have to fix the sign of the product $\sigma_s\sigma_p$. Using the ionic model of the molecule one can easily see that interference of s and p waves has to be destructive on the inner side and constructive on the outer side of the metal ion. If phases are fixed so that $a_l > 0$ and quantization axis is directed from Yb to F, then, taking into account that s orbital has one extra node, we come to a conclusion that $\sigma_s\sigma_p < 0$.

So, the final result of this section is

$$\sigma_s\sigma_p = -0.067 \quad . \tag{18}$$

Let us repeat the main steps of the treatment made above.

(1) Existence of the quantum number λ reduces the number of independent coefficients in expansion (1). Role of the spin-orbit interaction which mixes levels with different λ is discussed in the next section of the paper.

(2) Rapid decrease of the contributions of higher spherical waves to the hyperfine constants together with the normalization condition for the expansion coefficients means that only s and p waves are important for the hyperfine structure.

(3) Experimental values of the hyperfine constants A and A_d determine σ_s and σ_p up to the signs.

(4) Simple ionic-bond model of the molecule allows one to fix the sign of the product of these constants.

Let us try to compare our results with the *ab initio* calculations [18]. There are two reasons why it isn't easy to do. First, our method does not allow us to determine coefficients $C_{l,j}$ with the same accuracy as coefficients σ_i. Second, spherical waves from Eq. (2) can be only roughly associated with the valence orbitals of the ytterbium. Nevertheless, with the help of Eqs. (7), (15), and (17) we have the following estimates for the weights of s and p orbitals: $C_{0,1/2}^2 \approx 0.63, C_{1,1/2}^2 + C_{1,3/2}^2 \approx 0.23$. These numbers have to be compared with 0.84 and 0.15 from Ref. [18].

III. SPIN-ORBIT INTERACTION

Spin-orbit interaction mixes states with the same ω but different λ and determines splittings of the sublevels with $\omega = \lambda \pm 1/2$ of the state λ. The main admixture to the ground state can be expected from the first excited state with $\lambda = 1$ and energy 18 000 cm^{-1} [15]. Comparison of the spin-orbital splitting for substates with $\omega = 1/2$ and $\omega = 3/2$ of this state which is equal to 1370 cm^{-1} with that for the $6p$ state of Yb$^+$ shows that the $6p$ orbital contributes about 60% to the $\lambda = 1$ state. Above, we estimated contribution of the $6p$ orbital to the ground state at approximately 23%. Then, spin-orbital mixing of these states

$$\begin{aligned} \xi &= \frac{\langle \lambda = 1, \omega | H_{\rm SO} | \lambda = 0, \omega \rangle}{E_0 - E_1} \\ &= (0.6 \cdot 0.23)^{1/2} \frac{\langle 6p, \lambda = 1, \omega | H_{\rm SO} | 6p, \lambda = 0, \omega \rangle}{18000 \text{ cm}^{-1}} \\ &\approx -0.03 \quad . \end{aligned} \tag{19}$$

An alternative way to calculate ξ was used in [12]. It is based on the influence of the spin-orbital mixing on the electronic G tensor. One can find ξ from the experimental values for $G_\parallel$ and $G_\perp$ measured in [17]. This method gives an even smaller value for ξ, but there is uncertainty caused by the unknown contribution of the d wave, which is not suppressed in this case.

Both methods prove that λ is a good quantum number in a sense that the accuracy of Eq. (7) is about 3% or better. At this point we want to stress that relativistic effects are actually much more important than one can expect from Eq. (19). Indeed, though (7) holds true, for the small distances from the origin two waves with the same l but different j become quite different. As it follows from Eq. (8), the wave with $j = l - 1/2$ strongly dominates in this region. For this reason, for example, selection rules associated with quantum number λ do not hold for the singular operators.

IV. *P*- AND *T*-ODD INTERACTIONS

In an experimental search for P and T violation in atoms and molecules, the measured quantity is the EDM of a system correlated with its angular momentum. In the case of YbF one can look for the EDM correlated with the nuclear spin $\mathbf{I}$ of the ytterbium atom and for the EDM correlated with the electron angular momentum $\mathbf{J_e}$. For the former there is no advantage in comparison with experiment on the TlF molecule [5]. The latter has to be compared with atomic experiments on Tl [3] and Cs [2], where enhancement factors are much smaller. So, interactions which cause this type of EDM are of particular interest.

First of all, it is interaction of the EDM of the electron d_e with the molecular electric field $(-\nabla\phi)$ [16]:

$$H_d = 2d_e \begin{pmatrix} 0 & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} (-\nabla\phi) \quad . \tag{20}$$

Another one is the electron-nuclear scalar interaction

$$H_S = i\frac{G\alpha}{\sqrt{2}} Zk_S \gamma_0 \gamma_5 n(\mathbf{r}) \quad , \tag{21}$$

where G is the Fermi constant, γ_i are the Dirac matrices, and $n(\mathbf{r})$ is the nuclear density normalized to unity. Dimensionless factor Zk_S is the sum for all nucleons: $Zk_S = Zk_{S,p} + Nk_{S,n}$. Current status of different models of the CP violation and corresponding predictions for d_e and k_S are discussed in [1].

One more source of P and T violation is the interaction of the nuclear magnetic quadrupole moment M with the molecular magnetic field [19]. This interaction depends on both $\mathbf{I}$ and $\mathbf{J_e}$:

$$\begin{aligned} H_M &= -\frac{M}{4I(2I-1)} T_{i,k} \frac{3}{2r^5} \gamma_0 \gamma_j r_l (\epsilon_{j,l,i} r_k + \epsilon_{j,l,k} r_i) \quad , \\ T_{i,k} &= I_i I_k + I_k I_i - \frac{2}{3} I(I+1)\delta_{i,k} \quad . \end{aligned} \tag{22}$$

One can also look for P-odd, T-even interaction of the nuclear anapole moment with valence electron:

$$H_A = \frac{G\alpha}{\sqrt{2}} k_A \mathbf{I} \gamma_0 \gamma n(\mathbf{r}) \quad , \tag{23}$$

where k_A is the anapole moment constant for the ytterbium nucleus [16]. This interaction is interesting because at present there are no reliable measurements of the anapole constants k_a. However, in [20], the needed accuracy of the experiment was almost reached for cesium. For the YbF molecule enhancement is several orders of magnitude larger.

With the help of formula (3) electron matrix elements of the operators (20)–(23) are easily expressed in terms of the constants σ_i. For example,

$$\langle \lambda, \omega | H_d | \lambda, \omega \rangle = W_d d_e \omega \quad , \tag{24}$$

$$\begin{aligned} W_d &= 8 \sum_i C_{-i} C_i \int_0^\infty g_{-i} g_i \frac{d\phi}{dr} r^2 dr \\ &= 16\alpha^2 Z^3 \left(\frac{\sigma_s \sigma_p}{\gamma_{1/2}(4\gamma_{1/2}^2 - 1)} \right. \\ &\quad \left. - \frac{\sqrt{2}\sigma_p \sigma_d}{\gamma_{3/2}(4\gamma_{3/2}^2 - 1)} + \ldots \right) \\ &= 174\sigma_s\sigma_p - 15\sigma_p\sigma_d + \cdots = -11.7 \quad , \end{aligned} \tag{25}$$

where γ_j is defined in (5). Again, as for the hyperfine structure, contributions of waves with $l > 1$ are strongly suppressed.

Let us note here, that $\frac{1}{2}W_d$ is simply the averaged electric field on the electron in the state $|\lambda, \omega\rangle$ [averaged in the sense of Eq. (20)]. From Eq. (25) this field is equal to 3×10^{10} V/cm. This has to be compared with approximately 500×100 kV/cm $= 5 \times 10^7$ V/cm for Tl [3], 120×4 kV/cm $= 5 \times 10^5$ V/cm for Cs [2] and 1×10^{11} V/cm for HgF [12,13].

Other matrix elements are calculated in a similar way. Numerical values are given in the following section.

V. SPIN-ROTATIONAL HAMILTONIAN

In the preceding section we discussed electron matrix elements. It was shown that the unpaired electron feels the field $\sim 3 \times 10^{10}$ V/cm. But this field is directed along the molecular axis and for a rotating molecule is averaged to zero. One needs to apply an external electric field to polarize the molecular axis along it. Total polarization takes place in the field $\sim 10^3$–10^4 V/cm.

Quantitative description of the molecular dynamics in the external fields can be made with the help of an effective spin-rotational Hamiltonian. This Hamiltonian is defined in the subspace of spin and rotational degrees of freedom. It is convenient to introduce effective electron spin $\mathbf{S}$, $S = 1/2$ defined in the subspace of two degenerate states $\omega = \pm 1/2$. Then, as was shown in [21,13],

$$\begin{aligned} H_{\mathrm{SR}} &= B\mathbf{N}^2 + \gamma \mathbf{S} \cdot \mathbf{N} + \mathbf{S} \cdot \mathbf{A} \mathbf{I} + \mathbf{S} \cdot \mathbf{A}' \mathbf{I}' \\ &\quad + \mu_0 \mathbf{S} \cdot \mathbf{G} \mathbf{B} - D\mathbf{n} \cdot \mathbf{E} \\ &\quad + W_A k_A \mathbf{n} \times \mathbf{S} \cdot \mathbf{I} + (W_S k_S + W_d d_e)\mathbf{S} \cdot \mathbf{n} \quad . \end{aligned} \tag{26}$$

In this expression $\mathbf{I}$ and $\mathbf{I}'$ are the spins of Yb and F nuclei; $\mathbf{N}$ is the rotational angular momentum; B and γ are the rotational and the spin-doubling constants. Tensors $\mathbf{A}$ and $\mathbf{A}'$ correspond to the hyperfine structures on two nuclei. Interactions with the external fields $\mathbf{B}$ and $\mathbf{E}$ are described by G tensor and constant D; μ_0 is the Bohr magneton; $\mathbf{n}$ is the unit vector directed along the molecular axis from Yb to F. Terms with the constants W_A, W_S, and W_d in (26) correspond to the anapole moment, the scalar P,T-odd interaction and to the EDM of the electron.

Parameters of H_{SR} are known from the experiments for the isotopes ^{171}Yb and ^{19}F [15,17]:

$$\begin{aligned} B &= 7237 \text{ MHz}; \\ A_{\parallel} &= 7822 \text{ MHz}, \quad A_{\perp} = 7513 \text{ MHz} \quad (I = 1/2); \\ A'_{\parallel} &= 220 \text{ MHz}, \quad A'_{\perp} = 134 \text{ MHz} \quad (I' = 1/2); \\ G_{\parallel} &= 1.9975, \quad G_{\perp} = 1.9954 \quad . \end{aligned} \tag{27}$$

Constant γ can be estimated from the relation [23]

$$\gamma = -2B(G_{\perp} - G_{\parallel}) \approx 30 \text{ MHz} \quad . \tag{28}$$

It is more difficult to estimate D. We can do that only in a very rough manner within the ionic model. According to the ionic model one electron moves from Yb to F, while the other remains on Yb in the polarized state (1). Then

$$\begin{aligned} D &= -R_0 + 2C_{0,1/2}C_{1,1/2}\langle 6s|r|6p\rangle \\ &\approx -5.2 \times 10^{-18} \text{ cgs} \quad , \end{aligned} \tag{29}$$

where R_0 is the internuclear distance.

More accurate values for γ and D can be measured in the molecular beam experiment with even isotopes of Yb. In this case all terms of H_{SR} proportional to I vanish and spin-rotational spectrum is simplified.

On the other hand, for ^{173}Yb ($I = 5/2$) there are additional terms which correspond to the electric quadrupole moment Q and the magnetic quadrupole moment M of the nucleus

$$H'_{\mathrm{SR}} = \frac{-1}{4I(2I-1)} T_{i,k} \left(\frac{1}{2} Q q_0 n_i n_k + 2 M W_M S_i n_k \right) \quad . \tag{30}$$

Constant q_0 here is defined as in [24]. Contribution of coupled electrons to q_0 doesn't vanish, but is probably smaller than that of the unpaired electron. The latter is readily calculated using Eqs. (3) and (17). For $Q = 2.8 \times 10^{-24} e\,\mathrm{cm}^2$

$$Q q_0^{\mathrm{val}} = 1880 \text{ MHz}. \tag{31}$$

Our results for the constants W_i are as follows:

$$\begin{aligned} W_A &= 0.73 \text{ kHz}; \\ W_S &= -48 \text{ kHz}; \\ W_d &= -1.5 \times 10^{25} \frac{\mathrm{Hz}}{e\,\mathrm{cm}}; \\ W_M &= -2.1 \times 10^{33} \frac{\mathrm{Hz}}{e\,\mathrm{cm}^2}. \end{aligned} \tag{32}$$

VI. DISCUSSION

In this section we are going to dwell on the accuracy of the numbers given in Eq. (32) and on the perspectives of the experiment with the YbF molecule.

The accuracy of our method is mainly determined by the approximation (3) for the radial functions and by the neglect of the higher terms of the expansion (1). Other possible sources of errors, such as single-electron approximation, spin-orbital mixing, and experimental errors in the hyperfine constants A and A_d must be much smaller. It is known that functions (3) give the accuracy for matrix elements of interest about 15%. Contribution of higher spherical waves was estimated above to be about a few percent. So, we expect the total errors for the constants W_i to be about 20% or less.

As was mentioned earlier, molecular beam of the YbF molecule was recently obtained in Yale university [14]. The intensity of the beam as well as population of the lower spin-rotational levels can be increased by using the beam source described in [22]. So, it is likely that the EDM experiment on the YbF will be possible in the near future. Let us discuss what can be measured in this experiment.

Almost 70% of natural isotopes of Yb are spinless. Then the spin-rotational spectrum consists of the simple rotational structure with small splittings caused by the spin-doubling and the magnetic hyperfine interaction with fluorine nucleus. Polarization rate depends on the single parameter $|DE/2B|$ which turns to unity in the field $E \approx 5.5$ kV/cm. Experiment with the spinless isotopes can give information on d_e and k_S [note that sometimes another constant $C_S = Z/(Z+N)\ k_S$ is used]. For both of them corresponding frequency shifts are about three orders of magnitude larger than in experiment with Tl. Note also that for the YbF experiment one needs much weaker external electric field. Probably, these advantages will be partly compensated by the lower statistics available in the molecular experiment in comparison with the atomic one. But still, this possibility looks very attractive.

There is also isotope ^{171}Yb with $I = 1/2$ (it's natural abundance is 14%). In this case the lower part of the spin-rotational spectrum is significantly changed by the large hyperfine structure on ytterbium nucleus. This isotope can be used to look for P-odd effects caused by the anapole moment. Some of these effects were discussed in [25,21], but the best way to measure the anapole constant k_a is still to be worked out.

At last, there is isotope ^{173}Yb with $I = 5/2$. For this isotope it is possible to look for the molecular EDM caused by the magnetic quadrupole moment of the nucleus. Connection between the latter and the constant of P,T-odd nucleon-nucleon interaction was established in [19]. But, the low natural abundance together with the higher density of spin-rotational levels [$\sim (2I+1)$] results in more than an order of magnitude lower statistics in comparison with spinless isotopes. So, this experiment will be more complicated.

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