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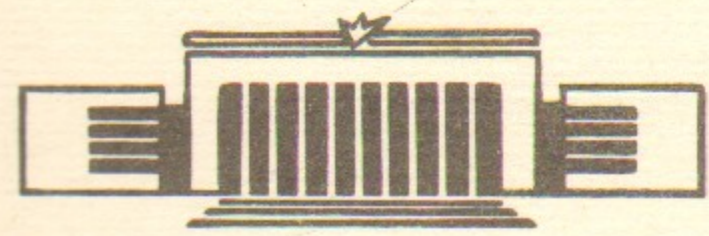
ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ СО АН СССР

V.L.Flambaum, I.V.Khriplovich

ON THE ENHANCEMENT OF
PARITY NONCONSERVING EFFECTS
IN DIATOMIC MOLECULES

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ON THE ENHANCEMENT OF PARITY NONCONSERVING
EFFECTS IN DIATOMIC MOLECULES

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Abstract

Effects of parity nonconservation in molecules with the $^2\Sigma$ electron state can be used to detect the anapole (P-odd) nuclear moments. The magnitude of circular polarization of radiation in microwave range reaches 10^{-4} being 10^4 times larger than in the 2s state of hydrogen. Considerable enhancement arises as well in optical transitions. T-odd effects are also discussed.

It is known, that there are close rotational levels of opposite parity in diatomic molecules. This circumstance can be used to enhance the effects of time (T) /1-3/ and space (P) /4,5,2/ parity violation. The effects of P-nonconservation prove to be enhanced only in the molecules with non-zero electron angular momentum, just the P-odd nuclear spin dependent interaction being enhanced /5,2/. In Refs. /6,7/ it has been shown that this interaction is due mainly to the P-odd nuclear forces leading to the appearance of a nuclear anapole moment \vec{a} directed along the spin \vec{I} of the nucleus. The electromagnetic vector-potential created by the anapole moment is equal to

$$\vec{A} = \vec{a} \delta(\vec{r}).$$

Ref. /5,2/ deal with the molecules in which Λ - or Ω - doubling of the rotational levels takes place (Λ and Ω are the projections of the electron orbital and total angular momenta on the axis of the molecule). However, the molecules with the $^2\Sigma$ electron state have a number of advantages. For instance, the LuO, LaO and LaS molecules possess a high binding energy that makes them thermodynamically stable. There is a lot of experimental information about these molecules /8/. They are suitable for both the radiofrequency and optical experiments due to convenient position of the excited states. The P-odd effects grow rapidly with the nuclear charge which is fairly large in La and Lu ($Z = 57$ and 71 , respectively). And, finally, due to the compensation of a hyperfine and rotational splitting a very small interval arises in these molecules between the levels of opposite parity (0.2 cm^{-1} in LaO, $< 0.01 \text{ cm}^{-1}$ in LaS, and 0.05 cm^{-1} in LuO). This interval between the opposite parity levels can be made even smaller by applying an external magnetic field.

Relatively simple structure of the lower rotational states of such molecules is also convenient. The interaction of the spin with the rotation of a molecule in the $^2\Sigma$ state is small /9/, much smaller than that between the electron and nuclear spins, which has the same order of magnitude as in the atoms. Therefore, the angular momenta coupling scheme is here as follows. The spins of an unpaired electron and nucleus, \vec{S} and \vec{I} , are coupled into the angular momentum $\vec{F} = \vec{S} + \vec{I}$. The

interaction of \vec{F} with the molecular rotation is so weak that it is broken by a magnetic field of about 100 G.

The coordinate wave function of the unpaired electron near a nucleus is expanded in the orbitals of a heavy atom:

$$|\beta\rangle = \beta_s |s\rangle + \beta_p |p\rangle + \beta_d |d\rangle + \dots \quad (1)$$

Since the \sum -term is considered, in the expression (1) even the constituents with a non-zero orbital angular momentum possess $l_z = 0$. The electron interaction with the nuclear anapole moment is conveniently written as follows [6,7]:

$$H_a = e \vec{\alpha} \vec{\alpha} s(\vec{r}) \equiv \frac{G}{\sqrt{2}} \frac{K \vec{I} \vec{\alpha}}{I(I+1)} \chi_a s(\vec{r}) \quad (2)$$

where e is the proton charge, $\vec{\alpha}$ are the Dirac matrices for an electron, G is the Fermi constant, $K = (-1)^{I+\frac{1}{2}-l} (I+\frac{1}{2})$, l is the orbital angular momentum of an external unpaired nucleon, and χ_a is the dimensionless constant proportional to the anapole moment of the nucleus. In spherical nuclei [7]

$$\chi_a = \frac{g}{10} g \frac{\alpha M_N}{m r_0} [A^{2/3} - 0.4 I(I+1)] = 1.1 \cdot 10^{-3} g M_N [A^{2/3} - 0.4 I(I+1)] \quad (3)$$

Here A is the atomic number of a nucleus, $\alpha = 1/137$, m_p is the proton mass, $r_0 = 1.2 \cdot 10^{-13}$ cm, M_N is the magnetic moment of the external nucleon in nuclear magnetons ($M_p = 2.8$;

$M_n = -1.9$), and g is the dimensionless constant characterizing the strength of the weak nucleon-nucleus interaction. For the unpaired proton, $g_p = 4.5$, and for neutron $|g_n| \approx 1$ [7]. As a result, for the ^{139}La nucleus $\chi_a = 0.3$. As for the ^{175}Lu nucleus, it is not a spherical one so that the expression (3) is not strictly speaking applicable to it. Nevertheless, as an estimate, we take $\chi_a = 0.35$ for ^{175}Lu (this value follows from formula (3)).

Calculating the matrix element of the interaction (3) between the molecular states $|II_z\rangle |SS_z\rangle |\beta\rangle$ by means of the quasiclassical wave functions presented, e.g., in Ref. [10] (as it was done in [11] for a T-odd interaction) we find

$$H_{\text{eff}} = \xi (\vec{s} \times \vec{I}) \vec{n} \quad (4)$$

$$\xi = \frac{\beta_s}{\gamma_s^{3/2}} \frac{\beta_p}{\gamma_p^{3/2}} Ry \frac{2\sqrt{2}}{13\pi} G m^2 \alpha^2 Z^2 R_w \frac{K}{I(I+1)} \chi_a \quad (5)$$

Here \vec{n} is the direction of the molecular axis pointed from the heavy atom to the light one, $Ry = 13.6$ eV, m is the electron mass, R_w is the relativistic factor for a weak interaction,

$$R_w = \frac{2\gamma+1}{3} \left(\frac{\alpha_B}{2Z r_0 A^{1/3}} \right)^{2-2\gamma} \frac{4}{[\Gamma(2\gamma+1)]^2}, \quad \gamma = \sqrt{1 - (Z\alpha)^2},$$

α_B is the Bohr radius. At $Z \rightarrow 0$ $R_w \rightarrow 1$, $R_w(Z=57) = 3$ and $R_w(Z=71) = 5$. γ_s and γ_p denote the effective quantum numbers of the lower s and p states of an external electron in the heavy atom ($E = -Ry/\gamma^2$). In the La and Lu atoms these are the $6s$ and $6p$ states. The quantity $\beta_s/\gamma_s^{3/2}$, through which the wave function $|\beta\rangle$ is expressed at $Z \rightarrow 0$, enters also the hyperfine structure constant of a molecule:

$$b = \frac{\beta_s^2}{\gamma_s^3} Ry \frac{8}{3} \frac{M}{I} Z \alpha^2 \frac{m}{m_p} R_{\text{hf}}, \quad R_{\text{hf}} = \frac{3}{8(4\gamma^2-1)}, \quad (6)$$

where M is the magnetic moment of a nucleus. Since the hyperfine splitting in the LaO, LaS, and LuO molecules is known [8], for the determination of ξ it is necessary to estimate, at $Z \rightarrow 0$, the quantity $\beta_p |p\rangle$ proportional to $\beta_p/\gamma_p^{3/2}$. It can be made, for example, by using the normalization condition for $|\beta\rangle$. The value of γ_s in the La and Lu atoms is about the same: $\gamma_s = 1.38$. The comparison of the expression (5) with experiment [8] yields $\beta_s \approx 0.75$ in LaO, LaS and LuO. If we set $\beta_p = \beta_d$ as an estimate, it then follows from the condition $\beta_s^2 + \beta_p^2 + \beta_d^2 = 1$ that $\beta_p \approx 0.5$. Estimation of the mixing of s and p states by an internal electric field of the polar molecule results in the same order of magnitude of β_p (see Ref. [11]). Assuming $\gamma_p = 1.6$, as in the La and Lu atoms, we find

$$\xi(LaS) \approx \xi(LaO) = -2.5 \cdot 10^{-9} \text{ cm}^{-4} \chi_a \quad (7)$$

$$\xi(LaS) \approx \xi(LuO) = -7 \cdot 10^{-9} \text{ cm}^{-1} \alpha_a \quad (8)$$

In this calculation we use the expansion in atomic orbitals (1) together with the atomic effective principal quantum numbers γ . Meanwhile, in the molecules under consideration two electrons are shifted from heavy atoms towards oxygen. In principle, for an unpaired electron, it is possible, therefore, to use the ion characteristics instead of the atomic ones. One can check easily that such a modification would lead only to a small increase of the calculated values of ξ .

The Hamiltonian (4) causes the mixing of the rotational molecular states $|L, F, \eta\rangle$ and $|L' = L \pm 1, F' = F \pm 1, \eta\rangle$ ($\vec{\eta} = \vec{F} + \vec{I}$) of opposite parity. In the LaO and LuO molecules, the mixing coefficient of the $|L=0, F=3, \eta=4\rangle$ and $|L=1, F=3, \eta=4\rangle$ states is the maximal one because of a small energy denominator: $E_{0,4} - E_{1,3} = 4b - 2B$ (the energy of molecular rotation amounts to $B L(L+1)$). This coefficient is equal to

$$\xi = -i \sqrt{\frac{I(2I+1)}{12}} \frac{\xi}{E_{0,4} - E_{1,3}} \quad (9)$$

Its numerical values are:

$$\xi(LaO) = -i \cdot 2 \cdot 10^{-8} \alpha_a, \quad \xi(LuO) = -i \cdot 2 \cdot 10^{-7} \alpha_a \quad (10)$$

The mixing, larger than in LaO, occurs between the $|L=1, F=4, \eta\rangle$ and $|L=2, F=3, \eta\rangle$ states in the LaS molecule. According to Ref. /8/, the energy denominator in this case, vanishes within experimental accuracy, but it is probable that the accuracy itself in the measurement of the constant b in LaS constitutes 0.01 cm^{-1} . In LuS, the constant b has not been measured.

It is easy now to find the magnitude of the parity violating E1-amplitude in the transition between the hyperfine components $F=3$ and $F=4$. For example,

$$A_-(E1) \equiv \langle L=0, F_2 = F = I - \frac{1}{2} | D_- | L=0, F_2 = F = I + \frac{1}{2} \rangle = \frac{\partial \xi}{\sqrt{3}} \quad (11)$$

Here $|I\rangle$ is the state with a weak mixing taken into account, $D_- = \frac{1}{\sqrt{2}}(D_x - iD_y)$, $\vec{D} = D\vec{n}$, D is the electric dipole moment of the polar molecule. We have failed in finding the value of

D for the LaO and LuO molecules, but the value of D in the BaO molecule similar to them is known: $D = -3.14 e a_B$. The molecule BaO differs from LaO and LuO by the absence of an unpaired electron. Since the coupling energy and internuclear distances in LaO and LuO are close to those in BaO (and in LaS they are close to those in BaS where $D = -4.28 e a_B$), it is natural to assume that the dipole moments due to the shift of two electrons to oxygen, are close as well. Putting $D(LaO) = D(LuO) = -3 e a_B$ we find

$$\begin{aligned} LaO: A_-(E1) &= 3 \cdot 10^{-8} \alpha_a i e a_B \\ LuO: A_-(E1) &= 3 \cdot 10^{-7} \alpha_a i e a_B \end{aligned} \quad (12)$$

The amplitude of the corresponding M1-transition in both molecules is $A_-(M1) = -\frac{e}{2m} \sqrt{\frac{4I}{2I+1}}$. As a result, the degree of circular polarization of radiation $P = -2 \text{Im} A_-(E1) / A_-(M1)$ constitutes

$$\begin{aligned} P &= 1.3 \cdot 10^{-5} \alpha_a \text{ in LaO}, \quad P \approx 10^{-4} \alpha_a \text{ in LaS}, \\ P &= 1.3 \cdot 10^{-4} \alpha_a \text{ in LuO} \end{aligned} \quad (13)$$

We emphasize that the admixed E1-amplitude and the degree of circular polarization in LuO exceeds by a factor of 10^4 their values in the microwave transition in the 2s state of hydrogen and by a factor of 10^5 that in caesium ground state.

The larger magnitude of parity nonconserving effects can probably be obtained in the forbidden transition $|L=0, F=4\rangle \rightarrow |L=2, F=3\rangle$. The admixed E1-amplitude in it is comparable with (12), while without parity violation the transition is switched on, in practice, by external fields only.

The parity nonconserving effects can be additionally enhanced by reducing the interval between the opposite parity levels by a magnetic field about 1 kG. Since in contrast to the hydrogen 2p state, the natural width of the levels is negligible here, one could get, in principle, larger enhancement in the molecules than in hydrogen by means of magnetic field.

Note that the limitations on stray electric fields in LaO and LuO are also much weaker than in hydrogen. In addition to the fact that the P-odd interaction in the molecules is

stronger, of significance is the circumstance that an electric field does not mix directly the levels $|L=1, F=3\rangle$ and $|L=0, F=4\rangle$.

The parity nonconserving effects in the LaO, LuO and LaS molecules can be searched for in optical experiments as well, just as it was done in the experiments with Tl (Ref. /12/) and Cs (Ref. /13/) (for the PbF, BiO and BiS molecules see the discussion in Refs. /5,2/). The admixed E1-amplitude also reaches here $10^{-8}-10^{-7}$, being 10^2-10^4 times larger than its value in the atoms. Furthermore, in the $^2\Sigma \rightarrow ^2\Sigma$ transitions the M1-amplitude turns out to be suppressed because of the orthogonality of electron wave functions. This increases the magnitude of circular polarization. In this case, it is possible to switch on the transition, just as in Tl and Cs, by an electric field mixing the rotational molecular states of opposite parity. As to the experimental search for the optical activity of these molecules due to parity nonconservation (for BiO and BiS see the discussion in Ref. /2/), a serious difficulty for the compounds discussed is perhaps the high temperature necessary to obtain sufficient vapour pressure. According to /21/, for LaO and LaS a reasonable pressure (> 1 mm) is reached only at $T \approx 2500^\circ\text{C}$.

In the molecules under discussion the T-odd effects are also amplified. In particular, due to T-odd nuclear forces (or electric dipole moment of the external nucleon) a nucleus acquires a magnetic quadrupole moment. It induces in turn an electric dipole moment of the molecule with non-zero electron angular momentum in its stationary state. Using the formulae of Ref. /11/, we found that the parameter \mathcal{X} of the T-odd interaction $H_{\text{eff}} = \mathcal{X}_{L\alpha} \frac{F\hbar}{F} R y$ is equal to $\mathcal{X}_{L\alpha} = -3 \cdot 10^{-17}$ at $F = 3$, while the electric dipole moment, at $L = 0$, constitutes $D_T = -\frac{\mathcal{X} D}{3 B} R y = -5 \cdot 10^{-20} e \cdot \text{cm} \cdot \eta$ where η is the parameter characterizing the intensity of the T-odd nucleon-nucleus interaction. The LaS molecules has the same value of \mathcal{X} and a four times larger dipole moment, $D_T = -2 \cdot 10^{-19} e \cdot \text{cm} \cdot \eta$. An analytical formula for the magnetic quadrupole moment, derived in Ref. /11/, is applicable for spherical nuclei only. If, nevertheless, we use it for an estimate in the non-spherical ^{175}Lu nu-

cleus, we obtain twice larger values of the T-odd constants in Lu compounds: $\mathcal{X}_{Lu} = -6 \cdot 10^{-17} \eta$, $D_T(LuO) = -1 \cdot 10^{-19} e \cdot \text{cm} \cdot \eta$, and $D_T(LuS) = -4 \cdot 10^{-19} e \cdot \text{cm} \cdot \eta$. The latter value is 40 times larger than D_T of the TlF molecule, and the experiments with TlF has led to one of the two best bounds on η : $|\eta| \leq 1$ /11-17/. The molecular experiments offer also the possibility to obtain the bounds on the other T-odd characteristics (for example, on the electric dipole moment of electron /1-3/).

Note that in the Σ -states, the electric dipole moment arises due to the mixing of the states with equal F(Ref. /11/), which are separated by a normal rotational interval. Therefore, in such molecules there is no additional enhancement of T-odd effects due to partial compensation of energy intervals. It can be shown however that here also the effect may be enhanced by applying a magnetic field reducing the interval between the nearest opposite parity levels.

The parity violation effects, comparable with those considered above, occur in the compounds of Ba, Yb, Hg with H, F, Cl, Br, I atoms.

Previously, the parity violation effects have been analysed in the molecules with \overline{II} -terms (PbF, Ref. /5/; BiO and BiS, Ref. /2/). The lower rotational states in these molecules have rather complicated structure since the Coriolis and hyperfine interactions in them are comparable. However, these molecules are likely to have also the levels of opposite parity with the interval considerably smaller than the rotational one.

In conclusion, we wish to point out that the parity nonconservation in atoms, discovered in /18/ and then observed in /12,13,19,20/, is due to the nuclear spin-independent part of the weak electron-nucleon interaction. Meanwhile, in molecular experiments one can study the spin-dependent part of the P-odd interaction, which is mainly due to an interaction between the electron and the nuclear anapole moment. The nuclear anapole moment is of interest not only as a new, so far not observed nuclear characteristic. Its measurement would give unique information about the parity violating nuclear forces.

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К ВОПРОСУ ОБ УСИЛЕНИИ ЭФФЕКТОВ НЕСОХРАНЕНИЯ
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