Parity nonconservation in diatomic molecules in a strong constant magnetic field

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It is shown that the spin-rotational levels of opposite parity in the molecules PbF and HgF cross in magnetic fields $\sim 10^3$ G. This effect enhances many *P*-odd effects, governed by the anapole moment of a heavy nucleus.

1. INTRODUCTION

Parity nonconservation effects in atomic and molecular physics have become familiar in both experimental and theoretical investigations (see, for example, Ref. 1). The greatest progress has been made in the measurement of one of the constants of the effective *P*-odd weak interaction of electrons and nuclei—the "weak nuclear charge." Only preliminary reports are as yet available regarding measurements of the other constant— the so-called anapole moment of the nucleus.[2] All these experiments were performed on atoms. Until very recently experiments on molecules were performed exclusively in order to search for *P*, *T*-odd interactions. But, as has been pointed out repeatedly in theoretical work,[4-7] investigations of *P*-odd effects in diatomic molecules also look promising. Calculations have been performed for the molecules BiS,[5] PbF,[8] and HgF.[9] The important point is that the corresponding experiments would give information about the anapole moments of nuclei.

The use of a constant external magnetic field to enhance *P*-odd effects in atomic experiments has also been discussed (see, for example, Ref. 10). This has been achieved only for the hydrogen atom,[11-13] where the required magnetic fields are achievable experimentally, but the *P*-odd effect was found to be too weak owing to the large width of the $2p_{1/2}$ state. Diatomic molecules in the ground electronic state have close sublevels of opposite parity (components of Λ doublets, Ω doublets, or rotational sublevels of opposite parity). Mixing of such sublevels occurs only as a result of *P*-odd interaction, which is determined by the anapole moment of the nucleus. The imposition of a relatively weak magnetic field (10^3–10^4 G) can substantially enhance *P*-odd effects. The possibility of such enhancement was pointed out by Khriplovich,[1] but he did not discuss specific experiments.

We note that in his thesis work, performed at Leningrad University in 1983, Kopp proposed using a magnetic field for crossing close rotational levels of the states $^3\Pi_u$ and $^3\Sigma_g^+$ of the H_2 molecule. He showed that crossing occurs in fields of 10^5 G and the magnitude of the *P*-odd amplitudes is equal to $\sim 10^{-3}$ Hz.

In this paper we shall study several possible variants of experiments designed to search for *P*-odd effects in diatomic molecules.

In Sec. 2 an expression is presented for the effective spin-rotational Hamiltonian of diatomic molecules having the ground states $^2\Sigma_{1/2}$ and $^2\Pi_{1/2}$, taking into account the *P*-odd effective interaction (this pertains to molecular radicals). The parameters of this Hamiltonian are determined from existing experimental data and the results of calcula-

tions of the electronic structure of the molecules.

In Sec. 3 a numerical calculation of level crossing is performed, using the existing expressions for the spin-rotational Hamiltonian for the molecules PbF and HgF, and the optimal situations for experiments are selected.

The possible effects of splitting of an rf resonance line in the region of crossing of sublevels of opposite parity in a magnetic field are described in Sec. 4. The magnitude of the splitting in this case can reach 10–10^3 Hz in fields of the order of 10^4 G.

The usual question in experiments on *P*-odd phenomena—the rotation of the polarization plane of light accompanying absorption in vapors of diatomic molecules—is studied in Sec. 5. In the presence of level crossing this phenomenon combines in a unique way with the Faraday effect.

Finally, in Sec. 6 the *P*-odd Stark effect in the field of an intense plane-polarized laser wave is discussed. This effect consists of the fact that the resonance frequency depends on the propagation direction of the wave with respect to the magnetic field. This effect is significantly stronger in molecules than in atoms[14] and reaches a magnitude of 10^3 Hz for laser-field strengths of 10^4 V/cm. Here, however, additional experimental difficulties also arise.

2. SPIN-ROTATIONAL HAMILTONIAN

In Refs. 4–9 and 15 it was shown that polar molecules with one heavy nucleus and an unfilled shell are most suitable for studying *P*-odd effects. Examples of such molecules are HgF and PbF. These molecules have the ground states $^2\Sigma_{1/2}$ and $^2\Pi_{1/2}$, which we shall study below using the parametrization employed in Ref. 9.

The state $^2\Sigma_{1/2}$. In the overwhelming majority of the cases the $^2\Sigma_{1/2}$ states are related to Hund's *b*-type coupling, i.e., they are described by the following quantum numbers: Λ—the projection of the orbital angular momentum on the axis of the molecule, S—the spin of the electrons, and N—the rotational angular momentum of the molecule. Denoting the nuclear spins by I_1 and I_2 we can write the effective spin-rotational Hamiltonian in the following form:

$$H_{sr} = BN^2 + \gamma(\mathbf{N}, \mathbf{S}) + (\mathbf{I}_1, \mathbf{A}_1\mathbf{S}) + (\mathbf{I}_2, \mathbf{A}_2\mathbf{S}). \tag{1}$$

In this expression B is the rotational constant, γ is the spin doubling constant, and $\mathbf{A}_1$ and $\mathbf{A}_2$ are axial tensors of the effective electron-nucleus spin-spin interaction. The parameters appearing in Eq. (1) can be determined from existing experimental data.

The state $^2\Pi_{1/2}$. In this case a type of coupling intermediate between Hund's a and c types of coupling is usually realized. The rotational moment has the form

$$H_r = B(\mathbf{J}-\mathbf{J}_e)^2 = B\mathbf{J}^2 - 2B(\mathbf{J}_e, \mathbf{J}) + B\mathbf{J}_e^2, \qquad (2)$$

where $\mathbf{J}$ is the total angular momentum of the molecule and $\mathbf{J}_e$ is the electronic angular momentum. Averaging the operator $\mathbf{J}_e$ with respect to the electronic function, we can introduce the concept, which is convenient in this case, of the effective electron spin $\mathbf{s}$ defined as

$$\mathbf{s}_\pm |\omega\rangle = |-\omega\rangle, \quad \mathbf{s}_0|\omega\rangle = \omega|\omega\rangle, \qquad (3)$$

where $\omega = \pm 1/2$ is the projection of the total angular momentum $\mathbf{J}$ on the axis of the molecule. In this case the effective spin-rotational Hamiltonian is written as

$$H_{sr} = B\mathbf{J}^2 + \Delta(\mathbf{sJ}) + (\mathbf{I}_1, \mathbf{A}_1\mathbf{s}) + (\mathbf{I}_2, \mathbf{A}_2\mathbf{s}), \qquad (4)$$

where Δ is the ω-doubling constant.

For the $^2\Sigma_{1/2}$ states the operators $\mathbf{J}_e$ and $\mathbf{s}$ are identical, so that to within a constant the expression (1) reduces to Eq. (4). It is also necessary to take into account the fact that $\mathbf{J} = \mathbf{N} + \mathbf{s}$, and set

$$\Delta = -2B + \gamma. \qquad (5)$$

This makes it possible to use the operator (4) for both $^2\Sigma_{1/2}$ and $^2\Pi_{1/2}$ states. Table I gives the parameters of the operator H_{sr} for the molecules HgF and PbF. The tensors $\mathbf{A}$ are defined in the molecular coordinate system as follows:

$$(\mathbf{a}, \mathbf{Ab}) = A^\| a_0 b_0 - A^\perp (a_1 b_{-1} + a_{-1} b_1). \qquad (6)$$

We also need expressions for the operators of interaction with a constant external magnetic field as well as the effective P-odd interaction. These operators have the form[7]

$$H_F = -\mu_0(\mathbf{B}_0, \mathbf{Gs}), \qquad (7)$$

$$H_P = W\varkappa([\mathbf{ns}], \mathbf{I}_1). \qquad (8)$$

For the Σ terms the anisotropic components of the $\mathbf{A}$ tensors and the tensor $\mathbf{G}$, which replaces the g factor, are different from zero only owing to the spin-orbital interaction. In Eqs. (7) and (8) μ_0 is the Bohr magneton, $\mathbf{B}_0$ is the external magnetic field, $\mathbf{n}$ is a unit vector along the axis of the molecule, W is the effective weak-interaction constant

which is obtained by averaging the P-odd interaction over the electronic state, and

$$^1/_2\varkappa = -^2/_3\varkappa_{2p,\,n} + ^4/_3 k_a, \qquad (9)$$

where

$$\varkappa_{2p,\,n} = \mp^1/_2\lambda(1 - 4\sin^2\theta_W)$$

is the constant characterizing the axial-vector weak interaction of an electron with a proton (neutron),[1] the constant $\lambda \approx 1.25$ characterizes the renormalization of the weak interaction by the strong interaction, k_a is the anapole moment of the nucleus, and θ_W is the Weinberg angle. We also assume that the nucleus 2 is a light nucleus while the nucleus 1 is described by the shell model with one valence nucleon and has the spin $I_1 = \frac{1}{2}$. According to all of the modern experimental data taken together, $\sin^2\theta \approx 0.23$, and calculations give for the anapole moments of heavy nuclei values of k_a ranging from -0.1 (for ^{207}Pb) to $+0.31$ (for ^{209}Bi).[17]

The parameters appearing in Eqs. (7) and (8) are presented in Table II. The presentation given below is based on the formulas (4), (7), and (8).

3. CROSSING OF SPIN-ROTATIONAL SUBLEVELS IN A MAGNETIC FIELD

In order to calculate the levels of a molecule in a constant external magnetic field it is necessary to diagonalize the operator H_{sr} and H_F:

$$H_{sr} + H_F = B\mathbf{J}^2 + \Delta(\mathbf{J}, \mathbf{s}) + (\mathbf{I}_1, \mathbf{A}_1\mathbf{s}) + (\mathbf{I}_2, \mathbf{A}_2\mathbf{s}) - \mu_0 B_0(\mathbf{b}_0, \mathbf{Gs}), \qquad (10)$$

where $\mathbf{b}_0 = \mathbf{B}_0/|\mathbf{B}_0|$. We shall employ the following coupling scheme for classification of the states:

$$\mathbf{J} + \mathbf{I}_1 \equiv \mathbf{F}_1, \quad \mathbf{F}_1 + \mathbf{I}_2 \equiv \mathbf{F}. \qquad (11)$$

The basis functions are characterized by the following collection of quantum numbers: $|JpF_1FM\rangle$, where p is the parity and M is the projection of the total angular momentum of the molecule on the direction of the external magnetic field. Then

$$\langle JpF_1FM|H_{sr}|J'p'F_1'F'M'\rangle$$

$$= \frac{\delta_{pp'} \cdot \delta_{MM'} \delta_{FF'}}{(2F+1)^{1/2}} \langle JpF_1F\|H_{sr}\|J'pF_1'F'\rangle, \qquad (12)$$

TABLE I. The parameters of the spin-rotational Hamiltonian for the molecules PbF and HgF (all data are given in cm^{-1}).

Parameters	^{207}PbF ($^2\Pi_{1/2}$) [8]	HgF ($^2\Sigma_{1/2}$) [9,16]	
		^{199}Hg ($I_1 = \frac{1}{2}$)	^{201}Hg ($I_1 = \frac{3}{2}$)
B	0,2288	0,222 *	0,222 *
$\Delta\ (\gamma)$	−0,1388	0,0143 *	0,0143 *
$A_1^\|$	0,305	0,754	0,268
$A_1^\perp$	−0,262	0,729	0,258
$A_2^\|$	−0,0208	—	—
$A_2^\perp$	0,0240	—	—

*Data provided by A. V. Titov.

G, W	^{207}PbF ($^2\Pi_{1/2}$) [8]	HgF ($^2\Sigma_{1/2}$) [9,16]	
		^{199}Hg	^{201}Hg
$G^{\parallel}$	$-0,075$	$1,993$	$1,993$
$G^{\perp}$	$0,307$	$1,961$	$1,961$
$10^8 W$, cm^{-1}	$3,2$	$8,63$	$7,97$

$$\langle JpF_1 FM \mid -\mu_0 B_0(\mathbf{b}_0, \mathbf{Gs}) \mid J'p'F_1'F'M' \rangle = \frac{\delta_{pp'}\delta_{MM'}C^{FM}_{F'M'10}}{(2F+1)^{1/2}} \cdot$$

$$\cdot (-\mu_0 B_0)\langle JpF_1 F \| \mathbf{Gs} \| J'pF_1'F' \rangle. \quad (13)$$

Here $C^{FM}_{F'M'10}$ are Clebsch-Gordan coefficients. The matrix elements presented above and appearing in Eqs. (12) and (13) are given in Appendix 1.

The results of the numerical diagonalization of the operator H_{sr} and H_F for the molecules PbF and ^{199}HgF are shown in Figs. 1 and 2. The results of the calculation of the matrix element of the operator H_p between levels of opposite parity in the region of level crossing are given in Table III (the formulas are given in Appendix 2).

4. P-ODD rf RESONANCE ON CROSSING SPIN-ROTATIONAL SUBLEVELS

One possible experiment is to observe the splitting of the rf resonance lines near the pseudocrossing of levels having opposite parity in a magnetic field. We designate the crossing levels as the 1 and 2 levels. We designate the level with which the resonance is realized as level 3 (see Fig. 3). For definiteness we shall assume that the parity of level 1 is the same as that of level 3 (in the absence of weak interaction). When the operator H_p is included the crossing of levels 1 and 2 becomes a pseudocrossing. Denoting the splitting between levels 1 and 2 neglecting H_p as Δ ($\Delta \sim B_0 - B_*$, where B_* is the magnetic field at the crossing point), we obtain

$$\Delta_p = (\Delta^2 + 4\chi^2)^{1/2},$$

$$\chi_p = \frac{2^{1/2} i\chi}{[\Delta p(\Delta + \Delta p)]^{1/2}}. \quad (14)$$

Here $i\chi \equiv \langle 1/H_p|2\rangle$, Δ_p is the splitting between the levels 1 and 2 after H_p is taken into account, and χ_p is the admixture of the starting state 2 added to the starting state 1.

The frequency dependence of the intensity of the resonance as a function of the magnetic field near the crossing point will be different in the cases when H_p is taken into account and when H_p is neglected. Figure 4 shows this dependence in the case when H_p is neglected and Fig. 5 shows the dependence in the case when H_p is not neglected.

The splitting of the rf resonance line in Fig. 5 is at least 2χ and, according to Table III, is equal to 10–10^3 Hz.

We note that such experiments seem to be most practicable with a molecular beam. In this case Doppler line broadening is small and the only type of broadening that could be of hindrance—transit broadening—is equal to $\Gamma \sim 200$ Hz for a chamber 2 m long and beam velocity ~ 400 m/s, which gives a realistic possibility for observing splitting of the line.

The main source of interference is the constant electric field E, which also mixes the levels 1 and 2. A limit on E
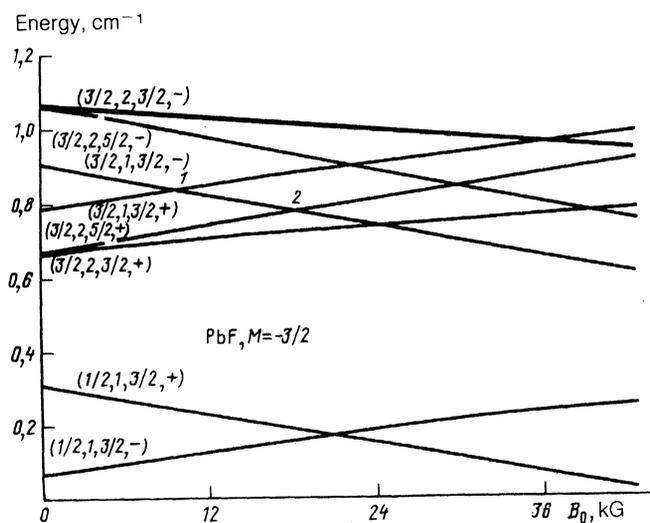

FIG. 1. The spin-rotational structure of the ground-state levels of the molecule PbF in a magnetic field. The quantum numbers $(JF_1 Fp)$ for $B_0 = 0$ (J and F_1 are approximate quantum numbers) are indicated in parentheses. The numbers 1 and 2 correspond to Table III.
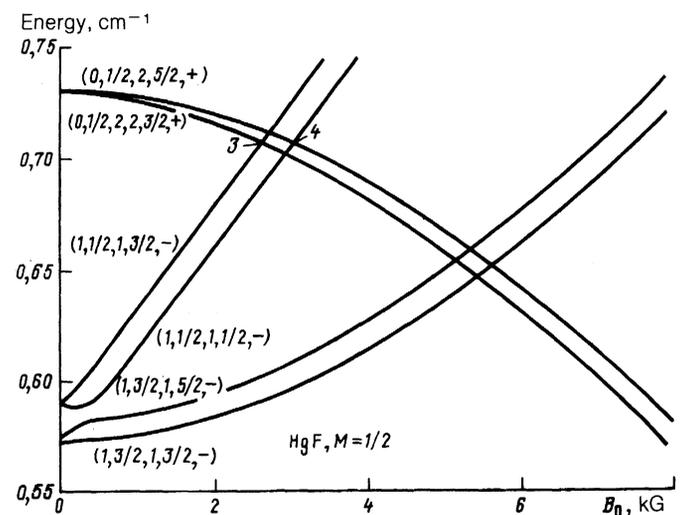

FIG. 2. The spin-rotational structure of the ground-state levels of the molecule HgF in a magnetic field. The quantum numbers $(F_1 F_2 Np)$ with $B_0 = 0$ in the coupling scheme $\mathbf{s} + \mathbf{I}_1 = \mathbf{F}_1$, $\mathbf{F}_1 + \mathbf{I}_2 = \mathbf{F}_2$, $\mathbf{F}_2 + \mathbf{N} = \mathbf{F}$—the approximate quantum numbers—are indicated in parentheses. The numbers 3 and 4 correspond to Table III.

TABLE III. The matrix elements of the operator H_p for some crossings of spin-rotational levels.

Molecule	N_i *	B_0, 10^3 G	$\dfrac{|\langle 1|H_p|2\rangle|}{\varkappa}$, Hz
PbF	1 2	9,78 20,70	359 112
HgF	3 4	2,23 2,99	113 87

*The numbers correspond to those marked in Figs. 1 and 2.

follows from the condition $dE \leqslant \chi$, which for $d \sim 1$ a.u. and $\chi \sim 10^3$ Hz gives $E \leqslant 10^{-4}$ V/cm (we note that the induced electric field arising as the molecules move in a magnetic field does not mix levels with identical values of M, because it is orthogonal to the magnetic field). This is a quite stringent condition. Aside from this, the magnetic field B_0 must be maintained constant with adequate accuracy. The limit on the variation of the magnetic field is

$$\mu_0 g \Delta B_0 \ll \chi. \tag{15}$$

Taking the g factor $g \sim 2$, we obtain $\Delta B_0 \leqslant 10^{-4} - 10^{-3}$ G, which for a field of $B_0 \sim 10^3$ G gives the following condition on the relative stability of the magnetic field:

$$\Delta B_0 / B_0 \leqslant 10^{-7} - 10^{-6}. \tag{16}$$

This is a very stringent condition. The weaker the field B_0 is, the easier it is to satisfy, so that crossings which are achievable with the minimum value of B_0 should be chosen for the experiment.

It should be noted that in this experiment the mixing by the weak interaction is 100%, while in the absence of the magnetic field $\chi_p = \langle H_p \rangle / \Delta E_{+-} \sim 10^{-6}$ (ΔE_{+-} is the splitting between the levels of opposite parity). In addition, if a beam is employed an attempt can be made to detect directly adiabatic transitions which are accompanied by a change in parity.
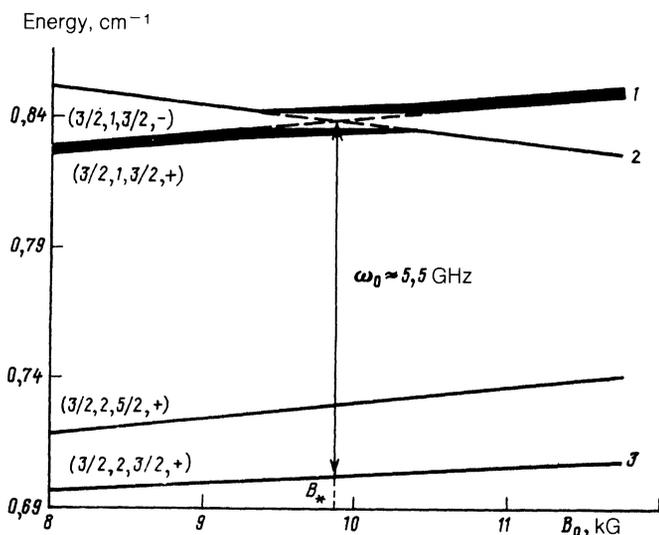
5. P-ODD FARADAY EFFECT

We now examine the conventional formulation of the question of the rotation of the polarization plane by a gaseous molecular medium. The "weak" nuclear charge was first measured in precisely such experiments in a medium consisting of atomic bismuth.[1] In contradistinction to the atomic approach we assume that states with different values of M are separated quite far from one another by the constant external magnetic field. The angle of rotation of the polarization plane near resonance is given by the following formula:[1]

$$\psi = -(\pi \omega l \mathcal{N}/\Delta_d) g(u, v)(|A^+|^2 - |A^-|^2), \tag{17}$$

where ω is the frequency of the absorbed photon; A is the amplitude for absorption of a right- or left-hand polarized photon: $\Delta_d = v_0 \omega_0$ is the Doppler width ($v_0 = (2kT/M)^{1/2}$, ω_0 is the resonance frequency); l is the path traversed by the light; $\mathcal{N}$ is the number density of particles; $u \equiv (\omega - \omega_0)/\Delta_d$; $v \equiv \Gamma/2\Delta_d$, where Γ is the collision width of the transition;

$$g(u, v) = \operatorname{Im}\{\pi^{1/2} e^{-w}[1 - \Phi(-iw)]\}, \tag{18}$$

$$w = u + iv,$$

$$\Phi(z) = \frac{2}{\pi^{1/2}} \int_0^z \exp(-t^2)\, dt.$$

FIG. 3. Transformation of the crossing of the levels which have opposite parity into pseudocrossing when H_p is taken into account (for the example of the crossing 1 in Fig. 1). The line thickness indicates the fraction of states with positive parity. The level shifts are not shown to scale.
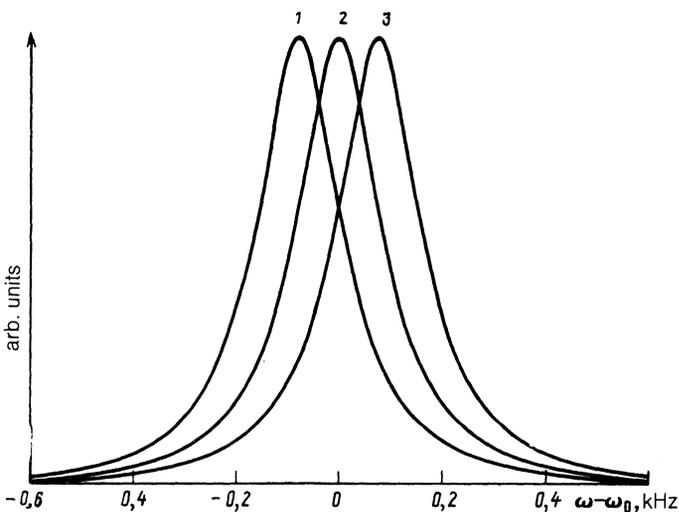
FIG. 4. The frequency dependence of the strength of the magnetic resonance as a function of the field B_0 near the crossing point taking H_p into account (for the example of the levels in Fig. 3): 1) $B_0 = B_* - \Delta B$, 2) $B_0 = B_*$, 3) $B_0 = B_* + \Delta B$, $\Delta B = 7 \cdot 10^{-4}$ G.
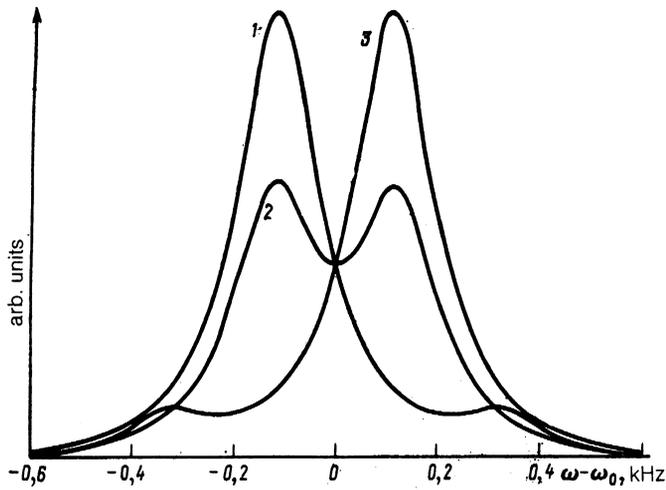
FIG. 5. The frequency dependence of the strength of the magnetic resonance as a function of the field B_0 near the crossing point taking H_p into account (for the example of the levels in Fig. 3): 1) $B_0 = B_* - \Delta B$, 2) $B_0 = B_*$, 3) $B_0 = B_* + \Delta B$, $\Delta B = 7 \cdot 10^{-4}$ G.

As in Sec. 3, we shall study a three-level system. The mixing ratio χ_p of the levels 1 and 2 is given by the formula (14). In this case

$$A^\pm = (1 - |\chi_p|^2)^{1/2} A_1{}^\pm + \chi_p A_2{}^\pm, \tag{19}$$

where

$$A_1{}^\pm = (2\pi\omega)^{-1/2}\langle 1 | (\mu, \, \mathbf{e}_B{}'^\pm) | 3\rangle, \tag{20}$$

$$A_2{}^\pm = (2\pi\omega)^{-1/2}\langle 2 | (\mathbf{d}, \, \mathbf{e}'^\pm) | 3\rangle.$$

Here $\mathbf{e}'^\pm$ and $\mathbf{e}_B'^\pm$ are the electric and magnetic polarization vectors of the right- or left-hand polarized photon. Let the photon be incident at an angle β to the direction of the constant magnetic field. Then

$$\mathbf{e}'^\pm = 2^{-1/2}(\mp \mathbf{e}_x - i\mathbf{e}_y \cos\beta + i\mathbf{e}_z \sin\beta_\cdot).$$

$$\mathbf{e}_B{}'^\pm = 2^{-1/2}(i\mathbf{e}_x \pm \mathbf{e}_y \cos\beta \mp \mathbf{e}_z \sin\beta). \tag{21}$$

Substituting Eq. (21) into Eq. (20) we obtain

$$(2\pi\omega)^{1/2}A^\pm = \begin{cases} \mp 2^{-1/2}\sin\beta[\,(1 - |\chi_p|^2)^{1/2}\langle 1|\mu_0|3\rangle \pm |\chi_p|\langle 2|d_0|3\rangle\,], \quad M' = M \\[4pt] {}^1\!/_2 i(1 \pm \cos\beta)[\,(1 - |\chi_p|^2)^{1/2}\langle 1|\mu_{-1}|3\rangle \mp |\chi_p|\langle 2|d_{-1}|3\rangle\,]. \\ M' = M - 1. \\[4pt] \mp {}^1\!/_2 i(1 \mp \cos\beta)[\,(1 - |\chi_p|^2)^{1/2}\langle 1|\mu_1|3\rangle \mp |\chi_p|\langle 2|d_1|3\rangle\,], \\ M' = M + 1. \end{cases} \tag{22}$$

In experiments performed with atomic systems summation over M' and averaging over M is usually presupposed. For $\beta = 0$ and $|\chi_p| \ll 1$ this gives

$$(2\pi\omega)^{1/2}\overline{A^\pm} = \pm i[\,\overline{\langle 1|\mu_{\pm 1}|3\rangle} \pm |\chi_p|\overline{\langle 2|d_{\pm 1}|3\rangle}\,]$$

and after substituting into Eq. (17) the interference term, which is proportional to χ_p, leads to the P-odd effect.

In our case, for $\beta = 0$ and $M' = M \pm 1$, 100% Faraday rotation arises. For $\beta \neq 0$ and $M' = M$, however, there is no such rotation and the rotation of the polarization plane is determined completely by the weak interaction:

$$\psi_{PNC} = \frac{l\mathcal{N}^2}{2\Delta_D}g(u, v)|\chi_p|(1 - |\chi_p|^2)^{1/2}\langle 1|\mu_0|3\rangle\langle 2|d_0|3\rangle\sin^2\beta. \tag{23}$$

Using the standard definition of the absorption length

$$L^{-1} = 2\omega\,\overline{\mathrm{Im}\,n} = 2\pi\mathcal{N}\frac{\omega}{\Delta_d}f(u, v)(|A^+|^2 + |A^-|^2), \tag{24}$$

where

$$f(u, v) = \mathrm{Re}\{\pi^{1/2}e^{-w}[1 - \Phi(-iw)]\} \tag{25}$$

[See Eq. (18)] an expression can be obtained for a convenient relative characteristic of the strength of P-odd effects—the angle of rotation of the polarization plane of light over the absorption length:

$$\psi_{PNC}^L = \frac{g(u, v)|\chi_p|(1 - |\chi_p|^2)^{1/2}\langle 1|\mu_0|3\rangle\langle 2|d_0|3\rangle}{4f(u, v)[\,|\chi_p|^2|\langle 1|\mu_0|3\rangle|^2 + (1 - |\chi_p|^2)|\langle 2|d_0|3\rangle|^2\,]}. \tag{26}$$

When setting up an experiment we must also take into account the Faraday rotation arising on the wings of transitions into states with $M' = M \pm 1$. Since the hyperfine interaction with a light nucleus is weak, one of the levels with $M' = M \pm 1$ lies near the level with $M' = M$. The splitting between these levels is $\sim 10^2$ MHz, while the Doppler width of the line is ~ 0.1–10^2 MHz with transition frequencies of ~ 1–10^3 cm^{-1}. The dependence on the angle β can be used to distinguish the P-odd rotation against the background of the Faraday rotation from the wings.

We note that aside from the correlation $(\mathbf{v}, \mathbf{s}_{ph})$ ($\mathbf{v}$ is the wave vector and $\mathbf{s}_{ph}$ is the spin of the photon) studied here, in an experiment it is also possible to observe another correlation, $(\mathbf{v}, \mathbf{b}_0)$, with constant polarization $\mathbf{s}_{ph}$ of the light.[18] Let the light be incident parallel to the external magnetic field ($\beta = 0$) and let, for example, $M' = M - 1$. In this case the light will undergo 100% Faraday rotation [see Eq. (22)], but when the propagating direction of the wave relative to the external magnetic field $\mathbf{B}_0$ is changed the absorption coefficient for the light changes and the following expression can be easily derived for the difference of the absorption lengths:

$$\frac{L_+{}^{-1} - L_-{}^{-1}}{L^{-1}} = \frac{|\chi_p|(1 - |\chi_p|^2)^{1/2}\langle 1|\mu_0|3\rangle\langle 2|d_0|3\rangle}{2[\,|\chi_p|^2|\langle 1|\mu_0|3\rangle|^2 + (1 - |\chi_p|^2)|\langle 2|d_0|3\rangle|^2\,]}. \tag{27}$$

We note that when the magnetic field is tuned exactly on crossing $|\chi_p| = 2^{-1/2}$ these effects will not contain the small contribution associated with the weak interaction and

therefore they will be three to six orders of magnitude stronger than the analogous effects in the absence of a magnetic field.[15] Formulas for the matrix elements appearing in Eqs. (21)–(25) are given in Appendix 2. In order to calculate the remaining electronic matrix elements of the magnetic and electric dipole moment operators it is necessary to have either experimental data on the oscillator strengths of the corresponding transitions or the results of calculations of the electronic structure of the corresponding states.

6. P-ODD STARK EFFECT

We now study an experiment analogous to the one which we proposed previously for atoms.[14] We assume that a molecule is placed in a constant magnetic field and a strong field of a plane-polarized wave. Because of parity nonconservation the correlation $(\mathbf{v}, \mathbf{b}_0)$ arises, where $\mathbf{v}$ is a unit vector pointing in the direction of propagation of the wave and $\mathbf{b}_0 = \mathbf{B}_0/|\mathbf{B}_0|$. When levels of opposite parity cross the magnitude of the shift of the quasi-energy levels $\propto (\mathbf{v}, \mathbf{b}_0)$ is once again significantly larger than in atoms. Because of the complicated structure of the spin-rotational states it is very difficult to calculate this effect, so that here we shall omit the formulas and give only an estimate. For $E \geqslant 10^4$ V/cm

$$\Delta W^{EB} \sim |\langle 1|H_p|2\rangle|, \tag{28}$$

where ΔW^{EB} is the shift occurring in the quasi-energy levels when the propagating direction of the wave is reversed. From the data of Table III we obtain

$$\Delta W^{EB} \sim 10^3 \text{ Hz}. \tag{29}$$

In the analogous atomic experiments the degree χ of uncontrollable circular polarization of the laser wave is severely restricted, thanks to which an imitation of the effect occurs. In this case this restriction is significantly weaker. Indeed, the linear Stark effect arising in the presence of χ is of the order of

$$\Delta W_\chi^{EE} \sim \frac{\chi E^2 \langle d\rangle^2 \omega}{\Delta E_{el}^2}, \tag{30}$$

where ΔE_{el} is the splitting between the electronic levels, E is the strength of the laser field, and $\langle d\rangle$ is the electric moment of the electronic transition. For diatomic molecules the typical values are $\langle d\rangle \sim 1$ a.u. and $\Delta E_{el} \sim 0.1$ a.u. Then the condition $\Delta W_\chi^{EE} \ll \Delta W^{EB}$ leads to

$$\chi \ll 10^{-1}-10^{-2}, \tag{31}$$

where we have set $\omega \sim 0.01$ a.u., which corresponds to a CO_2 laser.

In an experiment with molecules, however, there arises a different difficulty—imitation of the effect as a result of a shift of the levels owing to the standard Stark effect resulting from the instability of the laser field. The accompanying shift of the energy levels is of the order of

$$\frac{E\Delta E\langle d\rangle^2}{\Delta E_{el}},$$

whence

$$\frac{\Delta E}{E} \ll 10^{-2}-10^{-3}. \tag{32}$$

Apart from these conditions, the magnetic field must be tuned precisely on the crossing of the spin-rotational sublevels and the magnetic field must be highly stable, as we have already mentioned above.

CONCLUSIONS

We examined a number of P-odd effects in the molecules PbF and HgF. In order to observe these effects the constant magnetic field must be tuned precisely to the crossing of the levels. In addition, every experiment has its own difficulties and spurious effects. Some of them were discussed above, but a more detailed investigation is required.

It is hoped that the difficulties mentioned are not fundamental and can be overcome. We stress once again that the advantage of molecular experiments is that the magnitude of the effects is large.

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APPENDIX I. REDUCED MATRIX ELEMENTS FOR CALCULATING SPIN-ROTATIONAL SUBLEVELS IN A MAGNETIC FIELD

In the formulas presented below we assume everywhere that the nuclear spins are given by $I_1 = I_2 = \frac{1}{2}$. Then, using the standard angular-momentum apparatus[19] we can obtain the following expressions for the matrix elements appearing in Eqs. (12) and (13):

$$\langle JpF_1F\|BJ^2 + \Delta(\mathbf{sJ})\|J'pF_1'F\rangle$$

$$= \delta_{JJ'}\delta_{F_1F_1'}(2F+1)^{1/2}\{BJ(J+1)+{}^1\!/_4\Delta[1+\chi_J(2J+1)]\}, \tag{I.1}$$

where

$$\chi_J = \pm p(-1)^{J+1/2}.$$

Here the plus sign is taken for the ${}^2\Pi_{1/2}$ states and the minus sign is taken for the ${}^2\Sigma_{1/2}$ states;

$$\langle JpF_1F\|(\mathbf{I}_1, A_1\mathbf{s})\|J'pF_1'F\rangle = \delta_{F_1F_1'}(2F+1)^{1/2}(-1)^{F_1+J'+1/2}$$

$$\times \begin{Bmatrix} J & J' & 1 \\ {}^1\!/_2 & {}^1\!/_2 & F_1 \end{Bmatrix}\left(\frac{3}{2}\right)^{1/2}\langle J\|A_1\mathbf{s}\|J'\rangle, \tag{I.2}$$

$$\langle JpF_1F\|(\mathbf{I}_2, A_2\mathbf{s})\|J'pF_1'F\rangle$$

$$= [(2F+1)(2F_1+1)(2F_1'+1)]^{1/2}(-1)^{F+1}$$

$$\times \begin{Bmatrix} F_1 & F_1' & 1 \\ {}^1\!/_2 & {}^1\!/_2 & F \end{Bmatrix}\begin{Bmatrix} J' & {}^1\!/_2 & F_1' \\ F_1 & 1 & J \end{Bmatrix}\langle J\|A_2\mathbf{s}\|J'\rangle. \tag{I.3}$$

The matrix elements of the effective spin which appear here are given by the following formula:

$$\langle J\|A\mathbf{s}\|J'\rangle = \begin{cases} \dfrac{1}{4}\left[\dfrac{2J+1}{J(J+1)}\right]^{1/2}[A^\| + \chi_J A^\perp(2J+1)], & J'=J \\[3mm] \dfrac{1}{4}\left[\dfrac{(2J-1)(2J+1)}{J}\right]^{1/2}(A^\| + \chi_J A^\perp), & J'=J-1. \\[3mm] -\dfrac{1}{4}\left[\dfrac{(2J+1)(2J+3)}{J+1}\right]^{1/2}(A^\| - \chi_J A^\perp), & J'=J+1 \end{cases} \tag{I.4}$$

The reduced matrix element of the operator of the interaction with the constant magnetic field is as follows:

$$\langle JpF_1F\|\mathbf{Gs}\|J'pF_1'F'\rangle$$

$$= [(2F+1)(2F'+1)(2F_1+1)(2F_1'+1)]^{1/2}$$

$$\times (-1)^{F'+F_1+F_1'+J-1}\begin{Bmatrix} F_1' & 1/2 & F' \\ F & 1 & F_1 \end{Bmatrix}\begin{Bmatrix} J' & 1/2 & F_1' \\ F_1 & 1 & J \end{Bmatrix}\langle J\|\mathbf{Gs}\|J'\rangle,$$

(I.5)

and the reduced matrix element $\langle J\|\mathbf{Gs}\|J'\rangle$ is obtained analogously to Eq. (I.4).

APPENDIX II. MATRIX ELEMENTS OF THE EFFECTIVE WEAK INTERACTION AND OF THE MAGNETIC AND ELECTRIC DIPOLE MOMENTS

After diagonalizing the operator H_{sr} and H_F we obtain states which we write in the form

$$|n, pM\rangle = \sum_{JF_1F} C^n_{JF_1F}|JpF_1FM\rangle.$$

(II.1)

The coefficients $C^n_{JF_1F}$ are obtained by means of a numerical calculation. Then the matrix element of the operator $\hat{A}$ between two such states can be written as

$$\langle 1, pM|\hat{A}|2, p'M\rangle$$

$$= \sum_{JF_1F}\sum_{J'F_1'F'} C^1_{JF_1F}C^2_{J'F_1'F'}\langle JpF_1FM|\hat{A}|J'p'F'F_1'M\rangle. \quad (II.2)$$

For the operator $\hat{A}$ we shall study H_p, μ_α, and d_α. For the operator H_p appearing in Eq. (II.2) the matrix elements are given by the following formulas:

$$\langle JpF_1FM|H_p|J'-pF_1'F'M\rangle = -1/4 iW \varkappa \delta_{F_1F_1'}\delta_{FF'} \cdot$$

$$\cdot \left(\frac{3}{2}\right)^{1/2}\begin{Bmatrix} J & J_1 & 1 \\ 1/2 & 1/2 & F_1 \end{Bmatrix}(-1)^{F_1+J'+1/2}\chi_J X_{JJ'}, \quad (II.3)$$

where

$$X_{JJ} = (2J+1)[(2J+1)/J(J+1)]^{1/2},$$

$$X_{J, J-1} = X_{J-1, J} = [(2J+1)(2J-1)/J]^{1/2}. \quad (II.4)$$

We shall now examine the operator μ_α (analogous formulas are valid for the operator d_α). Now the states acquire an additional index $n(m)$ which labels the corresponding electronic state. Separating the dependence on the projections, we obtain

$$\langle nJpF_1FM|\mu_\alpha|mJ'pF_1'F'M\rangle$$

$$= \frac{C^{FM}_{F'M'1\alpha}}{(2F+1)^{1/2}}\langle nJpF_1F\|\mu\|mJ'pF_1'F'\rangle. \quad (II.5)$$

The dependence on the nuclear spins is also easily singled out (we neglect here the nuclear magneton):

$$\langle nJpF_1F\|\mu\|mJ'pF_1'F'\rangle$$

$$= [(2F+1)(2F'+1)(2F_1+1)(2F_1'+1)]^{1/2}$$

$$\times(-1)^{F+J+F_1+F_1'-1}\begin{Bmatrix} F_1' & 1/2 & F' \\ F & 1 & F_1 \end{Bmatrix}\begin{Bmatrix} J' & 1/2 & F_1' \\ F_1 & 1 & J \end{Bmatrix}\langle nJp\|\mu\|mJ'p\rangle.$$

(II.6)

In (II.6) we set $I_1 = I_2 = \frac{1}{2}$. To calculate the dependence of J we shall express the states with definite parity in terms of states with definite projection of the total angular momentum Ω on the molecular axis (using the phase conventions adopted in this paper):

$$|nJpM_J\rangle = 2^{-1/2}[|nJ; +|\omega|; M_J\rangle \pm p(-1)^{J+|\omega|}|nJ; -|\omega|; M_J\rangle],$$

(II.7)

where the plus sign is taken for $^2\Pi_{1/2}$ states and the minus sign is taken from $^2\Sigma_{1/2}$ and $^2\Pi_{3/2}$ states. The reduction of the matrix elements $\langle nJ\omega\|\mu\|mJ'\omega'\rangle$ to purely electronic matrix elements is made using formulas that are analogous to those presented in Ref. 20.

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