ant with respect to rotations of the plane, we have

$$F''-2u^2F=0, \quad u''+(F^2-u^2)u=0. \tag{8}$$

The fields which decrease at infinity have the following asymptotic behavior:

$$u=2^{1/2}/z, \quad F=kz^{-1}, \quad s=((17)^{1/2}-1)/2.$$

By means of a scale transformation the quantity k can be reduced to unity. The qualitative behavior of F and u in this case remains the same as for the preceding solution. The corresponding calcualtions carried out on a computer are represented in the figure by curves with the subscript 2. The values of the invariant energies for the first extrema are listed in the table.

Thus, the example we have considered proves the existence of multiple solutions for the YM equations for prescribed charges, solutions which differ from the Coulomb solution and contain a "magnetic" field, and illustrates the localization of the fields near the charges. The characteristic length of decay of the fields can be expressed in terms of the Planck constant and the fundamental YM charge g if one goes over from dimensionless quantities to dimensional ones:

$$l_0 = \left(\frac{\hbar c}{g^2}\right)^{1/2}\left(\frac{g}{\sigma}\right)^{1/2}$$

and decreases as the charge density is increased. Such a dependence is essential for an analysis of fields created by a point charge if the latter is considered as the limit of a charged sphere of radius R as $R \to 0$.

Since

$$\sigma = Q/4\pi R^2,$$

the fields will fall off at distances

$$l_0 = R(\hbar c/gQ)^{1/2} \tag{9}$$

and in the limit will become unobservable.

The expression (9) bears witness of the strongest self-screening of macroscopic charges (even if one assumes that there is no self-screening of elementary charges). Indeed, for elementary particles

$$\hbar c/g^2 \approx 1.$$

When the charge is created by a macroscopic ($Qg \gg 1$) number of charges, the field can be observed in a layer of thickness $l_0 \ll R$ (which in fact justifies the use of the plane results for a macroscopic sphere).

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Parity breaking effects in diatomic molecules

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It is shown that effects of nonconservation of time and space parities in molecules are considerably enhanced owing to the presence of closely spaced rotational levels of opposite parities. The enhancement factor of the intrinsic electric dipole moment of the electron reaches values of 10^7 to 10^{11}. The degree of circular polarization of the photons from allowed M1 transitions amounts to 10^{-3}, and the optical activity of molecular vapors to 10^{-7} rad/m. In such experiments, now quite feasible, the coupling constant for the weak interaction between the electronic vector current and the nucleonic axial-vector current can be measured. Experiments to measure this constant in heavy atoms are very complicated.

1. INTRODUCTION

As is well known, diatomic molecules have very closely spaced levels of opposite parities. This is the so called Λ or Ω doubling of rotational levels with given total angular momentum J. In the present paper it is shown that a mechanism based on this close spacing of levels enhances T-odd and P-odd effects. Recently we have seen a paper by Labzovskii[1] on the calculation of P-odd effects in molecules. In the part dealing with enhancement of these effects, our results in principle overlap to a considerable extent with those

of Labsovskiĭ. An important difference is that we discuss experiments of a different kind, more promising in our opinion, and also consider the enhancement of the electric dipole moment (EDM) of the electron.

In molecules there is enhancement of the part of the weak interaction caused by the product of the electronic vector and the nucleonic axial-vector currents. This interaction gives a contribution proportional to Z^2 (Ref. 2). The enhancement factor for the EDM of the electron increases in proportion to Z^3 (Refs. 3-5). Therefore we shall consider molecules in which one of

the atoms is heavy. The spin-orbit interaction in such molecules is comparable with the splitting between states with different values of Λ (the case intermediate between Hund's case a and c, Ref. 6, and it is convenient to carry out the classification of the electronic terms in terms of the component Ω of the total electronic angular momentum along the axis of the molecule.

Let us recall how the splitting of levels of opposite parity arises. We consider first the simplest case $|\Omega| = \frac{1}{2}$. For crude estimates we can suppose that the the total angular momentum of the electrons is also $j = \frac{1}{2}$ (Hund's case c). The levels with $\Omega = \frac{1}{2}$ and $\Omega = -\frac{1}{2}$ are degenerate, so that the electronic angular momentum is decoupled from the axis of the molecule; i.e., it can be quantized along any axis. Let L be the angular momentum of the rotation of the nuclei. It is obvious that for a given total angular momentum J there are two states: $L_1 = J - \frac{1}{2}$ and $L_2 = J + \frac{1}{2}$, which have different parities. The characteristic splitting is

$$\Delta E \sim BL_1(L_1+1) - BL_2(L_2+1) = 2B(J+\tfrac{1}{2}), \quad B = \hbar^2/2I,$$

where I is the moment of inertia of the molecule. For example, for the molecule BiS we have $\Delta E = 0.11 \times (J+\frac{1}{2})$ cm^{-1} (Ref. 7), which is four to six orders of magnitude smaller than the separation of levels of opposite parity in heavy atoms.

For accurate calculation it is convenient to write the wave function of a diatomic molecule in terms of the D functions of the symmetrical top[6-8]:

$$|JM\omega\eta\rangle = \left(\frac{2J+1}{8\pi}\right)^{1/2} \{ D_{-\omega M}^{J}(\varphi, \theta, 0)|\omega\rangle$$
$$+ \eta(-1)^{J-\omega} D_{-\omega M}^{J}(\varphi, \theta, 0)|-\omega\rangle\}, \quad \omega = |\Omega|. \tag{1}$$

Here J and M are the total angular momentum and its component along the z axis, Ω is the projection of the angular momentum along the axis of the molecule, and η is the parity of the state ($\eta = \pm 1$): $|\omega\rangle$ and $|-\omega\rangle$ are the corresponding internal states of the molecule. The operator of the centrifugal energy is given by

$$H_\mu = B(\mathbf{J}-\mathbf{j})^2. \tag{2}$$

The matrix elements for the states (1) are calculated by the standard method.[6,8] In first order in H_B the splitting between levels of opposite parity is

$$\Delta E = E_+ - E_- = 2(-1)^{J+\omega} B(J+\omega)\langle\omega|j_+|-\omega\rangle, \tag{3}$$

where $j_+ = j_x + ij_y$ is a component of the operator j in a system attached to the molecule. It is clear that $\Delta E \neq 0$ only for $\omega = \frac{1}{2}$. For $\omega > \frac{1}{2}$ the splitting is different from zero in a higher order in H_B (Ref. 6).

$$\Delta E \sim BJ^{2\omega}(B/\varepsilon)^{2\omega-1}, \tag{4}$$

where ε is the characteristic distance between electronic terms of the molecule, $\varepsilon/B \sim M_{\text{Mol}}/m_e$. We recall that we are dealing with molecules with strong spin-orbit interaction. In the opposite case there can be another reason for the splitting to be small.

2. T-ODD EFFECTS. ENHANCEMENT OF THE ELECTRIC DIPOLE MOMENT OF THE ELECTRON

The interaction of the EDM of the electron with the electric field of the molecule breaks T and P parity and leads to a mixing of the states (1) of opposite parity. The matrix elements of this interaction H_d, found for the states (1) by standard techniques,[6,8] reduce to the matrix elements for the states of the fixed molecule, $\langle\Omega|H_d|\Omega\rangle$ and $\langle\Omega|H_d|-\Omega\rangle$. Since the operator H_d is T-odd and is a pseudoscalar, we have

$$\langle\Omega|H_d|\Omega'\rangle \sim \delta_{\Omega\Omega'}\cdot\Omega = \delta_{\Omega\Omega'}(\mathbf{Jn}), \tag{5}$$

where $\mathbf{n}$ is the direction of the axis of the molecule. We carry out calculations for the specific molecule BiS ($\omega = \frac{1}{2}$), for which the spectrum is well known (Ref. 7). In this case only the T-odd interaction of the electron with the Bi nucleus is important. According to Ref. 7 we can consider that in the ground state of BiS there is one unpaired electron, concentrated mainly on the bismuth atom. The electric field of the other atom leads to a mixing of different electronic states:

$$|\tfrac{1}{2}\rangle = a|s_{\frac{1}{2}}, j_z = \tfrac{1}{2}\rangle + b|p_{\frac{1}{2}}, j_z = \tfrac{1}{2}\rangle + c|p_{\frac{3}{2}}, j_z = \tfrac{1}{2}\rangle + \dots \tag{6}$$

The coefficients a, b, and c are real, and $a \sim b \sim c$. Using the results of Ref. 5, we can write the matrix element of H_d in the form

$$\left\langle \frac{1}{2} \middle| H_d \middle| \frac{1}{2} \right\rangle \approx -2ab \frac{4(Z\alpha)^2 Z|e|d_e}{\gamma(4\gamma^2-1)a_B^2(\nu_s\nu_{p_{1/2}})^{3/2}}. \tag{7}$$

Here ν_i is the effective principal quantum number of the electron, $\gamma = [1 - (Z\alpha)^2]^{1/2}$, d_e is the dipole moment of the electron, e is its charge, and a_B is the Bohr radius.

The presence of the intrinsic dipole moment d_M of the polar molecule does not in itself lead to a linear Stark effect in a stationary state with fixed total angular momentum **J**. However, the P-odd and T-odd mixing of the rotational states (1) brings about a correlation between d_M and the total angular momentum **J**. Thus in the stationary state a dipole moment

$$\mathbf{d} = \frac{2\omega d_M\langle\omega|H_d|\omega\rangle}{\Delta E_{J,\eta}} \frac{\mathbf{J}}{J(J+1)} \tag{8}$$

arises. For the BiS molecule we have $\Delta E_{J,\eta} = (-1)^{J+1/2} (J+\frac{1}{2})\eta \cdot 0.11$ cm^{-1}. The matrix element for the mixing is given by Eq. (7). For the numerical estimates we set $-2ab = 1$, $d_M = 0.5|e|a_B$, and $\nu_s = \nu_p = 1.5$ (this is a typical value of ν for the external electrons in Bi). Then the enhancement factor of the dipole moment of the electron is given by

$$R = \frac{d}{d_e} = 3\cdot10^7 \frac{(-1)^{J+1/2}\eta}{(J+\frac{1}{2})(J+1)}. \tag{9}$$

A fact that may be important from the experimental point of view is that R changes sign on going to a level with different parity η or on changing J by unity.

Let us now consider the case $\omega > \frac{1}{2}$. The energy denominator ΔE in Eq. (8) decreases rapidly with increasing ω (see Eq. (4)). Therefore R can be as large as 10^{11} even for ω as small as 1. Naturally, there are limitations on the minimum possible value of ΔE. The

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most obvious of these is that for large ω the levels will be moved apart by the external electric field. For a given ΔE this puts a restriction on the field. For BiS we find that one must require $E \lesssim 10^4 J^2$ V/cm.

We note that there is a definite relation between the mechanism of enhancement of the EDM of the electron considered here and a method for measuring the EDM of the proton proposed by Sandars[9] (the measurements are reported in Ref. 10). Sandars' idea[9] was that if one polarizes the TlF molecule with an outside electric field, then the strong intramolecular electric field will be directed along the external field, so that in fact the outside field is increased. It is clear that the mechanisms of enhancement considered in Ref. 9 and in the present paper relate to the respective cases when the interaction with the external field is strong or weak compared with the rotational energy spacings.

Usually experiments searching for evidence of a dipole moment are done with atomic or molecular beams through measurements of the linear Stark effect. We call attention to the possibility in principle of detecting T-odd effects by observing an optical activity of an atomic or molecular vapor in an electric field (analog of the Faraday effect).

3. P-ODD EFFECTS. CIRCULAR POLARIZATION OF PHOTONS AND OPTICAL ACTIVITY OF MOLECULAR VAPORS

Like the T-odd effects, the P-odd effects in molecules are also enhanced owing to the mixing of rotational states (1) of different parities. Considering that the weak-interaction Hamiltonian H_w is T-even and Hermitian, it is not hard to verify that $\langle \Omega | H_w | \Omega \rangle = 0$. On the other hand, the nondiagonal matrix element $\langle \Omega | H_w | - \Omega \rangle$ is different from zero. The operator H_w contains parts dependent on and independent of the nuclear spin,[2] i.e.,

$$H_w = s + \mathbf{V} \mathbf{I}_{nuc}. \tag{10}$$

It is clear that the matrix element $\langle \Omega | H_w | - \Omega \rangle$ is different from zero only for $\omega = \frac{1}{2}$, and that the only contribution is that of the second term, which is a vector in the electronic variables.[1] Accordingly, in molecules there is enhancement of the part of the weak interaction involving the product of the electronic vector current and the nucleonic axial-vector current.

Using the wave functions (6) and the results of Ref. 2, we can write the matrix element of the weak interaction in the following form:

$$\left\langle \frac{1}{2} \left| V_+ \right| - \frac{1}{2} \right\rangle = 2iabg_1 \frac{2\gamma+1}{3} \frac{Gm_e^2 \alpha^2 Z^2 R}{\pi (\nu_x \nu_{p_{1/2}})^{3/2}} \frac{m_e e^4}{2\hbar^2}. \tag{11}$$

Here $V_+ = (-V_x - iV_y)/2^{1/2}$, $G = 10^{-5}/m_p^2$ is the Fermi constant,

$$R = 4 \left(\frac{2r_0 Z}{a_B} \right)^{2\gamma-2} \Big/ [\Gamma(2\gamma+1)]^2$$

is a relativistic factor, r_0 is the radius of the nucleus, $g_1 = \kappa_N \langle \sigma_N \rangle$, $\langle \sigma_N \rangle$ is the mean value of the spin of the outer nucleon, and κ_N is the quantity to be determined in the experiment, the constant of the weak interaction

between the electronic vector current and the nucleonic axial-vector current. In bismuth $R = 9.4$, $\langle \sigma_p \rangle = 2/11$; in the Weinberg model, $\kappa_p = (2\sin^2\theta - \frac{1}{2})\lambda$, where $\lambda = 1.25$ is the renormalization constant for the axial current and $\sin\theta$ is a parameter of the model.

The further calculations are carried out with standard technique.[8] With the level with fixed J, η and total angular momentum $F (F = J + I)$ there are admixed states with the same F but parity $-\eta$, and with angular momenta $J - 1$, J, $J + 1$. We do not write out the expressions for the mixing coefficients because they are cumbersome.

Let us now consider transitions between the hyperfine-structure components of the ground state X ($\omega = \frac{1}{2}$) and the first excited state A ($\omega = \frac{1}{2}$) of the BiS molecule. The wave lengths of these transitions lie in the range 5500–8000 Å (Ref. 7), depending on the vibrational and rotational levels between which a transitions occurs. According to the electronic selection rules the transition $X \to A$ can occur either as $E1$ or as $M1$. If we consider a transition between rotational levels of the same parity ($\eta \to \eta$), it is an $M1$ transition. A transition $\eta \to -\eta$ is $E1$. Let us consider the optical activity of BiS vapor near $M1$ transitions. Owing to the already discussed mixing of levels of the opposite parity with the group state of the BiS molecule, a small amount of $E1$ is added to the $M1$ amplitude. Numerical estimates show that in the excited state the mixing is small and can be neglected. The calculations of the $M1$ and $E1$ amplitudes can be carried out by means of standard techniques of the theory of angular momentum.[8] For the numerical calculations we take the following values of the electronic matrix elements:

$$\langle A, \tfrac{1}{2} | D_z | X, \tfrac{1}{2} \rangle = ea_B \qquad \langle A, \tfrac{1}{2} | M_+ | X, -\tfrac{1}{2} \rangle = \mu_B \tag{12}$$

The matrix elements $\langle A, \frac{1}{2} | M_z | X, -\frac{1}{2} \rangle$ and $\langle A, \frac{1}{2} | D_+ | X, -\frac{1}{2} \rangle$ in BiS are markedly suppressed owing to the structure of the electronic states.[7] The largest value of the square of the overlap of the vibrational wave functions (the Franck-Condon factor) is ~ 0.2 (transitions $v_x = 0, 1 \to v_A = 6$, 7, 8). As to the rotational and hyperfine states, the most favorable transitions for observing the optical activity are $|X, J, F = J + I\rangle \to |A, J \pm 1, F = J \pm 1 + I\rangle$. The degree of circular polarization is

$$P = -2 \operatorname{Im} \frac{\langle D \rangle}{\langle M \rangle}. \tag{13}$$

In these transitions $P \sim 5 \cdot 10^{-4} \kappa_p/(J+1)$. The angle of rotation of the plane of polarization of light in BiS vapor for large J does not depend on J and amounts at temperature $1200°$ C and pressure 100 mm Hg to $\psi \sim 0.7 \cdot 10^{-7} \kappa_p$ rad/m.[2]

We call attention to the fact that the optical activity of BiS vapor turns out to be an order of magnitude smaller than that of Bi vapor,[11] although the degree of circular polarization is BiS is 3 to 4 orders of magnitude larger than in Bi. This is due to the fact that the $T = 1200°$ C many rotational levels of the molecule are excited:

$$Z = (2I+1) \sum_v e^{-\hbar\omega v/T} \sum_J (2J+1) e^{-BJ(J+1)/T} = 2.8 \cdot 10^5, \tag{14}$$

and therefore each particular level from which a transition occurs has a small population.

The BiS molecule, which we have considered as an example, is evidently not the best one from the experimental point of view, even among molecules with $\omega = \frac{1}{2}$. In it the effect is suppressed by about an order of magnitude because of the large angular momentum of the Bi nucleus. Most molecules, indeed, have $\omega = 0$ in the ground state. However, if the excited state to which the transition goes has $\omega = 1$, the case is one in which the effect will be of the same order as in a molecule with $\omega = \frac{1}{2}$. In fact, for $\omega = 1$ the matrix element of the mixing is of the form

$$\frac{\langle 1|H_w|0\rangle\langle 0|H_s|-1\rangle}{E_1 - E_0} \sim \left\langle \frac{1}{2}|H_w|-\frac{1}{2}\right\rangle \frac{B}{\varepsilon} J, \tag{15}$$

where H_B is the centrifugal energy operator; Eq. (2). However, the smallness of the factor B/ε in the matrix element is compensated by a similar smallness of the splitting of levels of different parities (see the Introduction).

We call attention to the fact that the optical activity of molecules can also be studied in the rf range in transitions between rotational levels and between hyperfine-structure levels.

In conclusion we remark that a two-center system similar to a molecule in a definite rotational state is formed during nuclear fission. In such a system, as shown in this paper, T-odd effects are greatly enhanced. As for P-odd effects in fission, the mechanism we have considered here cannot be directly transferred to this phenomenon because of the strong spin-spin interaction.

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[1] We point out that if, owing to nonsphericity of the nucleus, there is a tensor interaction $H_w = T_{ik} I_i I_k$, it may be enhanced relative to the vector interaction by 4 or 5 more orders of magnitude. The point is that $\langle \Omega | T_{ik} | -\Omega \rangle \neq 0$ for $\omega = 1$, and the splitting for a level with $\omega = 1$ is 5 orders of magnitude smaller than that of one with $\omega = \frac{1}{2}$.

[2] In these calculations we have assumed that the collision broadening of the lines is smaller than the Doppler broadening.

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Dielectronic recombination of electrons in collisions with ions

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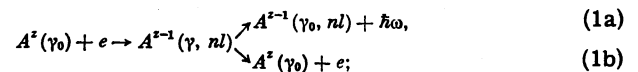(Submitted 10 January 1978)
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A simple expression is obtained for the dielectronic recombination coefficient of electrons colliding with partly ionized ions. The results are in good agreement with numerical calculations of the dielectronic recombination coefficients carried out by other authors.

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1. INTRODUCTION

Dielectronic recombination (DR) is known[1-5] to occur in the course of radiative stabilization [described by Eq. (1a) below] of an autoionizing state of an ion $A^{z-1}(\gamma, nl)$ formed on collision of an electron with an ion in a state $A^z(\gamma_0)$:

$$A^z(\gamma_0) + e \to A^{z-1}(\gamma, nl) \begin{cases} \nearrow A^{z-1}(\gamma_0, nl) + \hbar\omega, & \text{(1a)} \\ \searrow A^z(\gamma_0) + e; & \text{(1b)} \end{cases}$$

here, z is the ionic charge; γ_0 and γ are the quantum numbers of the ground and excited states of the A^z ion.

The important role played by DR in a high-tempera-