Energy difference between right-hand and left-hand molecules, due to parity nonconservation in weak interactions of electrons with nuclei

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Possible manifestations of parity nonconservation, due to weak interaction of electrons with nuclei, are widely discussed in atomic and moleceular phys-

ics. [1–3] Principal attention is being paid to the difference between the optical properties of light with right-hand and left-hand circular-polarization.

In this paper we ascertain the extent to which this interaction can lead to a difference between the energies of the right and left modifications of molecules capable of existing in two such forms. [1]

The Hamiltonian of the P-odd weak interaction of an electron with a nucleus will be written in the form (see[2])

$$W = - \frac{G\hbar^3 q}{2\sqrt{2}\, mc^2} Z [(\vec{\sigma}\, \mathbf{p})\delta\, (\mathbf{r}) + \delta(\mathbf{r})(\vec{\sigma}\, \mathbf{p})] , \tag{1}$$

where $G = 10^{-5}/m_p^2$ is the Fermi constant, m_p and m are the masses of the proton and electron, Z is the charge of the nucleus, $\frac{1}{2}\sigma, \mathbf{p}, \mathbf{r}$ are the spin, momentum, and coordinate of the electron, and $q \approx -0.9$ is a factor. We are interested in the correction of first order in W to the molecule energy. It is easy to verify that this correction can differ from zero only for molecules that have neither a symmetry center nor a symmetry plane, nor any other mirror-rotation symmetry axis, i.e., for molecules having right-hand and left-hand modifications. In the latter case, the correction to the energy, which is proportional to W, has opposite signs for the right and left forms of the molecules. We recall that inversion of the coordinates of all nuclei (or reflection in a plane) transforms a right-hand molecule into a left-hand molecule and vice versa.

The sought splitting must depend explicitly on the magnetic interactions involving the electron spin, particularly by spin-orbit interaction. This is seen from the fact that in the absence of such interactions the wave function takes the form of a product of a coordinate function and a spin function and the coordinate part of the diagonal matrix element of the operator $\sigma[\mathbf{p}\delta(\mathbf{r}) + \delta(\mathbf{r})\mathbf{p}]$ vanishes. Indeed, although W is invariant to time reversal, only the coordinate part of W reverses sign when t is replaced by $-t$.

In accordance with[1–3], the role of the interaction of W in the atom increases rapidly with increasing Z, approximately $\propto Z^3$. The largest splittings should therefore be expected in molecules containing a heavy atom. For heavy atoms, as is well known, the main contribution to the magnetic interaction is made by the coupling of the electron spin with the charge of the heavy nucleus—the spin orbit interaction V_{s0} which is of the order of $\mathrm{Ry}\,\alpha^2 Z^2$, where $\alpha = 1/137$ and $\mathrm{Ry} = me^4/2\hbar^2$. It is seen from the foregoing that, for example for the singlet term, the correction ΔE should be of the form $\langle S | W | T \rangle \langle T | V_{so} | S \rangle \Delta E_{ST}^{-1}$, where $\langle S |$ and $\langle T |$ are the singlet and the triplet states, respectively. Further calculation calls for expansion of the functions $\langle S |$ and $\langle T |$ in the atomic states and for estimates of the coefficients of this expansion. It is more convenient to make these estimates by considering an atom in an arbitrary electrostatic field.

Let us see what electrostatic-field structure should be produced by the other atoms of the molecule in order for the resultant correction to the energy to be different from zero. We consider the motion of an electron in a centrally-symmetric field of a heavy atom, and take the electrostatic field

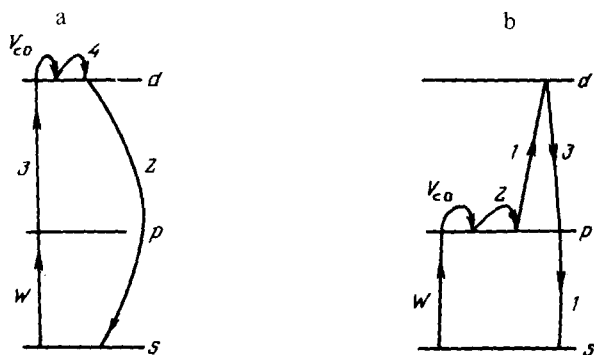$$\phi (\mathbf{r}) = \sum_{\kappa\, m} r^\kappa\, Y_{\kappa m}(\mathbf{r}/r)\, A_{\kappa m} \tag{2}$$

FIG. 1. The arrows joining the levels s, p, and d are labeled by the successive-ly turned-on perturbations: W—weak, V_{so}—spin orbit, $1, 2, 3, 4$—electrostatic multiple of the corresponding rank.

into account within the framework of perturbation theory. The correction of first order in W, of first order in V_{so}, and of kth order in the electrostatic field should contain the product of k multipole-expansion constants $A_{\kappa m}$ from (2). Owing to the invariance to rotations and to the fact that W is a pure scalar, the answer should contain a pseudoscalar combination of products of $A_{\kappa m}$. It turns out that this requirement can be satisfied by regarding only the third and high-er orders of perturbation theory in ϕ from (2). For example, in third order we have

$$\Delta E \sim \sum_{m_1 m_2 m_3} A\kappa_1 A\kappa_2 A\kappa_3 \begin{pmatrix} \kappa_1 & \kappa_2 & \kappa_3 \\ m_1 & m_2 & m_3 \end{pmatrix}, \qquad \kappa_1 + \kappa_2 + \kappa_3 = 2g + 1 . \tag{3}$$

Equation (3) contains a $3j$-symbol with an odd value of the sum $\kappa_1 + \kappa_2 + \kappa_3$. It is important that all three values κ_1, κ_2, κ_3 must be different, for otherwise the sum (3) vanishes by virtue of the symmetry properties of $3j$ symbols. The choice of the lowest multipolarities κ_1, κ_2, κ_3, satisfying these requirements is 2, 3, 4. In fourth order in ϕ, the pseudoscalar can be constructed with a lower sum of multipolarities $(\kappa_1, \kappa_1, \kappa_2, \kappa_3) = (1, 1, 2, 3)$. In order of magnitude we have $A_{\kappa m} \sim eR^{-\kappa-1}$, where e is electron charge and R is the characteristic linear di-mension of the charges making up the field ϕ. Using the known results of the calculations of the matrix elements $\langle s \mid W \mid p \rangle \sim \mathrm{Ry}\, 10^{-10} (Z/100)^3$ (see, e.g., [12]) and also estimates of the spin-orbit splitting in a state with orbital angular momentum l and effective principal quantum number n_*, [5] namely ΔE_{s0} $= \mathrm{Ry}\, \alpha^2 Z^2 [n_*^2 l(l+1)(l+\frac{1}{2})]^{-1}$, we can write down the following estimate of the ener-gy shift of interest to us:

$$\Delta E \sim 10^{-10} \mathrm{Ry} \left(\frac{Z}{100}\right)^5 [n_*^2 l(l+1)(l+\tfrac{1}{2})]^{-1} \left(\frac{\mathrm{Ry}}{E_{ik}}\right)^k \left(\frac{a}{R}\right)^{\sum_i \kappa_i} , \tag{4}$$

where E_{ik} are the energy denominators. It is seen that the largest values of ΔE are obtained by choosing such a chain of perturbation-theory virtual states, for which the spin-orbit splitting of the level enters with the lowest values of

$\iota_* l$. It turns out, however, that the choice of this level predetermines the same set of multiples $A_{\kappa m}$, which is represented in (4).

Figure 1 shows, by way of example, two chains of transitions through virtual level that arise when the s-level shift is calculated. In case a, the spin-orbit interaction is turned on at the level d and the lowest set of multipolarities turns out to be $(\kappa_1, \kappa_2, \kappa_3) = (2, 3, 4)$. In case b, the spin-orbit interaction is turned on at the level p, where it is approximately one order of magnitude larger, and the set of multipolarities corresponds to $(\kappa_1, \kappa_2, \kappa_3, \kappa_4) = (1, 1, 2, 3)$.

We shall use formula (4) to estimate the possible values of the energy difference ΔE between the right-hand and left-hand forms of the molecule. The most favorable is the situation wherein a heavy atom is bound to at least three different atoms that do not lie in one plane. In this case $(a/R)(\text{Ry}/E_{ik}) \sim 1$. This means that in the expansion of the molecular states in the atomic ones, the states s, p, and d are represented with approximately equal weight. Assuming also $[n_*^2 l(l+1)(l+\tfrac{1}{2})]^{-1} \sim 10^{-1}$ for the p states, we obtain

$$\frac{\Delta E}{2\pi\hbar} \sim 10^4 \left(\frac{Z}{100}\right)^5 \text{ Hz}. \qquad (5)$$

Thus, although the discussed effect arises only in relatively high orders of perturbation theory in the electrostatic interaction, and calls in each actual case for inclusion of a rather special set of multipoles of high rank and the spin-orbit interaction, the energy shift ΔE turns out to be far from very small. Owing to the Z^5 dependence, this pertains, of course, only to the heaviest atoms. In the case of molecules containing a heavy atom such as lead, one can count on a shift up to several kHz. Modern laser technology makes it possible, in principle, to determine frequency shifts of this size (see, e.g., [6]). We note also that the potential-well deformation due to the electron energy increment $\Delta E(R)$ leads for such molecules to a shift in the vibrational and rotational frequencies Ω_v and Ω_r by an amount $\Delta\Omega_v/\Omega_v \approx \Delta\Omega_r/\Omega_r \approx \Delta E/\text{Ry} \approx 10^{-12}$.

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[1] We note that the existence of such a difference between the energies of right-hand and left-hand molecules was postulated in [4] in connection with certain problems of chemistry and biology.

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