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ISOMERS CAUSED BY PARITY NON-CONSERVATION
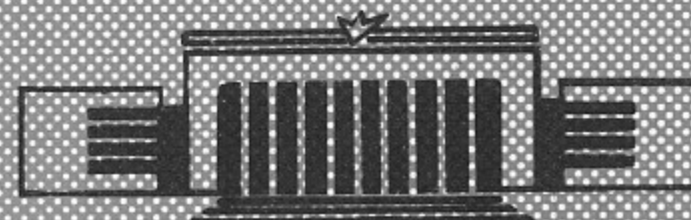
ON ENERGY DIFFERENCE BETWEEN OPTICAL
ISOMERS CAUSED BY PARITY NON-CONSERVATION

I.B.Khriplovich

Institute of Nuclear Physics
630090, Novosibirsk 90, USSR

A b s t r a c t

A model is considered demonstrating how energy difference
between optical isomers arises due to parity non-conserving
weak interaction of electrons with nucleus. The splitting of
Mössbauer line in mirror image crystals is discussed.

The discovery of neutral current weak interaction of electrons with nucleons, made at Novosibirsk [1] by observing optical activity of atomic bismuth vapour, is of course only the first positive result in the investigation of the weak interactions structure by the methods of atomic and molecular spectroscopy. The studies, both theoretical and experimental, in this direction are pursued now by many groups. One of the most beautiful manifestations of the weak interactions in atomic and molecular physics is energy difference between optical isomers caused by parity non-conservation. This effect of neutral currents which still has not been observed experimentally was predicted in the refs. [2-4]*).

The mentioned phenomenon is so surprising and unusual that even recently doubts in the very possibility of its existence were expressed. In the present work a relatively simple model of the effect discussed is considered. It allows one to trace explicity how the effect arises. The splitting of Mössbauer line in mirror image crystals is also discussed.

2. We start the exposition from simple order of magnitude estimates for the effect expected. Its origin becomes quite obvious if one takes into account that parity non-conserving weak interaction between electron and nucleus leads to helix structure in the spin orientation of atomic electron [6,7]. It is quite natural that the energy of a molecule is different in the cases when its structural, coordinate helix is the same as the spin one and when these helices are opposite. It can be said

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*) I take the opportunity to note that the definition of charged and neutral currents of weak interactions, given in the refs. [4,5], differs considerably from the common one.

that the spin helix is a peculiar asymmetric testing object with which one can tell a right-handed molecule from a left-handed one. By the way, it is clear from this picture that the level splitting can arise only due to interaction between spin and coordinate degrees of freedom, i.e., due to spin-orbit coupling. This fact was for the first time discovered by means of somewhat other considerations in the ref.[3]. However, in heavy molecules the connection of the phenomenon discussed with spin-orbit coupling does not lead to additional suppression in the magnitude of the effect since fine structure splitting is quite comparable in them with the electrostatic interaction.

The magnitude of the splitting is determined by the matrix element of weak parity-violating electron-nucleus interaction. This matrix element does not vanish only if it is taken between $s_{1/2}$ and $p_{1/2}$ states. By an order of magnitude it is

$$\delta E \sim \frac{Gm^2\alpha^2 Z^3 R}{\pi}\, \frac{m\alpha^2}{2} \qquad (1)$$

Here $G=10^{-5}/m_p^2$ is the Fermi weak interaction constant; m_p and m are proton and electron masses; $\alpha = 1/137$ is the fine structure constant; Z is the nucleus charge; the enhancement factor $R=4(2Z\alpha mr_0)^{2\gamma-2}/\Gamma^2(2\gamma+1)$ is caused by relativistic effects, it grows rapidly at large Z reaching values ~ 10 at $Z \sim 80$; r_0 is the radius of nucleus; $\gamma = \sqrt{1-Z^2\alpha^2}$. The system of units where $\hbar = 1$, $c = 1$ is used. It is natural to expect however that the relative distortion of a wave function due to the asymmetry of the environment is considerably smaller than unity. Therefore, the true splitting should be perhaps by 1÷2 orders of magnitude smaller than the estimate (1). Taking into account this circumstance, we find that in molecules containing heavy atoms with $Z \sim 80$ the value of δE can reach $10^4 \div 10^5$ Hz.

In light molecules the dependence of the effect on spin-orbit interaction leads to additional suppression in its value - the ratio of a typical fine structure interval to atomic energy, Rydberg, known (see, e.g., [10], §72) to be equal by order of magnitude to $Z^2\alpha^2$. In this case the estimate given in the refs. [11,12]

$$\delta E \sim \frac{Gm^2\alpha^4 Z^5 R}{\pi}\, \frac{m\alpha^2}{2} \qquad (2)$$

is valid. However, the true value of the splitting again should be much smaller. According to numerical calculations [13], the additional suppression factor reaches here three-four orders of magnitude. ~~Therefore, in the ground state of a molecule the energy splitting of mirror isomers δE even at $Z \sim 80$ does not perhaps exceed~~

The splitting δE of electron energy leads to difference in vibrational potential energies of optical isomers and hence to splitting of vibrational frequencies [4] of relative magnitude

$$\delta\omega/\omega \sim \delta E/m\alpha^2 \qquad (3)$$

At $Z \sim 80$ this ratio is about 10^{-10}. Such a deformation of potential energy through the change of equilibrium states and moments of inertia causes as well splitting of rotational frequencies [4] of the same relative value $\delta E/m\alpha^2$.

The experimental possibilities of the search for the discussed effect are considered by example of the molecule CHFClBr in the ref. [5]. Carried out experimental search for the frequency splitting of the transition with the wavelength $\lambda \approx 9500$ between vibrational levels of the ground state of camphor optical isomers has led to upper bound on the effect magnitude at the level of 300 kHz [14]. Since the most heavy atom in the camphor molecule is oxygen with $Z = 8$, from the above estimates this bound is seen to exceed by about ten or-

ders of magnitude the expected value of the effect.

3. We shall consider now a model of optical isomers level splitting caused by parity-violating weak interaction. Let a heavy atom have three neighbours-atoms different from it and from each other. It can be easily seen that a molecule of four non-complanar atoms is the simplest structure that can possess optical isomers. Then let external electron of the heavy atom have angular momentum $j \geq 3/2$, and its interaction with one of the three atoms of environment, marked by the index 3, be taken into account by the fact that the levels with different projections μ of the angular momentum of the axis going through the heavy atom and the atom 3 are not degenerate. The field of the atom 3 causes such a splitting of the levels of the heavy atom, e.g. due to tensor polarizability of the last one (see [10], § 76); the levels with the same $|\mu|$ stay degenerate. In other words, we mean the angular momentum-axis interaction in molecule (see[10], § 78,83) that leaves degenerate the levels with the same sign of the angular momentum projection. The field of two other atoms (rather, ions) of the environment, 1 and 2, is assumed to be a Coulomb one:

$$V(\vec{r}) = - \frac{Z_1 \alpha}{|\vec{r} - \vec{r}_1|} - \frac{Z_2 \alpha}{|\vec{r} - \vec{r}_2|} \qquad (4)$$

At last, let non-perturbed state of the heavy atom electron be $|p_{3/2}, \mu\rangle$. For the expectation value of P -odd electron-nucleon weak interaction not to vanish, the Coulomb perturbation (4) should at any rate admix to the initial state two new ones: $|s_{1/2}\rangle$ and $|p_{1/2}\rangle$. Taking into account addition rules for angular momentum, both orbital and total, as well as parity conservation in the interaction (4), one can see at once that the admixture of $|s_{1/2}\rangle$ to $|p_{3/2}\rangle$ is caused by dipole part of

Coulomb interaction only and that of $|p_{1/2}\rangle$ to $|p_{3/2}\rangle$ by quadrupole one. Direct calculation leads to the following result for the state perturbed in this way with the account of $s_{1/2}$ and $p_{1/2}$ admixtures which are of interest to us:

$$|p_{3/2}, \mu\rangle +$$

$$+ \frac{4}{3} \frac{\sqrt{4\pi}}{2E_s} m\alpha^2 \sum_{i=1,2} Z_i Q_1(r_i) \sum_{q,\mu'} (-1)^{1/2 - \mu'} \begin{pmatrix} 3/2 & 1 & 1/2 \\ \mu & q & -\mu' \end{pmatrix} V^*_{1q}(\vec{n}_i) |s_{1/2}, \mu'\rangle +$$

$$+ \frac{4}{5} \frac{\sqrt{4\pi}}{2E_p} m\alpha^2 \sum_{i=1,2} Z_i Q_2(r_i) \sum_{q,\mu'} (-1)^{1/2 - \mu'} \begin{pmatrix} 3/2 & 2 & 1/2 \\ \mu & q & -\mu' \end{pmatrix} V^*_{2q}(\vec{n}_i) |p_{1/2}, \mu'\rangle \qquad (5)$$

Here $E_s(E_p)$ is the energy of the admixed $s(p)$ state counted off the initial level $p_{3/2}$; V_{kq} are spherical functions; $\begin{pmatrix} j & k & j' \\ \mu & q & -\mu' \end{pmatrix}$ are $3j$ - symbols;

$$Q_k(r_i) = \frac{1}{m\alpha} \int_0^\infty drr^2 \left[f'(r)f(r) + g'(r)g(r) \right] \times$$

$$\times \left[\theta(r - r_i) \frac{r_i^k}{r^{k+1}} + \theta(r_i - r) \frac{r^k}{r_i^{k+1}} \right] \qquad (6)$$

$f(r)$ and $g(r)$ ($f'(r)$ and $g'(r)$) are upper and lower components of radial Dirac wave function of initial (final) state. Note that the expression (5) is valid also in nonrelativistic case. It is sufficient only to make the substitution $f'f + g'g \rightarrow R'R$ where R' and R are non-relativistic radial wave functions of the final and initial states. Of course in the non-relativistic approximation as well one should remember about fine structure of the levels.

Using the expression (5) and taking into account the exact value of the mixing matrix element for the states $s_{1/2}$ and $p_{1/2}$ [8, 9] (it differs from the estimate (1) by the factor

$$\frac{iq}{\sqrt{2}(\nu_s \nu_p)^{3/2}}$$ where ν_s and ν_p are the effective principal quantum numbers of corresponding states and q is a quantity close to $-N/2Z$, N being the number of neutrons in nucleus), the correction to energy can be written as

$$\frac{Gm^2\alpha^2 Z^3 Rq(m\alpha^2)^3}{\sqrt{2\pi}(\nu_s \nu_p)^{3/2} 8E_s E_p} \cdot \frac{16}{15} \cdot 4\pi i \sum_{q,q';\mu'} \begin{pmatrix} 3/2 & 1 & 1/2 \\ \mu & q & -\mu' \end{pmatrix} \begin{pmatrix} 3/2 & 2 & 1/2 \\ \mu & q' & -\mu' \end{pmatrix} \cdot$$

$$\cdot \sum_{i,j=1,2} Z_i Z_j Q_1(r_i) Q_2(r_j) [Y_{1q}(\vec{n}_i) Y^*_{2q'}(\vec{n}_j) - Y^*_{1q}(\vec{n}_i) Y_{2q'}(\vec{n}_j)] \qquad (7)$$

By means of standard transformations the expression (7) can be rewritten in a more transparent form:

$$(\mu^2 - 5/4) \cdot \frac{4}{5} Z_1 Z_2 ([\vec{n}_1 \times \vec{n}_2] \cdot \vec{n}_3)([Q_1(r_1) Q_2(r_2) \vec{n}_2 -$$

$$\qquad (8)$$

$$- Q_1(r_2) Q_2(r_1) \vec{n}_1] \cdot \vec{n}_3) \frac{Gm^2\alpha^2 Z^3 Rq}{\sqrt{2\pi}(\nu_s \nu_p)^{3/2}} \frac{(m\alpha^2)^3}{8E_s E_p}$$

Transition from a right isomer to a left one corresponds to change of sign of coordinates for all atoms at which the sign of the expression (8) also changes. Therefore, the calculated correction to energy has indeed different sign for right and left molecules so that the isomer energy splitting δE is equal to doubled quantity (8). The agreement with the estimate (1) is evident.

Note that it is clear from the expression (8) that every of the three atoms of environment is necessary for arising of the correction. In particular, since the effect vanishes after averaging over $|\mu|$ (indeed, $\mu^2 - 5/4 = +1$ at $|\mu|=3/2$ and -1 at $|\mu|=1/2$), the role of the interaction with the third atom, lifting the degeneracy of the initial state in $|\mu|$, is seen.

By the same example it can be easily demonstrated how essential is the spin-orbit interaction for the discussed level splitting. If it is neglected, initial states with different spin orientation, e.g.,

$$|p, 1_z = 1\rangle \ |\uparrow\rangle \quad \text{and} \quad |p, 1_z = 1\rangle \ |\downarrow\rangle$$

will be degenerate. Coulomb interaction is spin-independent and hence the mixing coefficients of the first state with $|s\rangle \ |\uparrow\rangle$ and $|p\rangle \ |\uparrow\rangle$ are the same as those of the second one with $|s\rangle \ |\downarrow\rangle$ and $|p\rangle \ |\downarrow\rangle$. As to the weak interaction matrix element, being linear in the Pauli matrices $\vec{\sigma}$, it changes sign at spin-flip:

$$\langle \downarrow | \langle s|H|p\rangle |\downarrow\rangle = - \langle \uparrow | \langle s|H|p\rangle |\uparrow\rangle$$

Therefore, after averaging over spin the effect indeed vanishes.

However, in heavy molecules where spin-orbit interaction is comparable with the electrostatic interaction between atoms the magnitude of the effect is not proportional to fine structure interval.

4. Another manifestation of the same effect could be the splitting of Mössbauer line in mirror image crystals. Mere existence of parity violating weak interaction of nucleus with electrons of crystal is unsufficient here for the effect to arise. Evidently the magnitude of this interaction should be necessarily different for the upper and lower nuclear levels.

Such a situation takes place for the part of weak interaction that depends on the nuclear spin. Since here contribution to the effect is given not by all nucleons, but only by one of them, that with non-paired angular momentum, the order of magnitude of the splitting will be roughly Z times smaller than previous estimates*). If we are interested in the contribution to the effect from the interaction independent of nuclear spin, it can be non-zero here only due to change of nuclear radius from the initial state to the final one. And again we lose in comparison with the above estimates the factor Z in the magnitude of the effect. Therefore, if there are electrons with non-paired spin in a lattice knot, simple estimate of the Mössbauer line splitting is (see (1)):

$$\delta E \sim \frac{Gm^2\alpha^2Z^2R}{\pi}\ \frac{m\alpha^2}{2}$$

The nucleus, most appropriate for experiment of the kind, seems to be now tantalum Ta_{73}^{181} (natural line-width $\Gamma = 6.7 \cdot 10^{-14}$ keV, transition energy $E = 6.25$ keV, quantum numbers of the nuclear ground state $7/2^+$, of the excited one — $9/2^-$). The expected splitting value is in this case

$$\delta E(Ta_{73}^{181}) \sim (10^{-15} \div 10^{-14})\ keV$$

Unfortunately, the effective line-width is here about 20 times larger than the natural one, and worse of all, the accuracy with which the position of line is reproduced under the transition from one sample to another is no better than $4 \cdot 10^{-13}$ keV.

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*) In the unified model of electromagnetic and weak interactions by Weinberg [15] and Salam [16] confirmed by all existent experimental data, at the value of the parameter of the theory $\sin^2\theta \approx 0.23$ that follows from experiment, the dimensionless constant, that characterizes parity-violating interaction dependent on nuclear spin, is numerically small. Therefore, such an effect will be here additionally suppressed.

5. In conclusion, I would like, as it is customary in articles on the discussed topic, to dwell, at least shortly, on the hypothesis according to which the energy difference of right and left molecules due to the neutral current weak interaction is the cause of the fact that in natural conditions biological molecules exist in one isomeric form only. This explanation of the asymmetry of organic nature was first discussed in the ref. [2]. Afterwards the same hypothesis was strongly advocated in the refs.[4]. It seems to me, however, that, due to the extreme smallness of the discussed effect, such an assumption is clearly less feasible than other possible explanations of the asymmetry of living nature.

The explanation seems to be more natural according to which an accidentally, spontaneously arising asymmetry in a racemic (i.e., consisting of equal numbers of right and left molecules) system does not vanish, but increases, since it leads to more rapid metabolism, i.e., to more rapid chemical reactions [17,18]. Let us consider for illustration*) a process $A + B \to AB$ where every molecule A and B have both right and left isomers. It is clear that the velocity of this reaction depends in general on the "helicity" of initial molecules. In the limiting case when the left isomer A_l interacts with the left isomer B_l, and the right one A_r with the right one B_r, the number of produced molecules AB is proportional to $N(A_l)N(B_l) + N(A_r)N(B_r)$ where N is the concentration of corresponding isomer. In the racemic mixture where $N(A_l) = N(A_r) = \frac{1}{2}N(A)$, $N(B_l) = N(B_r) = \frac{1}{2}N(B)$, this quantity is evidently twice smaller than in the system consisting of left or right molecules only where $N(A_l) = N(A)$,
$N(B_l) = N(B)$, $N(A_r) = 0$, $N(B_r) = 0$ or $N(A_r) = N(A)$,
$N(B_r) = N(B)$, $N(A_l) = 0$, $N(B_l) = 0$.

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*) Although this example was already considered in the book [18], I would like to present it here, since unfortunately the considerations of this kind are evidently little known among physicists who discuss these questions.

On the other hand, the asymmetry of organic nature could be caused by external factors. It was found experimentally long ago for instance that circularly polarized light acts differently on right and left molecules [19], this fact being quite natural from the physical point of view. (Partial circular polarization of the Sun light at a given part of the Earth surface can arise, e.g., due to the dichroism of atmosphere caused by the magnetic field of Earth). The hypothesis explaining the origin of biological asymmetry by the action of circularly polarized light ascends to van't Hoff [20].

And at last weak interactions can be indeed involved in the discussed phenomenon, but not due to neutral currents. Immediately after the discovery of parity non-conservation in weak interactions, the hypothesis was put forward according to which the asymmetry of organic molecules is the result of parity violation in β -decay of natural radioactive elements [21]. Longitudinally polarized β - electrons also act in different way in general on right and left molecules. One can easily imagine the definite mechanism of this phenomenon. Due to the longitudinal polarization of electrons, their Bremsstrahlung is partially circularly polarized, and again the immediate cause of the effect is the difference in the interaction of circularly polarized quantum with left and right molecule. The search for such a selective action on right and left molecules is underway with β -decay electrons [22-25] and positrons [26-28], as well as with longitudinally polarized electrons from linear accelerator [29,30]. Unfortunately, in all the three groups of experiments the results are still contradictory.

Acknowledgements

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