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P-ODD LONG-BANGE INTERACTION OF IONS IN MAGNETO-ORDERED CRYSTALS

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A b s t r a c t

In crystals with magnetic structure the exchange interaction between ions and conduction electrons when parity nonconservation is taken into account, gives rise to P-odd long-range spin-dependent forces between ions. The energy of the P-odd interaction reaches ~ 100 Hz for the crystals of rare earth elements with helical spin structure. The feasibility of observing parity nonconservation in such crystals and in Bloch domain walls in ferromagnetic films is discussed.

1. Introduction

In our previous paper [1] where P-odd van der Waals forces were considered, it was pointed out that a parity nonconserving interaction between ions splits the energies of crystals with right and left helical spin structure. This effect is an analog of the difference of the energies of right and left molecules (or crystals) due to a weak interaction, the phenomenon repeatedly discussed previously, but not yet observed experimentally. The present work contains a theoretical study of the parity violation effects in magneto-ordered crystals. Although the parity nonconservation in atomic phenomena is reliably established now in the experiments performed by various groups [2-4], the observation of the P-odd effects in crystals would be certainly of great scientific interest.

A helical spin structure exists in alloys and compounds which contain the elements with incomplete d- and f-shells (MnO_2, $TbMn_2$, $CeFe_{17}$ etc.), as well as in rare-earth metals: Dy, Ho, Er [5]. Domain walls in ferromagnetics also have a helical spin structure. The main contribution to P-odd effects in metals will be shown below to come from the exchange interaction between conduction electrons and ions. Since there is no such an interaction in dielectrics, the P-odd effects are much smaller in them than in metals. And although it cannot be excluded that the observation of the discussed effects in dielectrics can prove nevertheless to be simpler, we restrict to the considerstion of metals.

Discussing particular mechanisms of the P-odd interaction between ions in crystals, we shall make all the numerical estimates for holmium. The advantage of holmium crystals consist in the stability of the helical structure at low temperatures, in large nuclear charge (Z=67), as well as in the large spin component forming the helix. Due to these circumstances, the magnitude of the P-odd energy of the holmium ion is higher than, say, that of dyspresium or erbium.

Metallic holmium structure is as follows [6]: ions Ho^{3+} are localized at the sites of the hexagonal close-packed lat-

tice (a=6.77; c=10.62 a.u.). At the temperature lower than 132K the angular momenta of ions located in the same basic plane lie in this plane and are parallel to each other. When going from one plane to another the angular momenta are rotated by an angle α_o dependent on the temperature. Below 20 K the magnetic moments of the ions acquire a small ferromagnetic component along the hexagonal axis, and this angle α_o is weakly temperature-dependent and close to 30º. The phase transition "ferromagnetic helix – simple helix" and "simple helix – paramagnetic" in holmium are not accompanied by a change in the lattice structure. The electronic structures of the holmium atom and its ion are as follows:

$$Ho: \quad 4f^{11}6s^2 \quad {}^4I_{15/2}$$

$$Ho^{3+}: \quad 4f^{10} \quad {}^5I_8$$
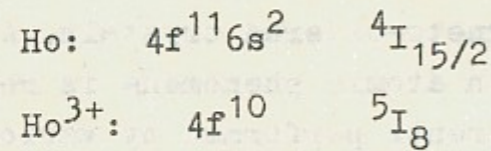
The nuclear spin of the most widespread isotope ^{165}Ho is equal to 7/2.

2. P-odd van der Waals interaction between ions

The energy of the P-odd van der Waals interaction between two identical ions with angular momenta $\vec{J}$ at the distance $\vec{R}$ is written as[1]:

$$U(\vec{R}) = U_\sigma(\vec{R}) + U_t(\vec{R})$$

$$U_\sigma(\vec{R}) = 4 \frac{\vec{N}(\vec{J_1} \times \vec{J_2})}{R^5} \frac{1}{2\pi i} \int \alpha_\sigma(\omega)\beta_\sigma(\omega)\omega\,d\omega \qquad (1)$$

$$U_t(\vec{R}) = 2\,\varepsilon_{kni}\frac{N_n}{R^5}(\delta_{\ell s} - 3N_\ell N_s)Q_{is}^{(1)}Q_{ek}^{(2)}\frac{1}{2\pi i}\int \alpha_t(\omega)\beta_t(\omega)\omega\,d\omega$$

where $\vec{N} = (\vec{R_1} - \vec{R_2})/|\vec{R_1} - \vec{R_2}|$; $Q_{ik} = J_i J_k + J_k J_i - \frac{2}{3}\delta_{ik}J(J+1)$; $\alpha_\sigma(\omega), \alpha_t(\omega), \beta_\sigma(\omega), \beta_t(\omega)$ are vector and tensor P-even and P-odd polarizabilities of ions such that

$$\alpha_{ik}(\omega) = \alpha_s(\omega)\delta_{ik} + i\varepsilon_{ikz}J_z\alpha_\sigma(\omega) + Q_{ik}\alpha_t(\omega)$$
$$\beta_{ik}(\omega) = i\beta_s(\omega)\delta_{ik} + \varepsilon_{ikz}J_z\beta_\sigma(\omega) + iQ_{ik}\beta_t(\omega) \qquad (2)$$

$\alpha_s(\omega), \beta_s(\omega)$ are scalar polarizabilities, and the polarizability tensors $\alpha_{ik}(\omega), \beta_{ik}(\omega)$ can be represented as follows:

$$\alpha_{ik}(\omega) = \sum_n \left\{ \frac{\langle o|d_i|n\rangle\langle n|d_k|o\rangle}{\omega_{no} - \omega - i\varepsilon} + \frac{\langle o|d_k|n\rangle\langle n|d_i|o\rangle}{\omega_{no} + \omega - i\varepsilon} \right\} \qquad (3)$$

$$\beta_{ik}(\omega) = \sum_n \left\{ \frac{\langle o|d_i|n\rangle\langle n|\mu_k|o\rangle}{\omega_{no} - \omega - i\varepsilon} + \frac{\langle o|\mu_k|n\rangle\langle n|d_i|o\rangle}{\omega_{no} + \omega - i\varepsilon} \right\} \qquad (4)$$

where $\vec{d}, \vec{\mu}$ are the electric and magnetic dipole moments of ions; $\omega_{no} = E_n - E_o$; E_o, E_n are the energies of the ground and excited states.

In calculating the sums (3) and (4) we shall describe the excited single-electron states $|n\rangle$ of the ion in a crystal by plane waves. The arguments in the favour of this approximation are as follows. In the method of orthogonalized plane waves

$$|n\rangle = |\vec{k}\rangle - \sum_\lambda |\lambda\rangle\langle\lambda|\vec{k}\rangle$$

where $|\vec{k}\rangle$ is a state with a given momentum and $|\lambda\rangle$ are occupied electron states. In the matrix elements of interest to us

$$\langle 4f|\vec{z}|n\rangle = \langle 4f|\vec{z}|\vec{k}\rangle - \sum_\lambda \langle 4f|\vec{z}|\lambda\rangle\langle\lambda|\vec{k}\rangle$$

$|\lambda\rangle = |4d\rangle$ dominate in the sum over λ. And the numerical calculations using Hartree-Fock wave functions[1] of the holmium atom[2] show that

$$|\langle 4f|\vec{z}|\vec{k}\rangle| \gg |\langle 4f|\vec{z}|4d\rangle\langle 4d|\vec{k}\rangle|$$

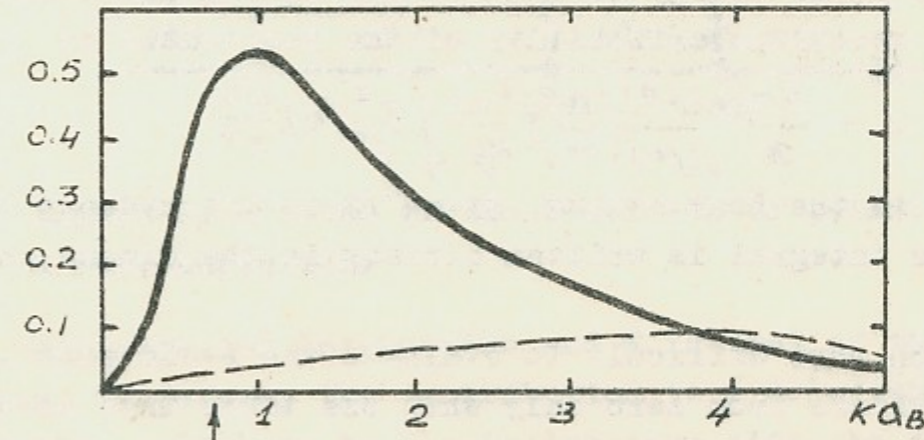in a broad interval of $|\vec{k}|$ (see Fig.1). Just this allows one

Figure 1. The dependence of $\langle 4f|z|k\rangle$ (solid line) and $\langle 4f|z|4d\rangle\langle 4d|k\rangle$ (dashed line) on k. The arrow marks the position of k_F in the model of free electrons.

[2]Since a crystal is quasineutral, it is more reasonable to use just the atomic wave functions rather than the ion ones.

to use simply the plane waves with $k > k_F$ as $|n\rangle$.

Begin with the calculation of the vector polarizability $\alpha_v(\omega)$ of the ion in the crystal. The contribution to it will be given only by the electrons of the incomplete shell $4f_{7/2}$. Substituting into (3) the relation

$$\langle 0|z_i|n\rangle = i\langle 0|p_i|n\rangle / m\omega_{nc}$$

(m is the electron mass; we use the units where $\hbar=c=1$), summing over all $f_{7/2}$ electrons and integrating over the orientation of $\vec{k}$, we obtain

$$\alpha_v(\omega) \simeq -\frac{2\alpha(\vec{j}\vec{\ell})}{\pi j(j+1)} \cdot \frac{m^*}{m} \int_{k_F}^{\infty} I_{j\ell}^2(k)\left(\frac{1}{E_k - \omega} - \frac{1}{E_k + \omega}\right)dk \qquad (5)$$

where $\alpha = 1/137$; j,ℓ are the total and orbital angular momenta of the electron; m^* is the effective mass;

$$I_{j\ell}(k) = \int_0^{\infty} R_{j\ell}(z)\, j_\ell(kz)\, z^2 dz \qquad (6)$$

$j_\ell(kz)$ is the spherical Bessel function, $R_{j\ell}(z)$ is the radial function of the 4f-electron. In deriving (5), we take into account that the Fermi energy is counted off E_0, in practice. At $\omega \to 0$ the vector polarizability of the ion equals to

$$\alpha_v(\omega) \simeq -\frac{8 a_B^3}{\pi} \cdot \frac{(\vec{j}\vec{\ell})}{j(j+1)} \left(\frac{m^*}{m}\right)^2 \frac{\omega}{Ry} \int_{k_F}^{\infty} I_{j\ell}^2(k)\frac{dk}{k^4} \qquad (7)$$

where $a_B = 1/m\alpha$ is the Bohr radius, $Ry = m\alpha^2/2$ is the Rydberg constant, and the integral is written already in the dimensionless variables.

It is much more difficult to evaluate the P-odd polarizability that differs from zero only when one takes into account the weak interaction between the electrons and nucleus. For the vector and tensor components we are interested in, these electrons should belong to an incomplete shell, in this case to f- one. However, the weak electron-nucleus interaction is of a local nature, is proportional to $\vec{p}\,\delta(\vec{z})$, and gives rise to the mixing only of the s- and p-electrons (see, e.g., Ref. [?]). Therefore, the functions $\beta_v(\omega)$ and $\beta_t(\omega)$ do not vanish here only due to the mixing of configurations. The relative magnitude of this mixing is $J/Ry \sim 10^{-1} \div 10^{-2}$. If one considers the P-odd polarizability of the f-shell arising as a result of the admixture of the s- and p-configurations, then it can be easily seen that $\beta_{v,t}(\omega)$ can arise only to the second order in J/Ry due to

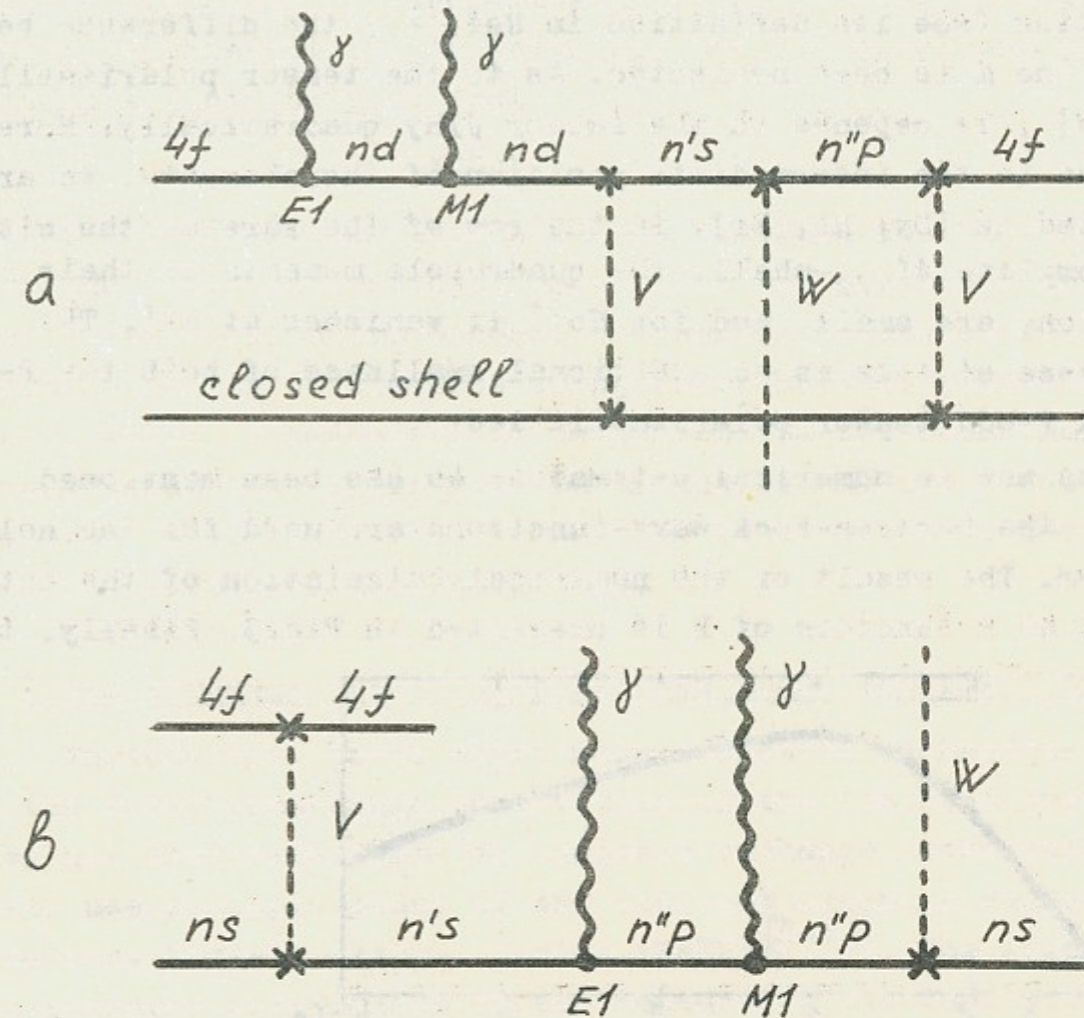the diagrams of the type "a" (Fig.2). Here V is the operator of

Figure 2. Arising of the P-odd vector polarizability of a rare-earth ion.

the configuration interaction and W is that of the weak interaction. Therefore, the contribution to $\beta_v(\omega)$ of the inner s- and p-shells, polarized by the interaction with the outer f-shell, turns out to be more important. It is sufficient to take into account such an interaction once, that results in the diagrams of the type "b" (Fig.2). But, being linear in the spin of the f-electrons, this mechanism contributes to the vector P-odd polarizability of the ion only.

Thus, the P-odd vector polarizability of a rare-earth ion contains, unlike the P-even vector polarizability, an extra small factor

$$\frac{Gm^2 \alpha^3 Z^3 R}{\pi} \cdot \frac{J}{Ry} \qquad (8)$$

where $G = 10^{-5} m_p^{-2}$ is the Fermi weak interaction constant, $R \sim 5$ is

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a relativistic enhancement factor for the weak electron-nucleus interaction (see its definition in Ref.[7]); the difference between m* and m is here neglected. As to the tensor polarizability $\beta_t(\omega)$, it depends on the factor J/Ry quadratically. Moreover, due to the intermediate position of the elements, we are interested in (Dy, Ho, Er), in the row of the rare-earths with the incomplete $4f_{7/2}$-shell, the quadrupole moments of their triple ions are small, and for Ho^{3+} it vanishes at all. The consequence of this is an additional smallness of both the P-even and P-odd tensor polarizabilities.

Pass now to numerical estimates. As has been mentioned already, the Hartree-Fock wave-functions are used for the holmium atom. The result of the numerical calculation of the integral (6) as a function of k is presented in Fig.3. Finally, the
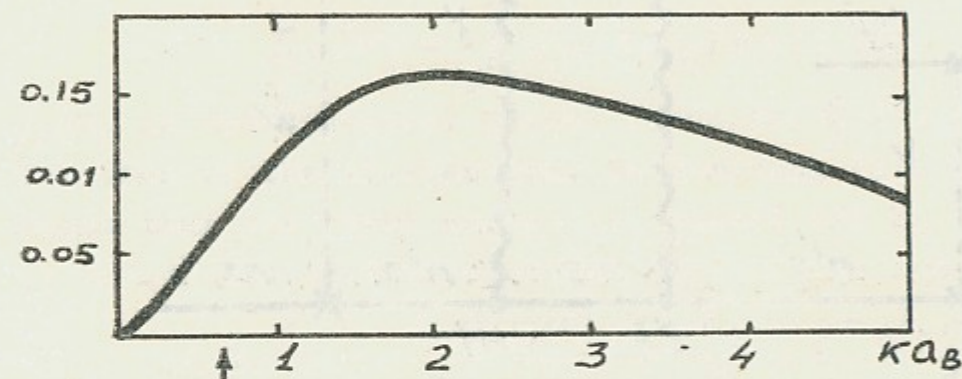

Figure 3. The dependence of $I_{7/2,3}$ on k. The arrow marks the position of k_F in the model of free electrons.

polarizability of the holmium ion does not exceed its dimensional estimate and for small ω

$$\alpha_\sigma(\omega) \lesssim a_B^3 \, \omega/Ry \qquad (9)$$

But then even an optimistic estimate for the interaction between two ions gives

$$U_\sigma \sim \frac{G Z^3 R \omega^2 d^4}{\pi} \frac{J}{Ry} \vec{N}_{12} (\vec{J}_1 \times \vec{J}_2) \left(\frac{a_B}{R_{12}}\right)^5 Ry \qquad (10)$$

And the energy per one ion in the crystal equals to

$$E_i \sim \frac{G Z^3 R \omega^2 d^4}{\pi} \frac{J}{Ry} \sum_j \vec{N}_{ij} (\vec{J}_i \times \vec{J}_j)(a_B/R_{ij})^5 Ry \qquad (11)$$

that constitutes for Ho (Z=67; R=4.5; $|\vec{J}|$=8; J/Ry~0.1)

$$E_i \sim (10^{-16} \div 10^{-17}) Ry \sim 0.1 \; Hz.$$

It is much smaller than the estimate in Ref.[1]. The disagreement is explained by the following factors. First, unlike the scalar polarizability, to which all the ion electrons can in principle contribute so that

$$\alpha_s \sim 10^2 a_B^3,$$

the vector polarizability (see (9)) contains no large coefficient, the contribution to it comes from the electrons of the incomplete shell only. Second, the specific structure of the electron shells of elements among which helical spin structures occur, makes it necessary to switch on the interconfiguration interaction, that gives rise to an additional small factor in the P-odd polarizability. Transition from the f- to d-metals does not eliminate this smallness.

3. P-odd exchange interaction between ions. The first order

Fortunately, there exist more effective mechanisms leading to the P-odd long-range interaction of the ion in a crystal. They are associated with an indirect exchange interaction. We shall use a simple model of the indirect exchange suggested by Ruderman, Kittel, Kasuya, Yosida (RKKY)[8-10]. The spin-dependent exchange interaction of the conduction electron with the electrons of incomplete shells of ions is described in this model by the operator

$$V(\vec{z}) = - J V_o \sum_i (\vec{s} \vec{S}_i) \delta(\vec{z} - \vec{R}_i) \qquad (12)$$

where $\vec{s}$ is the spin of the conduction electron; $\vec{S}_i$ is the spin of the ion located at the point $\vec{R}_i$; V_o is the volume per one ion in the crystal. For heavy rare-earth elements the exchange integral is positive and constitutes $\sim 10^{-2}$ of the Fermi energy E_F. To the second order of perturbation theory the operator (12) results in the following interaction between two ions (see, e.g., Ref.[6]):

$$E_{ij} = - \frac{9}{2} \pi n^2 E_F (J/E_F)^2 (\vec{S}_i \vec{S}_j) \phi(x_{ij}) \qquad (13)$$

where $x_{ij} = 2 k_F |\vec{R}_i - \vec{R}_j|$; $\phi(x) = j_1(x)/x^2$, $j_1(x) = -\frac{d}{dx}\frac{\sin x}{x}$ is the spherical Bessel function; n is the number of conduction electrons per ion; k_F is the Fermi momentum. The existence of

stable spin helices in crystals with helical structure is due just to this interaction[11,12]3). Note that the latter decreases with a distance between ions much slower ($\sim R^{-3}$) than the van der Waals forces ($\sim R^{-6}$).

Find now the correction to the crystal energy, due to the interaction (12) and to the weak P-odd interaction between the conduction electrons and the nuclei of ions. In these calculations it is convenient to use the non-relativistic limit of the operator of the weak P-odd interaction between the electron and nucleus. We write it as follows (see, e.g., Ref.[7]):

$$W(z) = \frac{G}{\sqrt{2}\,2m} \sum_i \left\{ Z_q \left[(\vec{\sigma}\vec{p}), \delta(\vec{z}-\vec{R}_i) \right]_+ + \right.$$

$$\left. + \varkappa \left[(\vec{I}_i \vec{p}), \delta(\vec{z}-\vec{R}_i) \right]_+ + i\varkappa' \left[(\vec{I}_i \times \vec{\sigma})\vec{p}, \delta(\vec{z}-\vec{R}_i) \right]_- \right\} \quad (14)$$

Here $[\ ]_-$ and $[\ ]_+$ denote a commutator and anticommutator, respectively; $\vec{p}$ is the operator of the electron momentum; $\vec{I}_i$ is the spin of the nucleus located at the point $\vec{R}_i$. In the dimensionless constant Z_q of the first structure the large factor Z has been made explicit to emphasize that it increases with the number of nucleons in the nucleus. In the standard model of weak interactions the value of q is for rare-earth elements $q \simeq -0.7$. Note that in the same model the constants $\varkappa$ and $\varkappa'$ are numerically small.

We shall consider the conduction electrons as free, possessing an effective mass m^*, and filling the sphere of radius k_F in the momentum space.

The correction to the energy of an electron with a momentum $\vec{k}$ and spin projection σ, linear in V and W, equals evidently to

$$E^{(1)}_{\vec{k}\sigma} = \sum_{\vec{k}'\sigma'} \frac{\langle \vec{k}\sigma|V|\vec{k}'\sigma'\rangle\langle\vec{k}'\sigma'|W|\vec{k}\sigma\rangle}{k^2 - k'^2} 2m^* + h.c. \quad (15)$$

The total correction $E^{(1)}$ to the crystal energy is obtained from the above expression by summation over $\vec{k}$, $|\vec{k}| \leq k_F$ and over σ. It is clear from the invariance arguments that the pseudoscalar correction should have the structure of the form

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3) Of course, in Bloch domain walls the spin helix arises for another reason, due to boundary conditions.

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$$\sum_{ij} (\vec{I}_i \times \vec{S}_j) \vec{R}_{ij} f(R_{ij})$$

Therefore, the first, leading term in (14), proportional to Z, but independent of $\vec{I}_i$, does not contribute to it. The term with $\varkappa$ in the operator (14), independent of the electron spin, also evidently cancels out after the summation over σ, σ'. Simple calculations result in

$$E^{(1)} = \frac{2G\varkappa'}{\sqrt{2}} \cdot \frac{m^*}{m} \, JV_0 \int_{|\vec{k}|\leq k_F} \frac{d\vec{k}}{(2\pi)^3} \int \frac{d\vec{k}'}{(2\pi)^3} \sum_{ij} (\vec{I}_i \times \vec{S}_j)\vec{\nabla} \frac{e^{-i(\vec{k}'-\vec{k})\vec{z}}}{k'^2-k^2} \Bigg|_{\vec{z}=\vec{R}_{ij}} \quad (16)$$

Integrating over $\vec{k}'$, $\vec{k}$ and introducing the factor Z^2R, which takes into account the difference of the density of conduction electrons on the nucleus from the average density over the crystal, one obtains

$$E^{(1)} = -\frac{G\varkappa'\alpha^2 Z^2 R\varkappa'}{\sqrt{2}\,\pi} \cdot \frac{J}{Ry} \cdot \frac{m^*}{m} (k_F a_B)^2 Ry \cdot 3n \sum_{ij} (\vec{I}_i \times \vec{S}_j) \frac{\vec{R}_{ij}}{R_{ij}} \cdot \frac{d\phi(x_{ij})}{dx_{ij}} \quad (17)$$

$$x_{ij} = 2k_F R_{ij}, \quad \phi(x) = j_1(x)/x^2 = -\frac{1}{x^2}\frac{d}{dx}\frac{\sin x}{x}$$

In the above expression the obvious relation $V_0 k_F^3 = 3\pi^2 n$ is taken into account. Note that, as it is seen from (17), the ion-ion interaction decreases at large distances ($k_F R \gg 1$) as $R^{-3}\sin(2k_F R)$.

If the hyperfine coupling is not broken, the energy of the interaction of one nuclear spin, found from (17), constitutes

$$E_i^{(1)} = -\frac{G\varkappa'\alpha^2 Z^2 R\varkappa'}{\sqrt{2}\,\pi} \cdot \frac{J}{Ry} \cdot \frac{m^*}{m} (k_F a_B)^2 Ry \cdot 6n \sum_j (\vec{I}_i \times \vec{S}_j) \frac{\vec{R}_{ij}}{R_{ij}} \cdot \frac{d\phi(x_{ij})}{dx_{ij}} \quad (18)$$

For a rough numerical estimate of the result, we replace the summation over the lattice sites by the integration over the whole space. Then the expression (18) reduces to the form

$$E_i^{(1)} \approx -\frac{G\varkappa'\alpha^2 Z^2 R\varkappa'}{\sqrt{2}\,\pi} \cdot \frac{J}{Ry} \cdot \frac{m^*}{m} (k_F a_B)^2 IS \cdot \frac{\alpha_0}{k_F c} \cdot \frac{1}{\pi} Ry \quad (19)$$

Besides the transition to integration, we neglect here a small ferromagnetic component of $\vec{S}$ and restrict to the first order in the parameter $\alpha/k_F c$, which is very small indeed. The numerical summation over the lattice sites leads to the result which is

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about twice as large as (19). Substituting into (19) the expe-rimental values (see Ref.[6], p.260)

$$J = 0.7 \cdot 10^{-2} Ry, \qquad m^* = 3m,$$

which correspond to the model of free electrons ($k_F a_B = 0.75$), one obtains, taking into account the mentioned correction from the numerical calculation,[4)]

$$E_i^{(1)} \approx -2 \cdot 10^{-15} \varkappa' \, Ry \approx -7 \varkappa' \, Hz \qquad (20)$$

Note once more that in the standard model of weak interactions the constant $\varkappa'$ is numerically small.

One more correction to the energy of the crystal could in general arise in the same order. We mean the deformation of the Fermi surface, due to the perturbation V and different for the opposite spin orientations, with subsequent taking into account of W. Or vice versa, W would deform the Fermi surface and then V would be taken into account. But in this case there is no such a correction. Indeed, the sums over the "exchange" and "weak" sites factorize here, and then it is impossible to con-struct a pseudoscalar, invariant with respect to translations. Thus, here the problem of the relation between this contribution and the usual second order correction disappears (see Refs.[10, 13]).

4. Second order effect effect in the exchange interaction

To the first order in the exchange interaction (12) the first, leading term in the P-odd Hamiltonian (14), which increa-ses with the number of nucleons in the nucleus, does not contri-bute. One can expect, therefore, that to the second order in V the smallness J/Ry will be compensated by the factor Z. The corresponding correction to the crystal energy is

$$E^{(2)} = (2m^*)^2 \sum_{\substack{|\vec{k}| \le k_F \\ \sigma}} \left\{ \sum_{\substack{\vec{k}' \vec{k}'' \\ \sigma' \sigma''}} \left[\frac{\langle \vec{k}\sigma | V | \vec{k}'\sigma' \rangle \langle \vec{k}'\sigma' | V | \vec{k}''\sigma'' \rangle \langle \vec{k}''\sigma'' | W | \vec{k}\sigma \rangle}{(\kappa^2 - \kappa'^2)(\kappa^2 - \kappa''^2)} + \right. \right.$$

[4)] For the enhancement factor we assume here the value R=4.5 which corresponds to the absence of derivatives in the relati-vistic Hamiltonian of the weak electron-nucleon interaction.

$$+ \frac{\langle \vec{k}\sigma | V | \vec{k}'\sigma' \rangle \langle \vec{k}'\sigma' | W | \vec{k}''\sigma'' \rangle \langle \vec{k}''\sigma'' | V | \vec{k}\sigma \rangle}{(\kappa^2 - \kappa'^2)(\kappa^2 - \kappa''^2)} +$$

$$+ \frac{\langle \vec{k}\sigma | W | \vec{k}'\sigma' \rangle \langle \vec{k}'\sigma' | V | \vec{k}''\sigma'' \rangle \langle \vec{k}''\sigma'' | V | \vec{k}\sigma \rangle}{(\kappa^2 - \kappa'^2)(\kappa^2 - \kappa''^2)} \left] - \right.$$

$$- \langle \vec{k}\sigma | V | \vec{k}\sigma \rangle \sum_{\vec{k}'\sigma'} \frac{\langle \vec{k}\sigma | V | \vec{k}'\sigma' \rangle \langle \vec{k}'\sigma' | W | \vec{k}\sigma \rangle + h.c.}{(\kappa^2 - \kappa'^2)^2} -$$

$$- \langle \vec{k}\sigma | W | \vec{k}\sigma \rangle \sum_{\vec{k}'\sigma'} \frac{\langle \vec{k}\sigma | V | \vec{k}'\sigma' \rangle \langle \vec{k}'\sigma' | V | \vec{k}\sigma \rangle}{(\kappa^2 - \kappa'^2)^2} \right\}. \qquad (21)$$

It is easy to show that the terms proportional to $\varkappa$ and $\varkappa'$ in the operator W do not contribute in this approximation. Then the diagonal matrix element of the remaining term in the weak interaction W evidently vanishes when taken over true stationa-ry states of an electron in a crystal - standing waves (in our problem there are no current states). This allows one to omit immediately the last term in the expression (21). As to the other terms, it can be easily seen in the limit of a large size of a crystal the running waves instead of the standing ones may be used, and they are much more convenient technically.

The next to last term in (21) could be nonvanishing only if a ferromagnetic component is present, when

$$\langle \vec{k}\sigma | V | \vec{k}\sigma \rangle = -J \frac{v_0}{V} \langle \vec{\sigma} \rangle \sum_i \vec{S}_i \ne 0 \qquad (22)$$

However, after the summation over the momenta and spins the result for the term under discussion should be from the invari-ance consideration of the form

$$\sum_i \vec{S}_i \sum_{j s} (\vec{S}_j \times \vec{R}_{js}) F(R_{js})$$

It is easy to see that by virtue of the symmetry of the problem the summation over s turns this expression to zero.

For the analogous reason the contribution to the energy associated with the deformation of the Fermi surface and similar to those discussed at the end of the preceeding section, vani-shes also.

In the result, the correction to the crystal energy reduces to the form

$$E^{(2)} = i\frac{G\bar{z}^3 Rqm}{\sqrt{2}}\left(Jv_o\frac{m^*}{m}\right)^2 \int\frac{d\vec{k}}{(2\pi)^3}\int\frac{d\vec{k'}d\vec{k''}}{(2\pi)^6}(k^2-k'^2)^{-1}(k^2-k''^2)^{-1}\times$$
$$|\vec{k}|\leq k_F$$

$$\sum_{ijs}(\vec{S_i}\times\vec{S_j})\{(\vec{k'}+\vec{k})\exp(i\vec{k''}\vec{R_{ij}}-i\vec{k'}\vec{R_{is}}+i\vec{k}\vec{R_{js}}) - \tag{23}$$
$$-(\vec{k}+\vec{k''})\exp(-i\vec{k}\vec{R_{ij}}+i\vec{k'}\vec{R_{is}}-i\vec{k''}\vec{R_{js}})+(\vec{k}+\vec{k''})\exp(i\vec{k'}\vec{R_{ij}}-i\vec{k}\vec{R_{is}}+i\vec{k''}\vec{R_{js}})\}$$

Besides the constant Zq, we have directly taken into account the already mentioned factor Z^2R, connected with the difference of the density of conduction electron near the nucleus from the average density over the crystal. Unfortunately, without further approximations neither analytic, nor even numerical calculation of the sum (23) proves to be possible.

Therefore, consider at first the contribution from the terms with s=i and s=j. The corresponding correction to the energy looks as the sum of two terms:

$$E_1^{(2)} = \frac{2G\bar{z}^3 Rqm}{\sqrt{2}}\left(Jv_o\frac{m^*}{m}\right)^2\int\frac{d\vec{k}}{(2\pi)^3}\int\frac{d\vec{k'}d\vec{k''}}{(2\pi)^6}(k^2-k'^2)^{-1}(k^2-k''^2)^{-1}\times$$
$$|\vec{k}|\leq k_F \qquad i(\vec{k}-\vec{k'})\vec{z}$$
$$\times\sum_{ij}(\vec{S_i}\times\vec{S_j})\,\vec{\nabla}e\Big|_{\vec{z}=\vec{R_i}}\,, \tag{24}$$

$$E_2^{(2)} = \frac{G\bar{z}^3 Rqm}{\sqrt{2}}\left(Jv_o\frac{m^*}{m}\right)^2\int\frac{d\vec{k}}{(2\pi)^3}\int\frac{d\vec{k'}d\vec{k''}}{(2\pi)^6}(k^2-k'^2)^{-1}(k^2-k''^2)^{-1}\times$$
$$|\vec{k}|\leq k_F$$
$$\times\sum_{ij}(\vec{S_i}\times\vec{S_j})\,\vec{\nabla}e^{i(\vec{k}-\vec{k''})\vec{z}}\Big|_{\vec{z}=\vec{R_i}} \tag{25}$$

In calculation of the first of them, when integrating over k'', we come across a divergence, natural for a calculation of the second order correction in a contact interaction. For regularization we introduce a cut-off integration momentum Q, which is naturally identified with the inverse radius of the ion f-shell. After that the expression (24) reduces by means of elementary transformations to the form

$$E_1^{(2)} = -\frac{Gm^2\alpha^2\bar{z}^3 Rq}{\sqrt{2}\,\pi}\cdot\frac{Q}{k_F}\left(\frac{Ju^*}{Ry\cdot m}\right)^2 Ry\cdot\frac{9n^2}{4}\sum_{ij}(\vec{S_i}\times\vec{S_j})\frac{\vec{R_{ij}}}{R_{ij}}\frac{d\phi(x_{ij})}{dx_{ij}} \tag{26}$$

very similar to (17). The corresponding contribution to the interaction energy of one spin is

$$E_{1i}^{(2)} = -\frac{Gm^2\alpha^2\bar{z}^3 Rq}{\sqrt{2}\,\pi}\cdot\frac{Q}{k_F}\left(\frac{Ju^*}{Ry\cdot m}\right)^2 Ry\cdot\frac{9n^2}{2}\sum_{j}(\vec{S_i}\times\vec{S_j})\frac{\vec{R_{ij}}}{R_{ij}}\frac{d\phi(x_{ij})}{dx_{ij}} \tag{27}$$

In fact, the sum here is the same as in the formula (18). Going again from summation to integration, one obtains

$$E_{1i}^{(2)} \approx -\frac{Gm^2\alpha^2\bar{z}^3 Rq}{\sqrt{2}\,\pi}\cdot\frac{Q}{k_F}\left(\frac{Ju^*}{Ry\cdot m}\right)^2 S^2\frac{\alpha_o}{ck_F}\cdot\frac{3n}{4\pi}Ry \tag{28}$$

Using the numerical value $Q = 1.3a_B^{-1}$ and taking into account the correction factor ~ 2 from the numerical summation, mentioned in the foregoing section, we find the magnitude of this contribution

$$E_{1i}^{(2)} \approx 1.1\cdot10^{-14}Ry \approx 35\ Hz \tag{29}$$

One can ascertain that in other terms in (23) the divergence at large momenta does not arise. Therefore, although a real ratio Q/k_F is not large (~ 1.7), the presence of this formal parameter in the found contribution allows one to believe that it is not cancelled out completely by other terms and hence can serve as a relatively reliable lower estimate of the effect under discussion.

No more complications arise when calculating the contribution (25). Performing the trivial integration over all $\vec{k}$, we get for the correction to the energy of the whole crystal $E_2^{(2)}$ and to the energy of one spin $E_{2i}^{(2)}$ the following expressions:

$$E_2^{(2)} = -\frac{Gm^2\alpha^2\bar{z}^3 Rq}{\sqrt{2}\,\pi}\left(\frac{Ju^*}{Ry\cdot m}\right)^2 Ry\cdot\frac{3\pi n^2}{16}\sum_{ij}(\vec{S_i}\times\vec{S_j})\frac{\vec{R_{ij}}}{R_{ij}}\times$$
$$\times\frac{d}{dx_{ij}}\left[\frac{1}{x_{ij}^2}+\frac{3}{x_{ij}^2}\frac{d}{dx_{ij}}j_1(x_{ij})\right], \tag{30}$$

$$E_{2i}^{(2)} = -\frac{Gm^2\alpha^2\bar{z}^3 Rq}{\sqrt{2}\,\pi}\left(\frac{Ju^*}{Ry\cdot m}\right)^2 Ry\cdot\frac{3\pi n^2}{8}\sum_{j}(\vec{S_i}\times\vec{S_j})\frac{\vec{R_{ij}}}{R_{ij}}\times$$
$$\times\frac{d}{dx_{ij}}\left[\frac{1}{x_{ij}^2}+\frac{3}{x_{ij}^2}\frac{d}{dx_{ij}}j_1(x_{ij})\right]. \tag{31}$$

Note that, as it is seen from the above formulae, the interaction between two ions at large distances contains in addition to the oscillating part the non-oscillating contribution falling off as R^{-3}.

For the numerical estimate the summation over j in (31) can be replaced by integration over the whole space. Neglecting as previously a small ferromagnetic component, to the leading

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order in α_o we obtain

$$E_{2i}^{(2)} \approx - \frac{Gm\alpha^2 Z^3 Rq}{\sqrt{2}\pi} \left(\frac{J \cdot \omega^*}{Ry \cdot m}\right)^2 S^2 \frac{\alpha_o}{|\alpha_o|} \cdot \frac{\pi n}{32} Ry \qquad (32)$$

This zeroth order in α_o contribution comes from the mentioned above non-oscillating term $\sim R^{-3}$ in the ion-ion interaction. The numerical summation over the lattice sites in (31) results in the value which is smaller by 15-20%. Thus, this contribution constitutes

$$E_{2i}^{(2)} \approx 1.6 \cdot 10^{-14} Ry \approx 50 \text{ Hz} \qquad (33)$$

And finally, to estimate the contribution to the correction (23) to the crystal energy $E^{(2)}$ from the terms with $s \neq i,j$, it is convenient to smear the weak interaction (14) over the whole crystal:

$$W \rightarrow \frac{GZq}{\sqrt{2}mV_o} (\vec{\sigma}\vec{p})$$

The eigenfunction of the obtained Hamiltonian

$$H = \frac{p^2}{2m^*} + \frac{GZq}{\sqrt{2}mV_o} (\vec{\sigma}\vec{p}) \qquad (34)$$

is

$$\widetilde{|\vec{k}\sigma\rangle} = \left[1 - i \frac{GZq}{\sqrt{2}V_o} \frac{m^*}{m} (\vec{\sigma}\vec{z}) \right] |\vec{k}\sigma\rangle \qquad (35)$$

and the eigenvalues of the true stationary states, the standing waves (see above), do not change: $\mathcal{E}_k = k^2/2m^*$. The correction to the crystal energy to the second order perturbation theory in V with the functions (35)

$$E_3^{(2)} = \sum_{\substack{\vec{k}\vec{k}' \\ \sigma\sigma'}} \frac{\widetilde{\langle \vec{k}\sigma|V|\vec{k}'\sigma'\rangle}\widetilde{\langle \vec{k}'\sigma'|V|\vec{k}\sigma\rangle}}{\mathcal{E}_k - \mathcal{E}_{k'}} \qquad (36)$$

is easily transformed into the form

$$E_3^{(2)} = \frac{Gm\alpha^2 Z^3 Rq}{\sqrt{2}\pi} \left(\frac{J \cdot \omega^*}{Ry \cdot m}\right)^2 Ry \cdot \frac{3n}{8} \sum_{ij} (\vec{S_i}\times\vec{S_j}) \frac{\vec{R_{ij}}}{R_{ij}} x_{ij} \phi(x_{ij}) \qquad (37)$$

Here again the additional factor $Z^2 R$, discussed above, is taken into account. The corresponding correction to the energy of one ion is equal to

$$E_{3i}^{(2)} = \frac{Gm\alpha^2 Z^3 Rq}{\sqrt{2}\pi} \left(\frac{J \cdot \omega^*}{Ry \cdot m}\right)^2 Ry \cdot \frac{3n}{4} \sum_{j} (\vec{S_i}\times\vec{S_j}) \frac{\vec{R_{ij}}}{R_{ij}} x_{ij} \phi(x_{ij}) \qquad (38)$$

It is seen from this expression that the most long-range part of the P-odd potential between two ions depends on the distance between them as $R^{-2}\cos(2k_F R)$.

For a crude numerical estimate pass from the summation over j to the integration over the spherically-symmetric region $x \geq x_o$. Assuming in the arising in this way expression

$$E_{3i}^{(2)} \approx - \frac{Gm\alpha^2 Z^3 Rq}{\sqrt{2}\pi} \left(\frac{J \cdot \omega^*}{Ry \cdot m}\right)^2 S^2 \frac{\alpha_o}{ck_F} \cdot \frac{x_o \sin x_o + 2\cos x_o}{24\pi} Ry \qquad (39)$$

that $x_o = 2k_F R_o$ where R_o is the minimal distance between the ions, we get $E_{3i}^{(2)} \approx -0.8$ Hz. Numerical summation over the lattice sites in the expression (38) leads to a larger result:

$$E_{3i}^{(2)} \approx -3 \text{ Hz} \qquad (40)$$

Thus, with (29), (33) and (40) taken into account the P-odd correction to the ion energy in the crystal constitutes

$$E_i^{(2)} = E_{1i}^{(2)} + E_{2i}^{(2)} + E_{3i}^{(2)} \approx 80 \text{ Hz} \qquad (41)$$

Of course, this result derived within a rather crude description of electrons in a crystal, is valid evidently only by an order of magnitude.

It is curious that in the used approximation of free electrons the sign of the effect is fixed unambiguously. In the standard model of weak interactions (where $q < 0$) the left spin structures are preferable than the right ones since their energy is lower.

Emphasize once more that the quantity $E_{2i}^{(2)}$ depends only on the sign of the angle of the spin rotation α_o, but not on its absolute value. Just due to the absence of the small parameter $\alpha/k_F c$ this contribution dominates in (41), although other numerical factors in it are disadvantageous.

5. Is it feasible to observe parity nonconservation in crystals with helical spin structure?

The natural question arises on the feasibility to observe the effects under discussion. The found value of the splitting of spin energy in the right and left helical structure ~ 100 Hz

by itself is not so far from the accuracy of $\sim 10^5$ Hz that is fairly common for the measurement of the constants of spin interaction in solid dielectrics by the paramagnetic resonance method [14]. Unfortunately, the exchange interaction in metals gives rise to strong broadening of the EPR lines.

As to the dielectrics with a helical spin structure, more favourable conditions for the EPR spectroscopy in them are accompanied by an additional suppression of P-odd effects. Indeed, the interaction responsible for magnetic ordering in dielectrics is undoubtedly not larger than the indirect exchange in metals. This follows from the comparison of the corresponding Neel points. And the P-odd interaction of d- or f-electrons in a dielectric must contain perhaps an additional smallness - the exchange interaction with s- and p-shells of the ion (see the discussion of the P-odd vector polarizability of holmium in Sect.2). Therefore, the value of the P-odd energy of a spin in a dielectric hardly exceeds 1 Hz.

Another manifestation of parity nonconservation can exist. Left spin structures that possess lower energy will be produced more frequently than the right ones when passing the Neel point if random factors fixing usually the sign of the produced helix are suppressed. This suggestion looks quite fantastic, but the following argument can be presented in its favour. It has been shown in Ref. [15] that by applying crossed electric and magnetic fields it is possible to fix effectively the sign of the arising spin helix in the compound $ZnCr_2Se_4$. The fields used in this experiment, E=2.5 kV/cm, H=12 kOe, are extremely small in the atomic scale. Moreover, an electric field influences a magnetic structure only via small spin-orbit interaction. In the result, the energy of the twisting interaction with these fields is according to a crude estimate only by a factor of 10 - 100 higher than the P-odd energy (41).

6. Bloch domain walls in ferromagnetic films

A usual Bloch domain wall in ferromagnetic can also serve as an example of a helical spin structure. Estimate the possibility for the weak interaction to influence the sign of a helix in the domain wall which is formed when a new domain is created by means of remagnetization of a part of a single-doma-

in film (see Fig.4).[5] The weak interaction gives rise to the twisting of the spins in the plane xy decreasing with the distance from the boundary z=0. Therefore, already in the equilibrium state there is a nucleus of a helical structure.
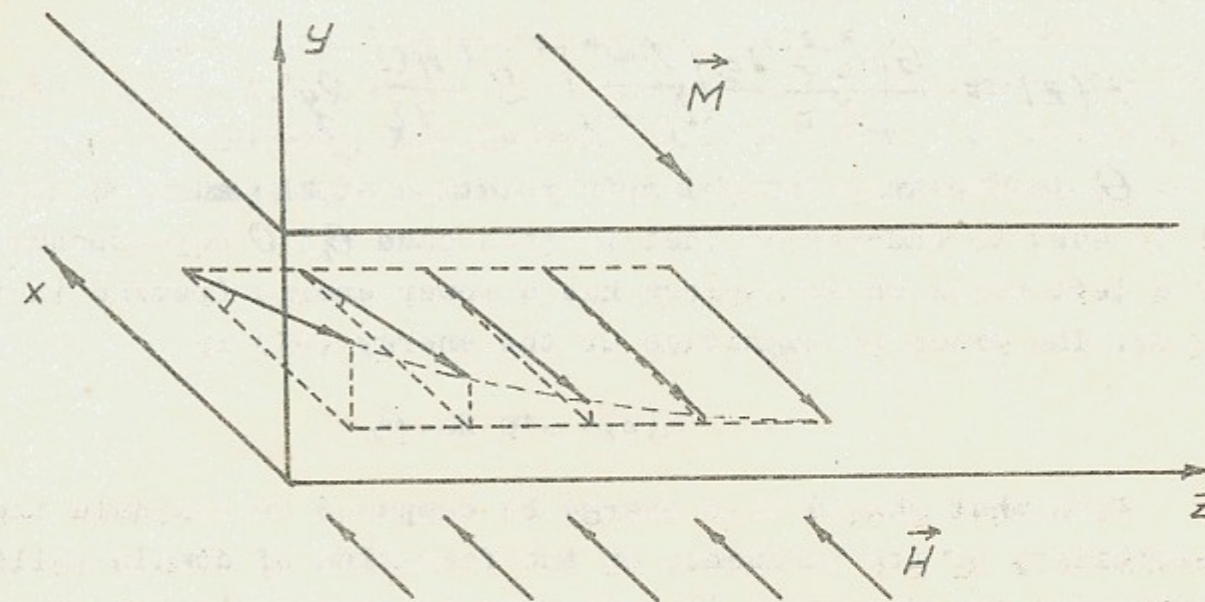

Figure 4. Arising of a spin helix near the boundary z=0 of a ferromagnetic film. $\vec{M}$ is the magnetization, $\vec{H}$ is the remagnetizing field.

Estimate the P-odd energy of an ion located sufficiently far from the boundary z=0. Since the angle of the spin rotation falls off with the distance from the boundary, a significant contribution to the effect can be given only by that part of the weak interaction in which the smallness of the rotation angle is compensated by a formal divergence of the remaining integral at large z. It can be easily seen that none of the expressions (18), (27) and (38) leads to such a divergence. As to the expression (31), only its first, non-oscillating term in the curly brackets possesses the needed property. Assuming that the spin $\vec{S}_i$ is located at the point z and the spin $\vec{S}_j$ is located at the point z', and taking into account the smallness of corresponding angles $\theta(z)$ and $\theta(z')$ of the spin rotation in the plane xy, we find that now $(\vec{S}_i \times \vec{S}_j)_z = -S^2[\theta(z) - \theta(z')]$. Substi-

tuting this expression into the formula (31) and assuming for a crude estimate

$$\theta(z) = \theta_o (1 - z/z_o), \quad z > 0, \quad z_o \text{ is a characteristic length,}$$

we get that in this case

$$E(z) \approx \frac{Gm^2 d^2 Z^3 Rq}{\sqrt{2}\,\pi} \left(\frac{J \cdot m^*}{Ry \cdot m}\right)^2 S^2 \frac{n\theta_o}{32} Ry \qquad (42)$$

Here θ_c is the angle of the spin rotation at the surface z=0. It is easy to understand that in this case $\theta_c > 0$ corresponds to a left helix whose nucleus has a lower energy (remind that q < 0). The order of magnitude of the energy (42) is

$$E(z) \sim -10 \text{ Hz} \cdot \theta_c$$

With what should this energy be compared to evaluate the possibility of its influence on the formation of domain walls? Begin with the fact that in soft magnetic materials the coercitive force, or the field necessary for remagnetization of a domain, constitutes $H_c \sim 10^{-2}$ Oe. The energy of interaction of a magnetic moment with such a field is equal to $E_c \sim \mu H_c \sim 10^{-10}$ eV $\sim 10^{-11}$ Ry $\sim 10^4$ Hz. However, in fact, the remagnetization is caused not by the coercitive force itself which is none other than the depth of a local minimum of the energy of the spin as a function of the angle of its rotation, but by the excess over zero of the spin energy in the field; and this excess can be made much smaller than E_c. In addition, the generalized momentum of the P-odd forces $K = -\partial E/\partial\theta$ is independent of the angle θ, meanwhile the momentum of the usual remagnetizing forces is proportional to a small initial deviation angle since switching on of the oppositely directed magnetic field leads to the arising of a local maximum of energy near $\theta = 0$. Hence, the attempt to observe parity violation in the domain formation, i.e., the obtaining dominantly of left-helical Bloch walls, does not seem hopeless. We would like to emphasize however that this problem requires at any rate sufficiently soft magnetic films with small number of defects and fairly accurate geometry of magnetic fields.

It should be noted that the hypothesis of a dominant for-

mation of Bloch walls with one sign of helix is being discussed already for a rather long time [16-18], although without any connection with the weak interactions.

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P-НЕЧЕТНОЕ ДАЛЬНОДЕЙСТВИЕ ИОНОВ В МАГНИТО-УПОРЯДОЧЕННЫХ КРИСТАЛЛАХ