P-odd long-range action of ions magnetically ordered crystals

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Account is taken of parity nonconservation; exchange interaction of ions with electrons leads, in crystals with magnetic structure, to spin-dependent long-range forces between the ions. The energy of the *P*-odd interaction reaches ~ 100 Hz for rare-earth crystals having a helicoidal spin structure. The possibility of observing parity nonconservation in these crystals, as well as in Bloch domain walls in ferromagnetic films, is discussed.

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1. INTRODUCTION

In our preceding paper, in which *P*-odd Van der Waals forces were considered, it was noted that a parity-nonconserving interaction between the ions splits the energies of crystals with right- and left-hand helicoidal spin structures. This effect, which is the analog of the energy difference between right and left molecules (or crystals), is due to weak interaction, a phenomenon discussed earlier many times, but not yet observed in experiment. The present paper is devoted to a theoretical investigation of effects of parity violation in magnetically ordered crystals. Even though parity nonconservation in atomic phenomena has been reliably established by now in experiments of various groups,[2–4] observation of *P*-odd effects in crystals would undoubtedly be of great scientific interest.

A helicoidal spin structure is encountered in alloys and compounds containing elements with unfilled *d* or *f* shells (MnO_2, $TbMn_2$, Ce_2Fe_{17}, and others), as well as in the rare-earth metals Dy, Ho, and Er.[5] A helicoidal spin structure is possessed also by domain walls in ferromagnets. We shall show below that the main contribution to *P*-odd effects is made by exchange interaction of conduction electrons with ions. Inasmuch as no such interaction takes place in dielectrics, the *P*-odd effects in them are much smaller than in metals. Although one cannot exclude the possibility that observation of the phenomena in question in dielectrics can nevertheless be simpler, we confine ourselves to metals.

When discussing actual mechansims of *P*-odd interaction of ions in crystals, all the numerical estimates will be made for holmium. The advantages of holmium crystals are the stability of the helicoidal structure at low temperatures, the rather large charge of the nuclear ($Z = 67$), as well as the large momentum that forms the helix. Therefore, the *P*-odd energy of the holmium ion is larger than, say, of dysprosium or erbium.

The structure of metallic holmium is the following[6]: the triply ionized Ho^{3+} ions are localized on sites of a hexagonal close-packed lattice ($a = 6.77, c = 10.62$ a.u.). At a temperature lower than 132 K the magnetic moments of the ions located in the same basal plane lie in the very same plane and are parallel to one another. On going in succession from plane to plane, the moments are rotated through an angle α_0 that depends on the temperature. Below 20 K the magnetic moments of the ions acquire a small ferromagnetic component along the hexagonal axis, and the angle α_0 depends little on temperature and is close to 30°. The phase transitions "ferromagnetic helix-simple helix" and "simple helix-paramagnet" in holmium are not accompanied by a change in the spatial lattice. The electronic structures of the holmium atom and ion are

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

$$\text{Ho}^{3+}:\quad (4f^{10})\quad {}^5I_8\,.$$

The spin of the most abundant isotope ^{165}Ho is 7/2.

P-ODD VAN DER WAALS INTERACTION OF IONS

The energy of the *P*-odd Van der Waals interaction of two identical ions with angular momenta **J** separated by a distance **R** is written in the form[1]:

$$U(\mathbf{R})=U_v(\mathbf{R})+U_t(\mathbf{R}),$$

$$U_v(\mathbf{R})=4\frac{\mathbf{N}[\mathbf{J}_1\times\mathbf{J}_2]}{R^5}\frac{1}{2\pi i}\int\alpha_v(\omega)\beta_v(\omega)\omega\,d\omega, \tag{1}$$

$$U_t(\mathbf{R})=2\varepsilon_{kni}\frac{N_n}{R^5}\times(\delta_{ls}-3N_lN_s)Q_{is}^{(1)}Q_{lk}^{(2)}\frac{1}{2\pi i}\int\alpha_t(\omega)\beta_t(\omega)\omega\,d\omega,$$

where

$$\mathbf{N}=(\mathbf{R}_1-\mathbf{R}_2)/|\mathbf{R}_1-\mathbf{R}_2|;\ Q_{ik}=J_iJ_k+J_kJ_i-{}^2/{}_3\delta_{ik}J(J+1);$$

$\alpha_v(\omega)$, $\alpha_t(\omega)$, $\beta_v(\omega)$, and $\beta_t(\omega)$ are the vector and tensor *P*-even and *P*-odd polarizabilities of the ions, such that

$$\begin{aligned}\alpha_{ik}(\omega)&=\alpha_s(\omega)\delta_{ik}+i\varepsilon_{ikr}J_r\alpha_v(\omega)+Q_{ik}\alpha_t(\omega),\\ \beta_{ik}(\omega)&=i\beta_s(\omega)\delta_{ik}+\varepsilon_{ikr}J_r\beta_v(\omega)+iQ_{ik}\beta_t(\omega),\end{aligned}\tag{2}$$

$\alpha_s(\omega)$ and $\beta_s(\omega)$ are the scalar polarizabilities, while the polarizability tensors $\alpha_{ik}(\omega)$ and $\beta_{ik}(\omega)$ can be represented in the form

$$\alpha_{ik}(\omega)=\sum_n\left\{\frac{\langle 0|d_i|n\rangle\langle n|d_k|0\rangle}{\omega_{n0}-\omega-i\varepsilon}+\frac{\langle 0|d_k|n\rangle\langle n|d_i|0\rangle}{\omega_{n0}+\omega-i\varepsilon}\right\}, \tag{3}$$

$$\beta_{ik}(\omega)=\sum_n\left\{\frac{\langle 0|d_i|n\rangle\langle n|\mu_k|0\rangle}{\omega_{n0}-\omega-i\varepsilon}+\frac{\langle 0|\mu_k|n\rangle\langle n|d_i|0\rangle}{\omega_{n0}+\omega-i\varepsilon}\right\}, \tag{4}$$

where **d** and **μ** are the electric and magnetic dipole moments

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of the ions: $\omega_{n0} = E_n - E_0$; E_0 and E_n are the energies of the ground and excited states.

In the calculation of the sums (3) and (4) we shall describe the excited single-electron states $|n\rangle$ of the ion in the crystal by plane waves. Arguments favoring this approximation are the following. In the orthogonalized plane wave method we have

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

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

$$\langle 4f|\mathbf{r}|n\rangle = \langle 4f|\mathbf{r}|\mathbf{k}\rangle - \sum_{\lambda}\langle 4f|\mathbf{r}|\lambda\rangle\langle\lambda|\mathbf{k}\rangle,$$

$|\lambda\rangle = |4d\rangle$ predominates in the sum over λ, and the numerical calculations using the Hartree-Fock wave functions of the holmium atom$^{1)}$ show that

$$|\langle 4f|\mathbf{r}|\mathbf{k}\rangle| \gg |\langle 4f|\mathbf{r}|4d\rangle\langle 4d|\mathbf{k}\rangle|$$

in a wide range of $|\mathbf{k}|$ (see Fig. 1). 2) It is this which enables us to use for $|n\rangle$ simply plane waves with $k > k_F$.

We begin with calculation of the vector polarizability $\alpha_v(\omega)$ of the ion in the crystal. It receives contributions only from the electrons of the unfilled shell $4f_{7/2}$. Substituting in (3) the relation

$$\langle 0|r_i|n\rangle=i\langle 0|p_i|n\rangle/m\omega_{n0}$$

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

$$\alpha_v(\omega)\approx-\frac{2\alpha(\mathbf{jl})}{\pi j(j+1)}\frac{m^*}{m}\int_{k_F}^{\infty}I_{jl}^2(k)\times\left(\frac{1}{E_k-\omega}-\frac{1}{E_k+\omega}\right)dk, \tag{5}$$

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

$$I_{jl}(k)=\int_0^{\infty}R_{jl}(r)j_l(kr)r^2\,dr, \tag{6}$$

$j_l(kr)$ is a spherical Bessel function and $R_{jl}(r)$ is the radial function of the $4f$ electron. In the derivation of (5) it was taken into account that the Fermi energy is reckoned in practice from E_0. As $\omega\to 0$ the vector polarizability of the ion is

$$\alpha_v(\omega)\approx-\frac{8a_B^3}{\pi}\frac{(\mathbf{jl})}{j(j+1)}\left(\frac{m^*}{m}\right)^2\frac{\omega}{\mathrm{Ry}}\int_{k_F}^{\infty}I_{jl}^2(k)\frac{dk}{k^4}, \tag{7}$$

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

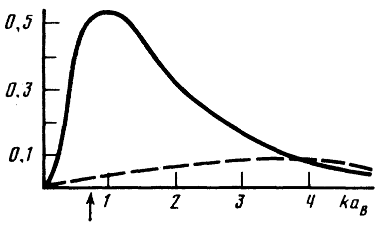

FIG. 1. Dependence of $\langle 4f|r|k\rangle$ (solid line) and $\langle 4f|r|4d\rangle\langle 4d|k\rangle$ (dashed line) on k. The arrow marks the position of k_F in the free-electron model.

It is much more difficult to estimate the P-odd polarizability $\beta_{ik}(\omega)$, which differs from zero only when account is taken of the weak interaction of the electrons with the nucleus. For the vector and tensor components of interest to us, these electrons should belong to an unfilled shell, in this case f. The weak interaction of an electron with a nucleus is, however, local in character, proportional to $\mathbf{p}\delta(\mathbf{r})$, and leads to mixing of only $s_{1/2}$ and $p_{1/2}$ electrons (see, e.g., Ref. 7). Therefore the functions $\beta_v(\omega)$ and $\beta_t(\omega)$ differ here from zero only because of the mixing of the configurations. The relative magnitude of this mixing is $J/\mathrm{Ry}\sim 10^{-1}$–$10^{-2}$. If we consider the f-shell P-odd polarizability that results from the admixture of the s and p configurations, it can be easily seen that $\beta_{v,t}(\omega)$ can appear only in second order in J/Ry on account of diagrams of the type in Fig. 2a. Here V is the operator of the interconfiguration interaction and W is that of the weak interaction. A more substantial contribution to $\beta_v(\omega)$ comes therefore from the inner s and p shells that are polarized by the interaction with the outer f shell. This interaction need be taken into account only once, and this leads to diagrams of the type 2b. However, since this mechanism is linear in the f-electron spin, it contributes only to the vector P-odd polarizability of the ion.

Thus, compared with the P-even vector polarizability, the P-odd one of a rare-earth element contains an additional small quantity

$$\frac{Gm^2\alpha^3Z^3R}{\pi}\frac{J}{\mathrm{Ry}}, \tag{8}$$

where $G\approx 10^{-5}mp^{-2}$ is the Fermi constant of the weak interaction, $R\sim 5$ is the relativistic factor of enhancement of the weak interaction of the electron with the nucleus (see its definition in Ref. 7); we neglect here the difference between m^* and m. As for the tensor polarizability $\beta_t(\omega)$, it depends quadratically on the factor J/Ry. In addition, owing to the intermediate position of the elements of interest to us (Dy, Ho, Er) in the series of rare earth elements with unfilled $f_{7/2}$ shell, their quadrupole moment is small, and even zero for holmium. The result is an additional smallness of the tensor polarizabilities, both P-even and P-odd.

We proceed now to the numerical estimates. We use, as already noted, the Hartree-Fock wave functions for the holmium atom. The result of the numerical calculation of the integral (6) as a function of k is shown in Fig. 3. As a result the polarizability of the holmium ion does not exceed its estimated value and for small ω we have

$$\alpha_v(\omega)\leqslant a_B^3\omega/\mathrm{Ry}. \tag{9}$$

But then even an optimistic estimate yields for the interac-

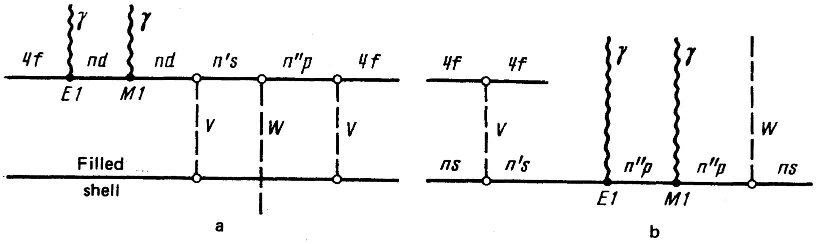

FIG. 2. Onset of *P*-odd vector polarizability of a rare-earth ion.

tion of two ions

$$U_v \sim \frac{GZ^3Rm^2\alpha^4}{\pi}\frac{J}{\mathrm{Ry}}\mathbf{N}_{12}[\mathbf{J}_1\times\mathbf{J}_2]\left(\frac{a_B}{R_{12}}\right)^5 \mathrm{Ry}. \qquad (10)$$

The energy per ion in the crystal is in this case

$$E_i \sim \frac{GZ^3Rm^2\alpha^4}{\pi}\frac{J}{\mathrm{Ry}}\sum_j \mathbf{N}_{ij}[\mathbf{J}_i\times\mathbf{J}_j]\left(\frac{a_B}{R_{ij}}\right)^5 \mathrm{Ry}, \qquad (11)$$

amounting for Ho ($Z = 67$; $R \approx 4/5$; $|\mathbf{J}| = 8$; $J/\mathrm{Ry} \sim 0.1$) to

$$E_i \sim 10^{-16} - 10^{-17}\,\mathrm{Ry} \sim 0.1\ \mathrm{Hz}.$$

This is much less than the estimate of Ref. 1. The discrepancy is explained by the following factors. First, in contrast to the scalar polarizability, a contribution to which is made by all the electrons of the ions, so that $\alpha_s \sim 10^2\, a_B^3$, the vector polarizability [see (9)] does not contain a large contribution and receives contributions only from the unfilled-shell electrons. Second, the features of the construction of the electron shells of the elements, among which helicoidal spin structures are encountered, lead to the necessity for including the interconfiguration interaction, so that an additional smallness is added to the *P*-odd polarizability. Going from *f* to *d* metals does not eliminate this smallness.

3. *P*-ODD EXCHANGE INTERACTION OF IONS. FIRST ORDER

Fortunately, there are more effective mechanisms that lead to *P*-odd long-range action of an ion in a crystal. They are connected with the indirect exchange interaction. We shall use the simple indirect-exchange, model proposed by Ruderman, Kittel, Kasuya, and Yosida (RKKY).[8–10] The spin-dependent exchange interaction between a conduction electron and the electron of the unfilled ion shells is described in this model by the operator

$$V(\mathbf{r}) = -JV_0\sum_i (\mathbf{s}\mathbf{S}_i)\,\delta(\mathbf{r}-\mathbf{R}_i), \qquad (12)$$

where s is the conduction-electron spin; $\mathbf{S}_i$ is the spin of an ion located at the point $\mathbf{R}_i$; V_0 is the volume per ion in the crystal. For heavy rare-earth elements the exchange integral J is positive and amounts to $\sim 10^{-2}$ of the Fermi energy E_F. In second-order perturbation theory the operator (12) leads to the following interaction between two ions (see, e.g., Ref. 6)

$$E_{ij} = -{}^9/_2\pi n^2 E_F (J/E_F)^2 (\mathbf{S}_i\mathbf{S}_j)\,\phi(x_{ij}), \qquad (13)$$

where

$$x_{ij} = 2k_F|\mathbf{R}_i-\mathbf{R}_j|, \quad \phi(x) = j_1(x)/x^2, \quad j_1(x) = -\frac{d}{dx}\frac{\sin x}{x},$$

$j_1(x)$ is a spherical Bessel function, n is the number of conduction electrons per ion, and k_F is the Fermi momentum. The onset of stable spin helices in crystals with helicoidal structure is due precisely to this interaction (Refs. 11 and 12).[3)] We note that it decreases with distance between the ions much more slowly (αR^{-3}) than the Van der Waals interaction (αR^{-6}).

Let us find the crystal-energy correction necessitated by the interaction (12) and by the weak *P*-odd interaction between the conduction electrons and the ion nuclei. It is convenient to use in these calculations the nonrelativistic limit of the *P*-odd weak interaction of the electron with the nucleus, whch we write in the form (see, e.g., Ref. 7)

$$W(\mathbf{r}) = \frac{G}{2^{1/2}\,2m}\sum_i \{Zq[(\boldsymbol{\sigma}\mathbf{p}),\delta(\mathbf{r}-\mathbf{R}_i)]_+ + \varkappa[(\mathbf{I}_i\mathbf{p}),\delta(\mathbf{r}-\mathbf{R}_i)]_+ + i\varkappa'[[\mathbf{I}_i\boldsymbol{\sigma}]\mathbf{p},\delta(\mathbf{r}-\mathbf{R}_i)]_-\}. \qquad (14)$$

Here $[\;]_-$ and $[\;]_+$ denote respectively the commutator and the anticommutator, $\mathbf{p}$ is the electron-momentum operator, and $\mathbf{I}_i$ is the nuclear spin of the ion at the point $\mathbf{R}_i$. In the dimensionless constant Z_q for the first structure the large factor Z was actually separated to emphasize that the constant increases with increasing number of nucleons in the nucleus. In the standard weak-interaction model, $q \approx -0.7$ for rare-earth elements. We note that $\varkappa$ and $\varkappa'$ are numerically small in the same model.

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

The correction to the energy of an electron with momentum $\mathbf{k}$ and with spin projection σ is linear in V and W and is obviously equal to

$$E^{(1)}_{\mathbf{k}\sigma} = \sum_{\mathbf{k}'\sigma'} \frac{\langle \mathbf{k}\sigma|V|\mathbf{k}'\sigma'\rangle\langle \mathbf{k}'\sigma'|W|\mathbf{k}\sigma\rangle}{k^2-k'^2}\cdot 2m^* + \mathrm{H.c.} \qquad (15)$$

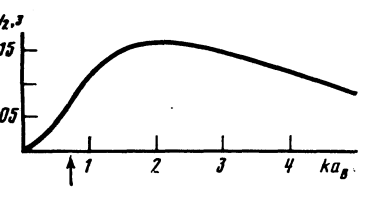

FIG. 3. Dependence of $J_{7/2,3}$ on k. The arrow marks the position of k_F in the free-electron model.

The total correction $E(1)$ to the crystal energy is obtained from this expression by summing over $\mathbf{k}$, $|\mathbf{k}| \leqslant k_F$, and over σ. From invariance considerations it is clear that the structure of the pseudoscalar correction should be

$$\sum_{ij} [\mathbf{I}_i \times \mathbf{S}_j] \mathbf{R}_{ij} f(R_{ij}).$$

Therefore the first, leading term in (14), which is proportional to Z but is independent of $\mathbf{I}_i$, makes no contribution to this correction. The term with $\varkappa$ in the operator (14), a term independent of the electron spin, obviously also drops out upon summation over σ and σ'. Simple calculations yield in the upshot

$$E^{(1)} = \frac{2G\varkappa'}{\sqrt{2}} \frac{m^*}{m} J V_0 \int\limits_{|\mathbf{k}| \leqslant k_F} \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\mathbf{k}'}{(2\pi)^3} \times \sum_{ij} [\mathbf{I}_i \times \mathbf{S}_j] \nabla \frac{\exp(-i(\mathbf{k}'-\mathbf{k})\mathbf{r})}{k'^2 - k^2} \bigg|_{\mathbf{r}=\mathbf{R}_{ij}} \tag{16}$$

Integrating with respect to $\mathbf{k}$ and $\mathbf{k}'$ and introducing the factor Z^2R that takes into account the difference between the conduction electron density at the nucleus and the average density over the crystal, we obtain hence

$$E^{(1)} = -\frac{Gm^2\alpha^2Z^2R\varkappa'}{2^{1/2}\pi} \frac{J}{\mathrm{Ry}} \frac{m^*}{m} (k_F a_B)^2 \,\mathrm{Ry} \cdot 3n \sum_{ij} [\mathbf{I}_i \times \mathbf{S}_j] \frac{\mathbf{R}_{ij}}{R_{ij}} \frac{d\phi(x_{ij})}{dx_{ij}},$$
$$x_{ij} = 2k_F R_{ij}, \quad \phi(x) = j_1(x)/x^2 = -\frac{1}{x^2} \frac{d}{dx} \frac{\sin x}{x}. \tag{17}$$

Account was taken here of the obvious relation $V_0 k_F^3 = 3\pi^2 n$. We recall that, as can be seen from (17). The interaction between two ions decreases at large distances ($k_F r \gg 1$) like $r^{-3} \sin(2k_F r)$.

If the hyperfine coupling is assumed unbroken, the interaction energy of one nuclear spin, obtained from (17), equals

$$E_i^{(1)} = -\frac{Gm^2\alpha^2R\varkappa'Z^2}{2^{1/2}\pi} \frac{J}{\mathrm{Ry}} \frac{m^*}{m} \times (k_F a_B)^2 \,\mathrm{Ry} \cdot 6n \sum_j [\mathbf{I}_i \times \mathbf{S}_j] \frac{\mathbf{R}_{ij}}{R_{ij}} \frac{d\phi(x_{ij})}{dx_{ij}}. \tag{18}$$

For a rough numerical estimate of the result we replace the summation over the lattice sites by integration over all of space. Expression (18) reduces then to

$$E_i^{(1)} \approx -\frac{Gm^2\alpha^2Z^2R\varkappa'}{2^{1/2}\pi} \frac{J}{\mathrm{Ry}} \frac{m^*}{m} (k_F a_B)^2 IS \frac{\alpha_0}{k_F c} \frac{1}{\pi} \mathrm{Ry}. \tag{19}$$

Besides changing to integration, we have neglected here the small ferromagnetic component S and confined ourselves to the first order in the parameter $\alpha_0/k_F c$, which is indeed very small. Numerical summation over the lattice sites leads to a result that is approximately twice as large as (19). Substituting in (19) the experimental values (Ref. 6, p. 260 of Russ. transl.) $J \approx 0.7 \times 10^{-2}$ Ry and $m^* \approx 3m$, which correspond to the free-electron model ($k_F a_B \approx 0.75$), we obtain when account is taken of the aforementioned correction from the numerical calculation[4)]

$$E_i^{(1)} \approx -2 \cdot 10^{-15} \varkappa' \,\mathrm{Ry} \approx -7\varkappa' \,\text{Гц}. \tag{20}$$

We note once more that in the standard weak-interaction model the constant $\varkappa'$ is numerically small.

Generally speaking, in this same order there could arise one more correction to the crystal energy. We have in mind the Fermi-surface deformation, which is different for opposite spin orientation and is due to the perturbation of V, with subsequent allowance for W. Conversely, W would deform the Fermi surface, and then V would be taken into account. In our case, however, there is no such correction. Indeed, the sums over the "exchange" and "weak" sites factor out here, and then it becomes simply impossible to construct a pseudoscalar that is invariant to translations. This eliminates, by the same token, the problem of the relation between this contribution and the usual second-order correction (see Refs. 10 and 13).

4. SECOND-ORDER EFFECT IN THE EXCHANGE INTERACTION

In first-order perturbation theory in the exchange interaction (12) the first leading term in the P-odd Hamiltonian (14), which increases with the number of nucleons in the nucleus, has dropped out. One can hope therefore that in second order in V the small quantity J/Ry will be offset by the factor Z. The corresponding correction to the crystal energy is

$$\begin{aligned} E^{(2)} = (2m^*)^2 \sum_{\substack{|\mathbf{k}| \leqslant k_F \\ \sigma}} \Bigg\{ \sum_{\substack{\mathbf{k}'\mathbf{k}'' \\ \sigma'\sigma''}} \Bigg[& \frac{\langle \mathbf{k}\sigma | V | \mathbf{k}'\sigma' \rangle \langle \mathbf{k}'\sigma' | V | \mathbf{k}''\sigma'' \rangle \langle \mathbf{k}''\sigma'' | W | \mathbf{k}\sigma \rangle}{(k^2 - k'^2)(k^2 - k''^2)} \\ & + \frac{\langle \mathbf{k}\sigma | V | \mathbf{k}'\sigma' \rangle \langle \mathbf{k}'\sigma' | W | \mathbf{k}''\sigma'' \rangle \langle \mathbf{k}''\sigma'' | V | \mathbf{k}\sigma \rangle}{(k^2 - k'^2)(k^2 - k''^2)} \\ & + \frac{\langle \mathbf{k}\sigma | W | \mathbf{k}'\sigma' \rangle \langle \mathbf{k}'\sigma' | V | \mathbf{k}''\sigma'' \rangle \langle \mathbf{k}''\sigma'' | V | \mathbf{k}\sigma \rangle}{(k^2 - k'^2)(k^2 - k''^2)} \Bigg] \\ & - \langle \mathbf{k}\sigma | V | \mathbf{k}\sigma \rangle \sum_{\mathbf{k}'\sigma'} \frac{\langle \mathbf{k}\sigma | V | \mathbf{k}'\sigma' \rangle \langle \mathbf{k}'\sigma' | W | \mathbf{k}\sigma \rangle + \mathrm{H.c.}}{(k^2 - k'^2)^2} \\ & - \langle \mathbf{k}\sigma | W | \mathbf{k}\sigma \rangle \sum_{\mathbf{k}'\sigma'} \frac{\langle \mathbf{k}\sigma | V | \mathbf{k}'\sigma' \rangle \langle \mathbf{k}'\sigma' | V | \mathbf{k}\sigma \rangle}{(k^2 - k'^2)^2} \Bigg\}. \end{aligned} \tag{21}$$

It is easy to show that the terms proportional to $\varkappa$ and $\varkappa'$ in the operator W do not work in this approximation. Next, the diagonal matrix element of the remaining term W on the true stationary states of the electron states in the crystal (standing waves, there are no current states in our problem) is obviously zero. This allows us to leave out immediately the last term of (21). As for the remaining terms, it can be easily verified that in the limit of large crystal dimensions it is possible to use traveling rather than standing waves, a technically much more convenient procedure.

The next-to-last term in (21) can differ from zero only in the presence of a ferromagnetic component, when

$$\langle \mathbf{k}\sigma | V | \mathbf{k}\sigma\rangle = -J\frac{V_0}{V}\langle\sigma\rangle\sum_i \mathbf{S}_i \neq 0. \qquad (22)$$

After summation over the momenta and spins, however, the answer for the term in question should, from invariance considerations, be of the form

$$\sum_i \mathbf{S}_i \sum_{js} [\mathbf{S}_j \times \mathbf{R}_{js}] F(R_{js}).$$

It can be easily seen that by virtue of the symmetry of the problem summation over s causes this expression to vanish.

For a similar reason, the contributions made to the energy by the deformation of the Fermi surface, similar to those discussed at the end of the preceding section, also vanish.

As a result, the correction to the crystal energy reduces to

$$E^{(2)} = i\frac{GZ^3Rqm}{2^{1/2}}\left(JV_0\frac{m^*}{m}\right)^2 \times \int\limits_{|\mathbf{k}|\leqslant k_F}\frac{d\mathbf{k}}{(2\pi)^3}\int\frac{d\mathbf{k}'\,d\mathbf{k}''}{(2\pi)^6}(k^2-k'^2)^{-1}(k^2-k''^2)^{-1}$$
$$\times\sum_{ijs}[\mathbf{S}_i\mathbf{S}_j]\{(\mathbf{k}'+\mathbf{k})\exp(i\mathbf{k}''\mathbf{R}_{ij}-i\mathbf{k}'\mathbf{R}_{is}+i\mathbf{k}\mathbf{R}_{js})-(\mathbf{k}'+\mathbf{k}'')$$
$$\times\exp(-i\mathbf{k}\mathbf{R}_{ij}+i\mathbf{k}'\mathbf{R}_{is}-i\mathbf{k}''\mathbf{R}_{js})+(\mathbf{k}+\mathbf{k}'')$$
$$\times\exp(i\mathbf{k}'\mathbf{R}_{ij}-i\mathbf{k}\mathbf{R}_{is}+i\mathbf{k}''\mathbf{R}_{js})\}. \qquad (23)$$

Besides the constant Z_q, we have taken directly into account here the already mentioned factor Z^2R connected with the difference between the conduction-electron density near the nucleus and the density averaged over the crystal. Without further approximations it is impossible to calculate the sum (23) analytically or even numerically.

We consider therefore first the contributions from the terms with $s = i$ and $s = j$. The corresponding energy correction takes the form of a sum of two terms:

$$E_1^{(2)} = \frac{2GZ^3Rqm}{2^{1/2}}\left(JV_0\frac{m^*}{m}\right)^2 \times \int\limits_{|\mathbf{k}|\leqslant k_F}\frac{d\mathbf{k}}{(2\pi)^3}\int\frac{d\mathbf{k}'\,d\mathbf{k}''}{(2\pi)^6}(k^2-k'^2)^{-1}(k^2-k''^2)^{-1}$$
$$\times\sum_{ij}[\mathbf{S}_i\mathbf{S}_j]\nabla e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}}|_{\mathbf{r}=\mathbf{R}_{ji}}, \qquad (24)$$

$$E_2^{(2)} = \frac{GZ^3Rqm}{2^{1/2}}\left(JV_0\frac{m^*}{m}\right) \times \int\limits_{|\mathbf{k}|\leqslant k_F}\frac{d\mathbf{k}}{(2\pi)^3}\int\frac{d\mathbf{k}'\,d\mathbf{k}''}{(2\pi)^6}(k^2-k'^2)^{-1}(k^2-k''^2)^{-1}$$
$$\times\sum_{ij}[\mathbf{S}_i\mathbf{S}_j]\nabla e^{i(\mathbf{k}'-\mathbf{k}'')\mathbf{r}}|_{\mathbf{r}=\mathbf{R}_{ji}}. \qquad (25)$$

When calculating the first of them, we encounter in the integration with respect to k'' the usual divergence in the calculation of the correction of second order in the contact interaction. For purposes of regularization, we introduce the limiting integration momentum Q, which can naturally be identified with the reciprocal radius of the ion f shell. Elementary transformations then reduce (24) to the form

$$E_1^{(2)} = -\frac{Gm^2\alpha^2Z^3Rq}{2^{1/2}\pi}\frac{Q}{k_F} \times\left(\frac{Jm^*}{\mathrm{Ry}\,m}\right)^2\mathrm{Ry}\frac{9n^2}{4}\sum_{ij}[\mathbf{S}_i\times\mathbf{S}_j]\frac{\mathbf{R}_{ij}}{R_{ij}}\frac{d\phi(x_{ij})}{dx_{ij}}, \qquad (26)$$

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

$$E_{1i}^{(2)} = -\frac{Gm^2\alpha^2Z^3Rq}{2^{1/2}\pi}\frac{Q}{k_F} \times\left(\frac{Jm^*}{\mathrm{Ry}\,m}\right)^2\mathrm{Ry}\frac{9n^2}{2}\sum_{i}[\mathbf{S}_i\times\mathbf{S}_j]\frac{\mathbf{R}_{ij}}{R_{ij}}\frac{d\phi(x_{ij})}{dx_{ij}}. \qquad (27)$$

The sum here is in fact the same as in (18). Again going from summation to integration, we obtain

$$E_{1i}^{(2)} \approx -\frac{Gm^2\alpha^2Z^3Rq}{2^{1/2}\pi}\frac{Q}{k_F}\left(\frac{Jm^*}{\mathrm{Ry}\,m}\right)^2 S^2\frac{\alpha_0}{ck_F}\frac{3n}{4\pi}\mathrm{Ry}. \qquad (28)$$

Using the numerical value $Q \approx 1.3a_B^{-1}$ and taking into account the correction factor ~ 2 due to the numerical summation, as mentioned in the preceding section, we obtain the value of this correction:

$$E_{1i}^{(2)} \approx 1{,}1\cdot 10^{-14}\ \mathrm{Ry} \approx 35\ \mathrm{Hz}. \qquad (29)$$

It can be verified that no divergence arises at large momenta in the ramaining terms of (23). Therefore, although the ratio Q/k_F is actually small (~ 1.7), the presence of this literal parameter in the obtained contribution suggests that it is not fully cancelled out by other terms and can therefore serve as a relatively reliable lower-bound estimate of the effect discussed.

No additional complications are encountered in the calculation of the contribution (25). A trival integration over all $\mathbf{k}$ gives for the corrections to the energy of the entire crystal $E_2^{(2)}$ and for the energy of one spin $F_{2i}^{(2)}$ the following expressions:

$$E_2^{(2)} = -\frac{Gm^2\alpha^2Z^3Rq}{2^{1/2}\pi}\left(\frac{Jm^*}{\mathrm{Ry}\,m}\right)^2\mathrm{Ry}\cdot\frac{3\pi n^2}{16}\sum_{ij}[\mathbf{S}_i\times\mathbf{S}_j] \times\frac{\mathbf{R}_{ij}}{R_{ij}}\frac{d}{dx_{ij}}\left[\frac{1}{x_{ij}^2}+\frac{3}{x_{ij}^2}\frac{d}{dx_{ij}}j_1(x_{ij})\right], \qquad (30)$$

$$E_{2i}^{(2)} = -\frac{Gm^2\alpha^2Z^3Rq}{2^{1/2}\pi}\left(\frac{Jm^*}{\mathrm{Ry}\,m}\right)^2\mathrm{Ry}\cdot\frac{3\pi n^2}{8}\sum_{j}[\mathbf{S}_i\times\mathbf{S}_j] \times\frac{\mathbf{R}_{ij}}{R_{ij}}\frac{d}{dx_{ij}}\left[\frac{1}{x_{ij}^2}+\frac{3}{x_{ij}^2}\frac{d}{dx_{ij}}j_1(x_{ij})\right]. \qquad (31)$$

We note that it can be seen from this that the interaction between two ions at large distances contains, besides an oscillating part, a nonoscillating contribution that decreases like r^{-3}.

For a numerical estimate, the summation over j in (31) can be replaced by integration over all of space. Neglecting, as before, the small ferromagnetic component, we obtain in principal order in α_0

$$E_{2i}^{(2)} \approx -\frac{Gm^2\alpha^2Z^3Rq}{2^{1/2}\pi}\left(\frac{Jm^*}{\mathrm{Ry}\,m}\right)^2 S^2\frac{\alpha_0}{|\alpha_0|}\frac{\pi n}{32}\mathrm{Ry}. \tag{32}$$

This contribution, which of zero order in α_0, stems from the aforementioned nonoscillating terms $\sim r^{-3}$ in the ion-ion interaction. Numerical summation over the lattice sites in (31) leads to a result smaller by 15–20%. This contribution is thus

$$E_{2i}^{(2)} \approx 1.6\cdot10^{-14}\,\mathrm{Ry} \approx 50\ \mathrm{Hz}. \tag{33}$$

Finally, to estimate the contribution made by the terms with $s \neq i, j$ to the correction (23) for the crystal energy $E(2)$, it is convenient to proceed as follows. We "smear out" the weak interaction over the entire crystal:

$$W \to \frac{GZq}{2^{1/2}mV_0}(\sigma\mathbf{p}).$$

The eigenfunction of the Hamiltonian obtained in this manner

$$H = \frac{p^2}{2m^*} + \frac{GZq}{2^{1/2}mV_0}(\sigma\mathbf{p}) \tag{34}$$

is equal to

$$|\widetilde{\mathbf{k}\sigma}\rangle = \left[1 - i\frac{GZq}{2^{1/2}V_0}\frac{m^*}{m}(\sigma\mathbf{r})\right]|\mathbf{k}\sigma\rangle, \tag{35}$$

and the eigenvalues for the true stationary states of the standing waves (see above) remain unchanged: $\varepsilon_k = k^2/2m^*$. The correction to the crystal energy in second order of perturbation theory in V with the functions (35)

$$E_3^{(2)} = \sum_{\substack{\mathbf{kk'}\\ \sigma\sigma'}} \frac{\langle\widetilde{\mathbf{k}\sigma}|V|\widetilde{\mathbf{k}'\sigma'}\rangle\langle\widetilde{\mathbf{k}'\sigma'}|V|\widetilde{\mathbf{k}\sigma}\rangle}{\varepsilon_k - \varepsilon_{k'}} \tag{36}$$

is easily transformed into

$$E_3^{(2)} = \frac{Gm^2\alpha^2Z^3Rq}{2^{1/2}\pi} \times\left(\frac{Jm^*}{\mathrm{Ry}\,m}\right)^2 \mathrm{Ry}\cdot\frac{3n}{8}\sum_{ij}[\mathbf{S}_i\times\mathbf{S}_j]\frac{\mathbf{R}_{ij}}{R_{ij}}x_{ij}\phi(x_{ij}). \tag{37}$$

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

$$E_{3i}^{(2)} = \frac{Gm^2\alpha^2Z^3Rq}{2^{1/2}\pi} \times\left(\frac{Jm^*}{\mathrm{Ry}\,m}\right)^2 \mathrm{Ry}\cdot\frac{3n}{4}\sum_{j}[\mathbf{S}_i\times\mathbf{S}_j]\frac{\mathbf{R}_{ij}}{R_{ij}}x_{ij}\phi(x_{ij}). \tag{38}$$

It is clear therefore that the longest-range part of the P-odd potential between two ions depends on the distance between them like $r^{-2}\cos(2k_Fr)$.

For a rough numerical estimate we replace the summation over j by integration over the spherically symmetric region $x \geqslant x_0$. Putting in the expression obtained in this manner

$$E_{3i}^{(2)} \approx -\frac{Gm^2\alpha^2Z^3Rq}{2^{1/2}\pi}\left(\frac{Jm^*}{\mathrm{Ry}\,m}\right)^2 S^2\frac{\alpha_0}{ck_F}\frac{x_0\sin x_0 + 2\cos x_0}{24\pi}\mathrm{Ry}, \tag{39}$$

and $x_0 = 2k_FR_0$, where R_0 is the minimum distance between the ions, we obtain $E_2^{(2)} \approx -0.8$ Hz. Numerical summation over the lattice sites in (38) leads to the large result.

$$E_{3i}^{(2)} \approx -3\ \mathrm{Hz}. \tag{40}$$

Thus, with allowance for (29), (33), and (40), the P-odd correction to the ion energy in the crystal amount to

$$E_i^{(2)} = E_{1i}^{(2)} + E_{2i}^{(2)} + E_{3i}^{(2)} \approx 80\ \mathrm{Hz}. \tag{41}$$

Of course, this result, obtained within the framework of a rather crude description of the electrons in the crystal, is apparently only an order-of-magnitude estimate.

It is curious that in the employed free-electron approximation the sign of the effect is uniquely determined. In the standard weak-interaction model (where $q < 0$) the left-hand spin structures are favored in energy over the right-hand ones.

We emphasize once more that E depends only on the sign of the spin rotation angle α_0, but not on its absolute value. It is precisely because of the absence of the small parameter α_0/ck_F that this contribution predominates in (41), notwithstanding the unfavorable remaining numerical factors.

5. CAN PARITY NONCONSERVATION BE OBSERVED IN CRYSTALS WITH HELICOIDAL SPIN STRUCTURE?

The natural question is whether the effects discussed are observable. The obtained spin energy difference ~ 100 Hz between the righ- and left-hand helicoidal structures is by itself not so far from the customary accuracy $\sim 10^5$ Hz of measurements of the spin-interaction constant in solid dielectrics by the paramagnetic-resonance method.[14] Unfortunately exchange interaction in metals leads to a strong broadening of the EPR lines.

As for dielectrics with helicoidal spin structure, the more favorable conditions for EPR spectroscopy are accompanied here by an additional suppression of the P-odd effects. Indeed, the interaction responsible for the magnetic ordering in dielectrics is known not to be larger than the indirect exchange in metals. This follows from a comparison of the corresponding Néel points. Furthermore the P-odd interaction of a d or f electron in a dielectric should contain also an additional small quantity—the exchange interaction with the s and p shells of the ions (see the discussion of the P-odd vector polarizability of holmium in Sec. 2). Therefore the P-odd energy of the spin in a dielectric can hardly exceed 1 Hz.

Another manifestation of parity nonconservation might be the predominant onset of left-hand spin structures having a lower energy, on going throught the Neel point, if the random factors that usually determine the sign of the produced helix are made weaker. No matter how fantastic this assumption may seem, the following argument can be advanced in its favor. It was shown in Ref. 15 that using an electric field crossed with a magnetic one it is possible to monitor effectively the sign of the resultant spin helix in the compound $ZnCr_2Se_4$. The fields $E = 2.5$ kV/cm and $H = 12$ kOe used in this experiment are quite negligible in atomic scale. Furthermore the electric field influences the magnetic structure only via the weak spin-orbit interaction. In the upshot the "warping" energy of the interaction with these field is roughly estimated to be only 10–100 times larger than the P-odd energy (41).

6. BLOCH DOMAIN WALLS IN FERROMAGNETIC FILMS

An example of the realization of a helicoidal spin structure is also the usual Bloch domain wall in a ferromagnet. Let us estimate the possibility of influencing with a weak interaction the sign of the helix in a domain wall produced when a new domain is produced by reversal of magnetization of a monodomain film (see Fig. 4).[5] Weak interaction leads to twisting of the spins in the xy plane; this twisting decreases with increasing distance from the wall $z = 0$. Thus, a germ of a helicoidal structure exists even in the equilibrium state.

Let us estimate the P-odd energy of an ion located far enough from the wall $z = 0$. Since the spin rotation angle decreases with the distance to the wall, a noticeable contribution to the effect can be made only by that weak-interaction part in which this smallness of the rotation angle is offset by the formal divergence of the remaining integral at large z. It is easy to verify that neither expression (18), (37), or (38) leads to such a divergence. As for expression (31), the necessary property is possessed in it only by the first nonoscillating term in the square brackets. Assuming the spin S_i to be located at the point z, and S_j at the point z', and taking into account the smallness of the corresponding angles $\theta(z)$ and $\theta(z')$ of the spin rotation in the xy plane, we find that now $[\mathbf{S}_i \times \mathbf{S}_j]_z = -S^2[\theta(z) - \theta(z')]$. Substituting this expression in (31) and assuming as a rough estimate

$$\theta(z) = \theta_0(1 - z/z_0), \quad z > 0,$$

where z_0 is the characteristic dimension, we find that in this case

$$E(z) \approx \frac{Gm^2\alpha^2Z^3Rq}{2^{1/2}\pi}\left(\frac{Jm^*}{\mathrm{Ry}\,m}\right)^2 S^2\frac{n\theta_0}{32}\mathrm{Ry}. \tag{42}$$

Here θ_0 the angle of the spin rotation on the surface $z = 0$. It can be easily imagined that in this case $\theta_0 > 0$ corresponds to a left-hand helix whose initiation energy is lower (we recall that $q < 0$). The order of magnitude of the energy (42) is $E(z) \sim -10$ Hz θ_0.

With what is this energy to be compared in order to assess the possibility of influence on the formation of domain walls? We begin with the fact that in soft magnetic materials the coercive force (i.e., the field necessary to reverse the domain magnetization) is $H_c \sim 10^{-2}$ Oe. The energy of the interaction between the magnetic moment and such a field is $E_c \sim \mu H_c \sim 10^{-10}$ eV $\sim 10^{-11}$ Ry $\sim 10^4$ Hz. Actually, however, the magnetization reversal is due not to the coercive force itself, which is none other than the depth of the local minimum of the spin energy with respect to its rotation angle, but by the amount by which the spin energy in the field exceeds zero; this excess, however, can be made much less than E_c. In addition, the generalized moment $K = -\partial E/\partial\theta$ of the P-odd forces does not depend on the angle θ, whereas the moment of the usual magnetization-reversing forces is proportional to a small deviation angle, since turning on an oppositely directed magnetic field leads to the appearance of a local energy maximum near $\theta = 0$. We therefore do not regard as hopeless and attempt to observe parity nonconservation in domain formation, i.e., to obtain predominantly left-hand-screw Bloch walls. We emphasize, however that this problem calls at any rate for the use of sufficiently soft magnetic films with few defects and sufficiently accurate magnetic-field geometry.

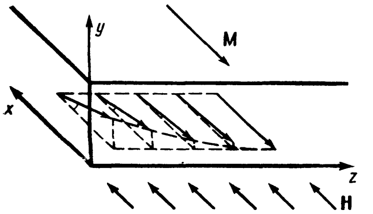

FIG. 4. Appearance of a spin helix near the boundary $z = 0$ of a ferromagnetic film; M is the magnetization direction and H is the magnetization-reversing field.

It must be noted that the hypothesis of predominant formation of Bloch walls with the same sign of the helix was discussed already long ago,[16–18] and incidently without any hearing on weak interactions.

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[1] In view of the quasineutrality of the crystal it is more reasonable to use the wave function of just the atom rather than the ion.

[2] We are grateful to V. A. Dzyuba, O. P. Sushkov, and V. V. Flambaum for kindly supplying us with their Hartree-Fock programs we used to perform all the atomic calculations.

[3] In Bloch domain walls, of course, the spin helix is the to an entirely different cause, namely the boundary conditions.

[4] For the gain we assume here the value $R \approx 4.5$ which corresponds to the absence of derivative in the relativistic Hamiltonian of the weak electron-nucleon interaction.

[5] We thank V. I. Shvetsov who called our attention to the possible parity violation in domain-wall formation.

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