

62

ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ
СО АН СССР

O.L.Zhizhimov

P-ODD LONG-RANGE INTERACTION
OF IONS IN MAGNETIC
SEMICONDUCTORS

PREPRINT 82-161

Новосибирск

P-ODD LONG-RANGE INTERACTION OF IONS
IN MAGNETIC SEMICONDUCTORS

O.L. Zhizhimov

Institute of Nuclear Physics
630090, Novosibirsk 90, USSR

A b s t r a c t

In semiconductors with magnetic structure the exchange interaction between ions and collective electrons when parity nonconservation is taken into account, gives rise to parity-violating long-range forces between ions. This spin-dependent interaction splits the energies of right and left helical spin structures. The magnitude of splitting is estimated.

1. The parity violation effects in magneto-ordered crystals mentioned for the first time in Ref. [1] have been discussed in detail in Ref. [2]. It was shown that the exchange interaction between conduction electrons and ions with allowance for the parity violation leads to P-odd long-range forces between ions in magnetic metals. Due to interaction energies of right and left helical spin structures split and the splitting amounts approximately to ~100 Hz per one ion in rare-earth metal.

In this paper P-odd long-range interaction between magnetic ions in nonmetal crystals and its dependence on electron structure and temperature are considered. A possibility of experimental observation of the parity violation effects in semiconductors is discussed.

In the paper the exchange mechanism of the origin of P-odd long-range forces is studied mainly. In semiconductors in distinction from metals there are some mechanisms of exchange interactions (see Ref. [3-4]), but we consider only the indirect exchange, which fits well into the frame of simple two-bands model of semiconductor. It cannot be excluded, however that other mechanisms of the exchange interaction in some cases will give a larger contribution to the P-odd interaction between ions. But then taking into account only the indirect exchange will serve as relatively reliable lower estimate for discussed effects, since complete cancelation of the contributions of different origin is unlikely.

2. Let us consider the model of semiconductor with intrinsic conduction. At zero temperature occupied electronic states form the valence band, separated from the wide conduction band by a narrow gap E_g . For the case of the direct gap in the centre of the Brillouin zone, for the nondege-

nerate semiconductors the dispersion law can be represented for small \vec{k} as follows

$$\epsilon_e(\vec{k}) = \epsilon_g + \vec{k}^2/2m_e, \quad \epsilon_h(\vec{k}) = -\vec{k}^2/2m_h \quad (1)$$

Here m_e and m_h are positive effective masses of electron and hole, respectively; we take $\hbar=c=1$. The exchange interaction of the collective electrons with the electrons of incomplete d- or f-shells we shall describe by operator

$$\hat{V} = -JV_0 \sum_i (\vec{S}_i \vec{s}) \delta(\vec{r} - \vec{R}_i) \quad (2)$$

where \vec{s} is the spin of the electron; \vec{S}_i is the spin of ion located at the point \vec{R}_i ; V_0 is the volume per one ion in the crystal; J is the exchange integral. To the second order of perturbation theory the operator (2) results in the following interaction between two ions in semiconductor ($T=0$) (see, e.g., Ref. [5-7]), $y_{ij} = k_0 R_{ij} \equiv k_0 |\vec{R}_i - \vec{R}_j|$

$$E_{ij}^{(s)} = -Ry (\vec{S}_i \vec{S}_j) \left(\frac{JV_0}{Ry a_0^3} \right)^2 \frac{(m_e m_h)^{3/2} (k_0 a_0)^4 K_2(y_{ij})}{m(m_e + m_h)^2 8\pi^3 y_{ij}^2}, \quad (3)$$

where $K_2(y)$ is the modified Bessel function; $Ry = m\alpha^2/2$ is the Rydberg constant; $\alpha = 1/137$; a_0 is the Bohr radius. The constant k_0 is

$$k_0^2 = 2\epsilon_g (m_e + m_h) \quad (4)$$

For comparison we present the analogous expression for the interaction between ions in metal (see, [8-10]),

$$E_{ij}^{(M)} = -Ry (\vec{S}_i \vec{S}_j) \left(\frac{JV_0}{Ry a_0^3} \right)^2 \frac{m^* (k_F a_0)^4 j_1(x_{ij})}{m 2\pi^3 x_{ij}^2}, \quad (5)$$

where $j_1(x)$ is the spherical Bessel function; k_F is the Fermi momentum; m^* is the effective mass of electron; $x_{ij} = 2k_F R_{ij}$. In contrast to (5) the function (3) has a constant sign. In the region $R_{ij} > k_0^{-1}$ the function (3) decreases exponentially, however, in the case $R_{ij} < k_0^{-1}$ the magnitude (3) can be quite comparable to that of (5).

Find now the effective interaction between ions, due to the interaction (2) and to the weak P-odd interaction between the collective electrons and the nuclei of ions (see, [2]),

$$\hat{W} = \frac{G}{2\sqrt{2}m} \sum_i \left\{ Zq [(\vec{p}\vec{\sigma}), \delta(\vec{z} - \vec{R}_i)]_+ + \right. \\ \left. + \kappa [(\vec{I}_i \vec{p}), \delta(\vec{z} - \vec{R}_i)]_+ + i\kappa' [(\vec{I}_i \times \vec{\sigma}) \vec{p}, \delta(\vec{z} - \vec{R}_i)]_- \right\} \quad (6)$$

Here $[\]_+$ and $[\]_-$ denote a commutator and anticommutator, respectively; $G \approx 10^{-5} m_p^{-2}$ is the Fermi weak-interaction constant; m_p is the proton mass; m is the true mass of electron, \vec{p} is the operator of the electron momentum; \vec{I}_i is the spin of the ion nucleus located at the point \vec{R}_i . In the dimensionless constant Zq (Z is the nuclear charge) 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 interaction $q \approx -0.7$ for rare-earth elements, and the constants κ and κ' are numerically small for all atoms (see Ref. [11]).

In one assumes that the collective electrons are described by plane waves, then the calculation of (2) and (6) in the framework of perturbation theory leads to the following effective interaction between ions

$$E_{ij}^{(1)} = -\frac{2G\kappa'}{\sqrt{2}} \frac{J}{V_0 N^2} (\vec{I}_i \times \vec{S}_j) \frac{1}{V} \sum_{\vec{k}, \vec{k}'} \frac{f_{\vec{k}}^\alpha (1 - f_{\vec{k}'}^{\alpha'})}{\epsilon_e(\vec{k}) - \epsilon_e(\vec{k}')} e^{i(\vec{k} - \vec{k}') \cdot \vec{z}} \Big|_{\vec{z} = \vec{R}_{ij}} \quad (7)$$

where α and α' mark the bands, $f_{\vec{k}}^\alpha$ is the Fermi distribution function, N is the complete number of ions. At zero temperature one can obtain from (7) taking into (1) for the semiconductor with the wide bands

$$E_{ij}^{(1s)} = \frac{G\kappa' d^2 Z^2 R \kappa' JV_0}{\sqrt{2}\pi Ry a_0^3} \frac{1}{(\vec{I}_i \times \vec{S}_j) N_{ij} Ry} \frac{(m_e m_h)^{3/2} (k_0 a_0)^5 d}{m(m_e + m_h)^2 \pi^2 dy_{ij}} \frac{K_2(y_{ij})}{y_{ij}^2} \quad (8)$$

where $N_{ij} = R_{ij}/R_{ij}$. The factor $Z^2 R$ is introduced here, which

takes into account the difference of the density of electrons on the nucleus from the average density over the crystal. The analogous expression for the interaction between ions of metal is (see. Ref. [2])

$$E_{ij}^{(1M)} = -\frac{6\pi d^2 Z^2 R \kappa' J V_0}{\sqrt{2} \pi R y a_B^3} (\vec{I}_i \times \vec{S}_j) N_j R y \frac{m^* 2(\kappa' a_B)^5 d}{m \pi^2} \frac{j_1(x_{ij})}{x_{ij}^2} \quad (9)$$

Note that for the nearest ions of metal $x_{ij} \gg 1$, and for narrow-gap semiconductors $y_{ij} \ll 1$, so (see. (3), (5), (8) and (9))

$$E_{ij}^{(1M)} \sim \frac{\cos x_{ij}}{x_{ij}^3}, \quad E_{ij}^{(5)} \sim \left(\frac{a_B}{R_{ij}}\right)^4,$$

$$E_{ij}^{(1M)} \sim \frac{\sin x_{ij}}{x_{ij}^3}, \quad E_{ij}^{(1S)} \sim \left(\frac{a_B}{R_{ij}}\right)^5,$$

i.e. in contrast to metal the P-odd interaction in semiconductors decreases faster than the usual one even for nearest ions. The point is that in the region $y_{ij} < 1$ since $k_0 < k_F$, in expression (8) it is necessary to differentiate the denominator (in expression (9) it is necessary to differentiate the numerator). This leads to the faster decrease of the P-odd interaction between ions in semiconductors and therefore to the additional smallness of the effects due to this interaction. If one recalls also that the constant κ' is numerically small, the contribution (8) to the P-odd interaction becomes negligibly small in comparison with the contributions of the next order in the interaction (2).

3. To the second order of perturbation theory in operator \hat{V} the effective P-odd interaction between ions can be represented as follows (see. Ref. [2])

$$E_{ij}^{(2)} = i \frac{6ZqJ^2}{2\sqrt{2}mV_0N^3} (\vec{S}_i \times \vec{S}_j) \sum_{\vec{k}\vec{k}'\vec{k}''} \sum_{\alpha\alpha'\alpha''} \frac{f_{\vec{k}}(1-f_{\vec{k}'}) (1-f_{\vec{k}''})}{[\epsilon_{\alpha}(\vec{k}) - \epsilon_{\alpha'}(\vec{k}')] [\epsilon_{\alpha}(\vec{k}) - \epsilon_{\alpha''}(\vec{k}'')]} \left\{ (\vec{k} + \vec{k}') e^{i\vec{k}'R_{ij} - i\vec{k}R_{is} + i\vec{k}R_{js}} - (\vec{k} + \vec{k}'') e^{-i\vec{k}R_{ij} + i\vec{k}R_{is} - i\vec{k}''R_{js}} + (\vec{k} + \vec{k}'') e^{i\vec{k}'R_{ij} - i\vec{k}R_{is} + i\vec{k}''R_{js}} \right\} \quad (10)$$

When summing over s there are the terms with $s=i$ and $s=j$. For these terms the replacement of the summation over \vec{k} by the integration at zero temperature reduces to the linearly divergent integrals. This divergence is natural for the higher orders of perturbation theory in a contact interaction. For regularization one can introduce a cut-off integration momentum Q which is naturally identified with the inverse radius of the ion f- or d-shell. At $k_0 \rightarrow 0$ the dimensional estimate gives

$$E_{ij}^{(2S)} (s=i,j) \sim Q/R_{ij}^5 \quad (11)$$

The fast decrease of the term (11) with the interspin distance makes it negligible in comparison with other terms in (10).

To estimate the contribution to (10) from the terms with $s \neq i, j$, it is convenient to smear the weak interaction (6) over the whole crystal

$$\hat{W} \rightarrow \frac{6Zq}{\sqrt{2}mV_0} (\vec{\sigma} \cdot \vec{p})$$

The eigenfunction of the obtained Hamiltonian

$$\hat{H} = \frac{\vec{p}^2}{2m_e m} + \frac{6Zq}{\sqrt{2}mV_0} (\vec{\sigma} \cdot \vec{p}) \quad (12)$$

is

$$|\vec{k}\sigma\rangle = \left[1 - i \frac{6Zq m_e m}{\sqrt{2}V_0} (\vec{\sigma} \cdot \vec{z}) \right] |\vec{k}\sigma\rangle, \quad (13)$$

where $|\vec{k}\epsilon\rangle$ is the nonperturbed wave function of the electron. The dispersion law (3) is still valid. Strictly speaking, it is necessary to add to (13) the correction, due to the influence of the other band. Evidently, this correction decreases with the increase of the gap, but even at $E_g=0$ the contribution of it to the discussed effects is $\sim 50\%$. Therefore for a rough estimate one can neglect the influence of the other band. At calculation of the correction to the energy of the second order in (2) the application of the wave function (13) gives

$$E_{ij}^{(2)} = -\frac{GZgJ^2}{\sqrt{2}mV_0N^2} (\vec{S}_i \times \vec{S}_j) \vec{R}_{ij} \sum_{\vec{k}, \vec{k}'} \frac{f_{\vec{k}}(1-f_{\vec{k}'})}{E_{\vec{k}}(\vec{k}) - E_{\vec{k}'}(\vec{k}')} e^{i(\vec{k}-\vec{k}')\vec{R}_{ij}} \quad (14)$$

For the wide bands at zero temperature one can obtain with (1)

$$E_{ij}^{(2S)} = \frac{G\omega d^2 Z^3 R_0 \left(\frac{J}{Ry}\right)^2}{\sqrt{2}\pi} \frac{(\omega_c \omega_v)^{3/2}}{m^2(\omega_c + \omega_v)} \frac{V_0 \kappa_0^3}{8\pi^2} (\vec{S}_i \times \vec{S}_j) N_{ij} \frac{K_2(y_{ij})}{y_{ij}} \quad (15)$$

where again the additional factor $Z^2 R$, mentioned above, is taken into account. In the region $y_{ij} < 1$ the interaction (15) decreases with the interion distance as R_{ij}^{-3} . In this sense the interaction (15) is analogous to the nonoscillating part of the interaction between ions in metal [2]

$$E_{2ij}^{(2M)} = \frac{G\omega d^2 Z^3 R_0 \left(\frac{J \cdot m^*}{Ry \cdot m}\right)^2}{\sqrt{2}\pi} \frac{3\pi n^2}{4} (\vec{S}_i \times \vec{S}_j) N_{ij} \frac{1}{R_{ij}^3} \quad (16)$$

Here n is the number of the conduction electrons of metal per one ion. However, in contrast to (16) the range of the interaction (15) is limited.

One can estimate the P-odd energy of the magnetic ion in the crystal with helical spin structure ("simple spiral"). Directing the z-axis along the wave vector \vec{g} of the helix and going from summation over j to integration, for the right helix one obtains

$$V_0 \sum_j (\vec{S}_i \times \vec{S}_j) N_{ij} \frac{K_2(y_{ij})}{y_{ij}} \rightarrow -\{S^z\} dR \frac{z}{R} \sin(gz) \frac{K_2(\kappa_0 R)}{\kappa_0 R} \quad (17)$$

where ξ is the relative concentration of the magnetic ions. The calculation gives

$$E_i^{(2S)} \approx -\frac{G\omega d^2 Z^3 R_0 \left(\frac{J}{Ry}\right)^2 (\omega_c \omega_v)^{3/2} \xi S^z g}{\sqrt{2}\pi m^2(\omega_c + \omega_v)} \frac{e^{-\rho_0 \sqrt{\kappa_0^2 + g^2}}}{8\pi (\kappa_0^2 + g^2)^{1/2}} Ry \quad (18)$$

where ρ_0 is the minimum distance between magnetic ions. For $g > \kappa_0$, $\rho_0 g < 1$ the P-odd energy of ion does not depend on g . In the metal there is also an independent on g contribution to the energy of ion. This contribution due to the interaction (16) dominates. The ratio of the independent on g contributions in the metal and in the semiconductor, other things being equal, is

$$\frac{E_i^{(2M)}}{E_i^{(2S)}} \sim \frac{m^*(\omega_c + \omega_v) \pi^2 n}{(\omega_c \omega_v)^{3/2} 4\xi} \quad (19)$$

As a rule this ratio exceeds appreciably unity. Even in the narrow-gap semiconductors with the heavy ions the value of the splitting of the energies of right and left helical spin structures hardly exceeds 0.1Hz per one ion¹⁾. Since in the standard model of weak interactions the sign of q is negative, in the semiconductors, as well as in the metals, the left spin structures are preferable than the right ones, their energy being lower.

4. If the temperature T exceeds the width of the forbidden band for intrinsic semiconductors or the corresponding energy of activation for impurity semiconductors, the electrons in conduction band and holes in valence band exist. As a result to the mechanism of the interband exchange considered before it is necessary to add the mechanism

1) In the semiconductors the typical values of the effective masses are $m_e \sim m_h \sim 0.1m$, while, for example, in the rare-earth metals $m^* \gtrsim m$.

of the intraband exchange. The influence of the intraband exchange on the interaction between magnetic ions is considered in Ref. [12]. The appropriate expression for the interaction energy is

$$E_{ij}^{(\tau)} = -R_{ij} (\vec{S}_i \cdot \vec{S}_j) \left(\frac{J}{R_{ij}} \right)^2 \frac{V_0}{a_0^3} \frac{\tilde{m}}{m} \frac{n}{4\pi} \frac{a_B}{R_{ij}} e^{-(\lambda R_{ij})^2}, \quad (20)$$

where $\lambda^2 = 2\tilde{m}T$, $\tilde{m} = m_e \approx m_h$; n is the number of the conduction electrons per one ion. For the intrinsic semiconductors the value n is

$$n = n_e = n_h = V_0 T^{3/2} \frac{(m_e m_h)^{3/4}}{\sqrt{2} \pi^{3/2}} e^{-\frac{E_g}{2T}}. \quad (21)$$

We assume here that the exchange integrals are equal for all bands.

Let us estimate the P-odd interaction between ions, due to the intraband exchange. For that one can apply (14) with $\alpha = \alpha'$ and $m_e = m_h$

$$E_{ij}^{(2T)} = -\frac{6ZgJ^2 2\tilde{m}}{\sqrt{2} V_0 N^2 m} (\vec{S}_i \times \vec{S}_j) \cdot \vec{R}_{ij} \sum_{\vec{k}, \vec{k}'} \frac{f_{\vec{k}} (1 - f_{\vec{k}'})}{\epsilon_{\alpha}(\vec{k}) - \epsilon_{\alpha}(\vec{k}')} e^{i(\vec{k}' - \vec{k}) \cdot \vec{R}_{ij}} \quad (22)$$

If $T \geq E_g$, the conduction electrons can be described by the Boltzman distribution function and the elementary calculation gives

$$\frac{1}{V_0 N^2} \sum_{\vec{k}, \vec{k}'} \frac{f_{\vec{k}} (1 - f_{\vec{k}'})}{\epsilon_{\alpha}(\vec{k}) - \epsilon_{\alpha}(\vec{k}')} e^{i(\vec{k}' - \vec{k}) \cdot \vec{R}_{ij}} = -\frac{n\tilde{m}}{2\pi R_{ij}} e^{-(\lambda R_{ij})^2}, \quad (23)$$

where the summation over \vec{k} and \vec{k}' is extended to the all space. Introducing again the discussed above factor $Z^2 R$, one obtains

$$E_{ij}^{(2T)} = \frac{6\tilde{m}^2 Z^2 R_{ij}}{\sqrt{2} \pi} R_{ij} (\vec{S}_i \times \vec{S}_j) \cdot \vec{N}_{ij} \left(\frac{J \tilde{m}}{R_{ij} m} \right)^2 \frac{n}{2} e^{-(\lambda R_{ij})^2} \quad (24)$$

It is interesting that in the region $R_{ij} < \lambda^{-1}$ the interaction between ions does not depend on the interion distance. Since (24) is valid for $T \geq E_g$, the order of magnitude λ is $\lambda \geq k_0$. Comparing (24) with (15) in the region $R_{ij} \lambda < 1$, $T \geq E_g$ when (21) is taken into account, one obtains

$$E_{ij}^{(2T)} / E_{ij}^{(2S)} \sim (\lambda R_{ij})^3 \ll 1$$

I.e. in spite of the weak dependence on the distance, the interaction (24) for intrinsic semiconductors is less effective, than interaction (15). For impurity semiconductors the interaction (24) is also suppressed, because even at the room temperature the electron concentration in conduction band (or that of holes in valence band) is small

$$n \sim 10^{-3} \div 10^{-4}$$

5. Thus, within the used model the interband interaction is most effective. It is proportional to the square of exchange integral and decreases with the distance between ions as R_{ij}^{-3} when $\kappa_0 R_{ij} < 1$. However, other things being equal, this interaction in helical spin structures leads to P-odd energy smaller than in metal. This is connected of the P-odd forces range in semiconductor

$$R_{max} \sim (2\tilde{m} E_g)^{-1/2}$$

but with the small values of effective masses $\tilde{m} \sim 0,1 m$. The conclusion of the suppression of P-odd interaction between ions in semiconductors is made for the model with wide bands. However, when, for example, the valence band decreases the increase of the effective mass m_h is accompanied by the exponential decrease of the interaction range. Therefore the transition to model with narrow bands probably does not change radically anything.

However, one cannot exclude, that the individual peculiarities of magnetic and electronic structure of semiconductors can enhance the P-odd interaction between nearest ions. We mean not only the direct exchange interaction, but also the anisotropic superexchange (see. Ref. [3,4]) with weak interaction between electrons and the nuclei of ions taken into account. The numerical predictions evidently depend here strongly on the details of the structure and cannot be made within some general model. At last one can note that in semiconductors the P-odd van der Waals interaction between magnetic ions [1,2] is quite comparable with the P-odd exchange interaction. Indeed, in spite of the faster decrease with the interion distance $\sim R^{-5}$, the van der Waals contribution to the magnitude of the P-odd energy of ion is ~ 0.1 Hz for crystal of rare-earth metal with helical spin structure. When passing from metal to semiconductor this estimate should not change essentially.

6. The effects of parity violation in semiconductors can be observed in crystals with helical spin structure: HgCr_2S_4 , ZnCr_2Se_4 etc. The striking demonstration of an effect would be the observation of preferential formation of structures with left spin helix which have lower energy (see. (18)). Effective control by the sign of spin helix in ZnCr_2Se_4 by means of crossed electric and magnetic fields reached in Ref. [13] is the argument in favour of this experiment (see. also [2]). Here it should be noted that the applied in Ref. [13] fields are small in the atomic scale and the interaction between electric field and magnetic structure is suppressed.

The analogous effect would be also the preferential formation of the left helix Bloch domain walls between two ferromagnetic domains that are formed when remagnetizing the single crystalline film. Obviously, in view of a prevalence of ferromagnetic compounds the choice of working substance here is much more rich than in case of a helical antiferromagnetic.

In conclusion the author is grateful to I.B.Khrilovich for constant interest to this work and for numerous helpful discussions.

References

1. Zhizhimov O.L., Khrilovich I.B. Zh.Eksp.Teor.Fiz. 1982, 82, 1026.
2. Zhizhimov O.L., Khrilovich I.B. Zh.Eksp.Teor.Fiz. 1983, 84, 342.
3. Methfessel S., Mattis D.C. Magnetic Semiconductors. Handbuch der Physik. Bd.XVIII/1, Springer-Verlag, 1968.
4. Nagaev E.L. Physic of Magnetic Semiconductors (in Russian), Moscow, Nauka, 1979.
5. Bloembergen N., Rowland T.J. Phys.Rev., 1955, 97, 1679.
6. Abrikosov A.A. J.Low Temp.Phys., 1980, 39, 217.
7. Liu L. Solid St.Comm., 1980, 35, 187; Phys.Rev.B., 1982, 26, 975.
8. Ruderman M.A., Kittel C. Phys.Rev., 1954, 96, 99.
9. Kasuya T. Prog.Theor.Phys., 1956, 16, 45.
10. Yosida K. Phys.Rev., 1957, 106, 893.
11. Khrilovich I.B. Parity Nonconservation in Atomic Phenomena (in Russian), Moscow, Nauka, 1981.
12. Karpenko B.V., Berdyshev A.A. Fiz.Tverd.Tel., 1963, 5, 3026.
13. Siratori K., Akimitsu J. et.al., J.Phys. Soc.Jap., 1980, 48, 1111.