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FERROMAGNETIC DOMAINS IN A SEMICONDUCTING ANTIFERROMAGNET

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It is energetically convenient for a conduction electron in a semiconducting antiferromagnet to produce around itself a region of ferromagnetic ordering with a radius of several lattice constants. The ground-state energy of such a quasiparticle, called a magnetic polaron is calculated. Domains with ferromagnetic ordering may also arise near non-ionized donors or acceptors. The low temperature transverse magnetic susceptibility of such defects may be comparable with the susceptibility of a perfect crystal. Under certain conditions the longitudinal susceptibility of the crystal is completely defined by the defects.

A preceding paper[1] considered the ground state of a conduction electron in a nonmetallic antiferromagnet. It was assumed that the spin of the magnetic atoms of the antiferromagnet greatly exceeds unity. It was shown that an energetically favored stated may be a self-consistant state of the system such, that in the antiferromagnetic ordering gives way to ferromagnetic ordering in a region of radius equal to several lattice constants. This ferromagnetic microregion is a potential well for the conduction electron, in which it becomes localized. The electron should move through the crystal together with the ferromagnetic microregion produced by it. Such a quasiparticle, in analogy with the polaron in ionic crystals[2,3], was called a magnetic polaron.

In the present paper we report a more detailed investigation of the possibility of capture of a conduction electron by magnetic polarization, including also the case of small spins. We obtain expressions for the energy of the ground state of the system at different relations between its main parameters. It is shown, in particular, that at small values of the spin the antiferromagnetic sd interaction is much more favorable for the production of the magnetic polaron than the ferromagnetic one. However, even if the magnetic polaron is not produced, the minimum energy of the system at small values of the spin is still much lower than the quasiclassical value[4].

Microregions with ferromagnetic ordering can occur also around defects that behave like donors or acceptors with respect to the electric properties of the crystal. The corresponding electrons or holes at these defects can be naturally interpreted as localized magnetic polarons. Recently numerous investigations, based on the Heisenberg model, were made of the influence of impurities on the magnetic properties of ferromagnets and antiferromagnets (see, for example,[5-7]). It is clear, however, that localized magnetic polarons cannot be described within the framework of this model, and the results of such investigations are not applicable to them. The "non-Heisenberg" defects considered here can possess anomalously large magnetic moments. At the practically attainable impurity concentrations, the impurity contribution to the transverse magnetic susceptibility can be comparable with the susceptibility of an impurity-free antiferromagnet. In definite cases, the longitudinal susceptibility is determined practically entirely by the defects.

1. FREE MAGNETIC POLARON

We investigate the ground state of a conduction electron in a nonmetallic antiferromagnet. To describe the system we use the sd-model. It is assumed that the crystal lattice is primitive cubic, and that both magnetic sublattices of the antiferromagnet are identical. We consider the case when the probability of observing the conduction electron near the magnetic atoms is much higher than near nonmagnetic atoms, so that the latter can be simply regarded as field sources. Accordingly, the Hamiltonian of the system under consideration is

$$\mathcal{H} = \sum [E_A \delta_{\sigma\sigma'} - A(\mathbf{s}\mathbf{S}_\mathbf{f})_{\sigma\sigma'}] a_{\mathbf{f}\sigma}^* a_{\mathbf{f}\sigma'} + B \sum a_{\mathbf{f}\sigma}^* a_{\mathbf{f}+\mathbf{g}\sigma} - \frac{I}{2} \sum (\mathbf{S}_\mathbf{f} \mathbf{S}_{\mathbf{f}+\mathbf{g}}). \tag{1}$$

Here $a_{f\sigma}^*$ and $a_{f\sigma}$ are the operators of creation and annihilation of the conduction electron with spin projection σ on the magnetic atom with number $f = (f_x, f_y, f_z)$; f and S_t are the operators of the spin of the conduction electron and of the f-th magnetic atom. Further, E_A is the "atomic" energy of the conduction electron, B is the Bloch integral, A is sd-exchange integral, and I is the integral of exchange between the magnetic atoms. We use the nearest-neighbor approximation, so that the index g, which numbers the neighbors, runs through six values.

A very important factor in what follows is that the quantities A and B are large compared with I: whereas the former two parameters are of the order of 0.1–1 eV, the exchange integral usually amounts to several hundredths or even thousands of an electron volt.

If we assume that the conduction electron leaves the antiferromagnetic ordering unchanged, then we obtain for the energy of the system, neglecting the zero-point oscillations of the spins, the following expressions[4]:

$$E = E_0 + E_A - \sqrt{(AS/2)^2 + B_\mathbf{k}^2}, \quad B_\mathbf{k} = 2B[\cos k_x a + \cos k_y a + \cos k_z a], \tag{2}$$

where E_0 is the energy of the ground state of the antiferromagnet, a is the lattice constant, and k is the quasimomentum.

It is seen from (2) that when $|A|S \gg 6|B|$ the antiferromagnetic ordering prevents the electron from gaining energy as it moves through the crystal. In the opposite limiting cases, it leads to a mutual cancellation of the contributions from the exchange interaction of this electron with the magnetic atoms. We can therefore expect the energetically more favored state to be one in which the antiferromagnetic ordering is replaced by ferromagnetic ordering in some region. The energy lost by the magnetic subsystem is compensated by the gain in the energy of the conduction electron, which can move freely inside the ferromagnetic microregion, acquiring inside this region a full gain in the energy of the sd-exchange.

We calculate below the energy of the magnetic polaron at rest. In the problem under consideration, the interaction Hamiltonian of the s-electron with the magnetic subsystem has a much more complicated structure than the Hamiltonian of the electron-phonon interaction in the polaron problem. In addition, the commutation rules of the spin operators are much more complicated than those of the Bose operators. It would therefore be apparently ineffective to employ here a field procedure similar to that developed in polaron theory.

We solve the problem by a direct variational method. It is assumed that the continuous-medium approximation is applicable. In constructing the trial function it is assumed that ideal ferromagnetic ordering is established in a region of radius R; when $r = R$ this becomes abruptly an antiferromagnetic ordering. The value of R serves as the variational parameter. Such a state of the magnetic subsystem will be denoted by the symbol $|0\rangle_R$. Since the ferromagnetic state is an eigenstate of the Heisenberg Hamiltonian, the state $|0\rangle_R$ with $R \gg a$ should lead to a groundstate energy which is close to the true energy. Such an approach is similar to that used by Pekar[2] in the polaron theory. A more accurate trial function, just as in[2], should take into account the fact that the center of the magnetic polaron may be located at any lattice site.

The detailed form of the trial function depends on the sign of the sd-exchange integral A. In ferromagnetic sd-coupling, the spin of the conduction electron inside the ferromagnetic microregion, obviously, is assumed to be polarized along the momentum of this region. Outside this region it is necessary to take into account both spin polarizations of the s-electron. We shall assume that the magnetic moment of the microregion is collinear with the antiferromagnetism vector. As is well known, in the ground state of an antiferromagnet, the magnetization of the sublattices is close to the limiting value even when $S = 1/2$. Therefore in that sublattice, in which the moment is parallel to the moment of the microregion, the s-electrons can also be regarded as fixed. In the other sublattice, at the magnetic atom closest to the s-electron, there is mixed in with the "correct" projection of the spin of this atom also an "incorrect one," which differs from it by unity. The limitation of the deformation of the magnetic ordering in the antiferromagnetic region to the atom closest to the conduction electron is justified by the condition $|A|S \gg |I|S^2$.

If we include in $|0\rangle_R$ also the vacuum electron function, then, in accordance with the foregoing, the trial wave function is constructed when $A > 0$ in the following manner:

$$\Phi = \Big\{ \sum_{|\mathbf{f}_1| \geqslant R/a} [c_{\mathbf{f}_1\uparrow} \overset{*}{a}_{\mathbf{f}_1\uparrow} + c_{\mathbf{f}_1\downarrow} \overset{*}{a}_{\mathbf{f}_1\downarrow} S^+_{\mathbf{f}_1}] + \sum_{|\mathbf{f}_1| < R/a} c_{\mathbf{f}_1\uparrow} \overset{*}{a}_{\mathbf{f}_1\uparrow} + \sum_{\mathbf{f}_2} c_{\mathbf{f}_2\uparrow} \overset{*}{a}_{\mathbf{f}_2\uparrow} \Big\} |0\rangle_R. \tag{3}$$

The indices $\mathbf{f}_1$ and $\mathbf{f}_2$ denote here atoms belonging respectively to sublattices 1 and 2. It is assumed that the moment of the ferromagnetic microregion is parallel to the moment of sublattice 2.

As to the antiferromagnetic sd-coupling, it is necessary here to take into account both projections of the conduction-electron spin and also inside the ferromagnetic microregion. At the same relative position of the moments of the microregion and of the sublattices, the wave function is chosen in this case in the form

$$\Phi = \Big\{ \sum_{|\mathbf{f}_1| \geqslant R/a} c_{\mathbf{f}_1\uparrow} \overset{*}{a}_{\mathbf{f}_1\uparrow} + \sum_{|\mathbf{f}_1| < R/a} [c_{\mathbf{f}_1\uparrow} \overset{*}{a}_{\mathbf{f}_1\uparrow} + c_{\mathbf{f}_1\downarrow} \overset{*}{a}_{\mathbf{f}_1\downarrow} S^+_{\mathbf{f}_1}] + \sum_{\mathbf{f}_2} [c_{\mathbf{f}_2\uparrow} \overset{*}{a}_{\mathbf{f}_2\uparrow} + c_{\mathbf{f}_2\downarrow} \overset{*}{a}_{\mathbf{f}_2\downarrow} S^+_{\mathbf{f}_2}] \Big\} |0\rangle_R. \tag{4}$$

The systems of equations for the determination of the coefficients of the functions (3) and (4), to which it is necessary to go over in the approximation of the continuous medium, are obtained in the standard manner. When $A < 0$ the set of amplitudes $c_{\mathbf{f}\sigma}$ can be regarded as a "bispinor" wave function, whose components are defined as follows:

$$\psi_1(\mathbf{r}) = c_{\mathbf{f}_1\uparrow}, \quad \psi_2(\mathbf{r}) = c_{\mathbf{f}_2\uparrow}, \quad \psi_3(\mathbf{r}) = c_{\mathbf{f}_1\downarrow}, \quad \psi_4(\mathbf{r}) = c_{\mathbf{f}_2\downarrow}. \tag{5}$$

Expansion of the coefficients $c_{\mathbf{f}\sigma}$ in a Taylor series makes it possible to make a substitution of the type

$$\sum_{\mathbf{g}} c_{\mathbf{f}_1+\mathbf{g}\uparrow} \to [6 + a^2\Delta]\, \psi_2(\mathbf{r}).$$

Taking the foregoing into account, the Schrödinger equation takes in the case of antiferromagnetic sd-coupling the form

$$\begin{gathered}
\Big\{\frac{AS}{2}[1 - 2\theta(r - R)] - E_R\Big\}\psi_1 + B(6 + a^2\Delta)\psi_2 - \\
- A\sqrt{\frac{S}{2}}\theta(R - r)\psi_3 = 0, \\
B(6 + a^2\Delta)\psi_1 + \Big(\frac{AS}{2} - E_R\Big)\psi_2 - A\sqrt{\frac{S}{2}}\psi_4 = 0, \\
-A\sqrt{\frac{S}{2}}\theta(R - r)\psi_1 + \Big[-\frac{A(S-1)}{2} - E_R\Big]\psi_3 = 0, \\
-A\sqrt{\frac{S}{2}}\psi_2 + \Big[-\frac{A(S-1)}{2} - E_R\Big]\psi_4 = 0, \\
\theta(x) = 1 \quad \text{for} \quad x \geqslant 0, \qquad \theta(x) = 0 \quad \text{for} \quad x < 0.
\end{gathered} \tag{6}$$

We use here the notation

$$E_R = E - E_A - 8\pi|I|S^2(R/a)^3. \tag{7}$$

The terms $\sim I/A$ were omitted from (6).

The system (6) is solved by transforming it into a single equation with respect to ψ_1. This component of the wave function is represented by a spherical wave with a real wave number k in the ferromagnetic microregion and an imaginary wave number $i\kappa$ outside this region. As a result we obtain the following system of transcendental equations for the determination of the energy:

$$(L^2(E_R) - B^2(6 - a^2k^2) = 0.$$

$$-(AS/2 + E_R)L(E_R) - B^2[6 + a^2k^2 \operatorname{ctg}^2 kR] = 0, \quad \operatorname{ctg} kR < 0, \tag{8}$$

where L(E) is given by

$$L(E) = \frac{AS}{2} - E + \frac{A^2S}{2}\left[E + \frac{A(S-1)}{2}\right]^{-1}. \tag{9}$$

In the case of ferromagnetic sd-coupling, the aggregate of the coefficients of the wave function (3) is regarded as a "vector" wave function with components

$$\psi_1(\mathbf{r}) = c_{\mathbf{f}_1\uparrow}, \quad \psi_2(\mathbf{r}) = c_{\mathbf{f}_2\uparrow}, \quad \psi_3(\mathbf{r}) = c_{\mathbf{f}_1\downarrow}. \tag{10}$$

When A > 0 the Schrödinger equation is of the form

$$\left\{\frac{AS}{2}[1 - 2\theta(R-r)] - E_R\right\}\psi_1 + B[6 + a^2\Delta]\psi_2 - A\sqrt{\frac{S}{2}}\theta(r-R)\psi_3 = 0,$$

$$B[6 + a^2\Delta]\psi_1 + [-AS/2 - E_R]\psi_2 = 0,$$

$$-A\sqrt{\frac{S}{2}}\theta(r-R)\psi_1 + \left[-\frac{A(S-1)}{2} - E_R\right]\psi_3 = 0. \tag{11}$$

It is solved in exactly the same manner as (6) and leads to the following equation for the energy:

$$-B(6 - a^2k^2) = AS - \frac{A^2S}{2B(6 - a^2k^2) + A} - \frac{B[6 + a^2k^2 \operatorname{ctg}^2 kR]^2}{6 - a^2k^2}, \tag{12}$$

$$E_R = -AS/2 - |B|[6 - a^2k^2], \quad \operatorname{ctg} kR < 0. \tag{13}$$

Proceeding to the analysis of (8), (12), and (13), it should be noted that they have solutions only when R exceeds a certain minimum value R_M. The energy levels E_R in the polaron well start with the lowest value at R = 0. This value is lower than the minimum energy of the band electron (2), inasmuch as when R = 0 the wave functions (3) and (4), unlike the band wave function, take into account the conservation of the projection of this spin of the s-electron, due to the exchange interaction with the magnetic atoms. If a magnetic polaron is produced, then its radius R should exceed R_M, in order that the gain of the electric energy compensate for the loss in the energy to the creation of the ferromagnetic microregion. When R tends to infinity, the polaron level tends, for A < 0 and A > 0 respectively, to

$$E_R = {}^1\!/_2 A(S+1) - 6|B|, \tag{14}$$

$$E_R = {}^1\!/_4[A - 12|B|] - {}^1\!/_4\{[A - 12|B|]^2$$

$$-48|B|A(S-1) + 4A^2S(S+1)\}^{1/2}. \tag{15}$$

Further, from (6) and (11) we see that at large values of S it is sufficient to use in place of the "bispinor" or (vector) wave function the "spinor" wave function with components ψ_1 and ψ_2. In this case (8), (12), and (13) reduce to (5) of [1].

Each of the systems of equations (8) and (12), (13) can be simplified in the limiting cases $|A|S \ll 6|B|$ and in the opposite case. In the first of these cases (weak sd-interaction) both systems lead to the same equation for the parameter k:

$$\frac{2}{\pi}kR_M = \sin kR, \tag{16}$$

where the minimum radius R_M is in this case

$$R_M = \frac{\pi}{2}a\left[\frac{2|B|}{|A|S} - \frac{|A|S^2(1 + 2/S)}{48B^2}\right]^{1/2}. \tag{17}$$

In some cases it is possible to obtain an approximate solution of (16):

$$k = \frac{\pi}{R}\left[1 - \frac{2}{\pi}\frac{R_M}{R}\right] \quad (R \gg R_M), \tag{18}$$

$$k = \frac{\pi}{2R_M}\left[1 - \left(\frac{2}{\pi}\right)^2\left(\frac{R - R_M}{R_M}\right)^2\right] \quad (R - R_M \ll R_M). \tag{19}$$

The energy E_R is expressed in terms of k with the aid of relation (13), where for A < 0 it is necessary to replace the sd-exchange integral by its modulus. If no magnetic polaron is produced, then the minimum energy of the system is equal to

$$E(0) = E_0 + E_A - 6|B| - \frac{A^2S^2}{48|B|}\left[1 + \frac{2}{S}\right]. \tag{20}$$

In the opposite case of strong sd-coupling with A > 0 and not too large values of S, the energy E_R and the parameter k are determined as before by Eqs. (13) and (16), but the minimum radius is given by the expression

$$R_M = \frac{\pi}{2}a\left[6\left(1 - \frac{1}{\sqrt{2S+1}}\right)\right]^{-1/2}, \tag{21}$$

and the energy of the system in the absence of a ferromagnetic microregion is equal to

$$E(0) = E_0 + E_A - \frac{AS}{2} - \frac{6|B|}{\sqrt{1+2S}} + \frac{6|I|S^2}{(2S+1)}. \tag{22}$$

On the other hand, if A < 0, then the energy is given by

$$E_R = \frac{A}{2}(S+1) - \frac{|B|2S}{1+2S}(6 - a^2k^2). \tag{23}$$

The parameter k is determined from (16) with the minimum radius

$$R_M = \frac{\pi}{2}a\left[\frac{|B|}{3(1+2S)|A|}\right]^{1/4}. \tag{24}$$

The value of E(0) is in this case

$$E(0) \approx E_0 + E_A + \frac{A(S+1)}{2} + \frac{144B^2S}{A(1+2S)^2} + \frac{6|I|S^2}{(1+2S)}. \tag{25}$$

It is possible to obtain an explicit expression for the value of R_0 of the parameter R at which the total energy of the system is minimal only if $R_0 \gg R_M$. Using (7), (13), (18) and (17), (21) we obtain

$$R_0 = a\left(\frac{\pi}{12}\frac{|B|}{|I|S^2}\right)^{1/5}. \tag{26}$$

In the case of a strong antiferromagnetic coupling, the value of |B| in (26) should be replaced by |B|2S/(1 + 2S).

Attention is called to the weak dependence of R_0 on B/I in (26). However, at smaller values of R_0 this dependence is much stronger. If the magnetic polaron is energetically favored, then in typical cases the value of R_0 amounts to 2–3 lattice constants.

It has been assumed so far that the energy of the system is minimal when the moment of the ferromagnetic microregion is collinear with the antiferromagnetism vector. In principle, it may turn out that the energy is even lower when these vectors are mutually orthogonal. A direct calculation shows, however, that the electronic part of the energy of the "parallel" configuration in the cases considered above is lower than the energy of the "perpendicular" configuration, with the exception of the case of a strong antiferromagnetic sd-coupling. However, even then the gain in that part of the energy is smaller than the loss in the surface magnetic energy due to spin rotation through an angle $\pi/2$.

The results obtained here for small spins differ most strongly from the results for large spins in the case of a strong ferromagnetic sd-coupling. This is connected with the strong decrease of the energy of the system due to the non-conservation of the s-electron spin projection on the atoms of the "energetically unfavored" sublattice. As a result, as seen from (22), the correction to the energy of the system due to the translational motion of the s-electron in the absence of a ferromagnetic microregion is of first order in B/A. On the other hand, in the case of large spins such a correction is of second order of smallness. Therefore the tendency to the formation of a magnetic polaron decreases with decreasing spin when $A > 0$.

In the case of antiferromagnetic sd-coupling, there is no such strong lowering of the energy of the system due to the "oscillations" of the spin of the conduction electron, and in the case of small spins the tendency to form the magnetic polaron remains sufficiently strong. The reason for this difference can be easily explained with $S = 1/2$ as an example. When $A > 0$, the ground state of the atom with the conduction electron on it is triply degenerate with respect to the direction of the total spin. Whereas in one sublattice this total spin is directed only to the magnetic moment of the sublattice, in the other sublattice it is perpendicular to this direction. These states are not orthogonal to each other with respect to the spin variables, since we are dealing with localization of the s-electron at different atoms. Thus, the s-electron going from atom to atom remains in states with the same energy, and the influence of the antiferromagnetic ordering reduces to a renormalization of the Bloch integral.

At the same value of the spin, but at the opposite sign of the sd-exchange integral, the ground state of the magnetic atom with the conduction electron on it is a singlet state. It is impossible to construct a singlet state with an s-electron on an atom of the other sublattice, which is not orthogonal to the first in the spin variables. Therefore for the conduction electron, the atoms of different sublattices are energetically not equivalent to each other, and antiferromagnetic ordering, as also in the case of large spins, hinders the translational motion of the s-electron.

2. LOCALIZED MAGNETIC POLARON

In this section we shall consider the state of an s-electron which is localized near a positively charged defect. We investigate also the magnetic properties of such defects. The consideration advanced in the preceding section concerning the state of the system can be repeated practically verbatim for the present case. The localized s-electron will tend to establish near the defect ferromagnetic ordering in place of antiferromagnetic ordering. If the disturbance of the antiferromagnetic ordering near the defect is energetically favored, then such a state can be interpreted as a localized magnetic polaron.

The ground state of the system is determined in the same manner as in the preceding section, but it is proposed to add to the Hamiltonian (1) a term that describes the field of the defect. The analysis is confined to the case of sufficiently large spins. We use the continuous-medium approximation and employ a variational principle. In the construction of the trial wave function it is assumed that at $r = R$, which plays the role of the variational parameter, the antiferromagnetic ordering changes jumpwise into ferromagnetic ordering. In the absence of an external field, the minimum of the energy is reached if the ferromagnetism vector M is parallel or antiparallel to the antiferromagnetism vector L. Which of these two orientations gives a lower energy depends on the exact position of the defect (the particular magnetic sublattice it belongs to etc.). In accordance with the results of the preceding section, the wave function of the system can be represented as the product of the electron wave function and the wave function of the magnetic subsystem. The electronic function is a two-component one with respect to the two magnetic sublattices (the spin of the conduction electron can be regarded here as fixed). The electronic Schrödinger equation takes the form

$$\left\{E_A + \frac{|A|S}{2}[1 - 2\theta(R-r)] - \frac{e^2}{\varepsilon r} - E_e\right\}\psi_1 + B[6 + a^2\Delta]\psi_2 = 0,$$

$$B[6 + a^2\Delta]\psi_1 + \left\{E_A - \frac{|A|S}{2} - \frac{e^2}{\varepsilon r} - E_e\right\}\psi_2 = 0, \tag{27}$$

where ϵ is the dielectric constant of the crystal and E_e is the electron energy.

A solution of (27) can be obtained in explicit form if it assumed that in the region $r > R$ the change of the Coulomb energy over the depth of penetration of the electron into the antiferromagnetic region is small compared with the energy of the sd-exchange. Under this condition we obtain for ψ_1 the solution:

$$\psi_1 = C_1 \exp\left\{-\frac{r}{\rho n}\right\}\Phi\left(1 - n, 2, \frac{2r}{n\rho}\right), \tag{28}$$

where

$$n = \sqrt{\frac{E_e'(\infty)}{E_e'(R)}}, \qquad E_e' = E_e + 6|B| + \frac{|A|S}{2} - E_A,$$

$\Phi(\alpha, \beta, z)$ is the confluent hypergeometric function, $\rho = 2|B|a^2\epsilon e^{-2}$ is the Bohr radius, $E_e(R)$ is the electron energy as a function of the radius R (solution inside the ferromagnetic microregion);

$$\psi_1 = C_2 e^{-\varkappa r}/r, \tag{29}$$

where the parameter κ is connected with the electron energy by the relation

$$B^2[6 + a^2\varkappa^2]^2 = [6|B| - E'_e][|A|S + 6|B| - E'_e] \tag{30}$$

(solution outside the ferromagnetic microregion).

The joining of the solutions (29) and (30) on the boundary of the microregion leads to the following transcendental equation for the determination of the electron energy:

$$\varkappa = -\frac{d}{dr}\left\{r \exp\left(-\frac{r}{\rho n}\right)\Phi\left(1 - n, 2, \frac{2r}{n\rho}\right)\right\}_{r=R}. \tag{31}$$

If $|A|S \gg 6|B|$, then (31) can be replaced with sufficient accuracy by

$$\Phi(1 - n, 2, 2R/n\rho) = 0. \tag{32}$$

The Schrödinger equation (27) can be solved also in the cases $R \gg \rho$ or $|A|S \ll e^2/\epsilon\rho$, using perturbation theory:

$$E_e(R) = E_e(\infty) + \frac{|A|S}{2} \langle 0|\theta(r-R)|0\rangle, \tag{33}$$

where the averaging is carried out over the ground state of the localized electron with $A = 0$.

The magnetic defect of the type under consideration has a moment

$$M \approx \frac{8\pi}{3}\mu_B S\left(\frac{R_0}{a}\right)^3. \tag{34}$$

Here μ_B is the Bohr magneton and R_0 is determined from the condition of the minimum of the total energy of the system. However, this moment is "bound" to the antiferromagnetism vector. If the external magnetic field is not strong enough to break this bond, then the magnetic susceptibility χ^p of such defects is unisotropic.

If the weak magnetic field **H** is parallel to **L**, then owing to the random distribution of the defect over the crystal their summary moment becomes equal to zero up to a field value at which the moment of the quasiparticle either changes by unity or is established along the field. It may turn out, however, that the critical field for the rotation of **L** by $\pi/2$ is smaller than the critical field indicated above. For defects that are arranged symmetrically with respect to the magnetic sublattices (anion vacancies etc.) we can expect the critical field that reverses the orientation of M to be equal to zero. In this case the longitudinal magnetic moment of the crystal in weak fields will be determined completely by the defects as $T \to 0$.

When $\mathbf{H} \perp \mathbf{L}$, the magnetic moment of each of the sublattices deviates from its position at $H = 0$ in the direction of the applied field, by an angle φ_1 or φ_2 respectively. The influence of the defects on the magnetic moment of the crystal becomes manifest not only by their anomalously large magnetic moments, but also by deviation angles that are anomalously large compared with the ideal lattice. Assume, for concreteness, that the magnetic moment of the defect at $H = 0$ is parallel to the moment of sublattice 2. Within the framework of the phenomenological theory[8], the energy E of a cubic crystal at small values of H can be represented as a functional of the sought angles $\varphi_1(r)$ and $\varphi_2(r)$ in the following manner:

$$E = E[l] + E[m], \quad l = \varphi_2 - \varphi_1, \quad m = \varphi_1 + \varphi_2, \tag{35}$$

$$E[l] = -\frac{S^2}{8}\int\limits_{r,\, r_1 \geqslant R}^{\infty} I(\mathbf{r}-\mathbf{r}_1)[l(r)-l(r_1)]^2\,d\mathbf{r}\,d\mathbf{r}_1 + \frac{bS^2}{2}\int\limits_{r \geqslant R}^{\infty} l^2(r)\,d\mathbf{r} - \frac{HM}{2}l(R), \tag{36}$$

$$E[m] = -\frac{S^2}{8}\int\limits_{r,\, r_1 \geqslant R}^{\infty} I(\mathbf{r}-\mathbf{r}_1)[m(r)+m(r_1)]^2\,d\mathbf{r}\,d\mathbf{r}_1 - \mu_B SH\int\limits_{r \geqslant R}^{\infty} m(r)\,d\mathbf{r} - \frac{HM}{2}m(R). \tag{37}$$

Here the quantities I(**r**) and b describe respectively the exchange interaction between the atoms from different sublattices and the anisotropic interaction that ensures stability of the configuration under consideration. In writing out (36) and (37) it is assumed that the moments of all the atoms in the ferromagnetic microregion $r < R$ are inclined by the same angle $\varphi_2(R)$, and that outside this microregion the interaction of the s-electron of the defects with the magnetic atoms can be neglected.

Let us assume (this is confirmed by further calculation) that the quantity $l(r)$ is a slowly varying function of the radius r. Taking into account the small radius of action of the exchange forces, the Euler equation for the functional $E[l]$ (36) takes the form

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{d}{dr}l(r)\right] - \varkappa_1^2 l(r) = 0, \tag{38}$$

where

$$\varkappa_1 = \frac{4b}{|J_1|}, \qquad J_1 = \frac{S^2}{3}\int\limits_0^\infty I(r)r^2dr.$$

The boundary conditions for this equation are obtained from an arbitrary variation of $l(r)$ at $r = R$ and $r = \infty$:

$$r^2\frac{dl(r)}{dr}\bigg|_{r=\infty} = 0, \quad r^2\frac{dl(r)}{dr}\bigg|_{r=R} = -\frac{HM}{2\pi|J_1|}. \tag{39}$$

The solution of Eq. (38) with boundary conditions (39) is given by expression

$$l(r) = \frac{HM\exp\{-\varkappa_1(r-R)\}}{2\pi|J_1|[1+\varkappa_1 R]r}. \tag{40}$$

It is clear from (40) that in order to consider the defects independently of one another, as was done here, it is necessary to satisfy the condition $\kappa_1 \gg n^{1/3}$, where n is the impurity concentration.

As regards the quantity $m(r)$, it cannot be regarded in general as a slowly varying function of r at distances on the order of the exchange-force radius, i.e., the lattice constant. This can raise doubts concerning the applicability of the phenomenological approach. We shall show below, however, that it is possible to neglect the rapid variations of $m(r)$ and to assume this quantity constant. Variation of the functional $E[m]$ (37) yields the following equation for its extremal value:

$$\int\limits_{r_1 \geqslant R} I(\mathbf{r}-\mathbf{r}_1)[\varphi(r)+\varphi(r_1)]d\Omega\,d\mathbf{r}_1 = -\frac{2HM}{R^2}\delta(r-R), \tag{41}$$

where

$$\varphi(r) = m(r) - \frac{2\mu_B HS}{|J|}, \quad J = \int I(\mathbf{r})\,d\mathbf{r},$$

$d\Omega$ is the solid-angle element corresponding to the vector **r**.

According to the condition $R \gg a$, Eq. (41) can be approximately replaced by the equation

$$\int\limits_0^\infty F(r-r_1)[\varphi(r+R)+\varphi(r_1+R)]\,dr_1 = -\frac{HM}{2\pi R^2}\delta(r),$$

$$F(r-r_1) \approx r_1^2\int I(\mathbf{r}-\mathbf{r}_1)\,d\Omega. \tag{42}$$

the kernel $F(r)$ of the integral equation (42) decreases rapidly over a distance on the order of a. Without limiting the generality of the obtained estimate, it is convenient to approximate it by means of an exponential

$$F(r) \approx K\exp(-r/a_1). \tag{43}$$

By direct verification we establish the equivalence of the integral equation (42) with the kernel (43) and the following differential equation:

$$\varphi''(r+R)-\frac{2}{a_1^2}\varphi(r+R)=-\frac{HM}{2\pi R^2 a_1 K}\left[\delta''(r)-\frac{\delta(r)}{a_1^2}\right]. \qquad (44)$$

The solution of (44), obtained by extending it to the region $r < 0$ and using a Fourier transformation, is of the form

$$m(r)=\frac{HM}{4\pi\sqrt{2}R^2 K a_1^2}\exp\left\{-\frac{\sqrt{2}}{a_1}(r-R)\right\}+\frac{2\mu_B HS}{|J|}. \qquad (45)$$

Thus, according to (45), the quantity $m(r)$ remains practically constant up to $r - R \sim a_1$, where it experiences an abrupt jump. However, from a comparison of (45) and (40) it follows that

$$m(R)\,/\,l(R)\ \sim\ a\,/\,R \ll 1,$$

i.e., the contribution of $m(R)$ to $\varphi_2(R)$ can be neglected compared with the contribution of $l(R)$.

From (45) and from the definition of the quantiy m it follows that the magnetic moment of an antiferromagnet is equal to its value in an ideal crystal already in the direct vicinity of the defect. We therefore obtain the following expression for the transverse susceptibility $\chi_\perp^p$ of the defect under consideration:

$$\chi_\perp^p \approx M^2 n\,/\,4\pi|J_1|R(1+\varkappa_1 R). \qquad (46)$$

An estimate of the effect showed that at a defect concentration $n \sim 10^{20}$ cm^{-3}, an effective electron mass $\hbar^2/|B|a^2$ equal to the true mass, a dielectric constant $\epsilon \sim 5$, and a Neel temperature ~0.01 eV we get $\chi_\perp^p \sim 10^{-4}S^2$ and $R_0 \sim 5$Å. Comparing the result (46) with the well-known expression for the susceptibility $\chi_\perp$ of an ideal antiferromagnet, we obtain $\chi_\perp^p/\chi_\perp \sim R_0^5 n a^{-2}$, i.e., $\chi_\perp^p$ amounts to several times 10% of $\chi_\perp$ under the conditions considered.

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