MAGNETIC POLARON IN A FERROMAGNETIC CRYSTAL

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We consider the motion of a conduction electron in a nonmetallic ferromagnetic crystal with allowance for s-d exchange interaction. If the sign of the s-d exchange integral is negative, the wave function contains an admixture of the polaron state, in which the motion of the electron is accompanied by a spin wave. The problem has a close analogy with the problem of the bound state of two spin waves, and is solved rigorously. The energy spectrum of the system is investigated numerically for a wide range of values of the parameters. We also calculate the electron spin averaged over the ground state, and the wave function of the bound state.

A conduction electron moving in a magnetically ordered nonmetallic crystal deforms the magnetic structure of the crystal. The mechanism coupling the electron with the localized atomic spins of the magnet is the s-d exchange interaction. Since this is practically a contact interaction, the electron-induced deformation of the magnetic structure can be localized near the electron and moves when the latter moves over the crystal. If such a localization takes place, the corresponding quasiparticle (electron accompanied by the deformation of the magnetic structure) is called a magnetic polaron. The conditions for the occurrence of a magnetic polaron in an antiferromagnetic crystal were investigated by Nagaev [1] by a variational method. Initially, in the analysis of the motion of a conduction electron in a ferromagnetic crystal, account was taken only of the fact that it becomes magnetized by the exchange field of the localized electrons, as manifest by the appearance of a definite orientation of the electron spin relative to the spontaneous magnetic moment of the crystal. This effect, however, is due only to the diagonal (with respect to the electric spin) part of the s-d interaction, with respect to which the magnetic lattice is absolutely rigid. Responsible for the deformation of the magnetic structure is the nondiagonal part of the s-d exchange, and if it is taken into account, then states of the polaron type can appear in a ferromagnet under certain conditions even at zero temperature. The present paper is devoted to the investigation of such states. It should be noted that in the limiting case of weak s-d exchange, this question was considered in [2-4], and in the limit of a strong s-d coupling it was investigated by Nagaev.[5]

Thus, let us consider a conduction electron in a ferromagnetic nonmetallic crystal, which can be described by the following Hamiltonian:[1]

$$\mathcal{H}=\sum_{m\sigma\sigma'}\{E_A\delta_{\sigma\sigma'}-A(\mathbf{sS}_m)_{\sigma\sigma'}\}a_{m\sigma}^{+}a_{m\sigma'}+B\sum_{m\Delta\sigma}a_{m\sigma}^{+}a_{m+\Delta,\sigma}-\frac{1}{2}I\sum_{m\Delta}(\mathbf{S}_m\mathbf{S}_{m+\Delta}). \quad (1)$$

Here $a_{m\sigma}$ is the operator of the annihilation of an electron at the site m with spin σ, $\mathbf{S}_m$ is the operator of the atomic spin of the quantity S, located at the site m. The energy parameters have the following meaning: E_A—atomic energy of the electron, B—Bloch transport integral, A—integral of exchange interaction of conduction electron and a localized atomic spin, $I>0$—exchange integral between the nearest neighboring atoms (Δ denotes summation over the nearest neighbors).

Let us direct the z axis of the coordinate system along the spontaneous moment of the crystal, and let us denote the directions of the electron spin along the z axis and in the opposite direction by $\uparrow$ and $\downarrow$, respectively. The operator of the z-projection of the summary spin of the crystal

$$S^0=\sum_m S_m^z+\frac{1}{2}\sum_m(a_{m\uparrow}^{+}a_{m\uparrow}-a_{m\downarrow}^{+}a_{m\downarrow}) \quad (2)$$

commutes with the Hamiltonian, and therefore the eigenstates of the Hamiltonian should be characterized by the eigenvalues of the Z-projection of the summary spin.

When $A>0$, obviously, the ground state corresponds to the summary spin $NS+\frac{1}{2}$, in which the conduction electron has a spin orientation along the spontaneous moment of the completely ordered localized spins. When $A<0$, the ground state of the system should be characterized by the z-projection of the summary spin, equal to $NS-\frac{1}{2}$. However, this value of the z-projection of the summary spin is obtained not only in the case when the electron spin is directed antiparallel to the summary spin of the ferromagnetic order, but also in the case of parallel orientation of the electron spin, provided that there is a single spin deflection in the system of localized spin.

In accord with the foregoing, the wave function of the system $\Psi_{NS-1/2}$ represents when $A<0$ a superposition of two states (we shall call them the trivial and the polaron states):

$$\Psi_{NS-1/2}=\Big\{\sum_m c(m\downarrow)a_{m\downarrow}^{+}+\sum_{mn}(2S)^{-1/2}b(m,n)a_{m\uparrow}^{+}S_n^{-}\Big\}|0\rangle, \quad (3)$$

with $|0\rangle$ the wave function of the state when there is complete ferromagnetic ordering in the spin system, and there is not a single electron in the conduction band. Such a state is defined uniquely by the conditions

$$S_n^{+}|0\rangle=0,\quad S_n^{z}|0\rangle=S|0\rangle,\quad a_{m\sigma}|0\rangle=0.$$

The Schrödinger equation for the state $\Psi_{NS-1/2}$ leads to

the following system of equations for the amplitudes of the wave function

$$-Bzc(n\downarrow)+B\sum_{\Delta}c(n+\Delta,\downarrow)-{}^1/_2A(2S)^{1/2}b(n,n)=Ec(n\downarrow),$$

$$-{}^1/_2A(2S)^{1/2}\delta_{np}c(n\downarrow)+[-Bz-{}^1/_2AS+ISz-{}^1/_2A(S-\delta_{np})]b(n,p)$$

$$+B\sum_{\Delta}b(n+\Delta,p)-IS\sum_{\Delta}b(n,p+\Delta)=Eb(n,p) \qquad (4)$$

with the normalization condition

$$\sum_{n}|c(n\downarrow)|^2+\sum_{np}|b(n,p)|^2=1. \qquad (5)$$

The energy E is reckoned from the level $E_A + {}^1/_2AS + Bz - {}^1/_2NzIS^2$, corresponding to the energy of the ground state of the spin system and the bottom of the conduction electron with spin ↓.

We seek the solution in the form of a Fourier expansion

$$b(n,p)=e^{i\mathbf{KR}}\frac{1}{N}\sum_{\mathbf{q}}b(\mathbf{K},\mathbf{q})e^{i\mathbf{qr}}, \qquad (6)$$

where

$$\mathbf{R}\equiv{}^1/_2(\mathbf{n}+\mathbf{p}),\quad \mathbf{r}\equiv\mathbf{n}-\mathbf{p}. \qquad (7)$$

As seen from (7), **K** corresponds to the summary momentum and **q** to the relative momentum of the two elementary excitations[1)] (the electron and the spin deflection), localized at the sites n and p (representing $c(n\downarrow)$) in the form

$$c(n\downarrow)=\frac{1}{N}c_{\downarrow}(\mathbf{K})e^{i\mathbf{Kn}},$$

we obtain in place of (4) the following system of equations:

$$c_{\downarrow}(\mathbf{K})=-\frac{A}{2}(2S)^{1/2}G_{\downarrow}{}^0(E,\mathbf{K})\sum_{\mathbf{q}}b(\mathbf{K},\mathbf{q}),$$

$$b(\mathbf{K},\mathbf{q})-\frac{E-\varepsilon_{\uparrow}(\mathbf{K})}{E-\varepsilon_{\downarrow}(\mathbf{K})}\cdot\frac{A/2}{E-\varepsilon_{\uparrow}({}^1/_2\mathbf{K}+\mathbf{q})-\varepsilon_m({}^1/_2\mathbf{K}-\mathbf{q})}\frac{1}{N}\sum_{\mathbf{q}'}b(\mathbf{K},\mathbf{q}')=0 \qquad (8)$$

and the normalization condition

$$\sum_{\mathbf{q}}|b(\mathbf{K},\mathbf{q})|^2+\frac{1}{2}\frac{A^2S}{[E-\varepsilon_{\downarrow}(\mathbf{K})]^2}\frac{1}{N}\Big|\sum_{\mathbf{q}}b(\mathbf{K},\mathbf{q})\Big|^2=1. \qquad (9)$$

Here

$$\varepsilon_m(\mathbf{K})=IS\Big(z-\sum_{\Delta}e^{i\mathbf{K}\Delta}\Big), \qquad (10)$$

$$\varepsilon_{\downarrow}(\mathbf{K})=-B\Big(z-\sum_{\Delta}e^{i\mathbf{K}\Delta}\Big), \qquad (11)$$

$$\varepsilon_{\uparrow}(\mathbf{K})=-B\Big(z-\sum_{\Delta}e^{i\mathbf{K}\Delta}\Big)-AS, \qquad (12)$$

where $\epsilon_m(\mathbf{k})$ is the energy of the spin wave in an ideal ferromagnetic crystal (in the absence of a conduction electron), $\epsilon\uparrow(\mathbf{K})$ and $\epsilon\downarrow(\mathbf{K})$ are the energies of the conduction electrons with momentum **K** and corresponding orientation, moving over the crystal with ideal ferromagnetic order; $G^0_{\downarrow}(E, \mathbf{K}) = (E - \epsilon_{\downarrow}(\mathbf{K}))^{-1}$ is the Green's function of the electron.

[1)] A distinguishing feature of the problem under consideration is that the state $\Psi_{NS-1/2}$ is neither a pure single-particle state nor a pure two-particle state (with respect to $|0\rangle$), but is a superposition of both. Therefore the quasimomentum **K** characterizing the level E turns out to be the quasimomentum of a quasiparticle forming the trivial state, and at the same time the quasimomentum of the mass center of the two-particle state. In the latter aspect, the problem has much in common with the problem of the bound state of two spin waves, solved by Wortis [6].

The second equation of (8) leads to the dispersion equation

$$1-\frac{AS}{E-\varepsilon_{\uparrow}(\mathbf{K})}=\frac{A}{2}\frac{1}{N}\sum_{\mathbf{q}}\frac{1}{E-\varepsilon_{\uparrow}({}^1/_2\mathbf{K}+\mathbf{q})-\varepsilon_m({}^1/_2\mathbf{K}-\mathbf{q})}, \qquad (13)$$

which defines the eigenenergies of the system E in the state $\Psi_{NS-1/2}$. We see from this expression that when $A \to 0$ the eigenenergies coincide with the band of the quasicontinuous levels of two-particle noninteracting excitations of the system, namely the conduction electron with spin ↑ and the spin waves. At each fixed **K**, this band contains N energy levels:

$$E=\varepsilon_{\uparrow}({}^1/_2\mathbf{K}+\mathbf{q})+\varepsilon_m({}^1/_2\mathbf{K}-\mathbf{q}), \qquad (14)$$

corresponding to N possible values of the relative quasimomentum **q**.

In the other limiting case $|A| \to \infty$ we have

$$E\approx{}^1/_2A. \qquad (15)$$

Inasmuch as $A < 0$, this means that a deep discrete level appears under the band of the quasicontinuous spectrum. At a finite value of the s-d exchange coupling parameter A, there exists for each **K** a band of the quasicontinuous spectrum of levels that lie (accurate to $\sim 1/N$) within the limits defined by (14), and a discrete level lying below this band can also appear. The latter level corresponds to a superposition of the trivial state of the conduction electron and the bound state of the conduction electron with spin ↑ and the spin wave.

Let us investigate first the structure of the spectrum at $\mathbf{K} = 0$. To find the energies lying outside the band, it is possible to replace in (13) the summation with respect to **q** by integration. The dispersion equation (13) is best rewritten then in the form:

$$\frac{B-IS}{A}=\frac{S}{2\mathscr{E}-z}+\frac{1}{4}G_{00}{}^0(\mathscr{E}), \qquad (16)$$

where

$$\mathscr{E}=\frac{E+(B-IS)z+AS}{2(B-IS)}, \qquad (17)$$

$$G_{nm}{}^0(\mathscr{E})=\frac{\Omega_0}{(2\pi)^3}\int d\mathbf{K}\,e^{i\mathbf{K}(\mathbf{n}-\mathbf{m})}\Big[\mathscr{E}-\frac{1}{2}\sum_{\Delta}e^{i\mathbf{K}\Delta}\Big]^{-1} \qquad (18)$$

(Ω_0 is the volume of the unit cell).

The last quantity is the real part of the single-particle Green's function in the node representation. It is tabulated in [7] for a primitive cubic lattice in the case of coinciding sites n and m (for which we used the symbol G^0_{00}), and also for the sites that are the nearest neighbors.

In order to obtain an idea of the behavior of the right-hand side of Eqs. (16) as a function of $\mathscr{E}$, we can write down Eq. (16) for the one-dimensional case, in which the integral (18) at n = m = 0 can be evaluated exactly:

$$\frac{B-IS}{A}=\frac{S}{2\mathscr{E}-2}+\frac{1}{4}\frac{1}{\sqrt{\mathscr{E}^2-1}},\qquad \mathscr{E}>1. \qquad (19)$$

In the three-dimensional case, however, $G^0_{00}(\mathscr{E})$ is finite everywhere, and the singularity of the expression in the right side of (16) is connected only with the first term. At $\mathscr{E} = z/2$ this singularity, as can be readily seen from (17), corresponds to an energy E = – AS, representing the bottom of the band of the electron with spin ↑ (dashed line in Fig. 1). It is seen from the figure that at all posi-

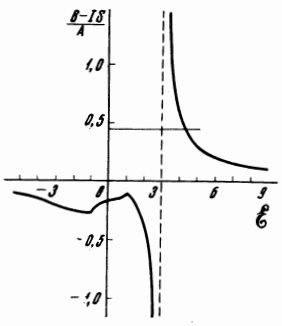

FIG. 1

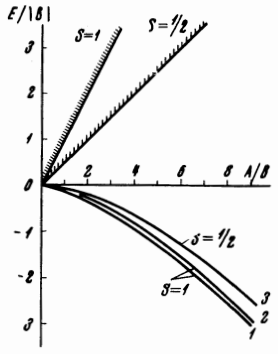

FIG. 2

FIG. 1. Graphic solution of Eq. (16) for the eigenvalues of the energy at K = 0 and S = 1.

FIG. 2. Dependence of the energy E at K = 0 on the value of A. Curves: 1–S = 1, |I/B| = 0.01; 2–S = 1, |I/B| = 0.1; 3–S = ½, |I/B| = 0.01.

tive values of the parameter (B – IS)/A (these are the only values of interest to us, since A < 0 and B < 0), there is one solution of Eq. (16), and we always have $\mathscr{E} > 3$. In order to understand the physical consequences of this result, let us rewrite Eq. (17), which connects $\mathscr{E}$ with E, in the form

$$\mathscr{E} - \mathscr{E}_{\downarrow} = \frac{E}{2(B - IS)}, \qquad \mathscr{E}_{\downarrow} = 3 + \frac{AS}{2(B - IS)}, \qquad (20)$$

where $\mathscr{E}_{\downarrow}$ corresponds to the energy E = 0, i.e., the energy of the electron with spin ↓ (trivial state). It is seen from the last relation that the energy of the trivial state can be obtained from the solution of (16), in which the last term with G_{00}^0 is discarded. The curve representing the first term in the right side of (16) lies below the curve shown in Fig. 1, and therefore at a given value of the parameter (B – IS)/A we always have $\mathscr{E} > \mathscr{E}_{\downarrow} > 3$. Taking (20) into account, we conclude that at all values of A the true energy of the system E, for K = 0, lies below the energy of the trivial state.

The dependence of the energy E at K = 0 on the different parameters is shown in Fig. 2. As before, the zero point is the energy of the trivial state. The straight lines in the upper part of the figure show the limits of the quasicontinuous spectrum at the corresponding values of the spin S. It is seen from Fig. 2 that all the values of A the discrete level becomes separated from the band of the two-particle stages, and the depth of the level increases strongly with increasing A.

To investigate the structure of the spectrum at K ≠ 0, we take into account the fact that I/B is a small parameter. In first approximation in this parameter, the dispersion equation (13) can be represented in the form

$$1 - \frac{AS}{B}\left[2\tilde{\mathscr{E}} - \sum_{\Delta}\cos(K\Delta)\right]^{-1} = \frac{A}{4B}\left\{G_{00}^0(\tilde{\mathscr{E}}) - \frac{IS}{2B}\frac{d}{d\tilde{\mathscr{E}}}(zG_{00}^0(\tilde{\mathscr{E}}) - G_{01}^0(\tilde{\mathscr{E}})\sum_{\Delta}\cos(K\Delta))\right\} \qquad (21)$$

where the unknown $\tilde{\mathscr{E}}$ is connected with the true energy E of the following relation:

$$\tilde{\mathscr{E}} = \frac{E + Bz + AS}{2B}. \qquad (22)$$

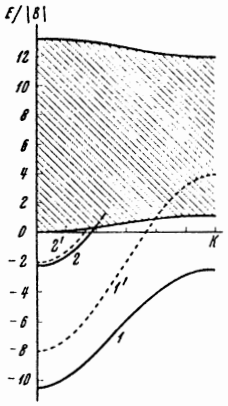

FIG. 3. Structure of the energy spectrum for a wave vector K in the direction [111]. Parameter-: S = 1, |I/B| = 0.1. Curve 1 and dashed curve 1′–A/B = 8; curve 2 and dashed curve 2′–A/B = 2. The dashed curves represent the energy of the trivial state at the corresponding values of the parameters.

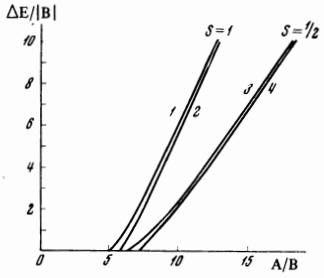

FIG. 4. Dependence of the gap ΔE between the band corresponding to the discrete level for the wave vector direction [111] and the band of the quasicontinuous spectrum, on the quantity A/B: curves 1 and 3–|I/B| = 0.01; 2 and 4–|I/B| = 0.1.

The results of the graphic solution of this equation at particular values of the parameters are shown in Fig. 3. We see here the energy of the system as a function of the wave vector in the direction [111] of the Brillouin zone. The shaded area corresponds to the quasicontinuous spectrum of the two-particle states, calculated in accordance with formula (14). Curves 1 and 2 correspond to the discrete spectrum. The system of discrete levels represented by curve 1 lies in its entirety below the quasicontinuous spectrum at all values of K, and therefore corresponds to a band containing an admixture of only bound states. Curve 2 represents the case when, starting with a certain finite wave vector, the discrete level falls in the band of the continuous spectrum and the motions of the conduction electron with spin ↑ and of the spin wave become uncoupled.

Thus, depending on the value of the parameter A, we can have either an overlap of the band corresponding to discrete spectrum with the quasicontinuous band, or a gap. Figure 4 shows the value of the gap ΔE as a function of the parameter A for two values of the localized spin.

In two limiting cases it is possible to obtain an analytic expression for the energies corresponding to isolated solutions of Eq. (13). In the case |A| ≪ z|B|, iteration of Eq. (13) yields

$$E = \varepsilon_{\downarrow}(K) + \frac{A^2S}{2}\frac{1}{N}\cdot \times \sum_{q}\frac{1}{\varepsilon_{\downarrow}(K) - \varepsilon_{\uparrow}(\tfrac{1}{2}K + q) - \varepsilon_m(\tfrac{1}{2}K - q)},$$

which coincides with the results of [3,4].

In the other limiting case |A| ≫ z|B| we have

$$E = \frac{A}{2} + \frac{(|B| + IS)z}{2S + 1} + \frac{1}{1 + 1/2S}|B|\left(z - \sum_{\Delta} e^{iK\Delta}\right). \qquad (23)$$

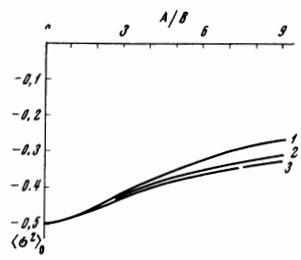

FIG. 5. Dependence of the average z-projection of the electron spin in the ground state on the parameters of the system. Curves: 1–S = ½; |I/B| = 0.01; 2–S = 1, |I/B| = 0.01; 3–S = 1, |I/B| = 0.1.

The width of the polaron band, given by formula (23), agrees with the results of Nageev.[5]

Let us calculate now the wave function of the system. A solution of the second equation of (8) in conjunction with the normalization condition (9) yields

$$b(\mathbf{K},\mathbf{q})=\frac{1}{\sqrt{N}}\frac{E-\varepsilon_\uparrow(\mathbf{K})}{E-\varepsilon_\uparrow(\tfrac{1}{2}\mathbf{K}+\mathbf{q})-\varepsilon_m(\tfrac{1}{2}\mathbf{K}-\mathbf{q})}\cdot \times\left\{(E-\varepsilon_\uparrow(\mathbf{K}))^2\frac{1}{N}\sum_{\mathbf{q}'}\frac{1}{[E-\varepsilon_\uparrow(\tfrac{1}{2}\mathbf{K}+\mathbf{q}')-\varepsilon_m(\tfrac{1}{2}\mathbf{K}-\mathbf{q}')]^2}+2S\right\}^{-1/2}. \quad (24)$$

Substituting this result in (6) and integrating with respect to q, we can obtain, in principle, the spatial distribution of the polaron component of the eigenstate of the system. It is seen already from (24) that for the energies E corresponding to the discrete spectrum (at a chosen value of **K**) the denominator $E - \epsilon_\uparrow(\frac{1}{2}\mathbf{K} + \mathbf{q}) - \epsilon_m(\frac{1}{2}\mathbf{K} - \mathbf{q})$ remains negative at all values of q, and therefore integration with respect to q in (6) gives rise, at sufficiently large |r|, to an exponential factor that points out the localized character of the bound state of the electron and the spin wave.

Formula (24) makes it possible to calculate the mean value of the electron spin in a specified state of the system with energy E and momentum **K**:

$$\langle\sigma^z\rangle_{E,\mathbf{K}}=(\Psi_{NS-1/2}(E)\,|\,\sigma^z\,|\,\Psi_{NS-1/2}(E)), \quad (25)$$

where σ^Z is determined by the second term in (2). Calculating this matrix element with the functions (3), we get

$$\langle\sigma^z\rangle_{E,\mathbf{K}}=\frac{1}{2}\left\{\sum_{\mathbf{q}}|b(\mathbf{K},\mathbf{q})|^2-\frac{1}{2}\frac{A^2S}{(E-\varepsilon_\downarrow(\mathbf{K}))^2}\frac{1}{N}\left|\sum_{\mathbf{q}}b(\mathbf{K},\mathbf{q})\right|^2\right\}. \quad (26)$$

Substituting here the relation (24), we obtain finally

$$\langle\sigma^z\rangle_{E,\mathbf{K}}=\frac{1}{2}-2S\Big/\left\{2S+[E-\varepsilon_\uparrow(\mathbf{K})]^2\frac{1}{N}\times\sum_{\mathbf{q}}[E-\varepsilon_\uparrow(\tfrac{1}{2}\mathbf{K}+\mathbf{q})-\varepsilon_m(\tfrac{1}{2}\mathbf{K}-\mathbf{q})]^{-2}\right\}. \quad (27)$$

It is easy to obtain asymptotic values of this quantity in two limiting cases in the ground state:

$$\langle\sigma^z\rangle_0=-1/2 \qquad (A\to 0); \quad (28)$$

$$\langle\sigma^z\rangle_0=-1/2(2S-1)\,/\,(2S+1) \qquad (|A|\to\infty). \quad (29)$$

The first case correponds to a purely trivial state, while the second to an extremely large contribution of the polaron state with one spin deflection to the eigenstate of the system.

At finite A, the results of a numerical calculation for the ground state of the system in accordance with formula (27) are shown in Fig. 5. We see from this that with increasing |A| the mean value of the z-projection of the electron spin changes monotonically from the value (28) to the value (29), owing to the increase of the contribution of the polaron state.

Note added in proof (23 June 1970). It should be noted that the state with a summary spin NS–½ will be the ground state of the system in the limit as $|A|\to\infty$ only if S = ½. If S > ½, the ground state of the system in the limit as $|A|\to\infty$ is characterized by a spin NS + ½–2S, and this calls for taking into account several spin deflections in the crystal. For intermediate values of A in the ground state there will be realized values of the summary spin S^0 from the interval $NS-\frac{1}{2}\leqslant S^0\leqslant NS+\frac{1}{2}-2S$.

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