Problem of the ground state of conduction electrons in antiferromagnets subjected to a strong magnetic field

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A translation-invariant quantum theory is developed for the motion of a conduction electron in an antiferromagnet subjected to a strong magnetic field. The cases of strong and weak coupling of the electron to the magnetic system of the crystal are considered. Critical values of the external magnetic field for which the conduction electron undergoes a transition to a self-localized state are obtained. The effective mass of carriers is calculated in the limits of strong and weak coupling.

It was shown in Ref. 1 that a self-localized state of conduction electrons can be created in an antiferromagnet subjected to a quantizing magnetic field. In such a case, the configuration of the spin system of the antiferromagnet changes, which leads to a reduction in the total energy of the system consisting of an electron plus atomic spins. It is important to note that no potential barrier needs to be overcome to achieve self-localization, which facilitates experimental investigation of the effect.

According to Ref. 1, self-localization of conduction electrons in strong magnetic fields leads to a reduction in the energy for arbitrary values of the Heisenberg exchange integral but this does not mean that the electron invariably undergoes a transition to a self-localized state in strong fields. To clarify the type of motion realized in antiferromagnets, we need to solve a quantum problem In which atomic spins are regarded as operators and not o-numbers. In this sense, the problem is analogous to the problem of a polaron in the cases of weak and strong coupling.[2,3] It should be noted that the Interaction of an electron with the magnetic lattice in an antiferromagnet is governed not only by the ratio of the exchange constant of the interaction of a conduction electron with the spins of magnetic atoms to the constant of the mutual exchange of magnetic atoms, but also by the magnetic field strength. Another important distinction in this case is that the interaction of a carrier with the spin system in a quantizing external field cannot be, in general, described by a single universal coupling constant.

1. QUANTUM DESCRIPTION OF AN ELECTRON IN AN ANTIFERROMAGNETC

The most general form of a Hamiltonian describing electron motion in an isotropic antiferromagnet subjected to a magnetic field is given by

$$H = H_e + H_{\text{int}} + H_M$$

$$H_e = \frac{1}{2m^*}\left(\mathrm{p} + \frac{e}{c}\mathrm{A}\right)^2, \qquad H_{\text{int}} = -\sum_{m,m'} A(R_m - R_{m'})(S_m, \sigma_{m'}),$$

$$H_M = -\frac{1}{2}\sum_{m,m'} I(R_m - R_{m'})(S_m, S_{m'}) - H\sum_m S_m, \tag{1}$$

where H, describes electron motion in a magnetic field with a vector potential A; H_{ist} corresponds to the s-f interaction of a conduction electron with the magnetic subsystem of the crystal; finally, H_{M} is the Hamiltonian corresponding to the interaction of lattice spins subjected to a magnetic field H (H is measured in energy units). The following notation is used in Eq. (1): S_m is the spin of an atom located at R_m; $\sigma_{m'}$ is the electron spin; $I(R_m\text{-}R_{m'})$ and $A(R_m\text{-}R_{m'})$ are, respectively, the Heisenberg and s-f exchange integrals.

The spin operators in the spin wave approximation are replaced by the Bose creation and annihilation operators of spin deviations and, in the system of coordinates connected with the spin of a magnetic atom, we obtain

$$S_m^{\pm} = S - b_m^+ b_{m'}, \qquad S_m^+ = \sqrt{2S}\,b_{m'}, \qquad S_m^- = \sqrt{2S}\,b_m^-, \tag{2}$$

where $S_m^{\pm} = S_m^x \pm S_m^y$. Assuming that the electron spin is completely polarized in the direction of the magnetic field, i.e., setting $\sigma_m = \sigma^s\delta(R_m - r)$ and taking into account the fact that the s-f exchange Interaction has a short range, $A(R_m\text{-}R_{m'}) = A\delta(R_m\text{-}R_{m'})$, we can use Eq. (2) to obtain the following expression for the interaction Hamiltonian

$$\left.\begin{aligned} H_{\text{int}} &= \frac{A}{2}S_r^z, \qquad S_r^z = \sum_m S_m^z\delta(r-R_m), \\ S_m^z &= \left(S - b_m^+ b_m\right)\cos\theta_m + \sqrt{\frac{S}{2}}\sin\theta_m\left(b_m + b_m^+\right). \end{aligned}\right\} \tag{3}$$

The quantization axis is chosen to be parallel to the magnetic field (for a general system of coordinates, θ_m denotes the angles between the spin S_m and the external magnetic field).

The assumption that the electron spin is parallel to the magnetic field is justified for crystals with a wide conduction band W » AS/2 provided the energy of the electron spin in a magnetic field $-\mu H$ exceeds the shift in the electron energy due to the lattice deformation stimulated by the spin moment, 'This condition is clearly equivalent to the condition under which the external magnetic field can be regarded as quantizing. Passing in Eqs. (1) and (3) from the operators of spin deviation (2) to the representation of the magnon creation and annihilation operators ζ^+ and ζ and using the Bogolyubov-Tyablikov canonical transformation

$$b_m = \sum_q \left(u_{mq}\zeta_q + u_{mq}^*\zeta_q^+\right) \tag{4}$$

which diagonalizes the quadratic form H_M, we obtain the following expression instead of Eq. (1):

$$\left.\begin{aligned} H &= H_e + H_{\text{int}}^{(1)} + H_{\text{int}}^{(2)} + H_M^{(1)}, \\ H_{\text{int}}^{(1)} &= \sum_q C_q e^{iqr}\left(\zeta_{1q} + \zeta_{1(-q)}^+\right), \\ H_M^{(1)} &= \sum_q \hbar\omega_{1q}\zeta_{1q}^+\zeta_{1q} + \sum_q \hbar\omega_{2q}\zeta_{2q}^+\zeta_{2q}. \end{aligned}\right\} \tag{5}$$

Here, ω_{1q} and ω_{2q} correspond to two different branches in the elementary excitation spectrum of an antiferromag-net. The form of the Hamiltonian $H^{(2)}_{\text{int}'}$ quadratic in the magnon operators can be found in the Appendix. In the long-wavelength limit ($q\to 0$), we obtain

$$\left.\begin{aligned} \hbar\omega_{1q} &= J\frac{(qa)}{2S}\sqrt{1-h^2} + O\left(q^3a^3\right), \\ \hbar\omega_{2q} &= Jh/S + O\left(q^2a^2\right), \\ C_q &= \frac{A}{4\sqrt{2}}\sqrt{\frac{S}{N}}(qa)^{1/2}\left(1-h^2\right)^{1/4} + O(qa), \end{aligned}\right\} \tag{6}$$

where $h = H/H_{sf}$, where H_{sf} is the spin flopping field of (he sub-lattices; $J= ZIS^2$; Z is the number of nearest neighbors) a is the lattice constant. Consequently, the part of the transformed Hamiltonian $H^{(1)}_{\text{int}}$ which is linear in the magnon operators describes only the Interaction of an electron with the acoustic branch of the excitations in the antiferromagnet. The electron interaction with the optical branch appears only in the terms quadratic in the operators ζ^+ and ζ in the transformed Hamiltonian. The explicit form and importance of such terms in the cases considered below are discussed in the Appendix.

2. PARTICLE ENERGY AND MASS FOR WEAK COUPLING

Summarizing the results of Sec. 1, we can write the total Hamiltonian describing electron motion in an antifer-romagnet subjected to a magnetic field in the form

$$H = \frac{1}{2m^*}\left(\mathrm{p} + \frac{e}{c}\mathrm{A}\right)^2 + \sum_q C_q e^{iqr}\left(\zeta_q + \zeta_{-q}^+\right) + \sum_q \hbar\omega_q \zeta_q^+ \zeta_q, \tag{7}$$

where ω_q and C_q are defined by Eq. (6), where, according to the results of Sec. 1, $\zeta_q \equiv \zeta_{1q}$. We shall now consider the case T=0 when the modification of the spectrum due to the interaction with "acoustic" magnons is small and can be regarded as a perturbation. Since Eq. (7) has the standard "polaron" form, we can conveniently use the we known results of perturbation theory. In the second order of perturbation theory, the electron energy is given by:

$$\varepsilon_{\alpha\alpha''}^{(2)} = \sum_{\alpha'} \frac{\left(H_{\mathrm{int}}\right)_{\alpha\alpha'}\left(H_{\mathrm{int}}\right)_{\alpha'\alpha''}}{\varepsilon_\alpha^{(0)} - \varepsilon_{\alpha'}^{(0)}} \tag{8}$$

The index α in Eq. (8) labels the electron eigenfunctions in a magnetic field and it includes the quantum num-bars n, k_z, and k_y, where n is the number of a Landau level and k_z and k_y are the components of the electron momentum in the corresponding directions (we use the gauge $A_x = 0$, $A_v = Hx$, and $A_Z = 0$). The matrix elements

$$I_{\alpha\alpha'}(q) = \int \Psi_\alpha^{(0)}(r) e^{iqr} \Psi_\alpha^{(0)}(r) dr \tag{9}$$

which appear in Eq. (8) evaluated with respect to the wave functions of Landau oscillators are given by

$$\left|I_{\alpha\alpha'}\right| = \delta_{ky\alpha',ky\alpha+qy}\delta_{kz\alpha',kz\alpha+qz}\left(\frac{1}{n!\,n'!}\right)^{1/2} \times \exp\left(-\frac{q_\perp^2\rho_0^2}{4}\right)\left(\frac{q_\perp^2\rho_0^2}{2}\right)^{\frac{|n'-n|}{2}} L_n^{|n'-n|}\left(\frac{q_\perp^2\rho_0^2}{2}\right), \tag{10}$$

where $q_\perp^2 = q_x^2 + q_y^2$; $L_n^{|n'-n|}$ is a generalized Laguerre polynomial; and $\rho_0 = \sqrt{2\mu_B c\hbar / eH}$.

To evaluate the spectrum in the vicinity of the bottom of the conduction band in a quantizing magnetic field, we can restrict ourselves to the approximation of the first Landau band (n = n' = 0). In this case, Eqs. (8) and (9) yield the following expression for the electron energy:

$$\varepsilon_{kz}^{(2)} = \sum_q \frac{C_q^2 e^{-\rho_0^2 q_\perp^2/2}}{\varepsilon_{kz} - \varepsilon_{kz+qz} - \omega_q}, \tag{11}$$

where the summation with respect to q is carried out over the first Brillouin zone (π/a, π/a, π/a). Expanding the expression (10) in powers of k in the neighborhood of k = 0 and carrying out the corresponding Integrations, we obtain the following expression for the electron energy is the continuum limit (ρ_0/a » 1):

$$E_{kz} = \varepsilon_{kz}^{(0)} + \varepsilon_{kz}^{(2)} = \frac{\hbar\Omega}{2} - \mu H + \Delta E_0 + \frac{\hbar^2 k_z^2}{2m^{**}} + \ldots, \tag{12}$$

$$\Delta E_0 = -\frac{\sqrt{1-h^2}}{32\pi^2}\frac{A^2 S m^* a^2}{\hbar^2}\left(\frac{a}{\rho_0}\right)^2 \ln\left(1 + \frac{\pi S^2 \hbar^2 m^* a^2}{J\sqrt{1-h^2}}\right),$$

$$m^{**} = m^* / \left[1 - \frac{S^3}{4\pi^2} \frac{A^2}{J^2} \frac{1}{\sqrt{1-h^2}} \left(\frac{a}{\rho_0} \right)^2 \right]. \tag{13}$$

It follows from Eq. (11) that ΔE_0 represents the shi in the electron energy due to a deformation of the spin system and m^{**} is the effective mass of a particle which system along simultaneously with the spin deformation it stimulates.

If perturbation theory is applicable, the renormalized effective mass m^{**} should differ only slightly from the effective mass of a "bare" electron m^*:

$$\left(m^{**} - m^*\right) m^* << 1. \tag{14}$$

Taking into account Eq. (13), the inequality (14) can be interpreted as a criterion for the magnetic field strength which the weak-coupling approximation holds:

$$\left.\begin{array}{c} h << h_{1,} \\ h_1 \left[1 + \dfrac{S^5}{32\pi^4} \dfrac{A^4}{J^4} \left(\dfrac{a}{\rho_{0C}} \right)^4 \right]^{-1/2}, \qquad \rho_{0C} = \sqrt{h}\rho_0, \end{array}\right\} \tag{15}$$

where ρ_{0C} represents a critical magnetic length for which spin flopping of antiferromagnetic sublattices occurs.

3. PARTICLE ENERGY AND MASS FOR STRONG COUPLING

A self-consistent method of treatment of strong interactions of particles with a quantum field taking into account the translation degeneracy of the Hamiltonian (7) was developed by Bogolyubov and Tyablikov[4-6] on the basis of the adiabatic approximation. In the limit of adiabatic coupling, the magnon frequencies are low and, therefore, we can set $\hbar\omega_q = \varepsilon^2 \nu_q$, where ε is a small parameter. In the zeroth approximation with respect to ε, the Hamiltonian (7) yields the following functional which determines the electron energy and the electron part of the wave function $\Psi(r)$:

$$F[q'] = \frac{1}{2m^*} \int \Psi^* \left(\mathrm{p} + \frac{e}{c} \mathrm{A} \right)^2 \Psi d\tau - \frac{1}{2} \sum_q \frac{C_q^2 \nu_q \left| \int \Psi^* e^{iqr} \Psi d\tau \right|^2}{\nu_q^2 - (\hbar \mathrm{q} C)^2}, \tag{16}$$

where $C = v/\varepsilon^2$ and н is the velocity of the particle. Submitting Eq. (6) in Eq. (16) and setting $v = 0$, we obtain from Eq. (16)

$$F[q'] = \frac{1}{2m^*} \int \Psi^* \left(\mathrm{p} + \frac{e}{c} \mathrm{A} \right)^2 \Psi d\tau - \frac{\widetilde{A}^2}{8L} \int |\Psi|^4 d\tau. \tag{17}$$

The functional (17) is the same as the functional derived in Ref. 1 in a quasiclassical study of spins in a crystal.

Following Refs. 5 and 6, we obtain an expression for the longitudinal effective mass ($v = v_Z$):

$$m^{**} = \frac{\hbar^2}{\varepsilon^4} \sum_q \frac{C_q^2 q_\tau^2}{2\nu_q^3} \left| \int \Psi^* e^{iqr} \Psi d\tau \right|^2. \tag{18}$$

In the approximation of the first Landau band, using the wave functions corresponding to the ground state of the functional (16)

$$q_0' = \frac{1}{\sqrt{4\pi r_z \rho_0^2}} \exp\left\{-\rho^2 / 4\rho_0^2\right\} \mathrm{ch}^{-1}\left(z / r_z\right),$$

$$r_z = \frac{\hbar^2}{2m^*} 8\pi\rho_0^2 \frac{8L}{\widetilde{A}^2}, \qquad L = J / 2a^3, \qquad \widetilde{A} = AS / 2,$$

be obtain the following expression for the matrix elements which appear in Eq. (18):

$$\left| \int \Psi^* e^{iqr} \Psi d\tau \right| = e^{-\rho_0^2 q_\perp^2 2} \frac{\pi q_z r_z}{2\mathrm{sh}\left(\frac{\pi q_z r_z}{2}\right)}. \tag{19}$$

Replacing summation in Eq. (18) by Integration and using Eq. (19), we obtain an effective mass in the following form:

$$m^{**} = \frac{\hbar^2}{15\pi} \left(\frac{a^3}{\rho_0^2 r_z}\right) \frac{A^2 S^4}{J^3 a^2 \left(1 - h^2\right)} \frac{\rho_0^2}{r_z^2} \ln \frac{r_z^2}{\rho_0^2} + \vartheta\left(\rho_0^2 / r_z^2\right). \tag{20}$$

Equation (20) implies that the effective mass of a particle increases with increasing magnetic field. Because of our assumption of strong coupling of the particle to the field, the effective mass m^{**} of the particle should be much greater than the initial mass of a free particle

$$m^{**} >> m^*. \tag{21}$$

In particular, using the values of parameters employed in Ref. 1 in the calculation of self-localized states, i.e., $AS/2 \approx 0.5$ eV, $J \approx 0.5 \cdot 10^{-2}$ eV, $H_{sf} \approx 10^6$ Oe, $H \approx 0.5 \cdot 10^6$ Oe, and $a \approx 3$A, we find that the effective mass evaluated from Eq. (20) is $m^{**} \approx 10m^*$. Making use of Eq. (20), we can reformulate the criterion (21) in the following form:

$$h >> h_2$$

$$h_2 = \left[1 + \frac{S^5}{6(16\pi)^2} \frac{A^4}{J^4} \left(\frac{a}{\rho_{0e}}\right)^4\right]^{-1/2}. \tag{22}$$

Hence, as expected, the criterion of strong coupling derived from the condition (21) is opposite to the criterion of weak coupling [see the inequality (I5)]. Comparing the conditions (22) and (15), we note that, since $h_1 < h_2$, it is natural to regard the range of magnetic fields

$$h_1 < h < h_2 \tag{23}$$

as corresponding to intermediate coupling of an electron to the magnetic lattice of a crystal.

4. DISCUSSION OF RESULTS

Our results determine the conditions under which electrons in an antiferromagnetic crystal subjected to a quantizing magnetic field become self-localized. In particular, it is shown that, for an external field within a certain range defined by Eq. (23), electrons undergo a transition from a delocalized state to a self-localized state. The transition to a self-localized state is accompanied by an increase in the effective mass of carriers which can exceed the mass of an electron in a delocalized state by several orders of magnitude. As a result, an increase in the longitudinal magnetoresistance of the crystal with increasing magnetic field should be observable [if the increase in the mass as a function of the magnetic field

strength obeys the dependence (20) up to H = H_{sf}, the crystal should undergo a transition from a conducting state to an insulating state, since m** $\to \infty$]. For H > H_{sf}, in addition to the spin flopping of sublattices in the antiferromagnet, electron transition from a self-localized to a delocalized state also occurs: this results in a sharp reduction in the magnetoresistance (reverse transition from an insulating to a conducting state should take place in the limit $H_{LOC} \to H_{sf}$). This discussion is clearly purely qualitative and a rigorous analysis should be based on a calculation of the carrier mobility. This would require further study.

APPENDIX

We shall discuss the contribution to the ground state energy of the terms in the interaction Hamiltonian quadratic in the spin deviation operators. Using Eq. (4) for the part of the interaction Hamiltonian quadratic in the magnon operators, we obtain

$$H_{\text{int}}^{(2)} = \sum_{q,q',j} e^{i(q+q')r}\left[A_{qq'j}\zeta_{-q'}^{+}\zeta_{-q'j} + \frac{1}{2} B_{qq'j}\left(\zeta_{-qj}^{+}\zeta_{-q'j}^{+} + \zeta_{qj}\zeta_{q'j}\right)\right], \tag{A.1}$$

where j = 1, 2 corresponds to the acoustic and optical branches of the spectrum. In the long-wave length limit, we find that

$$\left.\begin{aligned} &A_{qq'1} = -B_{qq'1} = -Ah\sqrt{1-h^2}\,/\,2Na(qq')^{1/2}, \\ &A_{qq'2} \equiv A_2 = -A(1-h^2)4N, \quad B_{qq'2} \equiv B_2 = -A(1-h^2)4N. \end{aligned}\right\} \tag{A.2}$$

We shall show that, in the weak-coupling limit (A $\to$ 0), the contribution of the Hamiltonian defined by Eqs. (A.1) and (A.2) to the electron energy is proportional to A^3, i.e., it is of higher order in the email parameter than the contribution of the linear terms (12). We shall first write the chain of equations of motion for the Green functions of the electron operators a^+ and a:

$$\begin{aligned} E\left\langle\left\langle a_{k'}a_k^+\right\rangle\right\rangle &= \frac{i}{2\pi}\delta_{kk'} + \sum_{k''} T_{k'k''}\left\langle\left\langle a_{k'}a_k^+\right\rangle\right\rangle + \sum_q \widetilde{C}_q\left\langle\left\langle \zeta_q a_{k'}a_k^+\right\rangle\right\rangle + \sum_q \widetilde{C}_q\left\langle\left\langle \zeta_{-q}^{+} a_{k'}a_k^+\right\rangle\right\rangle + \\ &+ \sum_{q,q',j} B_{qq'j}\left\langle\left\langle \zeta_{qj}\zeta_{q'j}a_{k'}a_k^+\right\rangle\right\rangle + \sum_{q,q',j} B_{qq'j}\left\langle\left\langle \zeta_{-qj}^{+}\zeta_{-q'j}^{+}a_{k'}a_k^+\right\rangle\right\rangle + \sum_{q,\dot{q}} \widetilde{A}_{qq'j}\left\langle\left\langle \zeta_{-qj}^{+}\zeta_{-q'j}a_{k'}a_k^+\right\rangle\right\rangle. \end{aligned} \tag{A.3}$$

Carrying out the following decoupling:

$$\left\langle\left\langle \zeta_{-qj}^{+}\zeta_{-q'j}a_{k'}a_k^+\right\rangle\right\rangle \approx \delta_{qq'}\left\langle \zeta_q^{+}\zeta_q\right\rangle\left\langle\left\langle a_{k'}a_k^+\right\rangle\right\rangle,$$

in Eq. (A.3), we find that the contribution of the quadratic terms in the weak-coupling limit is proportional to A $(\zeta^{+}\zeta)$, where $(\zeta^{+}\zeta)$ are the average occupation numbers of magnons. In the absence of the electron-magnon interaction, $(\zeta^{+}\zeta)$ = 0 at T = 0. For a nonzero interaction, the average occupation numbers of magnons are nonzero. However, it is easy to verify that, in the limit A $\to$ 0, $(\zeta^{+}\zeta) \propto A^2$ holds and, therefore, the total contribution of the quadratic terms to the energy is proportional to A^3.

To estimate the contribution of $H^{(2)}{}_{\text{ist}}$ in the strong coupling limit, we shall transform Eq. (A.1) introduce complex field coordinates by

$$\left.\begin{aligned} &\zeta_q^{+} = \frac{1}{\sqrt{2}}\left(\frac{1}{\varepsilon}Q_{-q} - i\varepsilon P_q\right), \quad \zeta_q = \frac{1}{\sqrt{2}}\left(\frac{1}{\varepsilon}Q_q - i\varepsilon P_{-q}\right), \\ &P_q = -i\partial\partial Q_q, \qquad Q_q^{+} = Q_{-q}, \qquad P_q^{+} = P_{-q}. \end{aligned}\right\}$$

Substituting Eq. (A.4) in Eq. (A.1), we obtain

$$H_{\text{int}}^{(2)} = \varepsilon^2 \sum_{q,q'} A_{qq'1} e^{i(q+q')r} P_{-q1} P_{-q'1} + \sum_{q,q'} e^{i(q+q')r} \left[\frac{A_2 + B_2}{2\varepsilon^2} Q_{q^2} Q_{q'2} + \frac{\varepsilon^2}{2} (A_2 - B_2) P_{-q} P_{-q'2} \right].$$

It follows from Eq. (A.4) that the acoustic part of the Hamiltonian $H^{(2)}_{\text{ist}}$ contains only the field moment P_{q1} and, in the zero approximation in e, it does not modify the ground state energy (17). The part of $H^{(2)}_{\text{ist}}$, which includes the optical coordinates Q_{q2} together with $H^{(1)}_{\text{M}}$ forms a quadratic form which has a single minimum $Q_{q2} \equiv 0$ and also yields a zero contribution to the ground state energy. The operators of the field moment which appear in Eq. (A.5) should, in general, contribute to the effective mass defined by Eq. (18), but it follows from Eq. (19) that this contribution is $0(N^{-1})$.

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