New type of self-localized state of a conduction electron in an antiferromagnetic crystal subjected to a strong magnetic field

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It is well known that rather stringent conditions restrict the possibility of self-localized electron states in crystals with magnetic ordering (the Heisenberg exchange integral must be small and the constant describing the s-f exchange of an electron with magnetic atoms should be large) and, therefore, such states can occur only in crystals with low Neel temperatures. [1]

The situation is quite different if an electron moves in an antiferromagnet subjected to a strong external magnetic field H which does not exceed the critical field H_c for the spin flop of the antiferromagnetic sublattices (typical values of H_c are of the order 10^6-10^7 Oe). Even small deviations of the spins of magnetic atoms due to the interaction with conduction electrons can then lead to a localized electron state. In fact, this situation is analogous to the case studied in Ref. 2 where it was found that con-denson-type states in a covalent crystal which have normally high energies can occur in strong magnetic fields.

We shall consider a conduction electron in a cubic antiferromagnetic crystal in a strong external magnetic field. The electron interaction with the spins of magnetic atoms will be described within the s-f model and it is assumed that the conduction band width W is large compared with the s-f exchange energy AS/2. In the continuum approximation (i. e., if all the characteristic dimensions of the problem are much greater than the lattice constant), the directions of the atomic magnetic moments are distributed continuously and the total energy functional has the

$$F = E_e + E_M, \tag{1}$$

$$E_e = \frac{\hbar^2}{2m}\int \Psi^*\left(\mathrm{p} + \frac{e}{c}\mathrm{A}\right)^2 \Psi d\tau - \widetilde{A}\int \cos\varphi |\Psi|^2 d\tau, \tag{2}$$

where $\widetilde{A}$ = AS/2; **A** is the vector potential of the magnetic field; and φ is the angle between the magnetic field and the atomic magnetic moment. For an antiferromagnet with two equivalent sublattices at T= 0, the total energy of the mutual exchange interaction of magnetic atoms and of their interaction with the external magnetic field H is given by

$$E_M = L\int \cos 2\varphi\, d\tau - \overline{H}\int \cos\varphi\, d\tau. \tag{3}$$

Here, L= J/2a^3; J= Z|I|S^2; I is the exchange integral; Z is the number of nearest neighbors; S is the spin of a magnetic atom; *a* is the lattice constant; and H= HS/a^3 (H is the magnetic field in energy units).

The ground state of the whole system can be determined from the condition that the functional (l)-(3) reaches its minimum and will be evaluated by a variational method. The trial parameters in Eqs. (l)-(3) are the angle φ and the electron wave function Ψ.

The minimization of the functional (l)-(3) with respect to φ yields the following condition:

$$\cos\varphi = \frac{\widetilde{A}}{4L}|\Psi|^2 + \frac{\widetilde{H}}{4L}. \tag{4}$$

Equation (4) determines the maximum value of the external magnetic field such that $\varphi < 1$. We shall denote this field H_{loc}. It follows from Eq. (4) that the local field H_{loc} is always weaker than the field corresponding to the spin flop H_c (H_c= 27/S). We shall restrict ourselves to fields[1)] $H < H_{loc}$.

Substituting Eq. (4) in Eqs. (l)-(3), we obtain the following functional:

$$F = \frac{\hbar^2}{2m}\int \Psi^*\left(\mathrm{p} + \frac{e}{c}\mathrm{A}\right)^2 \Psi d\tau - \frac{\widetilde{A}^2}{8L}\int|\Psi|^4 d\tau - \frac{\widetilde{A}\widetilde{H}}{4L}\int|\Psi|^2 d\tau. \tag{5}$$

[The functional (5) does not include terms corresponding to the energy of a crystal without electrons.] The functional (5) was studied in Ref. 2. Following Ref. 2, we shall seek the wave function Ψ in the form

$$\Psi - \frac{1}{\sqrt{2\pi\rho_0^2}}\exp\left\{-\frac{\rho^2}{4\rho_0^2}\right\}\chi(z), \qquad \rho_0 = \sqrt{\frac{2\mu_B c\hbar}{eH}}, \tag{6}$$

which corresponds to the approximation of the first Landau band. Substituting Eq. (6) in Eq. (5) and minimizing the resulting functional with respect to χ(z) (bearing in mind that the function χ is normalized), we obtain the for χ(z):

$$\frac{\hbar^2}{2m}\frac{d^2\chi}{dz^2} + \frac{\widetilde{A}^2}{8L}\frac{1}{2\pi\rho_0^2}\chi^3 + \left(E_e + \frac{\widetilde{A}\widetilde{H}}{4L}\right)\chi = 0, \tag{7}$$

where E_e is the electron energy. The localized solution χ(z) Is given by

$$\left.\begin{aligned} \chi(z) &= \pm\left(\sqrt{2r_z}\cosh\frac{z-z_0}{r_z}\right)^{-1}, \\ E_e &= -\frac{\hbar^2}{2mr_z^2} - \frac{\widetilde{A}\widetilde{H}}{4L}, \quad r_z = \frac{\hbar^2}{2m}8\pi\rho_0^2\frac{8Z}{\widetilde{A}^2}, \end{aligned}\right\} \tag{8}$$

where z_0 is an arbitrary constant and r_z is the radius of the localized state. It follows that the net energy gain due to the creation of a localized state is equal to 1/3 |Δ E|, where $\Delta E = -\hbar^2/2mr_z^2$. Substituting the wave function defined by Eqs. (6) and (8) in Eq. (4) and setting φ = 1, we obtain the following value of the local field:

$$H_{\mathrm{loc}} = 32\pi^2\gamma^3 JS\left[\sqrt{1 + \frac{1}{8\pi^2\gamma^3 S^2}} - 1\right], \quad \gamma = \frac{\hbar^2}{m_0 a^2 \widetilde{A}}\left(\frac{m_0}{m}\right)^{1/3}, \tag{9}$$

where m_0 is the free-electron mass. It follows from Eq. (9) that, for most crystals, the value of H_{loc} is of the same order as the spin flop field H_c of the antiferromagnetic sublattices.

We shall obtain numerical estimates for the following values of the parameters: m= m_0, $\widetilde{A} \approx 0.5$ eV, J ≈ $0.5 \cdot 10^{-2}$ eV, and $a \approx 3$ A. We then find that, for the magnetic field strength

$H \approx 5 \cdot 10^5$ Oe ($H_c \approx 10^6$ Oe), the electron energy is $E^*_e = h^2/2mr^2_z \approx 0.7 \cdot 10^{-3}$ eV and the characteristic radius of the localization region is $r_z \approx 7 \cdot 10^{-7}$ cm. The characteristic length $p_0 = \sqrt{2}\,\mu_B c\hbar/eH$ is then $p_0 \approx 3.5 \cdot 10^{-7}$ cm. It follows that the continuum approximation is applicable for these parameters. On the other hand, we find that, for the above dimensions of the localization region r_z and magnetic lengths p_o, the condition $(p_0/r_z)^2 \ll 1$ holds and we can neglect the corrections due to higher Landau bands. [2] The local magnetic field H_{loc} then differs by less than 1% from the critical field H_c ($H_{loc}/H_c \approx 0.99$). It follows from Eq. (8) that $r_z \sim H_c$ and, therefore, the continuum approximation becomes more accurate for crystals with high Neel temperatures but, in this case, the energy gain due to the electron localization is reduced ($E^* \propto H^{-2}_c$).

[1)] For $H_C > H > H_{loc}$, there is a region where the atomic spins are aligned, i. e., $\varphi = 0$, and the diameter of such a region represents an additional trial parameter. When the field is increased, the diameter of such a region also increases and tends to infinity for $H \to H_C$.

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