New type of self-localization state of carriers in an antiferromagnetic semiconductor

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A self-localization of charge carriers can occur in antiferromagnetic semiconductors with high Néel temperatures in which different antiferromagnetic structures have approximately equal energies. This localization occurs in a microscopic region with a skewed antiferromagnetic order of a type different from that of the rest of the crystal.

The problem of high-T_c superconductivity has again attracted much interest to self-localization states of charge carriers in antiferromagnetic semiconductors. Three types of these states have been proposed. 1. de Gennes[1] has proposed a model in which a carrier is trapped by a single magnetic atom, whose spin is tilted away from the moment of the sublattice to which this atom belongs. 2. In the ferron model proposed in Ref. 2, a carrier creates a ferromagnetic microregion within an antiferromagnetic crystal and stabilizes this region by localizing in it. 3. A quasioscillator model was proposed in Ref. 3. In this model, which has come to be known as the "magnetic string" model, an electron or hole oscillates about an equilibrium position in the crystal, creating an antiphase antiferromagnetic order as it moves along its trajectory and then annihilating this order in its return motion.

The de Gennes model clearly could not work for realistic parameter values, as was shown in Ref. 4. A string could be realized only in systems in which the magnetic atoms have a spin $S = 1/2$ and very narrow carrier energy bands. Ferrons are possible in crystals with low Néel temperatures T_N, and this is indeed where they have been observed experimentally.[4] They could not exist at high Néel temperatures.

We show below that there is yet another type of self-localization carrier state in an antiferromagnetic semiconductor. It could be realized at high T_N's and at values of other parameters for which a ferron or string would be impossible. On the other hand, there are some necessary conditions: The energy of the stable antiferromagnetic structure must be close to the energy of the unstable antiferromagnetic structure, and the energy of the carrier in the unstable structure must be lower than that in the stable structure. A microscopic region of a normally unstable antiferromagnetic phase could then form within the stable antiferromagnetic phase, being stabilized by the self-localization of a carrier in itself. There would be a further lowering of the energy of this self-localization state because of a skewness of the moments of the sublattices within the carrier localization region, although the magnetization of such a quasiparticle would be vastly smaller than that of a ferron. We will call this quasiparticle an "afmon."

In the s–d model, the energy of a carrier is given by the following expression[4] when there is a skewed antiferromagnetic order with a structure vector $\vec{Q}$ and an angle 2φ between the moments of the sublattices:

$$\tilde{E}_{\vec{k}} = \frac{1}{2}\{E_{\vec{k}} + E_{\vec{k}+\vec{Q}} - [(E_{\vec{k}} - E_{\vec{k}+\vec{Q}} - AS\cos\varphi)^2 + A^2S^2\sin^2\varphi]^{1/2}\}, \quad (1)$$

$$E_{\vec{k}} = 2B\sum_i^d \cos k_i a, \quad m = (2|B|a^2)^{-1}, \quad (\hbar = 1), \quad (2)$$

where a is the lattice constant of a simple square lattice ($d = 2$) or a simple cubic lattice ($d = 3$), and A is the s–d exchange integral. For concrete estimates, we take the seed energy of the carrier in (2) in the nearest-neighbor approximation. Expression (1) holds if the spins of the magnetic atoms of magnitude S can be treated as fixed. We can do this not only as $S \to \infty$ but also at $|A|S \ll W = 12|B|$.

According to (1) and (2), the minimum carrier energy in a checkerboard structure ($Q_i = \pi/a$ for all i) is higher than in layered structure ($Q_1 = \pi/a$, with $Q_i = 0$ for all other values of i). Assuming $W = |A| = 3$ eV for an estimate (this figure corresponds to a carrier mass close to the actual mass of an electron), we find that the difference between these energies in the absence of a skewness ($2\varphi = \pi$) is extremely significant: 0.29 eV in $d = 2$ and 0.46 eV in $d = 3$.

To estimate the difference in the energies per atom, D_{LN}, of the layered and checkerboard structures which would permit the existence of an afmon, it is sufficient to use the results of Ref. 4 for $d = 3$ and those of Ref. 5 for $d = 2$. According to those results, a heterophase self-localization of charge carriers would be possible inside a region of altered phase, which constitutes a potential well of depth $U \ll W$, would be possible if the energy expended on the formation of this phase, D, satisfies the inequality

$$D/W \leq D_c/W = 0.2(4 - d)(U/W)^{1+d/2}. \quad (3)$$

For a ferron we would have $U \approx AS/2$, while for an afmon we would have $U_{LN} = (d+1)A^2S^2/8W$ under the conditions $AS \ll W$, according to (1) and (2). According to (3), the ratio of the critical values D^c_{LN} for an afmon and D^c_{FN} for a ferron with $AS/2W = 1/3$ reaches 0.25 in $d = 2$ and 0.35 in $d = 3$. The requirement that the energies of the Landau and Néel structures be approximately the same thus turns out to be not very restrictive in practice. It is relaxed even further when we note that the afmon energy is lowered by the skewness of the sublattice moments of the layered phase.

To take this skewness into account here, we use a variational method. We assume that a carrier is localized in a square ($d = 2$) or a cube ($d = 3$) of side L, and we assume that the wave function of this carrier vanishes at the boundaries of the region. Using (1) and (2), we then see that the optimum parameters of the afmon should be found by minimizing the following expression for the quasiparticle energy with respect to L and φ:

$$E_A = d\pi^2/2mL^2 - \frac{AS}{2}\cos\varphi - (3A^2S^2/4W)[\sin^2\varphi - 1/d] + (L/a)^d D_{LN}(\varphi), \quad (4)$$

$$D_{LN} = \{-(2d-1)J_1 + 2J_2(d-1) - [J_1 + 2(d-1)J_2]\cos 2\varphi$$

$$+ 4(d-2)J_3(1 - cos2\varphi)\}S^2.$$

Here J_i are the integrals of the d–d exchange between the neighbors which come ith in terms of nearness. From the Néel condition for stability of the structure we have $J_1 < 2J_2$ and $J_1 > 4J_3$.

At small values of $l = S^2(2J_2 - J_1)$, we find the following expression for the magnetization of the afmon:

$$\cos\varphi = K_d l^{d/d+2},$$

$$K_2 = 2^{1/2}\{(16J_1S^2/AS)^2(\pi^2/a^2m) - 4|J_1|S^2\}^{-1/2},$$

$$K_3 = (AS/8|3J_1 + 4J_3|S^2(4ma^2/\pi^2)^{3/5}. \quad (5)$$

According to (5), the magnetization of an afmon per atom vanishes as the $l = 0$ phase boundary is approached. This vanishing is a consequence of the divergence of the dimension L as $l \to 0$: $l \sim L^{-1/4}$ in the two-dimensional case and $L \sim l^{-1/5}$ in the three-dimensional case. Correspondingly, the molecular field of the carrier which is acting on the d spins vanishes. The total moment of the antiferron, however, remains nonzero at the phase boundary.

Interestingly, the existence of a solution in the $d = 2$ case, i.e., a real value of the magnetization in (5), is guaranteed by the inequality which is the opposite of (3) for a ferron. An afmon could thus be realized only when a ferron could not. This assertion has not previously been made in the three-dimensional case.

A self-localization of a charge carrier is also possible in the case of a helicoidal order in a crystal. The helicoid vector must be relatively low in the localization region, since a relatively low value lowers the energy of the carrier. A detailed calculation will be reported elsewhere.

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