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Instability of the homogeneous state in dilute ferromagnetic semiconductors

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Abstract

We consider the stability of the homogeneous magnetically ordered state in dilute ferromagnetic semiconductors, with Ruderman-Kittel-Kasuya-Yosida indirect exchange. It is shown that when the electron (hole) polarization exceeds some critical value, the maximum of the indirect exchange shifts to a nonzero wave-vector promoting a state with charge and spin modulation. The modulated state becomes stable, when the carriers are almost fully polarized.

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Dilute ferromagnetic semiconductors (DMS) are investigated extensively during the last decade, after the discovery of ferromagnetism in III-V and II-VI Mn-based compounds.

This effort is motivated by both their unique physical properties and by their potential application in spintronics, see, e.g., the review [1]. The exchange interaction between localized spins in DMS is mediated by the carriers. The Curie temperature T_c increases with the increase of the carrier concentration. E.g., T_c in $Ga_{1-x}Mn_xAs$, with $x = 0.053$ reaches 100 K at hole concentration 3.5×10^{20} cm^{-3} [1].

We have shown in previous papers [2] and [3] that the magnetically ordered state in such systems is unstable. At a temperature T_0, $T_0 < T_c$, the

system enters into a state in which both the carrier density and the magnetization are modulated, the modulation scale being fixed by the Coulomb screening of the carriers and the their Fermi wave-vector. We argued that at T_0 the carriers are almost polarized, while the mean value of the local spin, $\langle S_z \rangle$ is small. An external magnetic field, which aligns the localized spins, suppresses the modulated phase.

The possibility of an inhomogeneous equilibrium state in DMS was rediscovered recently by C. Timm [4]. Unlike Refs. [2] and [3], he starts from a Landau-type model for *non-polarized* carriers, with a magnetization depending on the electron concentration, and derived T_0, which appeared to be close to T_c: $(T_c - T_0)/T_c \ll 1$.

In this paper we consider the transition into the modulated state at any degree of the carrier polarization, and show that polarization of the carries is a necessary condition for the stabilization of the inhomogeneous state.

The Hamiltonian of the $s-d$ model is

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} - 2J \sum_i \mathbf{S}_i \cdot \mathbf{s}_i + \mathcal{H}_C, \tag{1}$$

where $c^{\dagger}_{\mathbf{k},\sigma}(c_{\mathbf{k},\sigma})$ is the creation (annihilation) operator for a carrier with spin σ, $\epsilon_{\mathbf{k}} = \hbar^2 k^2/2m$ is the electron (hole) kinetic energy, $\mathbf{S}_i$ is the spin, localized at the lattice site i, $\mathbf{s}_i$ is the carrier spin, and $\mathcal{H}_C$ is the Coulomb interaction between the carriers. We suppose that the $s-d$ coupling J satisfies the inequalities $\epsilon_F \ll J \ll W$, where ϵ_F is the carrier Fermi energy, and W is the width of the carriers band. In DMS J is of the order of 1 eV, and therefore these inequalities are always fulfilled.

From the Hamiltonian (1) the indirect Ruderman- Kittel-Kasuya-Yosida (RKKY) exchange between localized spins follows to the second order in J/W:

$$\mathcal{H}_S = -\frac{J^2}{2} \sum_{ij} \chi(ij) \mathbf{S}_i \cdot \mathbf{S}_j, \tag{2}$$

where $\chi(ij)$ is the carrier susceptibility. We have

$$\chi(\mathbf{q}) = \sum_{\mathbf{p}} \frac{f(\mathbf{p}+\mathbf{q}) - f(\mathbf{p})}{\epsilon(\mathbf{p}) - \epsilon(\mathbf{p}+\mathbf{q})} \tag{3}$$

for non-polarized carriers, i.e. in the paramagnetic phase, and [2, 5]

$$\chi(\mathbf{q}) = \frac{\Pi_{\uparrow}(\mathbf{q}) + \Pi_{\downarrow}(\mathbf{q}) + 4U(q)\Pi_{\uparrow}(\mathbf{q})\Pi_{\downarrow}(\mathbf{q})}{1 + U(q)\Pi_{\uparrow}(\mathbf{q})\Pi_{\downarrow}(\mathbf{q})} \tag{4}$$

for carriers in the ferromagnetic phase, with a finite degree of polarization.

Here $f(\mathbf{p})$ is the Fermi distribution function, Π_σ is given by the sum in the r.h.s. of Eq. (3) with f and ϵ replaced by f_σ and ϵ_σ, $\sigma = \uparrow, \downarrow$, and $U(q) = 4\pi/\varepsilon q^2$ is the carrier-carrier interaction energy, ε being the dielectric constant. We suppose that the carrier concentration is much smaller than the concentration of localized spins, as in the above example of manganese doped gallium arsenide. This guarantees that the RKKY exchange is ferromagnetic.

The correlation function of the localized spins coupled by the interaction (2) is [2, 6]

$$K(\mathbf{q}) = \frac{Tb'}{T - b'J^2x\chi(\mathbf{q})}. \tag{5}$$

Here x is the concentration per unit cell of the localized spins, $b(y)$ is the Brillouin function, $y = h/T$, where h is the molecular field acting on the localized spins: $h = J(n_\uparrow - n_\downarrow)$, n_σ is the number of carriers with spin σ per a localized spin, while $n_\uparrow + n_\downarrow = n$. $b'(y) = db/dy$. Note that at $x = 1$, i.e. for an ordered crystal, Eq. (5) coincides with the equation for $K(\mathbf{q})$ given in Ref. [2].

At small y the function $b(y)$ is

$$b(y) = ay - \frac{cy^3}{3}, \quad a = \frac{S(S+1)}{3}, \; c = \frac{3}{5}a^2 + \frac{a}{10}. \tag{6}$$

It follows from Eqs. (5), (6), and (3) that $K(q)$ diverges at

$$T = T_c = \frac{S(S+1)}{3}J^2x\mathcal{N}(\epsilon_F), \tag{7}$$

where $\mathcal{N}$ is the carrier density of states, $\mathcal{N} = 3n/2\epsilon_F$, the Fermi energy is $\epsilon_F = \hbar^2k_F^2/2m$, $k_f = (3\pi^2n^2/\Omega)^{1/3}$, and Ω is the unit cell volume.

At temperatures lower than T_c the carriers became polarized, and the susceptibility is given by Eq. (4). It appears (see below) that at some critical degree of polarization the function $\chi(q)$ has a maximum at a finite $q = q_0$, and the correlation function K diverges at some $T = T_0$ lower than T_c, i.e. the ferromagnet enters into an inhomogeneous state with typical modulation vector q_0.

To find T_0 and q_0 the following equations should be solved simultaneously:

$$\frac{\partial\chi(q,b)}{\partial q} = 0, \tag{8}$$

$$T_0 = J^2xb'(y)\chi(q_0, b(y)), \tag{9}$$

$$y = \frac{1}{T}\sum_q [f(\epsilon_k - Jb(y)) - f(\epsilon_k + Jb(y))], \tag{10}$$

with $b(y)$ given by Eq. (6) and χ given by Eq. 4.

The solution of Eq. (8) shows that the susceptibility reaches its maximum at $q = 0$ in the temperature interval $T^* < T < T_c$, where T^* is given by the equation

$$\frac{\mathcal{N}_\uparrow - \mathcal{N}_\downarrow}{\mathcal{N}_\uparrow + \mathcal{N}_\downarrow} = \frac{\sqrt{3}\kappa}{6k_F}, \tag{11}$$

where $\mathcal{N}_\sigma$ is the density of states of carriers with spin σ, κ is the inverse screening length, $\kappa^2 = 4\pi e^2 \mathcal{N}/\varepsilon\Omega$. We assume that the Coulomb interaction is weak, and hence the screening range is large, i.e. $\kappa \ll k_F$.

Thus, the inhomogeneous state can appear only at $T < T^*$. In the vicinity of T^*, when the carrier polarization is small, q_0 and $\chi(q_0)$ are given by

$$\begin{aligned} q_0^2 &= 6k_F^2\Big[\frac{(\mathcal{N}_\uparrow - \mathcal{N}_\downarrow)^2}{\mathcal{N}^2} - \frac{\kappa^2}{12k_F^2}\Big] \\ \chi(q_0) &= \chi(0)\Big[1 + \frac{q_0^4}{12k_F^2\kappa^2}\Big], \end{aligned} \tag{12}$$

where $\chi(0)$ is

$$\chi(0) = \frac{4\mathcal{N}_\uparrow\mathcal{N}_\downarrow}{\mathcal{N}_\uparrow + \mathcal{N}_\downarrow}. \tag{13}$$

This result shows that the possibility of phase separation in DMS is crucially related to the spin polarization of the carries neglected in Ref. [4]. The importance of the polarization is clear from the following physical arguments. In the inhomogeneous state the system gains energy, since the ferromagnetic correlations are enhanced in the carrier rich regions and suppressed in the carrier poor ones. But it looses energy, because of the spatial fluctuation of the carrier density. If the carriers are partially polarized, the fluctuation of the magnetization is accompanied by the redistribution of the number of carriers with spin up and down, and this reduces the loss of the energy related to the fluctuations of the full density of the carriers.

If the carrier polarization is not small, $|\mathcal{N}_\uparrow - \mathcal{N}_\downarrow|/(\mathcal{N}_\uparrow + \mathcal{N}_\downarrow) \approx 1$, the inhomogeneous scale is given by

$$q_0^2 = \frac{2\sqrt{3}\kappa|\mathcal{N}_\uparrow - \mathcal{N}_\downarrow|}{(\mathcal{N}_\uparrow + \mathcal{N}_\downarrow)^{1/2}}\Big(\frac{\mathcal{N}_\uparrow}{k_{F\uparrow}^2} + \frac{\mathcal{N}_\downarrow}{k_{F\downarrow}^2}\Big)^{-1/2}. \tag{14}$$

Here $k_{F\uparrow,\downarrow} = (6\pi^2 n_{\uparrow,\downarrow}/\Omega)^{1/3}$. One gets for fully polarized carriers, when $\mathcal{N}_\downarrow = 0$:

$$q_0^2 = 2\sqrt{3} k_{F\uparrow} \kappa \tag{15}$$

in agreement with the result obtained in Refs. [2] and [3].

It follows from Eqs. (12) and (15) that q_0 increases with the decrease of T and the increase of the carrier polarization, and reaches its maximum value for fully polarized carriers. According to Refs [2] and [3] this happens at τ of the order of 0.1.

To find the transition temperature T_0 into the inhomogeneous state Eqs. (9) and (10) should be solved. The analysis of these equations shows that they have no solution in the case of weak carrier polarization, even though at temperatures $T < T^*$ the maximum of $\chi(q)$ is at $q = q_0(T) \neq 0$. But when the carriers become polarized, and q_0 reaches its maximum value given by Eq. (15), a solution exists, the transition temperature T_0 being $T_0 = T_c/2^{2/3} + O(\kappa/k_F)$ [2, 3].

In conclusion, the transition into the inhomogeneous state in ferromagnetically ordered DMS was analyzed at arbitrary degree of carrier polarization. We showed that the maximum of the indirect exchange coupling between localized spins shifts from zero q to a finite q at some small but finite polarization of the carriers. However, the transition into the inhomogeneous state takes place only at lower temperatures, when the carriers are almost fully polarized.

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