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# Magnetic polarons in materials with colossal magnetoresistance

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## Abstract

We construct a phase diagram for the materials with colossal magnetoresistance. The basic model which describes these materials is a double-exchange model. We rigorously prove that a ground state of this model corresponds to a phase-separated state with small ferromagnetic polarons inside an antiferromagnetic matrix. The general picture of a percolative state, which emerges from our calculations, is in good agreement with recent experiments on doped manganites. © 2000 Elsevier Science B.V. All rights reserved.

*Keywords:* Colossal magnetoresistance; Double exchange; Strongly correlated electrons

Recent beautiful experiments on electron transport [1], NMR [2] and neutron scattering [3] strongly support a picture of phase-separated ground state in doped manganites. This state was also advocated in recent numerical investigations [4]. In the present paper we provide a coherent theoretical confirmation of this picture, proving that a polaronic phase-separated ground state corresponds to a global minimum of the energy in our system.

We consider the double-exchange model [5] with the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) - J_H \sum_i \mathbf{S}_i \sigma_i + J_{\text{ff}} \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j, \quad (1)$$

where  $J_H$  is the on-site FM exchange and  $J_{\text{ff}}$  is the AFM Heisenberg exchange. We work in the limit of large Hund's coupling:  $J_H S \gg zt \gg J_{\text{ff}} S^2$ .

We calculate at first an energy of homogeneous state as a function of the carrier's concentration  $x$ . We obtain that for  $x < x_{C1} = (8\pi^4/3)(J_{\text{ff}}(2S+1)^{3/2}/zt)^3$  a collinear AFM-state is realized [6,7].

For  $x_{C1} < x < x_{C2} \approx 13.5x_{C1}$  a quantum two-band canted state arises in the system [8], while for  $x_{C2} < x < x_{C3} = (8J_{\text{ff}}S\sqrt{2S+1})/t$  a quantum one-band canted state takes place [8]. For  $x > x_{C3}$  a quantum one-band canting transforms to a classical canting of De-Gennes type with an energy [5]:

$$E_{\text{clas.cant}} = -J_H \frac{S}{2} x - \frac{zt^2 x^2}{2J_{\text{ff}}} - \frac{z}{2} J_{\text{ff}} S^2. \quad (2)$$

Finally for  $x > x_{C4} = 2J_{\text{ff}} S^2/t$  a collinear FM state is realized in the system [5].

Let us now verify a homogeneous state on the instability towards phase separation. For  $x < x_{C1}$  the compressibility of the system  $\kappa^2 = d^2E/dx^2$  is positive. However for  $x_{C1} < x < x_{C4}$  the compressibility changes its sign and becomes negative. Especially simple is the expression for the compressibility for  $x_{C3} < x < x_{C4}$ , where a canted state becomes classical:

$$\kappa^2 = -\frac{zt^2}{J_{\text{ff}} S^2} < 0. \quad (3)$$

So, while collinear AFM and FM states at least correspond to a local minimum of an energy, a canted state is absolutely unstable. This fact reflects a tendency towards phase separation in the system. We can show that the most energetically beneficial phase-separated state corresponds to FM-polarons embedded into an

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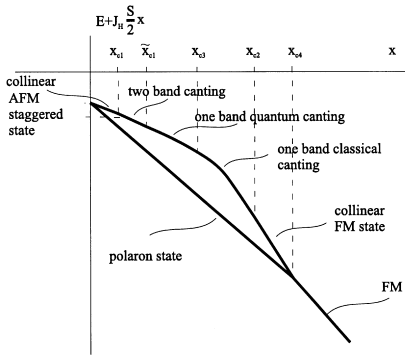


Fig. 1. Phase diagram of the double-exchange model.

AFM-matrix. To show this let us calculate an energy of a polaron state, assuming that each polaron is formed by one conduction electron localized inside a FM-bubble. A polaron energy for a spherical shape of a bubble reads [7–9]:

$$E_{\text{pol}} = -J_H \frac{S}{2} x - zt x + \frac{5\pi}{3} x (\pi t)^{3/5} (2zJ_{\text{ff}} S^2)^{2/5} - J_{\text{ff}} \frac{zS^2}{2}. \quad (4)$$

Note that in a layered situation FM-polarons have an ellipsoidal shape [10].

A direct comparison of the energies of a homogeneous state and a polaron state shows, that an energy of a polaron state corresponds to a global minimum of energy for all concentrations  $0 < x < x_{c5}$ . Note that at

$x = x_{c5} = 3/4\pi(a/R_{\text{pol}})^3 = 3/4\pi(2zJ_{\text{ff}} S^2/\pi t)^{3/5}$  the polarons start to overlap and all the sample becomes ferromagnetic. The resulting phase diagram of the double-exchange model is presented in Fig. 1.

In conclusion we have shown that the tendency towards a phase separation and a formation of a spatially inhomogeneous percolative state [11] is an inherent property of the double-exchange model.

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