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.

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

\begin{equation}
H = - t \sum_{\langle i,j \rangle} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) - J_H \sum_i S_i \sigma_i + J_H \sum_{\langle i,j \rangle} S_i S_j,
\end{equation}

where $J_H$ is the on-site FM exchange and $J_{\text{eff}}$ is the AFM Heisenberg exchange. We work in the limit of large Hund's coupling: $J_H S \gg z t \gg J_{\text{eff}} S^2$.

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

For $x_{C1} < x < x_{C2} \approx 13.5 x_{C1}$ a quantum two-band canted state arises in the system [8], while for $x_{C2} < x < x_{C3} = (8J_H S \sqrt{2S + 1}/zt)$ 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]:

\begin{equation}
E_{\text{cl-cant}} = - J_H \frac{S}{2} x - \frac{zt^2 x^2}{2J_{\text{eff}}} - \frac{z}{2} J_{\text{eff}} S^2.
\end{equation}

Finally for $x > x_{C4} = 2J_{\text{eff}} S^2/zt$ 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:

\begin{equation}
\kappa^2 = - \frac{zt^2}{J_{\text{eff}} S^2} < 0.
\end{equation}

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
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]:

\[
E_{\text{pol}} = -J_{tt} S x - ztx \\
+ \frac{5\pi}{3} x(\pi t)^{3/5}(2\pi J_{tt} S^2)^{2/5} - J_{tt} \frac{z S^2}{2}.
\]  

(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 \(0 < x < x_{CS}\). Note that at

\[x = x_{CS} = \frac{3}{4}\pi(a/R_{pol})^3 = \frac{3}{4}\pi(2\pi J_{tt} S^2/\pi t)^{3/5}\]

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.

Acknowledgements

M.Yu.K. acknowledges financial support from INTAS, grant 98-963 and RFBR, grant 98-02-17077.

References