University of Groningen

Magnetic polarons in materials with colossal magnetoresistance

Kagan, M.Y.; Mostovoy, M.V.; Khomskii, D.I

Published in:
Physica B: Condensed Matter

DOI:
[10.1016/S0921-4526\(99\)02666-6](https://doi.org/10.1016/S0921-4526(99)02666-6)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2000

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Kagan, M. Y., Mostovoy, M. V., & Khomskii, D. I. (2000). Magnetic polarons in materials with colossal magnetoresistance. *Physica B: Condensed Matter*, 284(35), 1209 - 1210. [https://doi.org/10.1016/S0921-4526\(99\)02666-6](https://doi.org/10.1016/S0921-4526(99)02666-6)

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Magnetic polarons in materials with colossal magnetoresistance

M.Yu. Kagan^{a,*}, M.V. Mostovoy^b, D.I. Khomskii^b

^a*P.L. Kapitza Institute for Physical Problems, Moscow 117334, Russia*

^b*University of Groningen, Nijenborgh 4, 9747 AG, Groningen, The Netherlands*

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_{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-banded state arises in the system [8], while for $x_{C2} < x < x_{C3} = (8J_{\text{ff}}S\sqrt{2S+1})/t$ a quantum one-banded canted state takes place [8]. For $x > x_{C3}$ a quantum one-banded 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

*Corresponding author.

E-mail address: kagan@kapitza.ras.ru (M.Yu. Kagan)

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]:

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

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.

Acknowledgements

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

References

- [1] N.A. Babushkina et al., Phys. Rev. B (1999), in press.
- [2] G. Allodi et al., Phys. Rev. B 56 (1997) 6036.
- [3] M. Hennion et al., Phys. Rev. Lett. 81 (1998) 1957.
- [4] S. Yunoki, J. Hu, A.L. Malvezzi, A. Moreo, N. Furukawa, E. Dagotto, Phys. Rev. Lett. 80 (1998) 845.
- [5] P.G. de Gennes, Phys. Rev. 118 (1960) 141.
- [6] J. Zaanen, A.M. Oles, P. Horsch, Phys. Rev. B 46 (1992) 5798.
- [7] E.L. Nagaev, Sov. Phys. Uspekhi 166 (1996) 833.
- [8] M.Yu. Kagan, D.I. Khomskii, M.V. Mostovoy, cond-mat/9804213.
- [9] T. Kasuya, A. Yanase, T. Takeda, Solid State Commun. 8 (1970) 1543.
- [10] M.Yu. Kagan et al., in preparation.
- [11] L.P. Gor'kov, V.Z. Kresin, JETP Lett. 67 (1998) 985.