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ScienceDirect
Journal of Magnetism and Magnetic Materials 320 (2008) e425–e427
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Ferromagnetic polarons in the one-dimensional double and super-exchange model

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Available online 23 February 2008

Abstract

We present an analytical and numerical study of the competition between double and super-exchange (SE) interactions with classical localized spins interacting with itinerant electrons in a one-dimensional (1D) model. A phase separation between ferromagnetic (F) and anti-ferromagnetic (AF) phases was found at low SE interaction energy. The F–AF phase separation consists of a large F polaron within an AF background. For large SE interaction energy, the conduction electrons are self-trapped within separate small magnetic polarons. These magnetic polarons contain a single electron inside two or three sites forming a Wigner crystal. A new phase separation is found between these small polarons and the AF phase.

PACS: 75.47.Lx; 75.30.Et; 75.10.Hk; 71.38.−k; 64.75.+g

Keywords: Manganites; Double and super-exchange model; Classical spin models; Polarons; Phase separation

1. Introduction

Magnetic ordering of localized spins mediated by non-magnetic conduction electrons, the so-called double exchange (DE), is the source of a variety of magnetic behavior in transition metal and rare-earth compounds [1]. Conversely this interplay affects the mobility of the carriers and may lead to interesting transport properties such as colossal magnetoresistance in manganites. The origin of the DE lies in the intra-atomic Hund's exchange coupling J_H of localized electrons with itinerant electrons and depends on the type of orbitals involved. Typically, the coupling is ferromagnetic (F) ($J_H > 0$), but it can be anti-ferromagnetic (AF) in more than half-filled shells [2]. The F tendency is expected to be thwarted by AF super-exchange (SE) interactions between localized spins S_i leading to interesting and unusual magnetic states [3]. This mechanism has been widely used in the context of manganites [2,4–6]. At low conduction electron density x, F polarons, the electron followed by an F local distortion, have been found for localized $S = \frac{1}{2}$ quantum spins [7]. "Island" phases, periodic arrangement of F polarons coupled anti-ferromagnetically, have been clearly identified at commensurate fillings both for quantum spins in one dimension [8] and for classical spins in two dimensions [9]. Phase separation and small F polarons have also been found for localized $S = \frac{3}{2}$ quantum spins [10]. It is of importance, therefore, to clarify the size of the polarons, and whether it is preferable to have island phases, separate small or eventually large polarons.

The DE Hamiltonian is originally of the form

$$H = -\sum_{i,j,\sigma} t_{ij}(c^{+}_{i\sigma}c_{j\sigma} + \text{h.c.}) - J_H \sum_i \vec{S}_i \cdot \vec{\sigma}_i. \quad (1)$$

$c_{i\sigma}{}^{+}(c_{i\sigma})$ are the creation (annihilation) operators of the conduction electrons at site i, t_{ij} is the hopping parameter. $\vec{\sigma}_i$ is the conduction band spin operator. This Hamiltonian simplifies in the strong coupling limit $J_H \to \infty$ (a limit commonly called itself the DE model), and for classical $S_i \to \infty$, localized spins. The complete DE + SE Hamiltonian in

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doi:10.1016/j.jmmm.2008.02.076

1D becomes $t_{ij} = t$:

$$H = \sum_i \left(-t \cos \frac{\theta_i}{2} c_i^+ c_{i+1} + \text{h.c.} \right) + J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}. \qquad (2)$$

Because of Hund's limit, electrons are indeed spinless electrons. In Eq. (2), θ_i, represents a relative angle between the classical localized spins at sites i and $i+1$. J corresponds to the SE energy.

The magnetic phase diagram was obtained at $T = 0$ K by using open boundary conditions on a linear chain of $N = 24$ sites. For a given conduction electron density x ($0 \leqslant x \leqslant 0.5$ because of the hole–electron symmetry) and an SE interaction energy J, 23 angles in the linear chain had to be optimized. For this goal, an analytical optimization [11] and a classical Monte Carlo method were used. The analytical solution was tested as a starting point in the Monte Carlo simulation.

2. Results and discussion

The most important result of this work is given in Fig. 1, where the magnetic phase diagram is presented.

Fig. 1 shows that when the SE interaction energy is small $JS^2/t \lesssim 0.12$, the F phase for a large conduction electron density and the AF phase for $x = 0$ can be found. The F–AF transition is given by the F–AF phase separation (AF + F in Fig. 1) consisting of one large F polaron within an AF background as can be seen in Figs. 2 and 3, for a typical value of $JS^2/t = 0.08$. All electrons are inside the polaron. The position of the polaron within the linear chain is not important because of translation degeneracy. These figures also show the charge distribution, n, inside the polaron and a spin configuration snapshot. In this region, the polarons' size diminishes with the conduction electron density (Figs. 2 and 3).

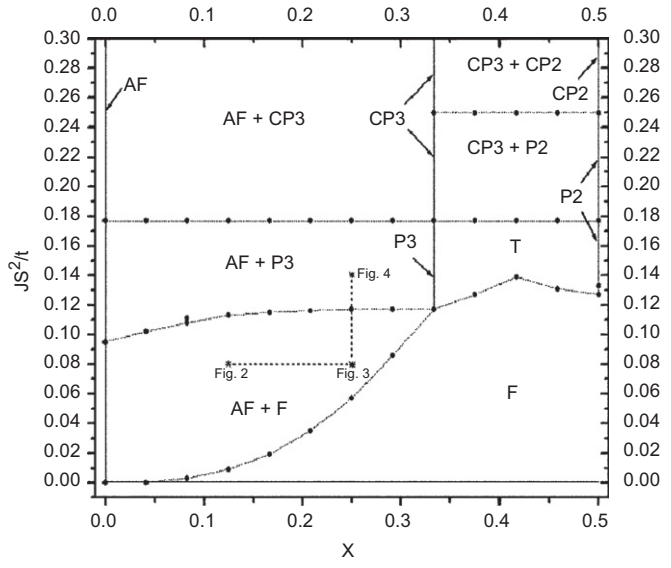

Fig. 1. Magnetic phase diagram as a function of the SE energy J and the conduction electron density x. A dotted line in this diagram represents a guide for the eyes. The different phases are described in the text.

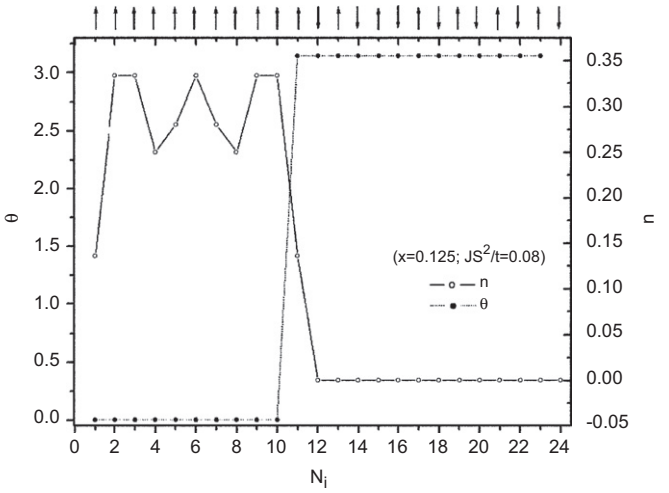

Fig. 2. AF + F phase at $x = 0.125$ (3 electrons) and $JS^2/t = 0.08$, showing 23 angles, charge distribution "n" in N_i sites and the spin configuration snapshot.

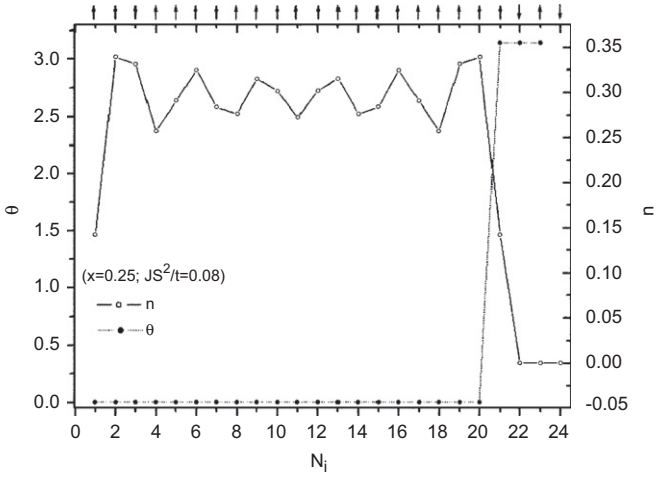

Fig. 3. The same as in Fig. 2, but at $x = 0.25$ (6 electrons).

For small SE interaction $JS^2/t \lesssim 0.09$, the F–AF phase separation has been reported in two dimensions [12], in one dimension by using classical localized spins and $J_H = 8$ [13] and in the one-dimensional (1D) F Kondo model [14]. Quantum results for $S = \frac{3}{2}$ show phase separation when Coulomb repulsion was taken into account [10]. In this limit, our results are in contradiction with the "spin-induced Peierls instability" mechanism proposed in Ref. [15].

If the SE interaction energy increases $0.12 \lesssim JS^2/t \lesssim 0.17$, electrons are self-trapped in small independent F polarons of two ($x = 0.5$) or three sites ($x \leq \frac{1}{3}$) forming a Wigner crystal. For instance, phases P2 and P3 consist of F polarons of two sites (P2≡$\cdots \uparrow \uparrow \downarrow \downarrow \uparrow \uparrow \downarrow \downarrow \cdots$) and three sites (P3≡$\cdots \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \cdots$ coupled AF. These "island" phases have been clearly identified by García et al. [8] for $x = 0.5$ and for $x = \frac{1}{3}$, respectively, by using quantum $S = \frac{1}{2}$ spins. In Ref. [13],

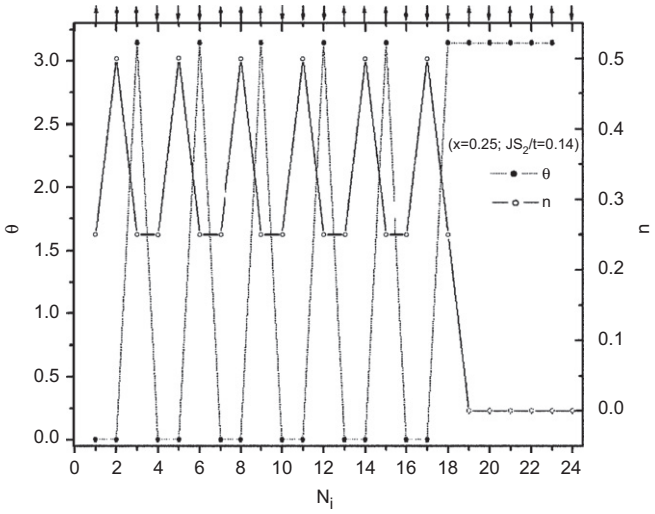

Fig. 4. AF + P3 phase at $x = 0.25$ (6 electrons) and $JS^2/t = 0.14$, showing 23 angles, charge distribution "n" in N_i sites and the spin configuration snapshot.

instead of P2 phase for $x = 0.5$, a spiral phase was proposed. In Fig. 1, a new phase separation between P3 and AF phases was found. This phase separation is formed by the P3 phase in an AF background, and is degenerate to a phase where: (a) the polarons can be ordered or not (due to translation and rotation degeneracy), or (b) to the phase obtained within the "spin-induced Peierls instability" [15]. A phase like AF + P3 was identified using $S = \frac{3}{2}$ quantum spins [10]. Fig. 4 shows the AF + P3 phase for a typical value of the SE interaction energy $JS^2/t = 0.14$.

The T phase in Fig. 1 is a general phase obtained by the Monte Carlo method and can be polaronic like or not. We found that the F → AF + F → AF + P3 transition is of first order. More details will be published elsewhere [16].

In Fig. 1, the line at $JS^2/t = 1/(4\sqrt{2}) \approx 0.176$ represents in general a second order transition. The full F character of the three-site polarons is unstable causing the apparition of two angles; we call this phase CP3 (canted P3 phase). An analytical exact degeneracy was found for this phase given by the following degeneracy condition:

$$\cos(\theta_1) + \cos(\theta_2) = \frac{1}{8(JS^2/t)^2} - 2, \tag{3}$$

where θ_1 and θ_2 are the angles inside the three-site polaron. The F character of the two-site polaron in the P2 phase is stable until $JS^2/t = 0.25$, above that limit, the F spins become canted and we call this phase CP2, see Fig. 1. In the SE interaction region $JS^2/t \geqslant 1/(4\sqrt{2})$, a new phase separation is identified between P2 and CP3 phases for $\frac{1}{3} \leq x \leq \frac{1}{2}$. We recovered the expected AF + CP3 phase separation for a low conduction electron density, $0 \leqslant x \leqslant \frac{1}{3}$. For $JS^2/t \geqslant 0.25$, we get P2 → CP2. The CP2 and CP3 phases evolve towards complete anti-ferromagnetism as $JS^2/t \to \infty$ (Eq. (3)). It is important to note that the size chosen for the linear chain ($N = 24$) and the boundary conditions do not change the nature of the phases involved in the phase diagram. The same phases are expected in the thermodynamic limit $N \to \infty$ and with periodic boundary conditions.

3. Conclusions

The complete phase diagram in one dimension of the DE + SE model was determined as a function of the SE interaction energy J and the conduction electron density x, using large Hund's energy and large localized spin parameters. The quantum results already published [7,8,10] were recovered and two types of phase separation were found. A phase separation between F and AF phases is obtained for low SE interaction energy. In the limit of large SE interaction we obtain a new phase separation between small polarons (one electron within a magnetic distortion of two or three sites) and AF regions. In the large SE limit a Wigner crystal and a spin-glass behavior can be identified. The analytical continuous degeneracy for this new phase Eq. (3) can be related to the spin-glass behavior in the nickelate compound $Y_{2-x}Ca_xBaNiO_5$ [15].

Acknowledgments

We want to acknowledge partial support from PAPIIT-IN108907-3, UNAM. E.V. would also like to thank CONACyT and DGAPA-UNAM for a postdoctoral fellowship.

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