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Double and super-exchange model in one-dimensional systems

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ABSTRACT

We present an analytical and numerical study of the competition between double and super-exchange interactions in a one-dimensional model. For low super-exchange interaction energy we find phase separation between ferromagnetic and anti-ferromagnetic phases. When the super-exchange interaction energy gets larger, the conduction electrons are self-trapped within separate small magnetic polarons. These magnetic polarons contain a single electron inside two or three sites depending on the conduction electron density and form a Wigner crystallization. A new phase separation is found between these small polarons and the anti-ferromagnetic phase. Spin-glass behavior is obtained consistent with experimental results of the nickelate one-dimensional compound $Y_{2-x}Ca_xBaNiO_5$.

1. Introduction

The double exchange (DE) or indirect exchange interaction is the source of a variety of magnetic behavior in transition metal and rare-earth compounds. DE has been widely used in the context of manganites [1–4]. The origin of the DE interaction lies in the intra-atomic coupling of the spin of the itinerant electrons with localized spins $\vec{S}_i$. In this coupling, localized and itinerant electrons belong to the same atomic shell. According to Hund's rule, the coupling is ferromagnetic (F) when the local spins have less than half-filled shells and anti-ferromagnetic (AF) for more than half-filled shells [2]. Independently of the sign of the coupling, the "kinetic" energy lowering, favors a F background of local spins. This F tendency is expected to be thwarted by AF super-exchange (SE) interactions between localized spins $\vec{S}_i$ as first discussed by de Gennes [5] who conjectured the existence of canted states. In spite of recent interesting advances, our knowledge of magnetic ordering resulting from this competition is still incomplete.

Although it may look academic, the one-dimensional (1D) version of this model is very illustrative and helpful in building an unifying picture. On the other hand, the number of pertinent real 1D systems as the nickelate one-dimensional metal oxide carrier-doped compound $Y_{2-x}Ca_xBaNiO_5$ [6] is increasing. In this compound, carriers are essentially constrained to move parallel to NiO chains. Spin-glass-like behavior was found at low temperature. Recently, it has been shown that three-leg ladders in the oxyborate system Fe_3BO_5 may provide evidence for the existence of spin and charge ordering resulting from DE and SE competition [7].

Naturally, the strength of the magnetic interactions depends significantly on the conduction band filling, x. At low conduction electron density, F polarons have been found for localized $S=\frac{1}{2}$ quantum spins [8]. F polarons in an AF background were also found in 2D [9]. "Island" phases, periodic arrangement of F polarons coupled anti-ferromagnetically, have been clearly identified at commensurate fillings both for quantum spins in one dimension [10] and for classical spins in one [11] and two dimensions [12]. Phase separation between hole-undoped anti-ferromagnetic and hole-rich ferromagnetic domains has been obtained in the Ferromagnetic Kondo model [13,14]. Phase separation and small ferromagnetic polarons have been also identified for localized $S=\frac{3}{2}$ quantum spins [15]. Therefore, it is of importance to clarify the size of the polarons, and whether it is preferable to have island phases, separate small polarons or eventually large polarons.

In this paper, we present an analytical and numerical study of the one-dimensional double and super-exchange model. Our results allow a straightforward explanation of the spin-glass-like behavior, which has been experimentally observed in the nickelate one-dimensional compound $Y_{2-x}Ca_xBaNiO_5$ [6]. The paper is organized as follows. In Section 2 a brief description of the model together with our results and a discussion are presented. Finally, conclusions are given in Section 3.

2. The model, results and discussion

Our one-dimensional double and super-exchange model will be described by the following Hamiltonian:

$$H=-t\sum_i \cos\left(\frac{\theta_{i,i+1}}{2}\right)(c_i^+c_{i+1}+h.c.)+JS^2\sum_i \cos(\theta_{i,i+1}),$$

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where t is the hopping parameter and $\theta_{i,i+1}$ is a relative angle between classical localized spins, $S \to \infty$, at sites i and $i+1$. $c_i^+(c_i)$ are the fermion creation (annihilation) operators of the conduction electrons at site i. A strong Hund's coupling limit is used in this work, $J_H \to \infty$. Because of this limit electrons are indeed spinless electrons. This part of the Hamiltonian represents the DE interaction [2]. On the other hand, J is the super-exchange interaction energy.

We determine the complete phase diagram of this model in one dimension as a function of the super-exchange interaction energy J and the conduction electron density x by using open boundary conditions on a linear chain of $N = 60$ sites (Fig. 1). For a given conduction electron density x ($0 \leqslant x \leqslant 0.5$ because of the hole-electron symmetry), we have to optimize all the $(N-1)$ angles $\theta_{i,i+1}$. For this goal, we use an analytical optimization and a classical Monte Carlo method. The analytical solution has been tested as a starting point in the Monte Carlo simulation. Besides the quantum results already published [8,10,15] we find two types of phase separation. In addition to the expected F–AF phase separation (AF + F in Fig. 1) appearing for small J consisting of one large ferromagnetic polaron within an AF background (all electrons are inside the ferromagnetic polaron) we obtain a new phase separation between small polarons (one electron within two or three sites, i.e. AF+P3) and AF regions at larger J. It is interesting to note that large polarons are never found stable in this limit. Above F phase for the commensurate fillings $x = \frac{1}{2}$ and $\frac{1}{3}$, we recover the "island" phases P2 (Fig. 2) ($\cdots\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\cdots$) and P3 (Fig. 3) ($\cdots\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\cdots$) identified previously for classical [11] and $S = \frac{1}{2}$ quantum [10] local spins. The electrons are self-trapped in small independent F polarons of two and three sites, respectively, each polaron contains one electron, forming in this way a Wigner crystallization see Figs. 2 and 3. In Ref. [16], a spiral phase has been proposed instead of the P2 phase for $x = \frac{1}{2}$. The ferromagnetic phase is stable for weak SE interaction below P2 phase, P2 phase becomes stable for $(2/\pi) - \frac{1}{2} < JS^2/t < \frac{1}{4}$.

For $JS^2/t > \frac{1}{4}$, P2 transforms into a canted phase CP2 in which the angle inside the F islands becomes finite (θ_1) while the angle between the polarons (θ_2) still keeps the value π. A complete analytical solution can be derived in this case. Similar phases P3 and CP3 are obtained for $x = \frac{1}{3}$. In CP3, two angles θ_1, θ_2 are finite inside the polaron while $\theta_3 = \pi$; this phase has a continuous degeneracy within each 3-site polaron given by the condition,

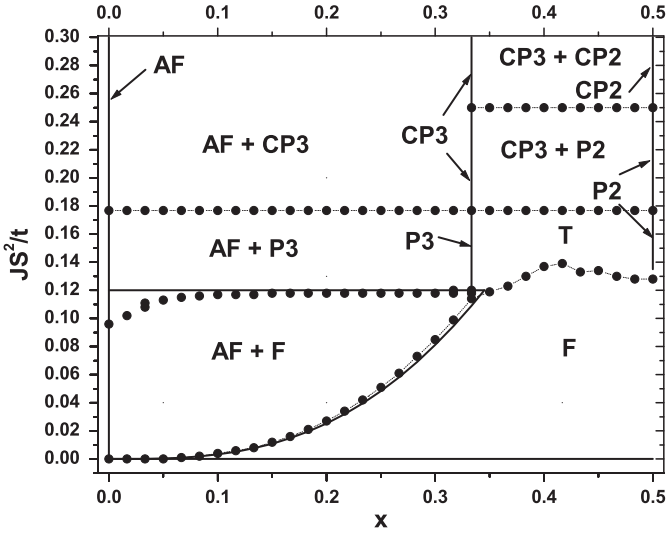

Fig. 1. Magnetic phase diagram as a function of the SE interaction energy J and the conduction electron density x. A dotted line in this diagram represents a guide for the eyes. The different phases are described in the text.

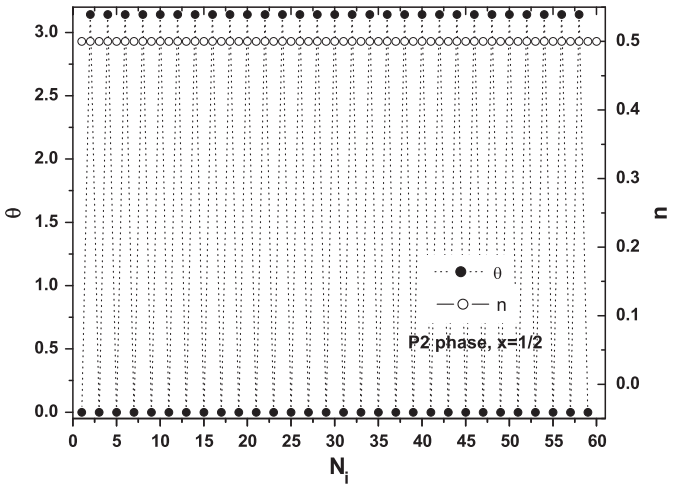

Fig. 2. P2 phase for $x = \frac{1}{2}$, showing $N-1$ angles θ and charge distribution n. Angles in this figure are 0 or π exactly.

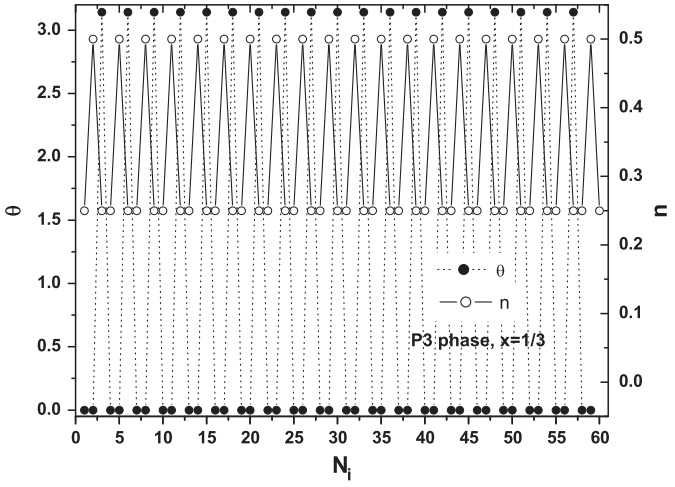

Fig. 3. P3 phase for $x = \frac{1}{3}$, showing the same as in Fig. 2.

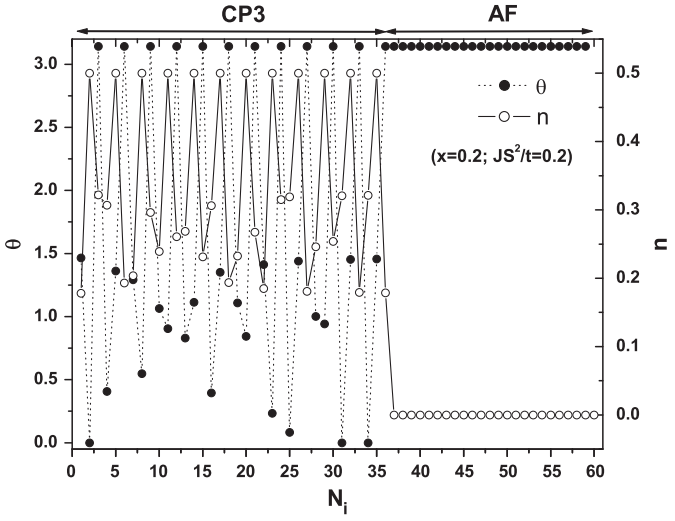

Fig. 4. AF + CP3 phase at $x = 0.20$ (12 electrons) and $JS^2/t = 0.20$. $N-1$ angles and charge distribution are presented.

$\cos(\theta_1)+\cos(\theta_2)=(1/8(JS^2/t)^2)-2$ see Fig. 4. Both CP2 and CP3 evolve towards complete anti-ferromagnetism as $JS^2/t\to\infty$. P3 $\to$ CP3 at $JS^2/t=1/4\sqrt{2}$. These phases result from the "spin-induced Peierls $2k_F$ instability" due to the modulation of the hopping with $I=1/x$ angles. For lower commensurate fillings $x<\frac{1}{3}$, such PI polaron phases are not found stable. Instead, above the F phase at low J we find AF–F phase separation. Of course, an anti-ferromagnetic phase always occurs at $x=0$.

Fig. 1 shows that when the SE interaction energy is small $JS^2/t\lesssim 0.12$, the F phase occurs for a large conduction electron density. At lower density, we obtain F–AF phase separation; the analytical optimization implies angles 0 and π exactly for the F and AF domains, respectively. For small SE interaction, the F–AF phase separation has been reported in two dimensions [17], in one dimension using classical localized spins and $J_H=8$ [16] and in the one-dimensional ferromagnetic Kondo model [14]. Quantum results for $S=\frac{3}{2}$, show phase separation when Coulomb repulsion was taken into account [15]. We can see that in this limit, our results differ from those of Koshibae et al. [11] within the "spin-induced Peierls instability" mechanism. At low concentration $x<\frac{1}{3}$, if the SE interaction energy increases $0.12\lesssim JS^2/t\lesssim 0.17$, we find a new phase separation between P3 and AF phases which transforms into AF + CP3 for $JS^2/t\gtrsim 0.17$ as P3 $\to$ CP3. Both phase separations are degenerate with respect to the position of the individual polarons while keeping the number of F and AF bonds fixed; the phase obtained within the "spin-induced Peierls instability" [11] belongs to this class. A phase like AF + P3 has been identified using $S=\frac{3}{2}$ quantum spins [15].

Phase separation also takes place for incommensurate fillings between $x=\frac{1}{2}$ and $\frac{1}{3}$ for SE interactions $JS^2/t\geqslant 1/4\sqrt{2}$. It is between CP3 and P2 or CP2 due to the canting inside the P2 polaron with increasing J. The transition between the two occurs for $JS^2/t=0.25$, where P2 $\to$ CP2.

Below CP3 + P2, the phase labeled T in Fig. 1 is a more general complex phase obtained by the Monte Carlo method and can be polaronic like or not. Of course, all the phase separations involving CP3 (AF + CP3, CP3 + P2, CP3 + CP2) present the spin configuration degeneracy (θ_1,θ_2) of the CP3 phase. This is clearly observed in Fig. 4 for the case of AF + CP3. This analytical continuous degeneracy in the spin configuration can be related to the spin-glass behavior as, for example, in the nickelate compound $Y_{2-x}Ca_xBaNiO_5$ [6]. It is interesting to note that such a possibility of ferromagnetic polarons immersed into an anti-ferromagnetic background has been invoked by Xu et al. [18] to fit their neutron data.

3. Conclusions

In this work we presented a unifying view for the magnetic phase diagram of the one-dimensional DE + SE model using large Hund's energy and classical localized spins. The solution is in general (a) phase separation between F and AF phases for low SE interaction energy and (b) phase separation between small polaronic and AF phases when the SE interaction is large. In this large SE limit a Wigner crystallization and a spin-glass behavior can be identified. We believe that the ground state of the nickelate one-dimensional compound $Y_{2-x}Ca_xBaNiO_5$ belongs to the phase, AF + CP3, providing a plausible explanation for the spin-glass-like behavior observed at low temperature.

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