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Analysis of Spin-polaron Formation in Hund Lattices

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We consider a one-dimensional Hund lattice model where a conducting band is coupled with localized spins $s = 1/2$ interacting antiferromagnetically, with coupling constant J, and investigate the ground state phase diagram as a function of both the exchange coupling J and the band filling, n. From spin structure factor measurements we found different evolving magnetic orderings in the ground state related to the particle distribution in the systems, although no charge density waves are formed, as found from density-density correlation function measurements. We study the quasi-particle formation and phase separation using the density-matrix renormalization group method, which is a highly efficient method to investigate quasi-one-dimensional strongly correlated systems.

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I. INTRODUCTION

The ferromagnetic Kondo lattice model, also known as Hund lattice model, is a well-established model to study the interplay between charge and spin degrees of freedom in strongly correlated fermionic systems such as transition-metal oxides. Examples of these materials are manganese oxides, nickelates and cuprates whose electronic, magnetic and transport properties have displayed interesting physics including giant or colossal magnetoresistance [1], multiferroicity [2] and high-temperature superconductivity [3]. Their properties as well depend strongly on the doping of the materials leading to formation of magnetically ordered regimes [4]. In our work, we consider a one-dimensional Hund lattice model where a conducting band is coupled with localized spins $s = 1/2$ interacting antiferromagnetically with coupling constant J. Even though the zero-temperature physics of such lattice model has been intensively studied under several selections of parameters [5–7], its phase diagram remains an open field. We investigate the ground state magnetic ordering as a function of the super-exchange coupling J and as a function of the particle density n away from half-filling and report measurements of static properties such as charge and spin structure factor for which we use the density-matrix renormalization group method (DMRG) [8,9].

II. HUND LATTICE MODEL AND SUPER-EXCHANGE INTERACTIONS

We consider the one-dimensional Hund lattice model along with super-exchange interactions between localized spins with total Hamiltonian:

$$\hat{H} = -t\sum_{i,\sigma} c^{\dagger}_{i,\sigma}c_{i+1,\sigma} + h.c. - J_H \sum_i \vec{S}_i\cdot\vec{\sigma}_i + J\sum_i \vec{S}_i\cdot\vec{S}_{i+1}, \quad (1)$$

where $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator with spin σ ($=\uparrow,\downarrow$) at site i and $t = 1$ is the nearest neighbor hopping matrix, which will set our energy scale. $\vec{S}_i$ is the localized spin operator on site i and $\vec{\sigma}_i$ is the electron spin operator, see Fig. 1. The Hund and super-exchange coupling, $J_H > 0$ and $J \geq 0$, respectively, are given in units of t. Eq. (1) has served as a model to

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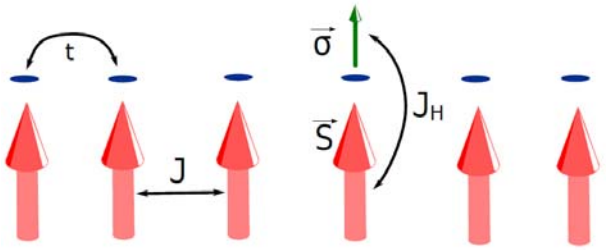

Fig. 1. (Color online) The Hund lattice model with antiferromagnetic interaction $J \geq 0$ between localized spins. The electrons in the conducting band are coupled ferromagnetically with the localized spins with coupling constant $J_H > 0$, which is the Hund coupling.

study, for example, diverse manganite compounds relevant due to their colossal magnetoresistance effect [10]. Because the Mn ions are placed in a crystalline environment of definite symmetry (a perovskite structure), their d orbitals, which in the free atom case are five fold degenerated, are no longer degenerate due to the effect of the crystal field which splits the d orbitals in three t_{2g} low-energy orbitals and two e_g high-energy state orbitals. Considering that in the case of manganites the d orbitals are not doubly-occupied, the t_{2g} orbitals generate a localized spin background of $\vec{S}_i$ with $S = 3/2$ in which electrons move in a linear combination of the two e_g orbitals obeying Hund's rule, which aligns electron spins ferromagnetically when they are on a $\vec{S}_i$ site. Electron mobility is then increased if the localized ions are ferromagnetically aligned or limited in an antiferromagnetic environment. Ordering in the charge sector has been found in close relation to the formation of magnetic structures [11]. Nevertheless, we have found an interval, in terms of the super-exchange coupling, for which no charge ordering is present yet spin structures are found. Measurement of ground-state properties is carried out using DMRG method, which is a very efficient method to handle an otherwise exponentially-increasing Hilbert space of a low-dimensional, many-body system [3,4]. We study a 24-site length chain with $J_H = 8t$ for different values of J and measure nearest-neighbor spin-spin correlation functions to investigate in detail the magnetic ordering away from the half-filled case. For the DMRG algorithm we set open boundary conditions and kept 512 matrix-density states, which rendered a maximum truncation error of approx. 10^{-6}.

III. SPIN-POLARON FORMATION

To investigate the ordering in the charge sector, we measured both the density-density correlation function $C(i, i_o)$, Eq. (2), and the charge structure factor $N(q)$, Eq. (3),

$$C(i, i_o) = \langle n_i n_{i_o} \rangle - \langle n_i \rangle \langle n_{i_o} \rangle, \tag{2}$$

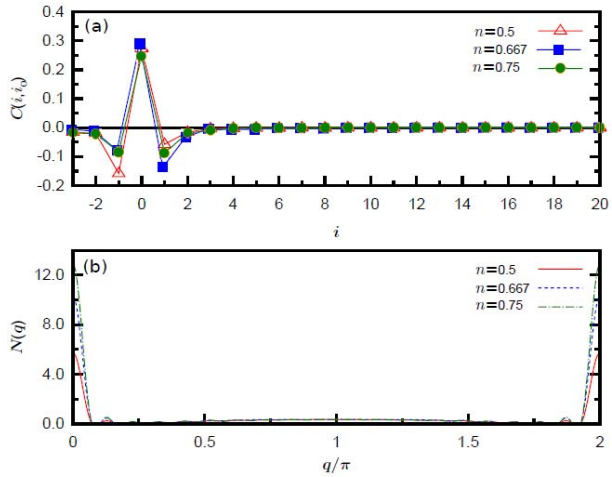

Fig. 2. (Color online) (a) Density-density correlation function $C(x, x_o)$, with $i_0 = 3$ and (b) Charge structure factor $N(q)$ as a function of the band-filling n and in both cases $J_H = 8.0$ and $J = 0.04$.

$$N(q) = \frac{1}{L} \sum_{i,j} e^{i(r_j - r_i)q} \langle\ n_i n_j\ \rangle, \tag{3}$$

where n_i refers to the on-site total number operator $n_i = n_{i,\downarrow} + n_{i,\uparrow}$. In Fig. 2(a) we show our results for $C(x, x_o)$ with super-exchange coupling $J/t = 0.04$ and for electronic densities away from half-filling. Such results hold also for $0 \leq J \leq 0.04$. From the density-density correlation function results as well as from the charge structure factor, see Fig. 2(b), we can rule out the formation of charge density waves for our systems. In fact, the charge sector remains independent of the interactions between the spins in the background of the system. Even though no charge ordering can be associated to the magnetic structures formation, we can see from Fig. 3 that, for particle densities above the quarter-filled case, the valleys in the charge oscillations, due to finite-size effects, can be related to the peaks in the spin-spin correlation function. In Fig. 4 we display in detail the results for the magnetic ordering at every position in the system, and in Fig. 5 we show our results for the static spin structure factor (SSF) S^{zz},

$$S^{zz}(q) = \frac{1}{L} \sum_{i,j} e^{i(r_j - r_i)q} \langle\ S_i^z S_j^z\ \rangle. \tag{4}$$

For low carrier concentrations the ground-state was found to be ferromagnetic in full agreement to the work by Sigrist *et al.* [12]. Furthermore, at quarter-filling, and for all the selected super-exchange coupling values, a uniform phase (both in the charge and spin sectors) of two-spin polarons antiferromagnetically aligned is observed also in agreement to previous reports [7]. In this case, the SSF, see Fig. 5(a), stabilizes quickly with increasing super-exchange coupling (the results for $J = 0.02, 0.04$ overlap) and peaks are found for commensurate values of

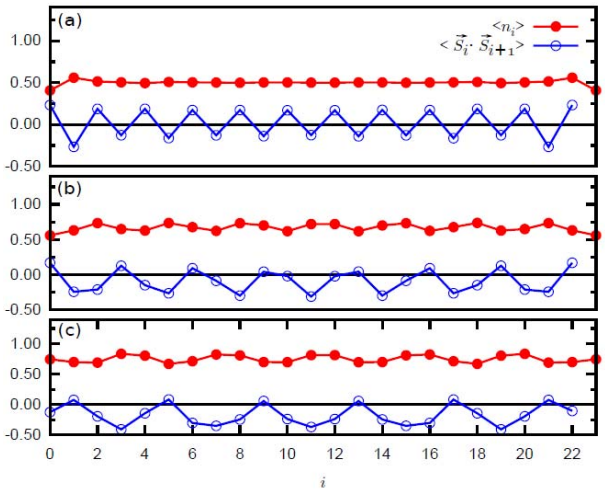

Fig. 3. (Color online) Particle density $< n_i >$ and nearest-neighbor spin-spin correlation function $< \vec{S}_i \cdot \vec{S_{i+1}} >$ with $J = 0.02$ for (a) $n = 0.5$, (b) $n = 0.667$ and (c) $n = 0.75$.

the momentum. For an electronic density of $n = 0.667$, the SSF, see Fig. 5(b) does not stabilize as quickly as in the former case and a gradual evolution of the magnetic order takes place with increasing J dividing the system in three sectors: a leftmost sector where two-spin polarons intercalate with single spins which align antiferromagnetically to the polarons, a middle sector where spin flips occur with changing J, and a rightmost sector similar to the first sector only the two-spin polarons are aligned in the other direction. The middle sector begins with a three-spins polaron and spin flips driven by J turn such sector in a completely antiferromagnetic one without altering the side sectors. In this case, and for $J = 0.02$, we found additional information, as compared to the results reported in [13], related to the rapid evolution of the magnetic structures and displayed in the form of peaks in the spin structure factor located at several incommensurate values of the momentum. For $J = 0$ and $J = 0.04$, we found peaks at $q = 0.667\pi$ and $q = 1.333\pi$. For a band-filling of $n = 0.75$, we found two different magnetic orderings: for $J = 0, 0.02$ a series of two-spin polarons alternate with pairs of antiparallel spins and the polarons themselves align antiferromagnetically to each other. Such phase displays SSF peaks at commensurate values of the momentum, for $q = 0.75\pi$ and $q = 1.25\pi$ (Fig. 5(c)). For a super-exchange coupling of $J = 0.04$, the spins order antiferromagnetically along the chain up to two-spin polarons right at the edges of the system and even though the ordering corresponds practically to an antiferromagnet, the peaks in the SSF indicate a phase other than the antiferromagnetic one, where the peaks deviate slightly from the commensurate value.

IV. FINAL REMARKS

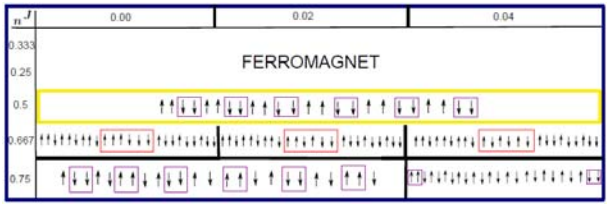

Fig. 4. (Color online) Magnetic ordering for the ground state of the model of Eq. (1) as a function of the band filling and the antiferromagnetic coupling J. Two- and three-spins polarons are found in these structures.

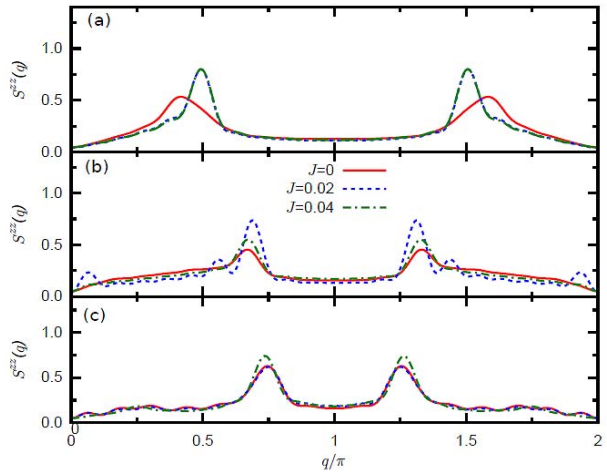

Fig. 5. (Color online) Spin structure factor for different values of the super-exchange coupling J and for (a) $n = 0.5$ (b) $n = 0.667$ and (c) $n = 0.75$. The phases found are further detailed in the text.

In this work we investigated the magnetic ordering in one-dimensional systems with a conduction band coupled to a spin background for which the ground-state phase diagram is not fully understood. Some key cases such as ferromagnetic and island phases, as reported in [5,7], were found. For the carrier concentration interval $0.5 < n < 1.0$ we observed the so called *island-like* and *spiral* phases with commensurate and incommensurate wave-vectors, respectively, as described by Garcia *et al.* in [7]. On the other hand, the relation between charge distribution and the formation of magnetic regimes, in the interval studied, seems to be true only in one direction, *i.e.*, an oscillating charge distribution due to particle densities away from half-filling in finite systems does not necessarily imply the formation of distinct polarized regions in the spin sector. For example, for low particle densities, there are position-dependent charge oscillations but the system remains ferromagnetic. However, polarons can be associated to holes, which seemed to pin down some of the magnetic structures. It is the super-exchange coupling between the localized spins which drives and shapes the ordering of the spins in the end.

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REFERENCES

[1] D. D. Sarma, P. Mahadevan, T. Saha-Dasgupta, S. Ray and A. Kumar, Phys. Rev. Lett. **85**, 2549 (2000).
[2] W. Eerenstein, N. D. Mathur and J. F. Scott, Nature **442**, 759 (2006).
[3] J.G. Bednorz, K.A. Müller and Zeitschrift für Physik B, **64**, 189 (1986).
[4] T. Kumar, M. Greenblatt. *Transition Metal Oxides: Magnetoresistance and Half-Metallicity.* Functional Oxides (Wiley & Sons Ltd., UK, 2010) p. 257.
[5] D.R. Neuber, M. Daghofer, H. G. Evertz, W. von der Linden and R. M. Noack, Phys. Rev. B **73**, 014401 (2006).
[6] E. Vallejo, F. Lopez-Urias, O. Navarro and M. Avignon, Solid State Commun. **149**, 126 (2009).
[7] D. J. Garcia, K. Hallberg, B. Alascio and M. Avignon, Phys. Rev. Lett. **93**, 177204 (2004).
[8] S. R. White, Phys. Rev. B. **48**, 10345 (1993).
[9] Y. Arredondo and H. Monien, Phys. Rev. B. **78**, 115425 (2008).
[10] K. I. Kobayashi, T. Kimura, H. Sawada, K. Terakura and Y. Tokura, Nature **395**, 677 (1998).
[11] D. J. Garcia, K. Hallberg, C. D. Batista, S. Capponi, D. Poilblanc, M. Avignon and B. Alascio, Phys. Rev. B **65**, 134444 (2002).
[12] M. Sigrist, K. Ueda and H. Tsunesugu, Phys. Rev. B **46**, 175 (1992).
[13] Y. Arredondo, E. Vallejo, O. Navarro and M. Avignon, J. Phys.: Condens. Matter **24**, 335601 (2012).