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Study Of Spin-Polaron Formation In 1D Systems

Y. Arredondo[a] and E. Vallejo[b] and O. Navarro[a]

[a] Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Apartado Postal 70-360, 04510 México D.F., México.
[b] Facultad de Ingeniería Mecánica y Eléctrica, Universidad Autónoma de Coahuila, Carretera Torreón-Matamoros Km. 7.5 Ciudad Universitaria, 27276 Torreón, Coahuila.

Abstract. We study numerically the formation of spin-polarons in low-dimensional systems. We consider a ferromagnetic Kondo lattice model with Hund coupling $\mathbf{J_H}$ and localized spins interacting antiferromagnetically with coupling constant $\mathbf{J}$. We investigate the ground state phase diagram as a function of the exchange couplings $\mathbf{J_H}$ and $\mathbf{J}$ and as a function of the band filling, since it has been observed that doping either on the ferromagnetic or antiferromagnetic regime lead to formation of magnetic domains [1]. We explore 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.

Keywords: Low-dimensional systems, quantum magnetism, super-exchange interactions.
PACS: 71.10.Fd, 75.10.Pq, 75.30.Et.

INTRODUCTION

The strong electron correlations present in low-dimensional structures along with large quantum fluctuations have revealed new and interesting quantum magnetic phases. The introduction of the spin as an additional degree of freedom has allowed the discovery of a rich variety of magnetic ordered phases in compounds such as manganese oxides with perovskite-type structure and has opened up a wide range of promising applications in the field of spintronics. Recently, the double perovskite oxide Sr_2FeMoO_6 (SFMO) has been subject of intense research due to its spin-dependent transport and magnetoresistive properties [2]. It has been suggested that the origin of magnetism in such compound is the result of the interplay between both charge (associated to the oxygen sites of SFMO) and localized spins (associated to 3d Fe sites) degrees of freedom along with a super-exchange mechanism taking place between the localized spins. Disorder in double perovskite materials plays as well a crucial role in determining their ground state properties. We will investigate numerically the ground-state of the ferromagnetic Kondo lattice model including an antiferromagnetic interaction between the localized spins in chains of fixed length L at different values of the band-filling, n.

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FERROMAGNETIC KONDO LATTICE MODEL WITH SUPER-EXCHANGE INTERACTIONS

We will consider a ferromagnetic Kondo lattice model with antiferromagnetically interacting localized *S=1/2*-spins. The corresponding model Hamiltonian is written in Eq. 1, where *t=1* is the nearest-neighbor hopping matrix, which we choose to set the energy scale and a cartoon of the model is depicted in Fig. 1.

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

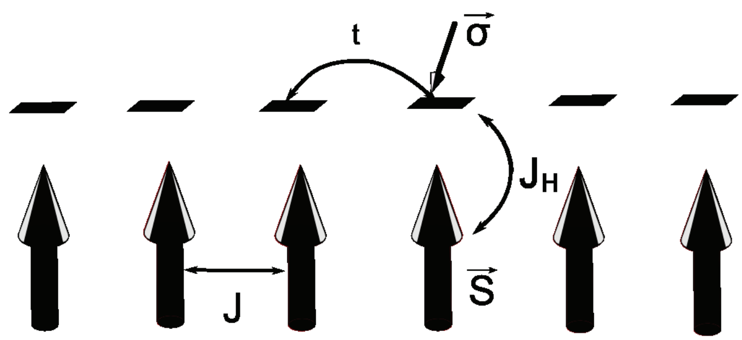

FIGURE 1. The Kondo lattice model with antiferromagnetic interaction J between localized spins $\vec{S}$. The electrons in the conducting band are coupled ferromagnetically with the localized spins with coupling constant J_H, which is the Hund coupling.

The measurement of ground-state properties is carried out using the density matrix renormalization group (DMRG), 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 $J_H = 8t$ and *J=0, 0.01t, 0.02t, 0.03t* and *0.04t*, and measure nearest-neighbor spin-spin correlation functions to find out the type of magnetic ordering away from the half-filled case. For the DMRG algorithm we used open boundary conditions and *512* matrix-density states, which rendered a maximum truncation error of approx. 10^{-6}.

SPIN-POLARON FORMATION

Spin-polaron structures have been identified in one-dimensional systems [5, 6, 7]. Our results show that in the low-carrier-concentration limit, i. e., for *n=1/4* and *n=1/3* the systems are ferromagnets, in accordance with the results of [8]. We also found out that the antiferromagnetic interaction, above the chosen interval, has no influence whatsoever on the magnetic ordering for such low-carrier densities. Upon increasing both the carrier concentration and the value of *J*, spin fluctuations become relevant and generate different ground states gradually turning the ferromagnetic state into an antiferromagnet. In Fig. 2 we show the nearest-neighbor spin-spin correlation function along with the particle density $< n_i >$ for *J=0.04t* and *n=1/2*, the localized spins order in pairwise antiferromagnetically aligned polarons such as $\cdots\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow \ldots$.

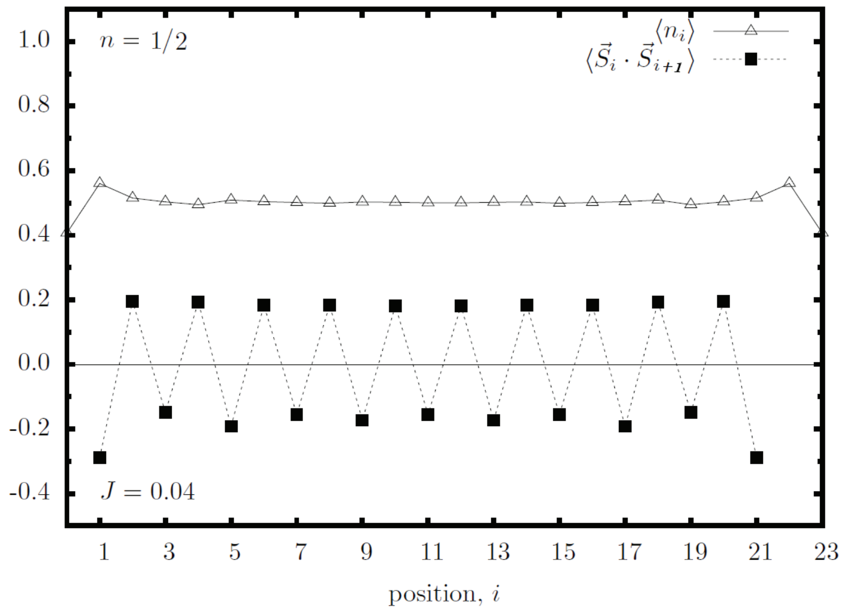

FIGURE 2. Particle density and nearest-neighbor spin-spin correlation function for *n=1/2* and *J=0.04*. The magnetic phase found is formed by pairwise polarons.

In Fig. 3, the corresponding correlation function for *J=0.04t* and *n=3/4* displays a full antiferromagnetic behavior, with the peaks of the correlation function associated to the positions of the minima of $< n_i >$.

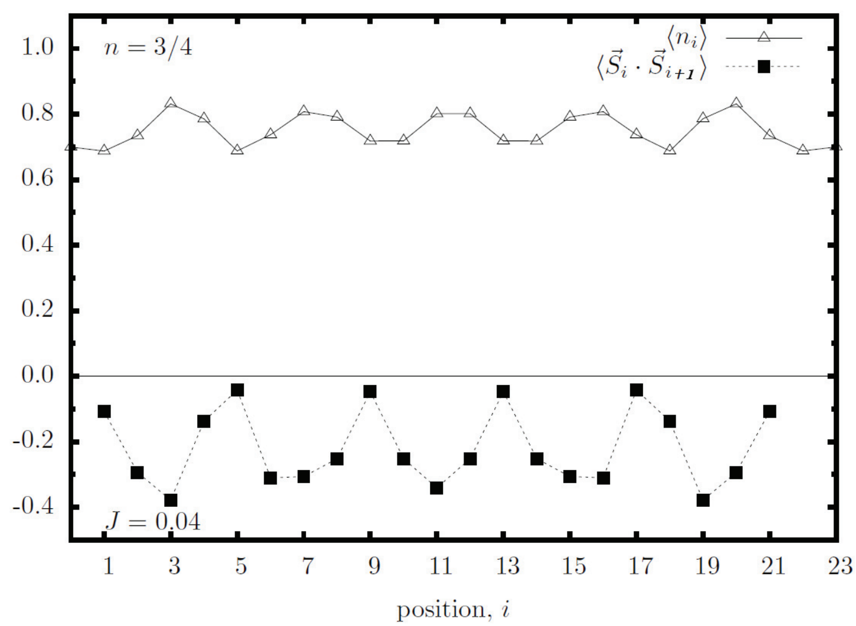

FIGURE 3. Particle density and nearest-neighbor spin-spin correlation function for *n=3/4* and *J=0.04*. The system displays an antiferromagnetic behavior.

In general, we do not expect our results to change with the chain length for electronic densities away from half-filling since our results can be compared to those reported in [7, 8]. We summarize our results in the phase diagram of Fig. 4, where both extremes of the magnetic behavior, the ferromagnet and the antiferromagnet, are separated by a region where spin-polarons arise. At the specific band-filling of *n=1/2*, i.e., with 12 holes in the system, the phase $\cdots\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\ldots$ appears for all the selected values of *J*. We observed as well that, once the value of *n* was fixed, the charge distribution remains the same for the values of *J* in the shown interval, i.e., the charge modulation is independent of the interactions between the localized spins. A study of the exact nature of such spin structures is left for future work. Previous results reported by Neuber et. al. using *S=3/2* localized spins show a different magnetic ordering [9].

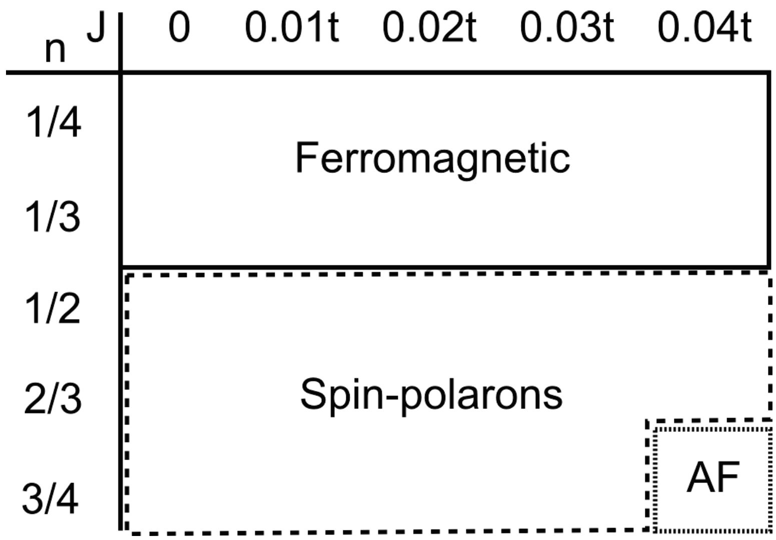

FIGURE 4. Phase diagram for the model of Eq. 1 as a function of the band filling and the antiferromagnetic coupling *J*. AF refers to the antiferromagnetic phase.

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