Local moments coupled to a strongly correlated electron chain

S. Moukouri, Liang Chen, and L. G. Caron

Centre de Recherche en Physique du Solide and Département de Physique, Université de Sherbrooke,
Sherbrooke, Québec, Canada J1K 2R1

A one-dimensional model Hamiltonian that is motivated by the recent discovery of the heavy-fermion behavior in the cuprates of the Nd_2CuO_4 type is studied. It consists of t-J interacting conduction electrons coupled to a lattice of localized spins through a Kondo exchange term J_K. Exact diagonalization and density-matrix renormalization-group methods are used. The latter method is generalized to arbitrary densities. At half filling, a spin gap opens for all $J_K > 0$. Away from half filling it is shown that, at strong J_K, the ground state is an unsaturated ferromagnet. At weak J_K the system is in a paramagnetic phase with enhanced Ruderman-Kittel-Kasuya-Yosida (RKKY) correlations. The importance of self-screening of the local moments in the depletion regime is discussed. We argue that these findings transcend the specifics of the model.

The study of quantum moments embedded in a metallic host is one of the most active fields of condensed matter physics. The main problem is the understanding of the low-temperature behavior of localized moments, which are typically rare-earth lanthanide or actinide ions, interacting with p or d bands of conduction electrons. It has been argued that there are two competing effects: the quenching of the local spins through the Kondo effect and their magnetic ordering due to the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction.[1] The canonical Hamiltonians of heavy-fermion compounds are the periodic Anderson lattice model (PAM) and the Kondo lattice model (KLM). The PAM and the KLM describe a lattice of local moments coupled to a wide conduction band. It is widely accepted that this situation prevails in the so-called heavy-fermion materials.[2]

The recent discovery of a heavy-fermion phenomenon in the Ce-doped Neodynium cuprate $Nd_{1.8}Ce_{0.2}CuO_4$ (Ref. 3) has led to an increasing interest in the study of strongly correlated electrons coupled to magnetic moments.[4] Although these compounds are at least two-dimensional (2D), as a first step towards their understanding, we report a study of a 1D Hamiltonian which retains the basic ingredients of their physics. This Hamiltonian describes the interplay between strongly correlated electrons and a lattice of local moments. The strongly correlated conduction-electron system is described by the 1D t-J model. The interaction between conduction electrons and the Nd ions is represented by a Kondo exchange term. Using standard notations, the Hamiltonian is written as follows:

$$H = -t \sum_{i\sigma} (c_{i\sigma}^{\dagger} c_{i+1\sigma} + \text{H.c.})$$
$$+ J_H \sum_i \left(\mathbf{S}_{ic} \cdot \mathbf{S}_{i+1c} - \frac{n_{ic} n_{i+1c}}{4} \right)$$
$$+ J_K \sum_i \mathbf{S}_{ic} \cdot \mathbf{S}_{if}. \tag{1}$$

The Hamiltonian (1) is a natural extension of the one-dimensional KLM in the limit of strongly correlated electrons. We recall that double occupancy is forbidden here. The indices c and f stand for conduction and localized electrons respectively. We set the hopping parameter t and the Heisenberg coupling J_H equal to 1. For those parameters, which are relevant for the cuprates, the ground state of the 1D t-J model is a Luttinger liquid.[5] We discuss the nature of the ground state as the band filling ρ of the conduction electrons and J_K are varied.

We use the density-matrix renormalization-group (DMRG) method of White.[6] The calculations are done using the infinite system method with three blocks instead of four as usual. One can immediately realize that there is a problem fixing the electron density at a given value at each iteration. To overcome this, we have targeted the two states whose electron number brackets the desired density when building the density matrix. This algorithm has been successfully checked for the one-dimensional t-J model.[7] In the present study, we have kept up to $m = 140$ states in the two external blocks. The states were labelled by the electron number and by the total z component of the spin. The maximum lattice size we have reached is 75. The truncation error defined as $1 - p(m)$, where $p(m)$ is the sum of the eigenvalues of the density matrix of the states kept, was of the order of 5×10^{-4}.

At half filling, the t-J chain reduces to a Heisenberg antiferromagnet. We have found that the singlet ground state is separated from the first excited triplet state by a gap for all $J_K > 0$. As shown in Fig. 1, the J_K dependence of this gap Δ is very close to that of the Kondo necklace model (KNM).[9] It is linear in the strong J_K limit and probably has a nonanalytic form for small J_K. We note that the values of the gap found here in the weak-coupling limit are much larger than that in the KNM. Thus, the interaction between the conduction electrons, represented here by the z part of the Heisenberg term after the Jordan-Wigner transformations, tends to enhance the gap. In order to understand the character of the gap, we have compared it with the binding energy per site which is defined as $E_B = [E_G(J_K=0,N) - E_G(J_K,N)]/N$, where $E_G(J_K,N)$ is the ground-state energy. It can be observed in Fig. 1 that in the strong-coupling limit, Δ is larger than E_B: the excitations of the system are
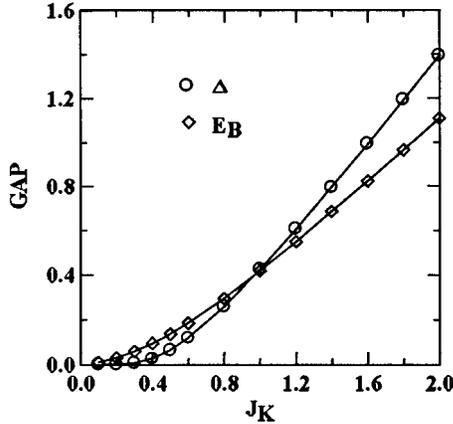
FIG. 1. The singlet triplet gap Δ (circles) and the binding energy E_B (diamonds) per site versus the Kondo coupling.

obtained by breaking up on-site singlets. In the weak-coupling regime, E_B becomes greater than Δ, this means that the system can be excited without the destruction of local singlets. The gap results from a collective effect. In the KNM,[9] as the coupling is decreased, the RKKY correlations become larger in magnitude. The situation is also similar here. Figure 2(a) displays the magnetic structure factors, $S_{f,c}(k) = (4/N)\Sigma_{l,m}\langle S^z_{f,c,l} S^z_{f,c,m}\rangle \exp[i(l-m)k]$, of localized and conduction electrons respectively. These structure factors have a maximum at $2k_{Fc} = \pi$ for $J_K = 0.2$. When the coupling is increased, the cusp flattens out, indicating the vanishing of the RKKY correlations. We emphasize that even in the RKKY regime there is no long-range order or even a power-
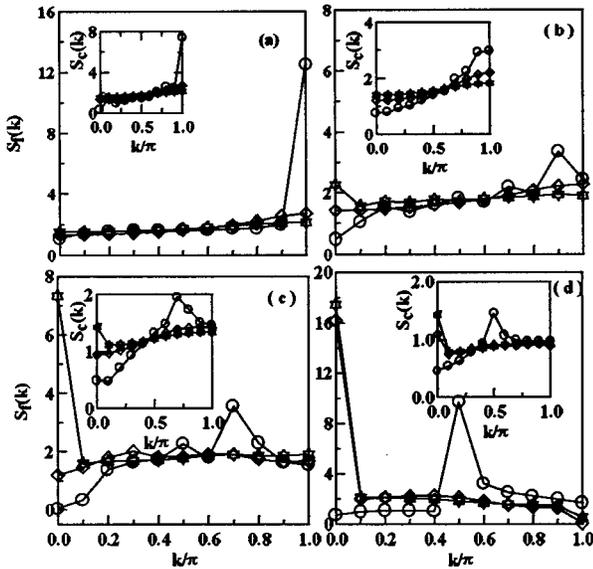

FIG. 2. The magnetic structure factor of the localized spins and of the conduction electrons (inset) for (a) $\rho=1$, (b) $\rho=0.9$, (c) $\rho=0.7$, (d) $\rho=0.5$ at $J_K=0.2$ (circles), $J_K=1$ (diamonds), and $J_K=2$ (stars).

law decay of the correlations because the tendency to magnetic order is thwarted by the gap induced by the Kondo mechanism. Finally, we note that our results are in agreement with those of Igarashi et al.[10] who also studied the effect of the lattice of local moments on a Heisenberg chain using an exact diagonalization method.

Away from half filling, the situation is less clear because the spin configuration of the ground state is not known. Actually, this information is important in a numerical calculation since it allows a significant reduction of the Hilbert space under study. There are, however, two limits where one can gain some insight. The first one is the situation with only one conduction electron, which is identical to the KLM with one electron. The theorem of Sigrist et al.[11] applies: the ground state is an unsaturated ferromagnet having a total spin $S_T = (N-1)/2$. The second one is the limit of infinite coupling in which all the conduction electrons form on-site singlets with the localized spins, so that $N-N_c$ spins remain free. The ground state has $2^{(N-N_c)}$-fold spin degeneracy. In this limit, the degrees of freedom consist in local singlets and unpaired f (up or down) spins. The spin degeneracy can be partially lifted by the introduction of the hopping term. The Heisenberg term has no role because there are no free conduction electrons. This situation is identical to the strong coupling limit of the KLM, where Sigrist et al.[12] have demonstrated that the ground state is a ferromagnet with $S_T = (N-N_c)/2$ for all $\rho \neq 1$. Their result also applies in the present case. In order to clarify the behavior of the system in the whole range of parameters, we have performed an exact diagonalization for lattice sizes of 4,5,6 sites with open boundary conditions. We have found that there is a critical value of the Kondo coupling J_c, which depends on the band filling. When $J_K \gtrsim J_c$, the ground state is always a ferromagnet at all $\rho \neq 1$. Below this transition point, the spin configuration of the ground state evolves from the maximum value of the spin to the minimum. There is a transition region where the spin of the ground state can have an intermediate value. But at smaller J_K, finite-size effects become important and trends are less clear. We display in Fig. 3 the energy difference δE between the triplet and the singlet lowest energy states for $N=4,5,6$ sites with $N_c=2,3,4$ electrons respectively. For the four sites case, δE is always positive below the transition point, while for five and six sites its sign is not constant reflecting the finite-size effects. We also present the interesting case of two electrons in six sites. It can help us understand the evolution from the maximum spin ground state $S_T=2$ to the minimum $S_T=0$. At strong coupling, the ground state has $S_T=2$, there is a narrow region near the transition point where the spin configuration of the ground state is $S_T=1$. Then it becomes $S_T=0$ at smaller couplings. One can also observe that when the density is reduced, the value of J_c decreases. Having in mind these results, we use the DMRG to compare the lowest energy states with $S_T=0$ and $(N-N_c)/2$. Since in the DMRG, the states are labelled by only the z component of the total spin, at each value of the coupling, we have calculated the lowest energy of the states with $S^z_T=0, \pm 1$ and $\pm(N-Nc)/2$, such that the last number is an integer. When these energies are all different, we have found that the lowest value is that of the state with $S^z_T=0$. It is thus reasonable to think that the ground state is a singlet. This occurs when $J_K < J_c$. But
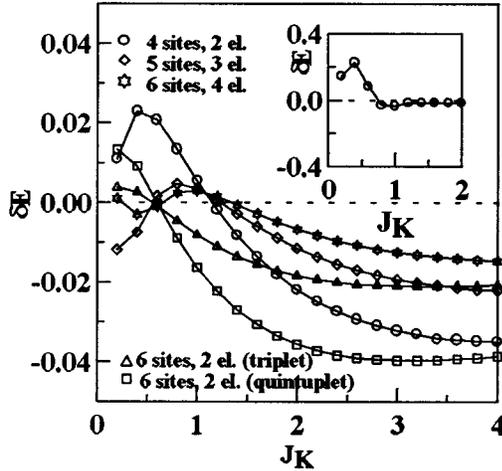
FIG. 3. Energy difference δE between the lowest states with $S_T = 1$ (or 2) and $S_T = 0$ for systems of 4, 5, and 6 sites with 2, 3, and 4 (or 2) electrons respectively. In the inset, δE between the lowest states with $S_T^z = 0$ and $S_T^z = (N - N_c)/2$ for $\rho = 1/2$.

FIG. 4. The on-site electron-spin correlation versus the Kondo coupling at $\rho = 1$ (circles), $\rho = 0.9$ (diamonds), $\rho = 0.7$ (stars), and $\rho = 0.5$ (triangles).

when $J_K > J_c$ all the states have the same energy (in the order of 10^{-3}) and we conclude that the ferromagnetic state is preferred. These findings corroborate the exact diagonalization calculations, namely that there is a crossover from a singlet ground state to a ferromagnet at the densities that we have investigated. We caution that in the finite-size study there is a transition region near J_c where the ground state can have an intermediate value of the total spin. A detailed study of this region is left for the future.

Let us now reexamine the magnetic structure factors of the f electrons shown in Fig. 2. In the strong coupling limit, $J_K = 2$, starting from half filling [Fig. 2(a)] where each f electron is screened by a conduction electron, the system is in a nonmagnetic state. The reduction of the density is equivalent to the insertion of $N - N_c$ free spins within N_c singlets. The problem is analogous to the insertion of holes in the strong U limit of the Hubbard model. At $\rho = 0.9$ [Fig. 2(b)], we found that the ground-state has $S_T = (N - N_c)/2$, thus, contrary to the strong U limit of the 1D Hubbard model, the ground state is an unsaturated ferromagnet; this extends the results of exact diagonalization to larger systems. Although the system is in the ferromagnetic state, the cusp at $k = 0$ is very small; we believe that this is due to the fact that the density of the singlets is still much larger than that of the unpaired f electrons, so that ferromagnetic correlations are hidden since the effective coupling between the unpaired f electrons is small.[12] As one decreases the band filling [Figs. 2(c) and 2(d)], the maximum at $k = 0$ steeply rises. The lower the density, the higher the maximum, since the number of the ordered spins is greater. At intermediate couplings, the FM state is destroyed for $\rho = 0.9$ around $J_c = 1.2$ and $\rho = 0.7$, around $J_c = 1$. One can clearly see that there is no dominant feature in $S_f(k)$ in these two cases when $J_K = 1$. But the FM state is still stable at $\rho = 0.5$ as indicated by the maximum at $k = 0$, the transition occuring only at $J_c = 0.8$. Thus, the FM-PM phase boundary is shifted towards smaller J_K when the band filling is decreased. This finding is consistent with the existence of ferromagnetism for all $J_K > 0$ of the case with one electron. In the small coupling regime, the ground
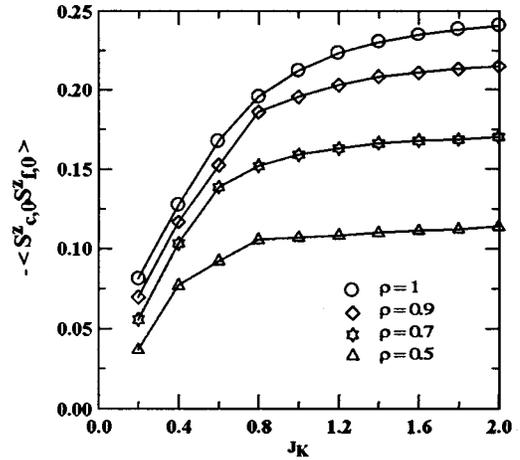
state is always a singlet. An incommensurate peak appears in $S_f(k)$ at $2k_{Fc} = \pi\rho$ at the three densities studied, showing that the RKKY correlations are dominant.

In the weak J_K region we see the ground state is still a singlet despite $N_c < N$. Nozières[8] has argued that at low temperatures there will not be enough conduction electrons to screen out all the localized spins. This incomplete Kondo screening could lead to an ineffective RKKY interaction. We see that in our case the nature of the screening process seems to be very different from that of the one-impurity case since a spin-compensated state exists even though $N_c < N$. A scenario discussed in Ref. 13 to avoid the Nozières exhaustion problem was that a significant part of screening is done by the f electrons themselves through the action of intersite RKKY correlations. Following Blankenbecler et al.[14] the condition for the quenching of a spin located at the origin gives rise to the compensation sum rule:

$$\langle S_{f,0}^{z2} \rangle = -\sum_{l \neq 0} \langle S_{f,l}^z S_{f,0}^z \rangle - \sum_l \langle S_{c,l}^z S_{f,0}^z \rangle. \qquad (2)$$

We have verified this relation for $J_K = 0.5$ where a Kondo state is expected since the ground state is a singlet and the magnetic correlations are short ranged . The left-hand side of (2) is always equal to 0.25. The first term of the right-hand side of (2) which gives the contribution of the f electrons to the screening slightly increases when the density is reduced. It takes the values 0.08, 0.08, 0.11, and 0.12 for $\rho = 1$, 0.9, 0.7, and 0.5, respectively, when the ten first neighbors are included. At the same time, the contribution of the conduction electrons which is measured by the second term decreases. It is equal, respectively, to 0.12, 0.11, 0.10, and 0.08. Even at half filling where the number of conduction electrons is equal to that of the local moments , the "self-screening" is non-negligible. However, when J_K is increased, strong on-site singlets are formed and this screening mechanism is no longer possible because RKKY correlations between f elec-

trons are suppressed. The major contribution to the compensation sum rule comes from the on-site electron-spin correlation—$\langle S^z_{c,0} S^z_{f,0} \rangle$ which is displayed in Fig. 4. This quantity is found to be very close to 0.25ρ in the strong coupling regime. Therefore, in the large J_K limit (2) is satisfied only at half filling, since the f electrons are FM ordered when $\rho \neq 1$. Thus the depletion effects occur because the formation of a coherent singlet ground state necessitates the action of the antiferromagnetic RKKY correlations.

So far, we have mainly discussed the action of the electrons on the lattice of local moments. We now wish to consider the inverse problem. For the conduction electrons we have found that $S_c(k)$ is flat at strong and intermediate couplings for $\rho = 0.9$ [Fig. 2(b)]. We note that for $\rho = 0.5$ and $\rho = 0.7$, a small peak arises at $k = 0$. This is a consequence of the f-spin induced ferromagnetic correlations of the conduction electrons [Figs. 2(c) and 2(d)]. Dominant structures appear in the structure factor $S_c(k)$ at $2k_{F_c}$ only for small J_K.

In summary, we have studied a model Hamiltonian which describes the physics of magnetic moments coupled to strongly correlated electrons in 1D. We have found that at half filling, the system is a spin gapped insulator for all nonzero values of the Kondo coupling. When the system is doped, a FM state is stable at strong coupling. We have argued that it is a consequence of the depletion effects. At weak coupling, the ground state is a collective singlet. We have shown that a significant part of the screening is made by the local spins themselves through the RKKY interaction. Finally, we have reached the same kind of conclusion as in a recent study of the ground-state properties of the one-dimensional KLM.[15] It seems that the Hamiltonian (1) and the KLM belong to the same universality class. Indeed, in the KLM there is no explicit interaction between the conduction electrons. However, it is well known that the Kondo exchange term induces an effective interaction between these electrons. It is thus likely that the Hamiltonian (1) and the KLM are not fundamentally different.

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