Spin Order in One-Dimensional Kondo and Hund Lattices

D. J. Garcia
Instituto de Fisica Gleb Wataghin, Unicamp, Campinas (6165), São Paulo, Brasil
Instituto Balseiro and Centro Atómico Bariloche, CNEA, 8400 San Carlos de Bariloche, Argentina

K. Hallberg and B. Alascio
Instituto Balseiro and Centro Atómico Bariloche, CNEA, 8400 San Carlos de Bariloche, Argentina

M. Avignon
Laboratoire d'Etudes des Propriétés Electroniques des Solides, CNRS, BP 166, 38042 Grenoble Cedex 9, France*
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We study numerically the one-dimensional Kondo and Hund lattices consisting of localized spins interacting antiferromagnetically or ferromagnetically with the itinerant electrons, respectively. Using the density-matrix renormalization group we find, for both models and in the small coupling regime, the existence of new magnetic phases where the local spins order forming ferromagnetic islands coupled antiferromagnetically. Furthermore, by increasing the interaction parameter $|J|$ we find that this order evolves toward the ferromagnetic regime through a spiral-like phase with longer characteristic wavelengths. These results shed new light on the zero temperature magnetic phase diagram for these models.

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The interplay between charge and spin degrees of freedom in strongly correlated systems has triggered enormous interest in recent years due to the rich variety of phases found in a plethora of compounds. Charge and spin superstructures with a doping dependent wave vector were found, for example, in $La_{2-x}Sr_xNiO_4$ using neutron scattering [1] and electron diffraction [2]. Stripe formation together with incommensurate spin fluctuations in high-T_c superconductors can also be regarded as a manifestation of similar phenomena [3] as well as the charge and spin ordering found in many of the doped manganese perovskites. Another large group of compounds, the heavy-fermion materials, presents various types of ground states including antiferromagnetically ordered states, the normal heavy-fermion state, as well as superconducting and insulating phases. Heavy-fermion systems and Kondo insulators are typical examples of systems in which the interactions between conduction electrons and quantum localized spins are essential [4,5]. Their physical properties result from an antiferromagnetic coupling J between these two types of particles, the so-called Kondo lattice model (KLM). The corresponding Hamiltonian has the well-known form

$$H = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - J \sum_i \vec{S}_i \cdot \vec{\sigma}_i. \quad (1)$$

The first term represents the conduction electron hopping between nearest-neighbor sites $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) being standard creation (annihilation) operators. In the second term the exchange interaction J is antiferromagnetic ($J < 0$), and $\vec{\sigma}_i = \frac{1}{2}\sum_{\sigma,\sigma'} c^\dagger_{i\sigma} \vec{\tau}_{\sigma\sigma'} c_{i\sigma'}$ ($\vec{\tau}_{\sigma\sigma'}$ are Pauli matrices).

It is interesting to note that, in recent years, the same model Hamiltonian with ferromagnetic coupling ($J > 0$) has been considered to contain the basic physics of manganites exhibiting the "colossal" magnetoresistance effect [6–9]. In this case, both localized spins and itinerant electrons originate from manganese d states. The system is assumed to contain essentially Mn^{4+} ions with three localized t_{2g} orbitals represented as local spins $\vec{S}_i$ and additional itinerant electrons in the e_g orbital. Because of the strong Hund coupling the spin of the e_g electron is constrained to be parallel to the local spin on that site. Hund's rule together with the hopping term gives rise to the "double-exchange" (DE) interaction that favors ferromagnetic ordering of the local spins [10]. In recent literature this model is often referred to as the ferromagnetic Kondo lattice; however, to avoid confusion with the Kondo model, we call it the Hund model (HM). The DE mechanism requires only that the system is away from half filling and is independent of the sign of J [11].

We will study the Hamiltonian (1) for both antiferromagnetic and ferromagnetic (FM) couplings, considering $S = 1/2$ localized quantum spins. To this end we use the density-matrix renormalization group (DMRG)[12] with open boundary conditions for chains of different sizes. We implemented the finite version of the DMRG algorithm reaching chains sizes of 36 sites (the discarded weight being less than 10^{-5}). The different phases are characterized through the local spin-spin correlation functions and its Fourier transform, the following spin structure factor:

$$S(q) = \frac{1}{L} \sum_{i,j} e^{iq(R_j - R_i)} \langle \vec{S}_i \cdot \vec{S}_j \rangle,$$

where L is the number of sites in the system and n is the number of conduction electrons per site.

In Fig. 1 we present the phase diagram of the one-dimensional Kondo and Hund models which we propose from our numerical results for several commensurate fillings (marked with dashed lines), improving previous results [5,13–18]. As can be seen, except for a scale factor, both phase diagrams present great similarities. The half-filled case $n = 1$ is pathological in both models whose ground state is very different from the $n \neq 1$ case: characterized by a spin gap, however, with a different behavior as a function of $|J|$ in the Kondo and Hund cases, it has been referred to as a "spin-liquid phase"[19]. For the Hund model it scales to the $S = 1$ chain with a Haldane gap. The transition to the FM phase in the Kondo model coincides with the previous work mentioned. However, for the Hund model we find that the border lies at slightly larger values of J as compared with Ref. [14] due to the larger system sizes considered here. We also include the phase separated regime [14].

At low $|J|$ a phase qualified as "paramagnetic" in the KLM and "incommensurate" in the HM had been identified with exact diagonalization and DMRG [13–15,18,20,21]; this phase is, however, much less understood than the ferromagnetic phase. In these references the local spin-spin correlations are calculated and $S(q)$ shows a peak at the wave number corresponding to $2k_F$ of the conduction electrons. However, no scaling was performed and the existence of what we call "island phases" (see below) was missed. Recently, the existence of a "spin dimerized" phase has been reported [22] for the Kondo model at quarter-filling ($n = 1/2$), through the order parameter $D(i) = \langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle$. The spin structure is of the island-type $\cdots \uparrow\uparrow\downarrow\downarrow \cdots$ similar to the one we have identified previously for the DE-superexchange model [23]. Our present calculations reproduce the results for $D(i)$. However, the absence of a spin gap [22] and our results on the long distance spin-spin correlation functions suggest a nonspontaneously broken translation symmetry state compatible with the generalization of the Lieb-Schultz-Mattis theorem [24]. We find that similar structures are present for other commensurate fillings $n = 1/4$, $1/3$, $2/3$, and $3/4$ as well. However, we do not find that the "island" phases stable at small $|J|$ transform directly into the FM phase [22]. Instead, they evolve toward the FM regime through an intermediate spiral-like phase with a wave vector q that changes from $q = 2k_F = \pi n$ (island) to $q = 0$ (FM) as $|J|/t$ increases. A spiral phase has been proposed analytically in a semiclassical model showing a similar evolution toward the FM phase [25].

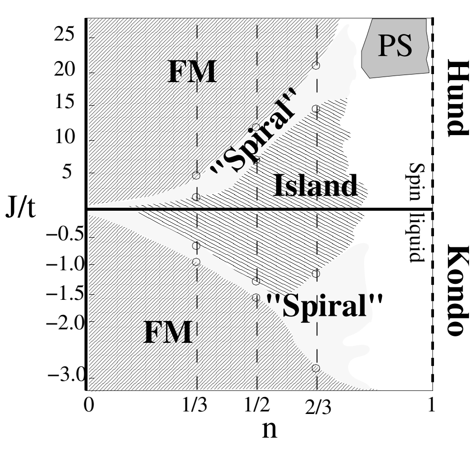

FIG. 1. Magnetic phase diagram for the KLM and HM. The various phases are described in the text. The circles indicate the crossover values.

Let us first present the quarter-filled case $n = 1/2$ (Fig. 2). For the Hund model and large J, i.e., $J/t \gtrsim 13$, the FM phase is clearly identified with a peak of $S(q)$ at $q = 0$, and the total spin (considering only localized spins) is $S_T = N_s/2$, where N_s is the number of localized spins in the system. Each electron forms a triplet state $S = 1$ with the localized spins and all localized spins are ferromagnetically ordered. For intermediate values of J ($6 \lesssim J \lesssim 10$) the FM phase gives rise to a "spiral" phase (Fig. 3), characterized by two broad peaks located at incommensurate values of q which evolve inwards (the momentum of the peak grows from $q = 0$ to larger values and another peak at a symmetric point with respect to $q = \pi$ moves towards smaller values). When J decreases further ($J/t \lesssim 6$) the spin structure transforms into an island structure with a more defined peak of $S(q)$ at $q = n\pi = \pi/2$ as shown in Fig. 2(f) indicating a four-site periodicity. This phase remains stable down to very small values of J/t; it has total spin $S_T = 0$ and zero spin gap.

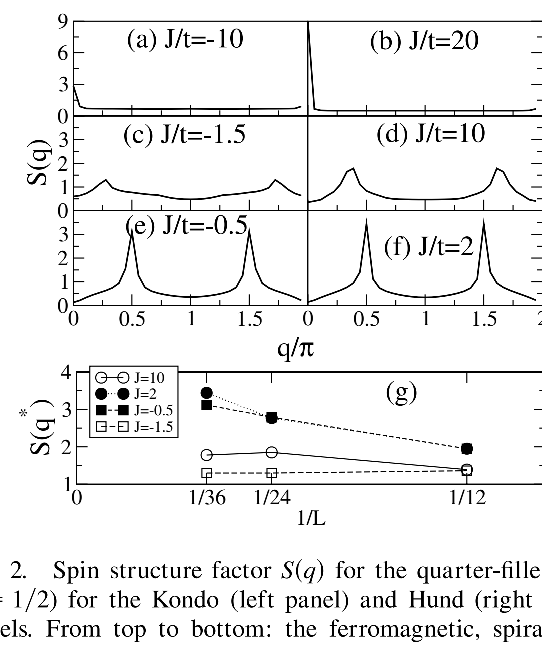

FIG. 2. Spin structure factor $S(q)$ for the quarter-filled case ($n = 1/2$) for the Kondo (left panel) and Hund (right panel) models. From top to bottom: the ferromagnetic, spiral, and island phases, appearing as $|J|$ is decreased. The lower panel shows the size dependence of the peak weight $S(q^*)$ in island (full symbols) and spiral phases (empty symbols).

Similar results are obtained in the Kondo case ($J < 0$). The island-type phase is conserved for a small Kondo coupling ($J/t \gtrsim -1.3$) and the ferromagnetic phase is recovered for $J/t \lesssim -1.6$ [Figs. 2(a), 2(c), and 2(e)]. In the strong Kondo coupling limit the ferromagnetic state differs from the Hund case in the sense that now, the conduction electrons form singlet states ($S = 0$) with the localized spins, so that the system contains $N_s/2$ singlets and $N_s/2$ unpaired localized spins. The unpaired spins are ferromagnetically coupled and the total spin is now $S_T = N_s(1 - n)/2 = N_s/4$. In the ferromagnetic phase, our results for the ground-state energy compare well with those obtained with the effective Hamiltonian in the strong coupling limit ($|J|/t \to \infty$) [26] i.e., $-J/8 - 2t/\pi$ in the Hund case and $3J/8 - t/\pi$ in the Kondo case. Triplet states in the Hund case conserve the hopping t while singlet states in the Kondo case acquire a reduced hopping $t/2$.

The weight of the peak of the spin correlation $S(q^*)$ for the island (and ferromagnetic) phases increases with the chain sizes indicating a quasi-long-range order in this case. Instead, for the spiral-like phase, this weight remains constant, indicating a short-range correlation. A similar behavior for these phases is found for the other fillings considered.

In order to visualize the order in real space we show in Fig. 3 the spin-spin correlation functions for the island and spiral phases. For the former case, the correlations change sign quite abruptly every two sites indicating that the structure is effectively of the island-type ⇈⇊ mentioned above with quasi-long-range ordering. The nearest-neighbor correlation $\langle \vec{S}(i) \cdot \vec{S}(i+1) \rangle$ changes abruptly from site to site, with a slight border effect. Here we reproduce the results of Ref. [22]. In the latter case, instead, the spiral order is clearly identified and differs qualitatively from the island order. The nearest-neighbor correlation $\langle \vec{S}(i) \cdot \vec{S}(i+1) \rangle$ remains ferromagnetic over the chain, with a small oscillation of period two suggesting a dominant spiral-like state with a remnant of the island order, which diminishes with J.

Similar island phases are clearly evidenced for $n = 1/3$ at intermediate values of the coupling for both models ($-0.5 \lesssim J/t \lesssim 1$). Typical examples are for $J/t = 1$ and $J/t = -0.3$ [see Figs. 4(c) and 4(d)]. $S(q)$ shows a clear peak at $q = n\pi = \pi/3$ and the spin correlation in real space presents an island structure of three ferromagnetic spins coupled antiferromagnetically between islands, basically ↑↑↑↓↓↓ (not shown). The ferromagnetic phase as discussed above is clearly recovered for $J/t \lesssim -1$ and $J/t \gtrsim 5$. In the intermediate region (for values of J between these intervals) we find again the spiral phase [Figs. 4(a) and 4(b)].

A similar behavior occurs for $n = 2/3$ as shown in Figs. 4(e)–4(h) . The island structure of the type ⇈⇂⇈⇂ is clearly identified for $-1 \lesssim J/t \lesssim 10$ in $S(q)$ with a peak at $q = 2\pi/3$. This island structure has a ferrimagnetic character [27] and we suggest that this configuration corresponds to the new "ferromagnetic" phase reported in Ref. [28]. For $15 \lesssim J \lesssim 21$ we observe a spiral phase. In the Kondo model we find that the island phase transforms into the FM regime through another intermediate phase, in the region $-3 \lesssim J \lesssim -1$, with a double wavelength (see below).

To illustrate the crossover between the different phases we plot in Fig. 5 the behavior of the wave vector where the spin structure factor is maximum, q^*, as a function of J for several fillings. Here it is clearly seen that for small $|J|$ the island phases show up with their characteristic wave vector $q^* = 2k_F = n\pi$. This phase is stable for a certain region until the spiral phase takes over for larger $|J|$. The wave vector of the spiral phase decreases to zero as $|J|$ increases, leading finally to the FM phase at sufficiently large values of the interaction parameter. We observe that

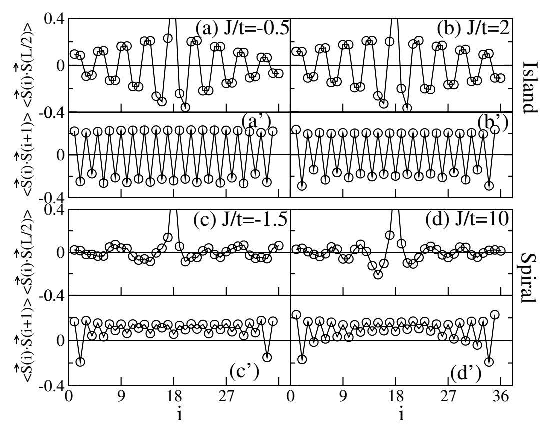

FIG. 3. Real-space local spin-spin correlations for $n = 1/2$ and the Kondo (left) and Hund (right) models. The qualitative difference between the island (top panel) and spiral (lower panel) phases can be seen.

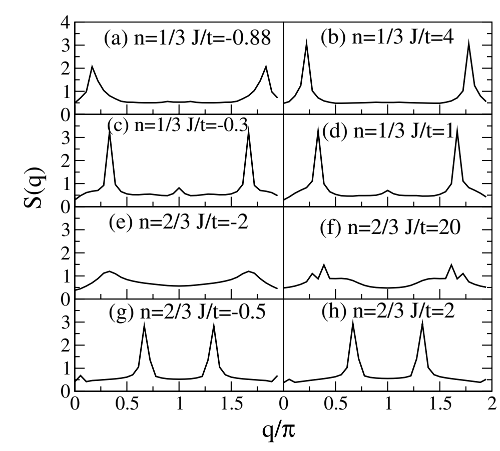

FIG. 4. Spin structure factors for both Kondo (left) and Hund (right) models showing the spiral [(a),(b) and (e),(f)] and island [(c),(d) and (g),(h)] phases for different fillings.

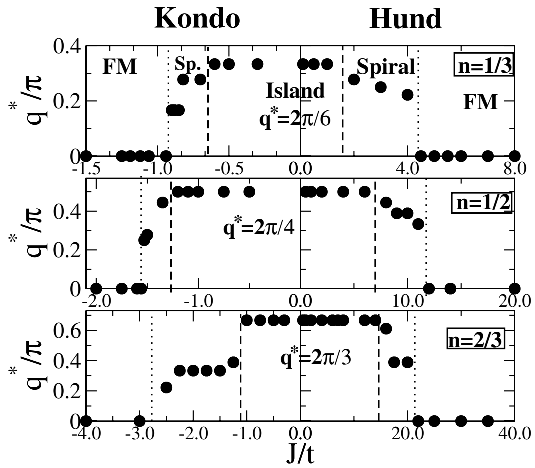

FIG. 5. Evolution of the momentum where the spin structure factor is maximum as a function of the interaction strength J covering both models for different fillings.

this behavior is qualitatively similar to the "unwinding" of the spiral phase towards the FM order obtained by Fazekas and Müller-Hartmann [25]. For $n = 2/3$ in the Kondo case we find that q^* remains fixed at $q = \pi/3$ in the region labeled as "polaronic liquid" in Ref. [28]. In this case, from the real-space spin-spin correlations it is difficult to distinguish clearly between a spiral and an island of type ↑↑↑↓↓↓ but with short-range order.

In conclusion, we have studied numerically, using the DMRG, the Kondo, and Hund models for localized spins interacting with itinerant electrons. In addition to the ferromagnetic phase at large $|J|$, we find the existence of island and spiral phases within the "paramagnetic regime" in these models. Both phases differ qualitatively as seen in different correlation functions. The island phase has quasi-long-range order and zero spin gap. Furthermore, we show how the ground state evolves from the low $|J|/t$ island $2k_F$ phase to the FM regime through a spiral-like phase at intermediate couplings. By carefully analyzing the finite-size scaling, we conclude that all phases obtained are *not due to Friedel oscillations* of the open boundaries. Based on the results for commensurate fillings we suggest the phase diagram shown in Fig. 1. We point out that the difference in the scale of J between the Kondo and Hund models has to be a consequence of the quantum nature of the localized spins, so that a complete understanding of the phase diagram requires a full quantum description of the Hamiltonian.

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*Associated with Université Joseph Fourier.

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