Spin-triplet solitons in the one-dimensional symmetric Kondo lattice

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By analyzing the Gutzwiller-projected, self-consistent mean-field solutions we demonstrate that for *all* coupling strengths of the half-filled, one-dimensional Kondo lattice (1) the spin excitations are local triplets, (2) the charge gap is *greater* than the spin gap, and (3) doping by Kondo holes induces residual spin-$\frac{1}{2}$ local moments. The implications of these results on a number of experiments and their relevance to the "Kondo insulators" will be discussed.

INTRODUCTION

The strongly correlated electronic states formed in rare-earth and actinide compounds have attracted much theoretical and experimental interest. Examples of such strongly correlated states include heavy-fermion metals, heavy-fermion superconductors, Ruderman-Kittel-Kasuya-Yosida (RKKY) metals, and the "Kondo insulators."[1] The Kondo insulators, like the ordinary band insulators, occur for an even number of electrons per unit cell and exhibit a band gap in low-temperature transport studies (although the gap can be 4 orders of magnitude smaller than that observed for the conventional band insulators). What is unusual about them, as we shall explain in this paper, is that their magnetic properties *cannot* be accounted for by a naive insulating band structure alone.[2]

In this paper, we study the lowest-energy states in various spin sectors of a one-dimensional half-filled (symmetric) Kondo lattice model by analyzing the Gutzwiller-projected[3] self-consistent mean-field solutions. We find that for *all* values of the antiferromagnetic Kondo coupling J (i) the spin excitations are local triplets, and (ii) the spin gap is less than the charge gap. As a result, (i) the low-frequency spin susceptibility should be almost independent of wave vector, (ii) substituting the magnetic rare-earth element by nonmagnetic ones creates localized charge-neutral spin $\frac{1}{2}$'s (i.e., localized spinons). These spinons can, in principle, be detected by low-temperature electron-spin-resonance measurement. Moreover, they can cause a low-temperature Curie component in the magnetic susceptibility. (iii) At zero temperature, an external magnetic field H induces magnetization for $H > H_c$, where H_c, the threshold field, is smaller than that expected from the transport gap. For medium to strong coupling, a magnetic field will induce a metal-insulator transition when the field-induced local triplets begin to overlap. (iv) Low-temperature transport and magnetic (e.g., NMR) measurements should exhibit a difference between the charge and spin gaps.

On the theoretical side, the half-filled one-dimensional Kondo lattice has also attracted much attention.[4] Among them, Tsunetsugu *et al.*[4(c)] have recently shown that a spin gap exists for all values of the antiferromagnetic Kondo coupling by performing numerical diagonalization. In this work we clarify the nature of the spin excitations by analyzing the Gutzwiller-projected self-consistent mean-field solutions.

The Hamiltonian for the Kondo lattice is given by

$$\mathcal{H}_{\mathrm{KL}} = -\sum_{ij} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \mathrm{H.c.}) - \mu\sum_i n_{ic} + \frac{J}{2}\sum_i \mathbf{S}_i \cdot c^{\dagger}_{i\sigma}\tau_{\sigma\sigma'}c_{i\sigma'} \,. \tag{1}$$

In Eq. (1), i,j label the unit cells of a crystalline lattice, t_{ij} is the conduction electron hopping integral, $c^{\dagger}_{\sigma}$ creates a conduction electron with spin σ, $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ is the conduction electron occupation number, $\mathbf{S}$ is a localized $S = \frac{1}{2}$ spin, τ denotes the Pauli matrices, J (>0) and μ are the antiferromagnetic Kondo coupling and the conduction-electron chemical potential, respectively. In the above and in the rest of the paper repeated spin indices are summed. In the following we shall represent the localized spins as the spins carried by auxiliary fermions via

$$\mathbf{S}_i = \tfrac{1}{2} f^{\dagger}_{i\sigma}\tau_{\sigma\sigma'}f_{i\sigma'} \,. \tag{2}$$

Here $f^{\dagger}_{i\sigma}$ creates an auxiliary fermion with spin σ in the ith unit cell. In order to remove the spurious charge degrees of freedom associated with the f electrons we impose the Hilbert-space constraints $n_{if} \equiv f^{\dagger}_{i\sigma}f_{i\sigma} = 1$ for all unit cells. Using this identity and

$$c_\alpha^\dagger \tau_{\alpha\beta} c_\beta \cdot f_\sigma^\dagger \tau_{\sigma\sigma'} f_{\sigma'} = 2n_{ic} - n_{ic} n_{if} - 2(c_\sigma^\dagger f_\sigma)(f_{\sigma'}^\dagger c_{\sigma'}) , \tag{3}$$

one can rewrite the Hamiltonian as

$$\mathcal{H} = -\sum_{ij} t_{ij}(c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - \frac{J}{2}\sum_i (c_{i\sigma}^\dagger f_{i\sigma})(f_{i\sigma'}^\dagger c_{i\sigma'}) - \mu' \sum_i n_{ic} , \tag{4}$$

where $\mu' \equiv \mu - J/4$. It is important to bear in mind that the Hamiltonian given by Eq. (4) is supplemented by the Hilbert-space constraint $n_{if} = 1$ for all i. By going to the standard coherent-state path integral[5] representation of the partition function $Z = \mathrm{Tr}\exp(-\beta\mathcal{H})$, we obtain $Z = \int D[c,f,b,\lambda]\exp(-S)$, where

$$S = \int_0^\beta d\tau \sum_i [\bar{c}_{i\sigma}(\partial_\tau - \mu')c_{i\sigma} + \bar{f}_{i\sigma}\partial_\tau f_{i\sigma}] - \sum_{ij} t_{ij}[\bar{c}_{i\sigma}c_{j\sigma} + \text{H.c.}] - \frac{J}{2}\sum_i [\bar{b}_i \bar{c}_{i\sigma} f_{i\sigma} + \text{H.c.}] + \frac{J}{2}\sum_i \bar{b}_i b_i + i\sum_j \lambda_j (n_{jf} - 1) . \tag{5}$$

In Eq. (5), b_i is an effective hybridization field introduced in the Hubbard-Stratanovich decoupling of the second term in Eq. (4), and λ_i, a time-independent field, is the Lagrange multiplier which enforces the constraint $n_{if} = 1$.

MEAN-FIELD SOLUTIONS

We have carried out mean-field analyses[6] by assuming b_i to be time independent, but allowing the full site dependence for both b_i and λ_i. Mean-field solutions are obtained by integrating out the fermions and minimizing the resulting free energy. The resulting mean-field equations are

$$b_i = \langle 0 | c_{i\sigma}^\dagger f_{i\sigma} | 0 \rangle , \quad \langle 0 | n_{if} | 0 \rangle = 1 , \tag{6}$$

where $|0\rangle$ is the self-consistent mean-field electronic state. In order to allow for the full site dependence, we have performed numerical self-consistent mean-field calculations for a one-dimensional lattice with nearest-neighbor hopping $t = 1$, with L, the length of the chain, up to 100. Since the total spin operator commutes with the Hamiltonian, we can obtain mean-field solutions for each spin sector. The results are summarized as follows. (1) The $S = 0$ sector: The global lowest-energy mean-field state lies in this sector. The corresponding solutions for λ_i and b_i are $\lambda_i = 0$ and $b_i = b_0 = \text{const}$ for all i. The electronic spectrum shows a hybridization gap Δ_c (which is equal to the charge gap in the mean-field theory) whose dependence on J is shown as the dashed line in Fig. 1. (2) The $S = 1$ sector: The lowest-energy spin-1 mean-field solution has $\lambda_i = 0$ (as a consequence of the particle-hole symmetry) for all i, *but* b_i shows a sharp minimum as shown in the inset of Fig. 2(a). When compared to the $S = 0$ ground state, the electronic spectrum associated with the $S = 1$ mean-field solution shows two midgap states which are both singly occupied. The spin-density

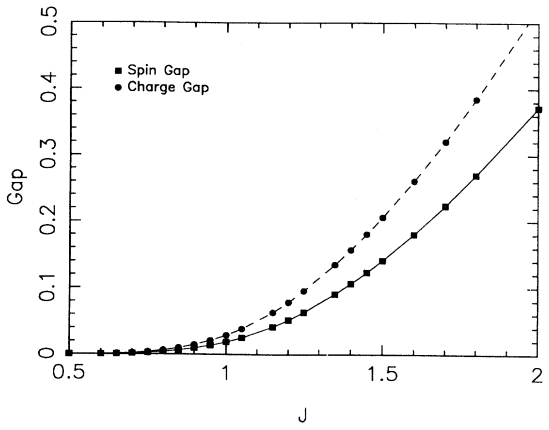

FIG. 1. Mean-field spin and charge gaps as a function of the Kondo coupling J.

distribution $S_z(x)$ associated with the $(S = 1, S_z = 1)$ state is shown in Fig. 2(a). The spin distribution remains localized for *all* values of the Kondo coupling $J > 0$. The character of this local triplet changes continuously from an f-f triplet in the weak-coupling limit to an f-c triplet in the strong-coupling limit. The shape of the local triplet changes from involving f electrons in three neighboring unit cells (with a central spin-$\frac{1}{2}$ f electron) in the weak-J limit to involving one c and one f electron in the same unit cell in the strong-coupling limit. The energy

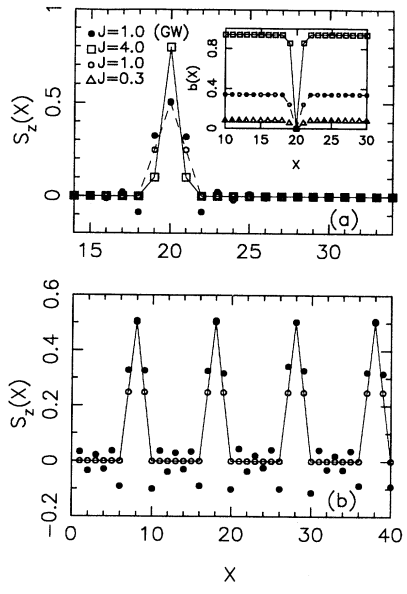

FIG. 2. (a) Spin-density distribution of the lowest-energy $(S = 1, S_z = 1)$ state. Inset: The self-consistent solution of the hybridization field $b(x)$. The soliton centers are fixed at the same position for comparison. (b) Mean-field (open circles) and Gutzwiller-projected (solid circles) spin-density distribution for the lowest-energy $(S = 4, S_z = 4)$ state at $J = 1$. In both (a) and (b), the error bars associated with the numerical Gutzwiller projection are less than the size of the symbol.

cost E_s to create such a localized spin-1 charge-neutral excitation, which we call a triplet soliton, is shown as the solid line in Fig. 1. Both Δ_c and E_s show the characteristic exponential behavior $\exp(-1/\gamma J)$ in the weak-coupling regime, and smooth crossover to linear J dependence in the strong-coupling regime. Moreover, $E_s < \Delta_c$ for *all* values of J. (3) The $S=M$ (M=integer) sector: The lowest-energy mean-field solution in this case has $\lambda_i = 0$ for all i, and b_i shows M localized minima which are maximally separated. This indicates that the residual interactions between the triplet solitons are repulsive in nature. The corresponding electronic spectrum shows $2M$ singly occupied midgap states. The $S_z(x)$ distribution associated with the ($S=M$, $S_z=M$) state configuration is shown in Fig. 2(b). Thus, the spin excitations in the one-dimensional (1D) half-filled Kondo lattice always appear in the form of triplet solitons.

GUTZWILLER-PROJECTED MEAN-FIELD SOLUTIONS

It is clear that the constraint $n_{if}=1$ is only satisfied on average in the above mean-field solutions. Do these results survive when we rigorously eliminate the spurious charge degrees of freedom? To answer this question we have performed Gutzwiller projections[3] on our mean-field wave functions $|\Phi^{\rm mf}\rangle$. The results are summarized as follows. (1) The $S=0$ sector: It is simple to show that after Gutzwiller projection, our mean-field $S=0$ ground-state wave function describes the exact ground state made of L independent local c-f singlets in the strong-coupling limit (the quality of our wave functions in the entire range of Kondo coupling is discussed below). The difference of the energy expectations between the Gutzwiller-projected lowest particle-hole band excitation and the Gutzwiller-projected $S=0$ ground state, i.e., the charge gap Δ_c, is plotted against J as the dashed line in Fig. 3(a). (2) The $S=1$ sector: The spin-density distribution $S_z(x)$ in the projected ($S=1$, $S_z=1$) local triplet state for $J=1$ is shown by the solid circles in Fig. 2(a). The effect of the projection is to attach a fast-dying oscillatory tail to the localized mean-field spin distribution. Although the extent of the oscillatory tail varies somewhat upon changing the Kondo coupling, the triplet core remains localized for *all* values of J.

In the presence of lattice translational symmetry, all eigenstates should have definite crystal momentum. To construct the $S=1$ crystal momentum eigenstates, we write $|\Psi_q\rangle = \sum_{x_c} \exp(iqx_c)|\Psi_{x_c}\rangle$, where $|\Psi_{x_c}\rangle = P_G|\Phi^{\rm mf}_{x_c}\rangle$ is the Gutzwiller-projected local triplet state with the center of the soliton located at x_c. Computing the energy expectation value

$$E_q^s = \frac{\langle \Psi_q | \mathcal{H}_{\rm KL} | \Psi_q \rangle}{\langle \Psi_q | \Psi_q \rangle} \tag{7}$$

using the Monte Carlo method and subtracting the corresponding projected ground-state energy in the $S=0$ sector, we obtain the dispersion relation for the creation energy of the triplet soliton ε_q^s which is shown in Fig. 3(b) for two values of J. The spin gap is given by $\Delta_s = \min(\varepsilon_q^s)$, which corresponds to $q=\pi$ for all values of J [see Fig. 3(b)]. The spin gap Δ_s as a function of J is shown in Fig. 3(a) by the solid line. Again, both Δ_c and Δ_s show the characteristic exponential J dependence $\exp(-1/\gamma_{c,s}\rho J)$ in weak coupling ($\rho = 1/4\pi t$) with $\gamma_s = 2.05 \pm 0.02$, $\gamma_c = 2.56 \pm 0.01$, and smooth crossover to linear J dependence in strong coupling. We have checked that in the thermodynamic limit both our spin gap and charge gap recover the exact results $\Delta_s = J$ and $\Delta_c = \frac{3}{2}J$ in the strong-coupling limit. Indeed, one can show that after the Gutzwiller projection, both our spin and charge-excited wave functions become exact in the strong-coupling limit. In order to get a feeling for the quality of our wave functions for weak and intermediate Kondo couplings, we compare our spin gap with that obtained by Tsunetsugu *et al.*[4(c)] from exact diagonalization [the open squares in Fig. 3(a)] and find excellent agreement over a wide range of J, indicative of a substantial overlap of our projected wave functions with the exact ones. As shown in Fig. 3(a), after Gutzwiller projection the spin gap Δ_s remains lower than the charge gap Δ_c for *all* values of J. As the result, the one-dimensional Kondo insulator exhibits *spin charge separation.* (3) The $S=M$ sector: After the projection the $S_z(x)$ distribution associated with the $S=M$, $S_z=M$ local triplet state is shown as the solid circles in Fig. 2(b).

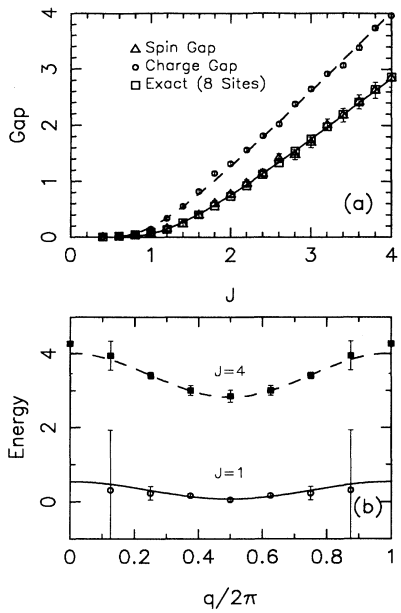

FIG. 3. (a) Gutzwiller-projected spin and charge gaps as a function of J. The open squares are the exact result of the spin gap on an eight-site chain from Ref. 4(c). (b) Dispersion of the triplet soliton creation energy ε_q^s.

EXPERIMENTAL IMPLICATIONS

The results presented above have several experimental implications.

(1) Dynamical spin susceptibility: The dynamical spin susceptibility $\chi(\mathbf{q},\omega)$ is given by

$$\chi(\mathbf{q},\omega)=-\sum_{\alpha}\frac{\langle 0|\mathbf{S}_q|\alpha\rangle\langle\alpha|\mathbf{S}_{-q}|0\rangle}{\omega-(E_q^{\alpha}-E_0)+i0^+}\ , \tag{8}$$

where the sum extends over all eigenstates $|\alpha\rangle$. Given the narrowness of the local triplet soliton dispersion, we anticipate the low-frequency spin susceptibility to be almost $\mathbf{q}$ independent. It is interesting to mention that a recent neutron-scattering experiment on CeNiSn (Ref. [7]) shows an $R\chi(\mathbf{q},\omega\rightarrow 0)$ which is almost $\mathbf{q}$ independent.

(2) Low-temperature magnetic susceptibility induced by doping with "Kondo holes:" As one substitutes a magnetic rare earth by a nonmagnetic one[8,9] (e.g., substituting Ce in CeNiSn by La), locally the Kondo spin disappears and hence a "Kondo hole" is created. In our model we simulate the Kondo-hole doping by raising the self-energy of an f orbital far above the chemical potential [i.e., by adding a term $\epsilon_f n_{0f}$ to Eq. (4)]. In that case we find that the lowest-energy mean-field state lies in the $S=\frac{1}{2}$ sector. The mean-field and the Gutzwiller-projected spin-density distribution associated with the ($S=\frac{1}{2}$, $S_z=\frac{1}{2}$) state is shown in Fig. 4. The electronic spectrum shows a single midgap state which is singly occupied in the mean-field solution. The character of this doping-induced spinon changes from purely f-like in weak coupling to purely c-like in strong coupling. Further studies show that λ_i and b_i profiles are identical to those of the $S=1$ local triplet in the stoichiometric system. Therefore, upon Kondo-hole doping the system nucleates an $S=1$ local triplet centered at the impurity Kondo hole, from which an f spin is subsequently removed. In the small-J limit, the energy of the system with a Kondo hole equals that of the local triplet state in the stoichiometric system since the center f spin in the latter can be freely removed, whereas in the large-J limit the Kondo hole gains a magnetic energy of $J/4$ by breaking the on-site f-c triplet. The spinons induced by Kondo-hole doping can in principle be detected via electron spin resonance experiment. Moreover, they will also contribute a Curie component to the low-temperature susceptibility.

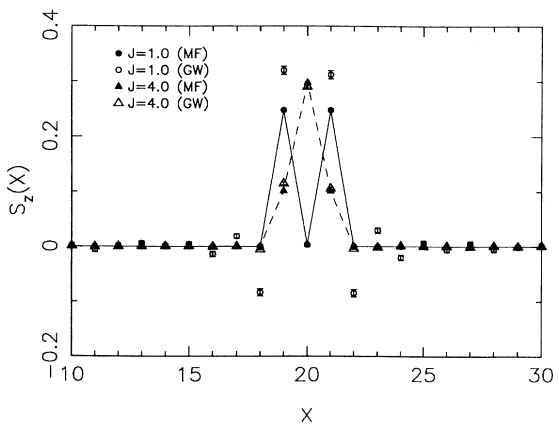

FIG. 4. The mean-field and Gutzwiller-projected ground-state spin-density distribution in the presence of a Kondo hole.

(3) External field-induced magnetic and metal-insulator transition: In an external magnetic field, the triplet solitons gain a Ziman energy $-g\mu_{\text{eff}}H$. As the result, when the field strength is greater than $H_c=\Delta_s/g\mu_{\text{eff}}$, it becomes energetically favorable to nucleate triplet solitons. For $H>H_c$, the repulsion among the triplet solitons due to the Kondo effect prevents the system from being fully polarized. Indeed, for small $H-H_c$, we find[11] that the magnetization is proportional to $H-H_c$.[8(c)] In the case where the soliton has an infinite size, a metal-insulator transition would directly occur at H_c. On the other hand, if the soliton has a finite extend, as in the one-dimensional Kondo lattice, the magnetic state remains insulating at H_c. As one increases the strength of the magnetic field, more triplet solitons are created and they begin to overlap at a field strength $H_c'>H_c$, at which point the system becomes metallic (as long as the Kondo coupling is finite, such that the c character of the triplet soliton is nonzero). For $H_c<H<H_c'$, the nature of the magnetic phase (itinerant vs localized ferromagnetism) is determined by the ratio of the soliton bandwidth and the strength of their repulsion.

(4) Manifestation of the spin charge separation: $\Delta_s<\Delta_c$ can, for example, be revealed by comparing the thermally activated transport studies and the low-temperature NMR studies. It is interesting to note that such a discrepancy is indeed observed for CeNiSn.[2] However, it is unclear whether such behavior is intrinsic. Furthermore, recent NMR studies performed on $Ce_3Bi_4Pt_3$ indicate a spin gap close to the charge gap extracted from thermal transport.[10] It should be emphasized, though, that the latter material is far into the mixed-valence regime characterized by a relatively large Kondo temperature compared to CeNiSn, which is thought to be close to the Kondo regime.

It is well known[12] that the heavy Fermi-liquid state in the Kondo lattice is unstable against the introduction of a *direct* RKKY interaction among the f spins, so long as the averaged RKKY coupling strength exceeds $k_B T_k$. A similar question can be asked about the stability of the Kondo insulating state against the RKKY interaction. For example, one can simulate the RKKY interaction by adding to Eq. (1) a direct nearest-neighbor Heisenberg antiferromagnetic exchange $J_H\mathbf{S}_i\cdot\mathbf{S}_j$. Such an interaction tends to decrease ε_q^s. In fact, a simple mean-field calculation in which one decouples both the Kondo coupling and the Heisenberg coupling leads to the conclusion that if $J_H>k_B T_k$ the mean-field ground state will be semimetallic. Therefore, like the heavy Fermi liquids, the Kondo insulators are also unstable against the large RKKY interaction.

All the results we report above are obtained for a one-dimensional Kondo lattice. A natural question is whether these results survive in higher dimensions. We have therefore looked at the two-dimensional square Kondo lattice. In that case we find that the mean-field solution the $S=1$ sector is also a local triplet. Although work is still in progress, we believe that most of the qualitative conclusions of this paper survive in two and three dimensions. This is not to say, however, that one should take

our results in quantitative sense. Effects such as higher-dimensionality, RKKY interaction, real crystalline structure, and finite Coulomb interaction among the conduction and the f electron can all change our results quantitatively. We have attempted to relate our results to the experiments on "Kondo insulators," bearing in mind that detailed comparisons are possible only after the above effects are taken into account.

Note added. After the completion of this work we were informed by Dr. Y. Hatsugai that the lowest spin triplet excitation does have crystal momentum $qa=\pi$ in agreement with our soliton dispersion.

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