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An RKKY-induced dimerized phase of the Kondo lattice model

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Abstract

We clarify the nature of the dimerized ground state found in the one-dimensional Kondo lattice model at quarter conduction electron filling. The conduction electrons mediate, through the RKKY mechanism, the long-range interactions among localized spins necessary to induce dimerization in that sub-system. On the other hand, the feedback of the local moments on the conduction electron fluid *does not* induce dimerization in the latter, whose spin sector remains gapless. The same feedback, however, is able to open a charge gap.

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The physics of heavy fermion materials is often described in terms of the Kondo lattice model [1]. Since a numerical analysis of the three-dimensional case is current beyond reach, most studies have focused on the one-dimensional case. Even though there is a good understanding of its phase diagram [2] some surprises remain. Recently, it has been demonstrated that the ground state at quarter conduction electron filling ($n = 1/2$) presents dimerization of the localized spins [3]. We give further details of these findings.

The model is described by the usual Hamiltonian of the spin-1/2 Kondo lattice chain

$$H = -\sum_{j=1,\sigma}^{L-1} \left(c^{\dagger}_{j,\sigma} c_{j+1,\sigma} + \text{H.c.}\right) + J \sum_{j=1}^{L} \mathbf{S}_j \cdot \mathbf{s}_j, \qquad (1)$$

where the notation is conventional, $\mathbf{S}_j$ is a spin-1/2 operator and $\mathbf{s}_j$ is the conduction electron spin density operator. We set the hopping and the lattice spacing to one. We treated the model with the density matrix renormalization group technique [4] with open boundary conditions. We used the finite-size algorithm for sizes up to $L = 120$ keeping up to $m = 800$ states per block. The discarded weight was typically about 10^{-5}–10^{-8} in the final sweep.

In Fig. 1 we show the dimer order parameter at $n = 1/2$ for localized spins $D_{\mathrm{l}}(j) = \langle \mathbf{S}_j \cdot \mathbf{S}_{j+1} \rangle$ and for conduction electrons $D_{\mathrm{c}}(j) = \langle \mathbf{s}_j \cdot \mathbf{s}_{j+1} \rangle$. In a uniform system $D(j)$ is j-independent, whereas it shows oscillations of period 2 in the presence of dimerization. It can be seen that the contribution of the localized spins is much more significant. In fact, the contribution from the conduction electrons is within the numerical error of the procedure and one cannot unambiguously state that there is long-range dimer order in the conduction electron fluid. By contrast, the localized spins show clear long-range dimer order. A finite-size scaling analysis in Ref. [3] shows that the dimerizationg does not die out as $L \to \infty$. The data therefore is consistent with long-range dimer order of the localized spins coexisting with quasi-long-range (power-law) dimer order of conduction electron spins.

This result is consistent with the picture presented in Ref. [3]. It was shown that the dimerization is induced in the localized spin sub-system by the RKKY interaction mediated by the conduction electrons. Indeed, the naive RKKY formula seems to favor a *classical* state of the localized moments with a $\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow \cdots$ type of order. This

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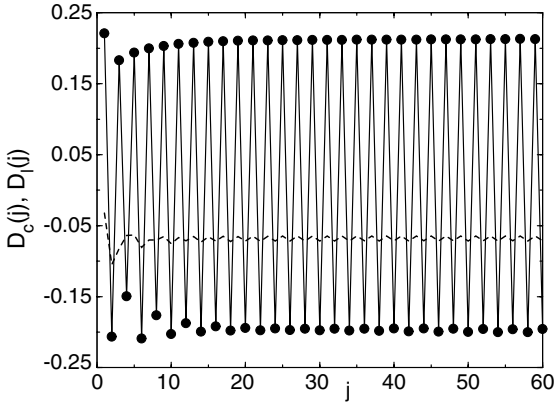

Fig. 1. The dimer order parameter for conduction electrons $D_c(j)$ and localized spins $D_l(j)$ vs lattice site for $J = 0.5$, $L = 120$ and density $n = 0.5$. Only half the chain is shown. The solid (dashed) line corresponds to $D_l(D_c)$.

conclusion is further corroborated by the amplitude of the oscillations of $D_l(j)$ in Fig. 1 $\sim$0.2. The above classical state would give an amplitude of 0.25, very close to observed value. Of course, quantum fluctuations restore the SU(2) invariance which cannot be spontaneously broken in one dimension. We conclude that the conduction electron fluid plays the part of the 'glue' that leads to dimerization and breaking of translation invariance.

On the other hand, the reverse is not necessarily true. The underlying dimer order of the local moments *does not* induce dimerization of the conduction electrons. It was shown by bosonization [3] that long-range dimer order of the localized spins generates a *staggered* nearest-neighbor exchange between conduction electrons at quarter-filling. Although this gives rise to a relevant perturbation in the charge sector (if $K_\rho < 1$), which opens a charge gap, it is only marginal in the spin sector and the conduction electron fluid can have a zero spin gap. This closes the self-consistent loop: the combined system is such that local moments are dimerized and gapped, whereas the conduction electrons have a charge gap but no spin gap. This is compatible with the picture emerging from Fig. 1.

It is interesting to note that a local picture, where one conduction electron binds to a triplet of nearest-neighbor local spins to form a spin-1/2 complex leads to a similar conclusion if these complexes are coupled like a spin-1/2 nearest-neighbor Heisenberg model (see Fig. 2).

Although the system is clearly dimerized at quarter-filling, it has only quasi-long-range, power law, antiferromagnetic order. This can also be confirmed numerically by plotting the spin-spin correlations as a function of the distance between spins, see Fig. 3. These correlations can be seen to die out with distance even at moderately small lattice sizes ($L = 40$). Therefore, the

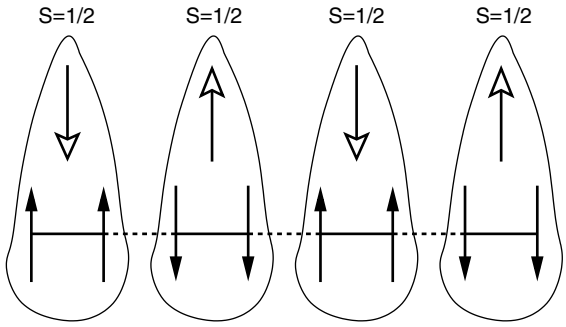

Fig. 2. Possible dimer structure at quarter-filling. The solid line connecting the localized spins denotes a triplet-like correlation while the dotted line a singlet-like one.

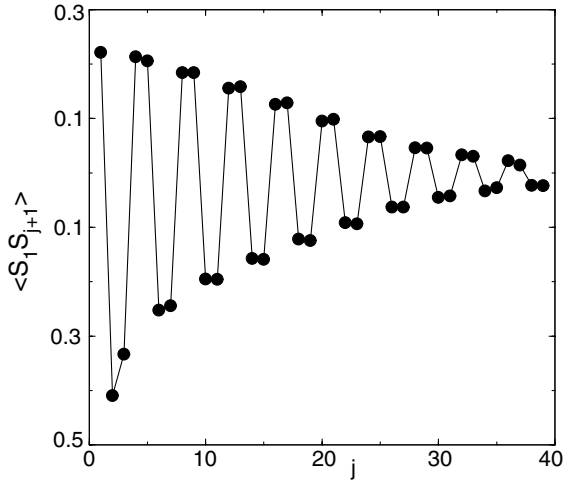

Fig. 3. Spin–spin correlation vs distance for $L = 40$, $J = 0.35$ and $n = 0.5$.

system exhibits long-range dimer order coexisting with quasi-long-range antiferromagnetic order, just like the J_1–J_2 Heisenberg model when $J_2 > 0.24J_1$ [5].

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