Available online at www.sciencedirect.com
SCIENCE DIRECT
Physica B 359–361 (2005) 102–104
PHYSICA B
www.elsevier.com/locate/physb

Ground state phases of the two-leg Kondo ladder

J.C. Xavier, E. Miranda*

Instituto de Física Gleb Wataghin, Unicamp/IFGW/DFMC, Caixa Postal 6165, 13083-970 Campinas, SP, Brazil

Abstract

We present the ground state phase diagram of the two-leg Kondo ladder obtained through the density-matrix renormalization group. At half-filling, the spin and charge gaps are non-zero. At other conduction electron densities, we have found fully and partially saturated ferromagnetism, paramagnetism, and dimerized phases at special commensurate fillings.

PACS: 75.30.Mb; 71.10.Pm; 75.10.−b

Keywords: Heavy fermions; Kondo model; Ladders

The Kondo lattice model is the simplest model believed to describe the essential physics of heavy fermion compounds [1]. The determination of its phase diagram in three dimensions is still an open question. It would be useful to do so with an unbiased numerical procedure. However, this is an impossible task in two or three dimensions with present computer power. A possible line of attack is then to consider the N-leg Kondo ladders (NKL). The NKL consist of N Kondo chains of length L coupled by the hopping term. The 2D system is obtained by taking both N and L to infinity.

Here, we are going to focus on the two-leg Kondo ladder with $M = 2 \times L$ sites with Hamiltonian

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

where $c_{j\sigma}$ annihilates a conduction electron in site j with spin projection σ, $\mathbf{S}_j$ is a localized spin $\frac{1}{2}$ operator, $\mathbf{s}_j = \frac{1}{2}\sum_{\alpha\beta} c^{\dagger}_{j,\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{j,\beta}$ is the conduction electron spin density operator and $\boldsymbol{\sigma}_{\alpha\beta}$ are Pauli matrices. Here $\langle ij\rangle$ denotes nearest-neighbor sites, $J>0$ is the Kondo coupling constant and the hopping amplitude was set to unity to fix the energy scale. We investigated the model with the density matrix renormalization group technique with open boundary conditions [2]. We used the finite-size algorithm for sizes up to $2 \times L = 80$,

*Corresponding Author. Tel.: +55 19 3788 5486; fax: +55 19 3788 4146.
E-mail address: emiranda@ifi.unicamp.br (E. Miranda).

0921-4526/$ - see front matter
doi:10.1016/j.physb.2005.01.003

keeping up to $m = 1200$ states per block. The discarded weight was typically about $10^{-5} - 10^{-9}$ in the final sweep.

We first focus on half-filling. In this case, the spin and charge gaps are non-zero for any Kondo coupling J [3], as can be seen in Fig. 1. These gaps are defined as $\Delta_s(L) = e(M,1) - e(M,0)$ and $\Delta_c(L) = e(M-2,0) - e(0,0)$, respectively, where $e(N_c, s)$ is the ground state energy of the system with N_c conduction electrons in the subspace of total spin s [4]. Similar results are found in the 1D case [4], as well in the 3KL [3]. These results suggest that the spin and charge gaps are non-zero for any number of legs and value of J at half-filling. Note that this behavior is quite different from the t-J ladders [5].

Away from half-filling we can probe the phase diagram by determining the Fourier transform of the spin–spin correlation function (the spin structure factor) $S(\vec{q}) = \frac{1}{2L}\sum_{\vec{r}_1,\vec{r}_2} e^{\vec{q}\cdot(\vec{r}_1-\vec{r}_2)}\langle \mathbf{S}^{\mathrm{T}}_{\vec{r}_1}\cdot\mathbf{S}^{\mathrm{T}}_{\vec{r}_2}\rangle$, where $\mathbf{S}^{\mathrm{T}}_{\vec{r}_1} = \mathbf{S}_{\vec{r}_1} + \mathbf{s}_{\vec{r}_1}$. In particular, the total spin S_{total} can be evaluated from the relation $S(\vec{q} = (0,0)) = 2L(S_{\mathrm{total}}(S_{\mathrm{total}}+1))$. We have found three distinct regions based on the values of the total spin, as shown in Fig. 2. The fully saturated ferromagnetic phase (FM) has $S_{\mathrm{total}} = (2L - N_c)/2$ while the paramagnetic (PM) one has $S_{\mathrm{total}} = 0$ [6]. We have also found a phase with partially saturated ferromagnetism (PFM) where $0 < S_{\mathrm{total}} < (2L - N_c)/2$ [6]. Note that, in the 1D case, ferromagnetism is present at any doping for large enough J [4]. It is intriguing that such a huge difference arises by coupling a single additional chain.

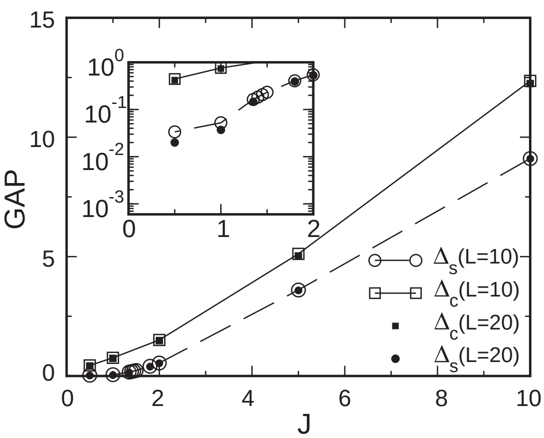

Fig. 1. The spin and charge gaps for the 2-leg Kondo ladder with $L = 10$ (open symbols) and $L = 20$ (closed symbols). The circles (squares) correspond to the spin (charge) gap. Inset: zoom of the region $0 < J < 2$.

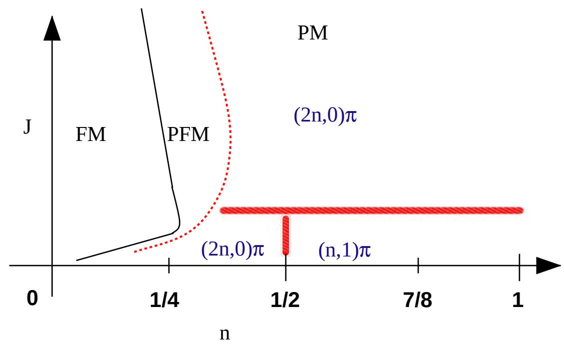

Fig. 2. Phase diagram of the 2KL. PM, FM, and PFM denote regions with paramagnetism, fully and partially saturated ferromagnetism, respectively. To the right of the dotted line, the thick lines separate three regions: small and large J, $n \geqslant 0.5$ and $n < 0.5$. These regions are characterized by the location of the spin–spin structure factor peak (see text). At half-filling, the spin and charge gaps are non-zero.

We have also found that in the PM phase the maximum of $S(\vec{q})$ can appear at three distinct positions, as indicated in Fig. 2. For small values of J, the maximum of $S(\vec{q})$ is located at $\vec{q} = (2n, 0)\pi$ for $n \lesssim 0.5$, while for $n \gtrsim 0.5$ it is at $\vec{q} = (n, 1)\pi$ [6]. For large values of J and $n \gtrsim 0.4$ $S(\vec{q})$ has only a small cusp at $\vec{q} = (2n, 0)\pi$ [6].

Recently spin dimerization was discovered in the 1D Kondo lattice model at quarter-filling [7]. We have found, at densities $n = \frac{1}{4}$ and $n = \frac{1}{2}$, that the spin correlations in the 2KL resemble the dimerization found in the 1D Kondo lattice model [6]. In order to illustrate this finding, we present in Fig. 3 the spin–spin correlations $\langle \mathbf{S}^{\mathrm{T}}_{\vec{r}_1}\cdot\mathbf{S}^{\mathrm{T}}_{\vec{r}_2}\rangle$ for nearest-neighbor sites of the 2KL at density $n = \frac{1}{4}$, $J = 0.8$ and $L = 32$. The solid (dashed) lines indicate that the correlation is negative (positive) and the line thickness is proportional to the amplitude of the correlations. As can be seen, along the legs the dimer order parameter $D(j) = \langle \mathbf{S}^{\mathrm{T}}_{(1,j)}\cdot\mathbf{S}^{\mathrm{T}}_{(1,j+1)}\rangle$ oscillates with period 2, while the rungs exhibit FM correlations. The origin of dimerization in the 1D Kondo lattice model was ascribed to the RKKY interaction [7]. A similar analysis, also suggests

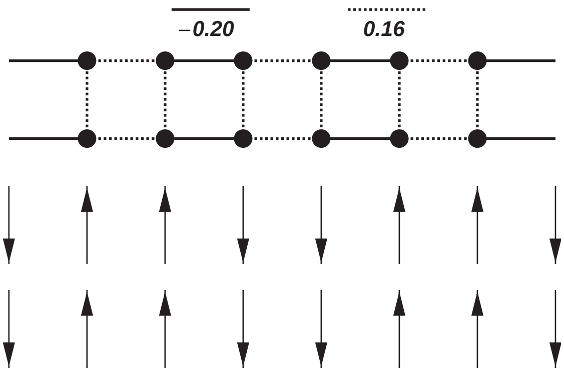

Fig. 3. Nearest-neighbor spin correlations of the 2KL for $L = 32$, $J = 0.8$, and $n = \frac{1}{4}$. Solid and dashed lines represent AFM and FM correlations, respectively. Only the central portion of the ladder is presented. Below the correlations, a classical configuration compatible with them is shown.

that this interaction is responsible for the spin arrangement shown in Fig. 3 [6].

In conclusion, we have obtained the phase diagram of the two-leg Kondo ladder and characterized its spin correlations as a function of Kondo coupling constant and conduction electron density.

This work was supported by grants from FAPESP (00/02802-7 (J.C.X.) and 01/00719-8 (E.M.)) and CNPq (301222/97-5 (E.M.)).

References

[1] A.C. Hewson, The Kondo Problem to Heavy Fermions, Cambridge University Press, UK, 1997.
[2] S.R. White, Phys. Rev. Lett. 69 (1993) 2863;
S.R. White, Phys. Rev. B 48 (1993) 10345.
[3] J.C. Xavier, Phys. Rev. B 68 (2003) 134 422.
[4] H. Tsunetsugu, M. Sigrist, K. Ueda, Rev. Mod. Phys. 69 (1997) 809.
[5] E. Dagotto, T.M. Rice, Science 271 (1996) 618.
[6] J.C. Xavier, E. Miranda, E. Dagotto, cond-mat/0405380.
[7] J.C. Xavier, R.G. Pereira, E. Miranda, I. Affleck, Phys. Rev. Lett. 90 (2003) 247 204.