The anisotropic Kondo necklace model

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Abstract

A real-space renormalization-group approach is used to investigate the zero temperature phase diagram of the Kondo necklace (KN) model in the presence of an Ising-like anisotropy parameter (δ). In the full anisotropic case, δ = 1, this approach yields a quantum critical point (QCP) separating an antiferromagnetic from a non-magnetic, Kondo-like, phase. The critical frontier of the phase diagram is presented as a function of the ratio between the coupling and the band with (J/W), and the anisotropic parameter (δ). We find for the KN model that a critical value δc of the anisotropy is required for the appearance of long range magnetic order at zero temperature.

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The study of the physical properties of heavy-fermions near the magnetic quantum critical point of these materials is an actual problem to which a lot of effort is being devoted both theoretically and experimentally. Heavy-fermions exhibit a variety of interesting phenomena and different ground states including antiferromagnetic, superconductor, Kondo-insulator and metallic [1,2]. Most of the properties of these systems can be attributed to their proximity to a magnetic quantum critical point (QCP) (see Ref. [3]). Recently, the effects of disorder in the Kondo lattice model have also been investigated [4–6] as this is an important ingredient in real systems. Using a non-perturbative RG approach, we have found that weak disorder is an irrelevant perturbation close to the magnetic QCP of the KN model [6]. The KN model was

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proposed by Doniach [7] to study heavy fermions and emphasizes magnetic degrees of freedom [8–11] neglecting charge fluctuations. It incorporates the essential physics of these systems, namely the competition between Kondo effect and magnetic ordering.

In this work we extend the previous renormalization group (RG) calculations to investigate the behavior of the one-dimensional KN model at zero temperature in the presence of an Ising-like anisotropy. As far as we know the phase diagram of the KN model in the whole space of the anisotropy parameter \(0 \leq \delta \leq 1\) has never been considered and the present letter represents a first step towards describing its effects in heavy fermions starting at a microscopic level. The anisotropic KN model is given by the Hamiltonian,

\[
H = \sum_{i=1}^{L-1} W_i (\sigma^x_i \sigma^x_{i+1} + (1 - \delta) \sigma^y_i \sigma^y_{i+1}) + \sum_{i=1}^{L-1} J \tilde{S}_i \tilde{\sigma}_i ,
\]

where \(\sigma^\mu\) and \(S^\mu, \mu = x, y, z\) are spin-1/2 Pauli matrices denoting the spin of the conduction electrons and those of the local moments, respectively. The sites \(i\) and \(i+1\) are nearest neighbors on a chain of \(L\) sites and \(W_i\) is an antiferromagnetic coupling which represents the hopping of the conduction electrons between neighboring sites. The Ising-like anisotropy parameter varies from 1 to zero. In the full anisotropic case \((\delta = 1)\), there is an unstable fixed point separating an antiferromagnetic phase from a spin compensated, Kondo-like phase, which can be fully characterized [6]. For the \(\delta = 0\) case, we have obtained that any interaction \(J\) gives rise to a dense Kondo state [6]. This result, \(J_c = 0\), is in agreement with the most recent density-matrix renormalization group [12] and quantum Monte Carlo calculations [13].

In the approximate decimation calculation used throughout this paper the linear chain may be viewed as \(b\) bonds in series, where \(b\) is the scaling factor \((b=2\) in Fig. 1). We define the renormalization transformation by referring the density matrix, for both the original and transformed systems, to a special basis. The introduction of the Ising-like anisotropy in the hopping terms leads us to consider the basis \(|m^x_1 m^y_2 \cdots m^x_L n^z_1 n^y_2 \cdots n^z_r\rangle\), where \(S^x \mid n^z_i\rangle = n^z_i \mid n^z_i\rangle, \sigma^x \mid m^x_i\rangle = m^x_i \mid m^x_i\rangle\) and \(\alpha = x, y\). At zero temperature the density matrix is essentially the ground state projector. The RG equations are obtained by the mapping of diagonal elements only. This approach has also been successfully applied to the transverse Ising model [14] and to quantum spin glasses [15].

![Fig. 1. The cells used in the renormalization group transformation, which correspond to a length scale factor \(b = 2\).](image-url)
a given configuration of on-site interactions and anisotropy parameter, \( K = J/W \) and \( \delta \), the RG transformation for the \( d = 1 \) system (Fig. 1) give us two matching conditions,

\[
\langle m^x_1 m^x_3 | \hat{\rho}'(K', \delta') | m^x_1 m^x_3 \rangle = \langle m^x_1 m^x_3 | \hat{\rho}(K, \delta) | m^x_1 m^x_3 \rangle
\]  

(2)

and

\[
\langle m^y_1 m^y_3 | \hat{\rho}'(K', \delta') | m^y_1 m^y_3 \rangle = \langle m^y_1 m^y_3 | \hat{\rho}(K, \delta) | m^y_1 m^y_3 \rangle
\]  

(3)

for the two unknowns \( K' = (J/W)' \) and \( \delta' \). The matrix elements,

\[
\langle m^x_1 m^x_3 | \hat{\rho}(K, \delta') | m^x_1 m^x_3 \rangle = \sum_{n_1, n_3} \langle m^x_1 m^x_3 n_1^2 n_3^2 | \rho(K, \delta) | m^x_1 m^x_3 n_1^2 n_3^2 \rangle
\]  

(4)

and

\[
\langle m^y_1 m^y_3 | \hat{\rho}(K, \delta) | m^y_1 m^y_3 \rangle
\]

\[
= \sum_{m_2, n_1, n_3} \langle m^y_1 m^y_3 m_2^2 n_1^2 n_3^2 | \rho(K, \delta) | m^y_1 m^y_3 m_2^2 n_1^2 n_3^2 \rangle,
\]

(5)

where \( x, y \) are obtained by performing the partial trace on the internal spins keeping those on the terminal sites (along the chain) fixed (see Fig. 1). The set of Eqs. (2), (3) yields two recursion relations which are formally given by,

\[
f'(K', \delta') = f(K, \delta)
\]

(6)

and

\[
g'(K', \delta') = g(K, \delta).
\]

(7)

The left-hand side of Eqs. (6), (7) are coupled analytical expressions for the primed variables in the renormalized cell but are too lengthy to be explicitly written here. For the original, larger cell, the right-hand side of these equations are written in a \( 64 \times 64 \) representation and the calculations have to be performed numerically. The matching of the quantities above, in the two cells, yields the RG equations which allow to obtain the phase diagram of the anisotropic \( KN \) model as a function of the anisotropic parameter \( \delta \) at \( T = 0 \).

For \( \delta = 1 \), we have only one equation and we recover our previous results for the full anisotropic \( KN \) model [6]. There is a quantum critical point at \( K_c = 0.21 \) separating an antiferromagnetic (\( AF \)) from a non-magnetic, Kondo singlet or spin-liquid phase. The critical exponents associated with this transition can be obtained in the usual way. For the correlation length, given by \( \xi \propto |\delta|^{-\nu} \), with \( \delta = K - K_c \), we obtain the exponent, \( \nu = 2.24 \approx 9/4 \). The dynamic exponent \( z \) is obtained from the finite size scaling relation for the gaps for excitations in the two cells, i.e., \( (\Delta E/\Delta E')_{K_c} = (L'/L)^z = b^z \), at the quantum critical point, where \( b = 2 \) is the length scale factor. We get \( z = 1.28 \). Using the quantum hyperscaling relation \( 2 - \alpha = \nu(d + z) \) we can also obtain the exponent \( \alpha = -3.12 \) which is negative but large in module. The spin-liquid, non-magnetic phase for \( K > K_c \) is characterized by a gap \( \Delta E = |\delta|^{\nu z} \) which vanishes at the QCP with the gap exponent, \( s = \nu z = 2.28 \). For \( \delta = 0 \), Eqs. (6), (7) are identical and we obtain the
Fig. 2. Schematic phase diagram of the anisotropic $KN$ model obtained from our renormalization method. The arrows give the flow of the RG equations.

original KN model. In this case any finite coupling $J$ gives rise to a non-magnetic, Kondo-like phase, i.e., $K_c = 0$ [6].

We next consider the Ising-like anisotropy parameter in the region $0 \leq \delta \leq 1$. In Fig. 2 we present our results for the zero-temperature $RG$ phase diagram, $K$ vs $\delta$. The system still exhibits two phases: the Ising anti-ferromagnetic phase and a non-magnetic, Kondo-like phase. The attractor of the antiferromagnetic phase in the presence of the anisotropy parameter is the same of the full anisotropic $AF$ phase. Therefore, the phase transition to the ordered magnetic phase is governed by the same critical exponents of the full anisotropic $\delta = 1$ case that we have calculated before. This is a consequence that the $RG$ flow along the critical line is towards the semi-stable fixed point of the Ising system at $K_c = 0.21$, $\delta = 1$, which therefore determines the universality class of the transition. We find for the $KN$ model that a critical value $\delta_c = 0.58$ of the anisotropy is required for the appearance of long-range magnetic order at zero temperature.

The existence of a finite and actually large value of $\delta$ to stabilize antiferromagnetic order in the system, even at $T = 0$ was not expected a priori. It shows the importance of quantum fluctuations in the Kondo necklace model which extends the spin liquid phase up to such large values of the anisotropy. Notice that the point $\delta_c$, $K = 0$ is not a fixed point. The line $K = 0$ corresponds to the $d = 1$, purely anisotropic $XY$ model which is ordered at $T = 0$ [16].

In conclusion, we have examined the phase diagram of the Kondo necklace model in the presence of an Ising-like anisotropy. The model is suitable to describe heavy fermion systems and emphasizes magnetic degrees of freedom neglecting charge fluctuations. The full anisotropic model is appropriate to describe systems where the ordered magnetic phase has a strong Ising character. In this case, the system presents a quantum critical point, at a finite value of $J/W$, separating the ordered magnetic phase from the spin liquid. We present the critical frontier separating the magnetic and non-magnetic phase as a function of the Ising anisotropy. We found a critical value for $\delta$ below which any interaction $J \geq 0$ gives rise to a dense Kondo state. The renormalization-group trajectories along the critical line flow towards the quantum critical point controlling the magnetic-spin liquid phase transition ($\delta = 1$). This implies that the exponents controlling the AF transition for finite $\delta$ are the same as those of the fully anisotropic $\delta = 1$ system.
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