Crossover from 2d to 3d in anisotropic Kondo lattices

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Abstract

We study the crossover from two to three dimensions in Kondo lattices (KLM) using the Kondo necklace model (KNM). In order to diagonalize the KNM, we use a representation for the localized and conduction electron spins in terms of bond operators and a decoupling for the relevant Green's functions. Both models have a quantum critical point at a finite value of the ratio (J/t) between the Kondo coupling (J) and the hopping (t). In 2d there is no line of finite temperature antiferromagnetic (AF) transitions while for $d \geqslant 3$ this line is given by, $T_N \propto |g|^{1/(d-1)}$ [D. Reyes, M.A. Continentino, Phys. Rev. B 76 (2007) 075114]. The crossover from 2d to 3d is investigated by turning on the electronic hopping $(t_\perp)$ of conduction electrons between different planes. The phase diagram as a function of temperature T, $J/t_\parallel$ and $\xi = t_\perp/t_\parallel$, where $t_\parallel$ is the hopping within the planes is calculated.
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1. Introduction

The study of low dimensional heavy fermions (HF) magnetic systems continues to be a focus of theoretical and experimental investigators [1–3]. Several theories were formulated to explain their unusual properties [4–6]. In this context the spin-density wave [5,6] (SDW) theory as well as the local quantum critical description [7] can account for the logarithmical divergent specific heat coefficients and quasi-linear resistivities only if the spin fluctuations are quasi-two dimensional. To take this into account we introduce an inter-layer coupling $t_\perp$. The idea is that turning it on leads to magnetic long range order to finite temperatures. We use the Kondo necklace model [8] as a simple Hamiltonian to explore this line of reasoning. It is given by

$$H = t_\parallel \sum_{\langle i,j \rangle} (\tau_i^x \tau_j^x + \tau_i^y \tau_j^y) + t_\perp \sum_{\langle i,j \rangle} (\tau_i^x \tau_j^x + \tau_i^y \tau_j^y) + J \sum_i \mathbf{S}_i \cdot \tau_i, \quad (1)$$

where τ_i are quantum spin-1/2 Pauli matrices representing the conduction electrons and $\mathbf{S}_i$ are localized spin operators. The sum $\langle i,j \rangle$ denotes summation over the nearest-neighbor sites. $t_\parallel$ is the hopping within the planes and $t_\perp$ the hopping between different planes. The $X - Y$ coupling term imitates the band energy of the conduction electrons and the third term represents the Kondo exchange via coupling J.

At strong coupling the ground state is an aggregate of intra-atomic Kondo singlets, the low-energy physics can be well described by triplet excitations from the Kondo singlet sea. To express this picture explicitly, we use the bond operators formalism [9], in which four creation operators are introduced to represent the four states in Hilbert space. This basis can be created out of the vacuum by singlet $|s\rangle$ and triplet $|t_\alpha\rangle = t_\alpha^\dagger|0\rangle$ $(\alpha = x, y, z)$ operators. In terms of these triplet and singlet operators the localized and conduction electron spin operators are given by $S(\tau)_{i,\alpha} = \frac{1}{2}(\pm s_i^\dagger t_{i,\alpha} \pm t_{i,\alpha}^\dagger s_i - i\varepsilon_{\alpha\beta\gamma} t_{i,\beta}^\dagger t_{i,\gamma})$, respectively. The restriction that the physical states are either singlets or triplets leads to the constraint $s^\dagger s + \sum_\alpha t_\alpha^\dagger t_\alpha = 1$.

Substituting the operator representation of spins into the original Hamiltonian (1), making $\langle s_i^\dagger \rangle = \langle s_i \rangle = \bar{s}$, in the strong coupling approximation and $t_{\mathbf{k},x} = \sqrt{N}\bar{t}\delta_{\mathbf{k},\mathbf{Q}} + \eta_{\mathbf{k},x}$ corresponding to introduce the antiferromagnetic (AF)

order parameter $\bar{t}$, we can obtain the mean field Hamiltonian. Using Green's function approach we obtain $\ll t_{\mathbf{k},x(y)}$; $t^{\dagger}_{\mathbf{k},x(y)} \gg_{\omega} = (1/2\pi)(\omega + \Lambda_{\mathbf{k}})/(\omega^2 - \omega_{\mathbf{k}}^2)$ and $\ll t_{\mathbf{k},z}; t^{\dagger}_{\mathbf{k},z} \gg_{\omega} = (1/2\pi)(1/(\omega - \omega_0))$ and consequently the excitations of the system. Above, $\omega_0 = (J/4 + \mu)$ is the dispersionless longitudinal spectrum of the spin triplet states and $\omega_k = \pm\sqrt{\Lambda_{\mathbf{k}}^2 - (2D_{\mathbf{k}})^2}$ correspond to the excitation spectrum of the transverse spin triplet states with two branches $\omega_x = \omega_y$. The other terms are $\Lambda_{\mathbf{k}} = \omega_0 + 2D_{\mathbf{k}}$, $\lambda(\mathbf{k})_{\parallel} = \cos k_x + \cos k_y$, $\Delta_{\mathbf{k}} = \frac{1}{4} t_{\parallel} \bar{s}^2 \lambda(\mathbf{k})_{\parallel}$, $\lambda(\mathbf{k})_{\perp} = \cos k_z$, $\Delta'_{\mathbf{k}} = \frac{1}{4} t_{\perp} \bar{s}^2 \lambda(\mathbf{k})_{\mathbf{z}}$, $D_{\mathbf{k}} = \Delta_{\mathbf{k}} + \Delta'_{\mathbf{k}}$, N is the number of lattice sites. The wave-vectors k are taken in the first Brillouin zone and the lattice spacing was assumed to be unity.

The Gibbs free energy can be directly obtained from the energy of the excitations given by the poles of Green's functions. It is given by

$$G_{AF} = \varepsilon_0 - \frac{2}{\beta} \sum_{\mathbf{k}} \ln[1 + n(\omega_{\mathbf{k}})] - \frac{N}{\beta} \ln[1 + n(\omega_0)] \quad (2)$$

with

$$\varepsilon_0 = N\left(-\frac{3}{4} J\bar{s}^2 + \mu\bar{s}^2 - \mu + (\omega_0 - \bar{s}^2(2t_{\parallel} + t_{\perp}))\bar{t}^2\right) + \sum_{\mathbf{k}}(\omega_{\mathbf{k}} - \omega_0) \quad (3)$$

being the ground state energy of the system. $\beta = 1/k_B T$, $n(\omega) = \frac{1}{2}(\coth(\beta\omega/2) - 1)$, $\bar{s}$ and $\bar{t}$ the singlet and triplet order parameter, respectively.

Since the parameter $\bar{s}$ is always nonzero [10] and $\bar{t} \neq 0$ in the AF phase, we minimize the ground state energy with respect to $\bar{t}$ to find, $\mu = t_{\parallel} \bar{s}^2/y - J/4$ and consequently, $\omega_{\mathbf{k}} = \frac{1}{y} t\bar{s}^2 \sqrt{1 + y(\lambda(\mathbf{k})_{\parallel} + \xi\lambda(\mathbf{k})_{\perp})}$ where $\xi = t_{\perp}/t_{\parallel}$ is the anisotropy ratio and $y = 1/(2 + \xi)$.

Minimizing the Gibbs free energy given by Eq. (2) using $(\partial\varepsilon/\partial\mu, \partial\varepsilon/\partial\bar{s}) = (0, 0, 0)$, we can easily get

$$\bar{t}^2 = 1 - \frac{J}{t_{\parallel}} \frac{y}{2} - \frac{1}{2N} \sum_{\mathbf{k}} \frac{1}{\sqrt{1 + y(\lambda(\mathbf{k})_{\parallel} + \xi\lambda(\mathbf{k})_{\perp})}} \coth\frac{\beta\omega_{\mathbf{k}}}{2} - \varsigma, \quad (4)$$

where $\varsigma = \frac{1}{4}(\coth(\beta\omega_0/2) - 1)$. Generally for $\xi = 0(1)$ at $T = 0$ the results of Ref. [10] to $2d(3d)$ are recovered.

The Neel line giving the finite temperature instability of the AF phase for $J/t_{\parallel} < (J/t_{\parallel})_c$ is obtained as the line in the T vs $(J/t_{\parallel})$ plane at which $\bar{t}$ vanishes ($\bar{t} = 0$). So for temperatures $k_B T \ll \omega_0$ ($\varsigma \sim 0$) and expanding close to the wave-vector $\mathbf{Q} = (\pi, \pi, \pi)$ associated with the AF instability we obtain

$$|g|\frac{y}{2} = \frac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} \frac{k_{\parallel} dk_{\parallel} dk_z}{\sqrt{\frac{y}{2}(k_{\parallel}^2 + \xi k_z^2)}} \left(\coth\frac{\beta\omega_{\mathbf{k}}}{2} - 1\right), \quad (5)$$
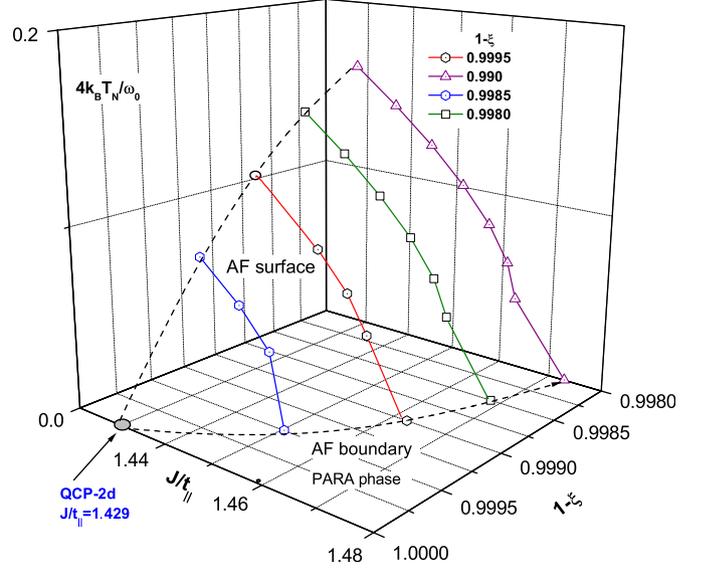
Fig. 1. (Color online) Sketch of Eq. (6) for $\xi \ll 1$. We can see that turning on ξ, there is a critical line of Neel that goes out from a new QCP that depends of ξ. The QCPs starting in QCP-$2d$ sketch a line that defines the AF boundary. Outside of the AF surface it is found the paramagnetic (PARA) phase.

where $g = |(J/t_{\parallel})_c - (J/t_{\parallel})|$ measures the distance to the quantum critical point (QCP).

In order to analyze the quasi-two dimensional regime, we consider $\xi \ll 1$, thereby $y \approx \frac{1}{2}(1 - \xi/2)$, so solving Eq. (4) with this approximation we obtain

$$|g|_{\xi \ll 1} = \frac{\sqrt{\xi}}{2(1 - \xi)} + \frac{1}{(1 - \xi)\pi} T\left[1 - \ln\left(\frac{2\pi\sqrt{\xi}}{T}\right)\right]. \quad (6)$$

This expression gives us the dependence between the critical line of Neel transitions and the anisotropy ratio ξ for temperatures $k_B T \ll \omega_0$, where ω_0 tracks J and $4k_B T_N \omega_0 = T$. It is sketched in Fig. 1.

In summary, we have obtained analytically the expression for the Neel line close to the QCP to quasi-two dimensional HF systems and we have shown that this line exists for values $\xi \ll 1$.

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