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Phase diagram of the Kondo necklace model at finite temperatures

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Abstract

A simplified version of the Kondo lattice model, the Kondo necklace model, is studied at finite temperature using a representation for the localized and conduction electron spins in terms of local Kondo singlet and triplet operators. We calculate the double time Green's functions to get the dispersion relation of the excitations of the system. We show that in 3-d there is an antiferromagnetic ordered state at finite temperatures, but in 2-d long-range magnetic order occurs only at $T = 0$.

Keywords: Kondo necklace; Quantum critical point

It is well known that the nature of the ground state of the dense Kondo compounds results basically from the competition between the Ruderman–Kittel-Kasuya–Yosida (RKKY) interaction and the Kondo effect. This is governed by a single parameter, the ratio J/t, where J is the effective exchange between localized moments and conduction electrons and t is the hopping term related to the bandwidth of the latter. The RKKY interaction is an indirect magnetic interaction between localized moments, mediated by the polarized conduction electrons, which produces a long-range-ordered magnetic ground state. On the other hand, the Kondo effect favors the formation of singlet states between localized moments and conduction electrons generating a non-magnetic ground state. As a result of the interplay between these two effects, some Kondo compounds are non-magnetic and are characterized by a heavy-fermion behavior (Fermi-liquid) at very low temperatures, while others order magnetically, generally antiferromagnetically. The study of this interplay is easily formulated using the Kondo lattice model (KLM), which emphasizes the importance of spin fluctuations neglecting charge

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fluctuations of the localized electrons [1]. The KLM is a theoretical model for heavy fermions that can be derived from the more fundamental Anderson lattice model in the case of well-developed local spin moments [2]. The KLM consists of two different types of electrons, the localized spins whose charge degrees of freedom are suppressed and the conduction electrons that propagate as charge carriers. It is described by

$$H = -t\sum_{\langle i,j\rangle}(c^{\dagger}_{i,\sigma}c_{j,\sigma} + \mathrm{h.c.}) + J\sum_{i}\mathbf{S}_i.c^{\dagger}_{i,\alpha}\sigma_{\alpha\beta}c_{i,\beta}. \tag{1}$$

The first term represents the conduction band ($c^{\dagger}_{i,\sigma}$, is a creation operator, t is the hopping between nearest neighbors) and the second term is the interaction between conduction electrons and localized moments $\mathbf{S}_i$ via the intra-site exchange J. σ_i are Pauli matrices. In order to study the interplay between Kondo screening and the RKKY interaction, Doniach proposed a simplified model related to the one-dimensional Kondo lattice, called the Kondo Necklace Model (KNM). In this model, the conduction electrons are replaced by a spin chain with XY coupling [1]

$$H = t\sum_{\langle i,j\rangle}(\tau^x_i\tau^x_j + \tau^y_i\tau^y_j) + J\sum_i \mathbf{S}_i.\boldsymbol{\tau}_i, \tag{2}$$

where $\boldsymbol{\tau}_i$ and $\mathbf{S}_i$ are independent sets of spin-$\frac{1}{2}$ Pauli operators. The first term mimics electron propagation and in one dimension can be mapped by the Jordan–Wigner transformation onto a band of spinless fermions. The second term is the magnetic interaction between conduction electrons and localized spins $\mathbf{S}_i$ via the coupling J, as in Eq. (1). Usually, for two $S=\frac{1}{2}$ spins τ_i and $\mathbf{S}_i$ placed on a lattice site, the local Hilbert space is spanned by four states consisting of one singlet and three triplet states defined by, $|s> = s^{\dagger}|0>$ and $|t_{\alpha}> = t^{\dagger}_{\alpha}|0>$ $(\alpha = x, y, z)$. A representation of the impurity spins and conduction electron spins in terms of these singlet and triplet operators is given by [3]

$$S_{n,\alpha} = \tfrac{1}{2}(s^{\dagger}_n t_{n,\alpha} + t^{\dagger}_{n,\alpha}s_n - i\varepsilon_{\alpha\beta\gamma}t^{\dagger}_{n,\beta}t_{n,\gamma}), \tag{3}$$

$$\tau_{n,\alpha} = \tfrac{1}{2}(-s^{\dagger}_n t_{n,\alpha} - t^{\dagger}_{n,\alpha}s_n - \mathrm{i}\varepsilon_{\alpha\beta\gamma}t^{\dagger}_{n,\beta}t_{n,\gamma}), \tag{4}$$

where α, β, γ represent components along the x, y and z axes, respectively, and ε is the antisymmetric Levi–Civita tensor. This type of spin representation in terms of singlet and triplet (bond) operators was first proposed by Sachdev and Bhatt to study the properties of dimerized phases [3]. Substituting this operator representation for the local and conduction electron spins and considering that the local Kondo spin singlets and triplets condense, the latter at the AF reciprocal vector $t_{\mathbf{k},x} = \sqrt{N}\bar{t}\delta_{\mathbf{k},Q} + \eta_{\mathbf{k},x}$. Finally using the Green's functions to obtain the thermal averages of the singlet and triplet correlation functions, we obtain for the total mean-field energy,

$$\varepsilon = \varepsilon' + \frac{\omega_0}{2}\sum_{\mathbf{k}}\left(\coth\frac{\omega_0}{2k_{\mathrm{B}}T} - 1\right) + \sum_{\mathbf{k}}\left(\omega_{\mathbf{k}}\coth\frac{\omega_{\mathbf{k}}}{2k_{\mathrm{B}}T} - \omega_0\right) \tag{5}$$

$$\varepsilon' = N\left(-\frac{3}{4}J\bar{s}^2 + \mu\bar{s}^2 - \mu + \left(\frac{J}{4} + \mu - \frac{1}{2}Zt\bar{s}^2\right)\bar{t}^2\right) \tag{6}$$

which generalizes the results of Ref. [4] to finite temperatures. Above ω_0 is the dispersionless energy level of the antiparallel spin-triplet excited state, $\omega_{\mathbf{k}} = \sqrt{\Lambda^2_{\mathbf{k}} - (2\Delta_{\mathbf{k}})^2}$ corresponds to the excitation spectrum of the parallel spin-triplet excited states, Z is the total number of the nearest neighbors on the hyper-cubic lattice and μ the Fermi energy. When the order parameter $\bar{t}$ is nonzero, minimizing Eq. (6) with respect to $\bar{t}$ yields $\mu = \frac{1}{2}Zt\bar{s}^2 - J/4$, which makes the parallel spin-triplet excitation spectrum gapless, $\omega_{\mathbf{k}} = \frac{1}{2}Zt\bar{s}^2\sqrt{1 + 2\lambda(\mathbf{k})/Z}$. The mean field $\bar{t}$ represents the AF order parameter. Finally, we derive the saddle-point equations, and obtain at finite temperatures

$$\bar{s}^2 = 1 + \frac{J}{Zt} - \frac{1}{2N}\sum_{\mathbf{k}}\sqrt{1 + 2\lambda(\mathbf{k})/Z}\coth\frac{\omega_{\mathbf{k}}}{2k_{\mathrm{B}}T} + \frac{1}{4Nk_{\mathrm{B}}T}\sum_{\mathbf{k}}\sqrt{1 + 2\lambda(\mathbf{k})/Z}\frac{\omega_{\mathbf{k}}}{\sinh^2\frac{\omega_{\mathbf{k}}}{2k_{\mathrm{B}}T}} + \xi,$$

$$\bar{t}^2 = 1 - \frac{J}{Zt} - \frac{1}{2N}\sum_{\mathbf{k}} \frac{1}{\sqrt{1+2\lambda(\mathbf{k})/Z}} \coth\frac{\omega_{\mathbf{k}}}{2k_B T} + \frac{1}{4Nk_B T}\sum_{\mathbf{k}} \frac{1}{\sqrt{1+2\lambda(\mathbf{k})/Z}} \frac{\omega_{\mathbf{k}}}{\sinh^2\frac{\omega_{\mathbf{k}}}{2k_B T}} + \xi,$$

where

$$\xi = -\frac{1}{4N}\sum_{\mathbf{k}}\left(\coth\frac{\omega_0}{2k_B T} - 1\right) + \frac{\omega_0}{8Nk_B T}\sum_{\mathbf{k}} \frac{1}{\sinh^2\frac{\omega_0}{2k_B T}}. \quad (7)$$

In 2-d, at zero temperature, we find an antiferromagnetic ground for $J/4t < 0.36$, but no long-range magnetic order at finite temperatures. In 3-d, the equation determining the AF order parameter close to zero temperature is given by

$$0.44 - \frac{6\sqrt{3}}{\pi^2}\left(\frac{k_B T}{\omega_0}\right)^3 = \frac{J}{6t}, \quad (8)$$

where $\omega_0 = 3t\bar{s}^2$. The phase diagram is shown in Fig. 1. There is a quantum critical point (QCP) at $x_c = (J/t)_c = 2.65$ and a line of finite temperature phase transitions which rises from the QCP as $T_N \propto |x - x_c|^{\psi}$, with a shift exponent $\psi = \frac{1}{3}$.

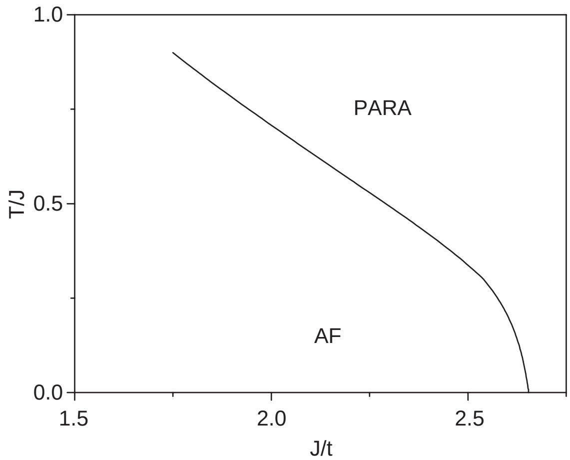

Fig. 1. Phase diagram for the Kondo necklace in three dimensions.

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