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PHASE DIAGRAM OF KONDO NECKLACE MODEL TO FINITE TEMPERATURE

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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.

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Keywords: Kondo necklace, quantum critical point, magnetic field.

Resumen

En el presente trabajo se presenta una versión simplificada del modelo de celda de Kondo, el llamado modelo del collar, a una temperatura finita usando una representación para los espines electrónicos de conducción localizados, en términos de los operadores de Kondo: singlete y triplete. Se calcula las funciones dobles de Green dependientes del tiempo para obtener la relación de dispersión de las excitaciones del sistema. Se demuestra que en tres dimensiones existe un estado ordenado antiferromagnético a temperaturas finitas, sin embargo, en dos dimensiones un orden magnética de alto rango ocurren solamente a T = 0.

Palabras claves: Collar Kondo, punto cuántico crítico, campo magnético.

It is well known that the nature of the ground stare of dense Kondo compounds results basically from the competition between the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction and the Kondo effect. It 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 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 emphasized the importance of spin fluctuations neglecting charge fluctuations of the localized electrons and has been well characterized by the Doniach phase diagram [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]. It 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

$$H = -t\sum_{<i,j>}\left(C^{\dagger}_{i,\sigma}C_{j,\sigma} + H\cdot c\right) + J\sum_{i} S_{i}\cdot C^{\dagger}_{i,\sigma}\sigma_{\alpha\beta}C_{i,\beta} \tag{1}$$

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The first term represents the conduction band ($C_{i,\sigma}^{\dagger}$, is the creation operator, t is the hopping between nearest neighbors) and the second term is the interaction between electrons and localized moment S_i via the intra-site exchange J, where σ are the 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 which eliminates charge fluctuations [1]:

$$H = t\sum_{<i,j>}\left(\tau_i^x\tau_j^x + \tau_i^y\tau_j^y\right) + J\sum_i S_i\cdot\tau_i \qquad (2)$$

where τ_i and S_i are independent sets of spins $-1/2$ 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 S_i via the coupling J, as in equation [1]. Usually, for two $s = 1/2$ spins τ_i and S_i placed on a lattice site, the local Hilbert spaced is spanned by four states consisting of one singlet and three triplet states defined by: $|s\rangle = s^{\dagger}|0\rangle$ and $|t_\alpha\rangle = t_\alpha^{\dagger}|0\rangle$ ($\alpha = x, y, z$). A representation of the impurity spins and conduction electron spins in terms of these singlet and triplet operators is given by

$$S_{n,\alpha} = \frac{1}{2}\left(s_n^{\dagger}t_{n,\alpha} + t_{n,\alpha}^{\dagger}s_n - i\in_{\alpha}\beta_{\gamma}\, t_{n,\beta}^{\dagger}t_{n,\gamma}\right) \qquad (3)$$

$$\tau_{n,\alpha} = \frac{1}{2}\left(-s_n^{\dagger}t_{n,\alpha} - t_{n,\alpha}^{\dagger}s_n - i\in_{\alpha}\beta_{\gamma}\, t_{n,\beta}^{\dagger}t_{n,\gamma}\right) \qquad (4)$$

where α, β, γ represents components along the x, y and z axes, respectively and $\in$ is the antysimetric 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 the operator representation of the impurity and conduction electron spins and considering that, the local Kondo spin singlets (s bosons) and local Kondo spin triplets (t_{kx}) condenses, as well on the AF reciprocal vector $t_{k,x} = \sqrt{N}\,\bar{t}\,\delta_{k,Q} + \eta_{k,x}$, it will lead considering at finite temperature.

$$\varepsilon = \varepsilon_g + \frac{\omega_0}{2}\sum_k\left(coth\frac{\omega_0}{2KT} - 1\right) + \sum_k\left(\omega_k\, coth\frac{\omega_k}{2KT} - \omega_0\right) \qquad (5)$$

$$\in_g = N\left(-\frac{3}{4}J\bar{s}^2 + \mu\bar{s}^2 - \mu + \left(\frac{J}{4} + \mu - \frac{1}{2}Zt\bar{s}^2\right)\bar{t}^2\right) \qquad (6)$$

where ω_0 is the dispersionless energy level of the antiparallel spin triplet excited state, $\omega_k = \sqrt{\Lambda_k^2 - (2\Delta_k)^2}$ corresponds to the excitation spectrum of the parallel spin triplet excited states and Z is the total number of the nearest neighbors on the cubic lattice. When the order parameter $\bar{t}$ is nonzero, the saddle point equation for $\bar{t}$ yields $\omega_k = \frac{1}{2}Zt\bar{s}^2\sqrt{1+2\lambda(k)/Z}$. The mean field $\bar{t}$ represent the AF order parameter. We derive the saddle-point equations, and finally obtain at finite temperature

$$\bar{s}^2 = 1 + \frac{J}{Zt} - \frac{1}{2N}\sum_k\sqrt{1+2\lambda(k)/Z}\, coth\frac{\omega_k}{2KT} + \frac{1}{4NKT}\sum_k\sqrt{1+2\lambda(k)/Z}\frac{\omega_k}{sinh^2\frac{\omega_k}{2KT}} + \xi \qquad (7)$$

$$\bar{t}^2 = 1 - \frac{J}{Zt} - \frac{1}{2N}\sum_k\frac{1}{\sqrt{1+2\lambda(k)/Z}}coth\frac{\omega_k}{2KT} + \frac{1}{4NKT}\sum_k\frac{1}{\sqrt{1+2\lambda(k)/Z}}\frac{\omega_k}{sinh^2\frac{\omega_k}{2KT}} + \xi \qquad (8)$$

where

$$\xi = -\frac{1}{4N}\sum_k\left(coth\frac{\omega_0}{2KT} - 1\right) + \frac{\omega_0}{8NKT}\sum_k\frac{1}{sinh^2\frac{\omega_0}{2KT}} \qquad (9)$$

Near to ground state, we have for 2D and 3D respectively,

$$0{,}35712-2\frac{\sqrt{2}}{\Pi}exp^{-\frac{\omega_0\sqrt{2}}{KT}}-\frac{1}{2}exp^{-\frac{\omega_0}{2KT}}\left(1-\frac{\omega_0}{KT}\right)=\frac{J}{4t} \qquad (10)$$

where $\omega_0 = 2t\overline{s}^2$

$$0{,}44234-\frac{6\sqrt{3}}{\Pi^2}\left(\frac{KT}{\omega_0}\right)^3-\frac{1}{2}exp^{-\frac{\omega_0}{2KT}}\left(1-\frac{\omega_0}{KT}\right)=\frac{J}{6t} \qquad (11)$$

where $\omega_0 = 3t\overline{s}^2$.

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