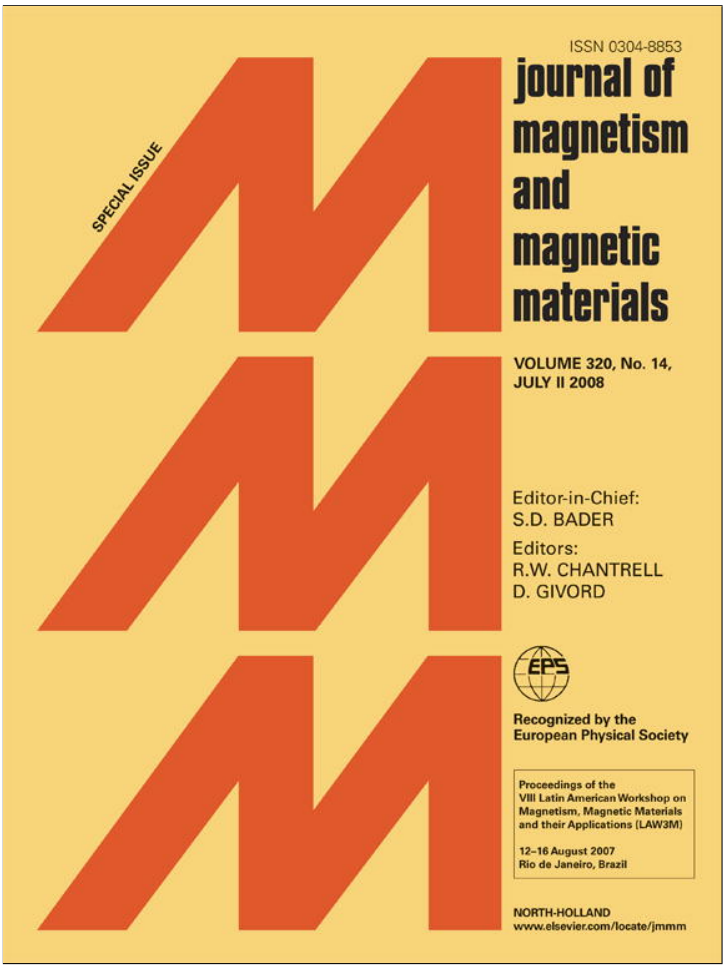

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Field induced magnetic quantum critical behavior in the Kondo necklace model

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Abstract

The Kondo necklace model augmented by a Zeeman term, serves as a useful model for heavy fermion compounds in an applied magnetic field. The phase diagram and thermodynamic behavior for arbitrary dimensions d has been investigated previously in the zero field case [D. Reyes, M. Continentino, Phys. Rev. B 76 (2007) 075114. [1]]. Here we extend the treatment to finite fields using a generalized bond operator representation for the localized and conduction electrons spins. A decoupling scheme on the double time Green's functions yields the dispersion relation for the excitations of the system. Two critical magnetic fields are found namely, a critical magnetic field called henceforth h_{c1} and a saturation field nominated h_{c2}. Then three important regions can be investigated: (i) Kondo spin liquid state (KSL) at low fields $h<h_{c1}$; (ii) destruction of KSL state at $h\geqslant h_{c1}$ and appearance of a antiferromagnetic state; and (iii) saturated paramagnetic region above the upper critical field h_{c2}.

Keywords: Kondo necklace model; Quantum phase transition; Kondo insulator

1. Introduction

The Kondo necklace model (KNM) [2] provides an approximate description of Kondo insulators [3] and heavy fermion (HF) materials. At half-filling, local singlet formation dominates whenever the Kondo coupling ratio J/t exceeds some value $(J/t)_c$ called quantum critical point (QCP); RKKY antiferromagnetism wins out otherwise. If a magnetic field is applied, this interferes with the singlet-RKKY competition by favoring triplet rather than singlet formation at each site. Accordingly, it suppresses the singlet amplitude and thus has the potential to stabilize an antiferromagnetic (AF) phase. Moreover, the Zeeman splitting lifts the degeneracy of the spin up and spin down bands, shifting them with respect to one another and potentially closing the spin gap. In this paper, we show by bond operator mean-field calculations that as the applied field is turned on the Kondo spin liquid ground state of the KNM with Zeeman splitting gives way to a AF phase at h_{c1}. At sufficiently large field, the localized spins become polarized and the system crosses over to a saturated paramagnetic regime. The KNM hamiltonian in a external magnetic field is given by

$$H = t\sum_{\langle i,j\rangle}(\tau_i^x\tau_j^x + \tau_i^y\tau_j^y) + J\sum_i \mathbf{S}_i.\boldsymbol{\tau}_i + h\sum_i(\mathbf{S}_i + \boldsymbol{\tau}_i), \quad (1)$$

where τ_i and $\mathbf{S}_i$ are independent sets of spin-$\frac{1}{2}$ Pauli operators, representing the conduction electron spin and localized spin operators, respectively. The sum $\langle i,j\rangle$ denotes summation over the nearest-neighbor sites. The first term mimics electron propagation. The second term is the magnetic interaction between conduction electrons and localized spins $\mathbf{S}_i$ via the coupling J. The last one is the Zeeman term where $h = g\mu_B H$, g the gyromagnetic ratio, μ_B the Bohr magneton and H a transversal magnetic field. We assume that the g factors of the conduction electron and localized spins are the same, and set $g\mu_B = 1$.

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2. Bond operator mean field formulation

For two $S=\frac{1}{2}$ spins, Sachdev and Bhatt [4] introduced four creation operators 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. However, the classic bond operators are not the eigenstates of an transversal magnetic field, and so we transform these to the operators [5], $t_x = 1/\sqrt{2}(d-u)$ and $t_y = -\mathrm{i}/\sqrt{2}(u+d)$, which create the triplet states, $u^\dagger|0\rangle = |\uparrow\uparrow\rangle$, $d^\dagger|0\rangle = |\downarrow\downarrow\rangle$ and $t_z^\dagger|0\rangle = 1/\sqrt{2}(|\uparrow\downarrow\rangle + |\uparrow\downarrow\rangle)$. On this basis the magnetic field term has the diagonal representation $h(S+\tau) = \mathrm{i}h(t_y^\dagger t_x - t_x^\dagger t_y) = h(u^\dagger u - d^\dagger d)$, ensuring that the operators $u^\dagger$, $d^\dagger$ and $t_z^\dagger$ reproduce the energy levels of the field eigenstates $S_z = +1,-1,0$, respectively. Further, the transformation conserves particle number by sites, $s_i^\dagger s_i + u_i^\dagger u_i + d_i^\dagger d_i + t_{iz}^\dagger t_{iz} = 1$. In terms of these operators the localized (conduction electron) spin operator is given by

$$S(\tau)^+ = \frac{1}{\sqrt{2}}(\pm s^\dagger d \mp u^\dagger s + t_z^\dagger d + u^\dagger t_z),$$

$$S^-(\tau) = (S^+(\tau))^\dagger,$$

$$S^z(\tau) = \tfrac{1}{2}(\pm s^\dagger t_z \pm t_z^\dagger s + t_z^\dagger d + u^\dagger t_z). \tag{2}$$

At zero field, as for all magnetic fields below the critical field h_{c1}, the system is in the quantum disordered regime with a spin gap between the singlet and triplet states on each site. This situation, for which the bond-operator technique is most directly applicable, is represented by neglecting the dynamics of the singlet operator and replacing s_i everywhere by a c-number $\bar{s}_i$, corresponding to a condensate of singlets. Proceeding within a mean-field approximation, the operators s_i and the site-dependent chemical potentials μ_i are replaced by uniform, global average values $\langle s_i\rangle = \bar{s}$ and $\mu_i = \mu$. Substituting the operator representation of spins defined in Eq. (2) into the original Hamiltonian and making a Fourier transformation we obtain

$$\begin{aligned} H_{mf} = {} & N\left(-\frac{3}{4}J\bar{s}^2 + \mu\bar{s}^2 - \mu\right) + \left(\frac{J}{4}+\mu\right)\sum_{\mathbf{k}} t_{\mathbf{k},z}^\dagger t_{\mathbf{k},z} \\ & + \sum_{\mathbf{k}} [(\Lambda_{\mathbf{k}} + h)u_{\mathbf{k}}^\dagger u_{\mathbf{k}} + (\Lambda_{\mathbf{k}} - h)d_{\mathbf{k}}^\dagger d_{\mathbf{k}}] \\ & + \sum_{\mathbf{k}} [\Delta_{\mathbf{k}}(u_{\mathbf{k}} d_{-\mathbf{k}} + d_{\mathbf{k}} u_{-\mathbf{k}} + \text{h.c.})], \end{aligned} \tag{3}$$

where $\Lambda_{\mathbf{k}} = \omega_0 + 2\Delta_{\mathbf{k}}$,

$$\lambda(\mathbf{k}) = \sum_{s=1}^{d} \cos k_s,$$

$\Delta_{\mathbf{k}} = \frac{1}{4}t\bar{s}^2\lambda(\mathbf{k})$, N is the number of lattice sites, Z is the total number of the nearest neighbors on the hyper-cubic lattice. The wavevectors k are taken in the first Brillouin zone and the lattice spacing was assumed to be unity. Diagonalization of the Hamiltonian (3) using the Green's functions gives us the thermal averages as

$$\begin{aligned} U = \langle \mathscr{H}_{mf}\rangle = {} & \varepsilon_0 + \frac{\omega_0}{2}\sum_{\mathbf{k}}\left(\coth\frac{\beta\omega_0}{2} - 1\right) \\ & + \sum_{\mathbf{k}}\left(\frac{\omega_{\mathbf{k}}+h}{2}\right)\left(\coth\frac{\beta(\omega_{\mathbf{k}}+h)}{2} - 1\right) \\ & + \sum_{\mathbf{k}}\left(\frac{\omega_{\mathbf{k}}-h}{2}\right)\left(\coth\frac{\beta(\omega_{\mathbf{k}}-h)}{2} - 1\right), \end{aligned} \tag{4}$$

where

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

is the ground state energy of the system and $\beta = 1/k_B T$. In this phase exist three modes with dispersion relations $\omega_k + h$, $\omega_k - h$ and ω_0, where $\omega_k = \pm\sqrt{\Lambda_{\mathbf{k}}^2 - (2\Delta_{\mathbf{k}})^2}$ is the dispersion relation for the field-free system and $\omega_0 = (J/4+\mu)$ the dispersionless spectrum of the longitudinal spin triplet states. In the disordered regime the triplet modes do not change the form of their dispersion, and are merely split by the magnetic field due to the Zeeman interaction.

3. Kondo spin liquid state ($h < h_{c1}$)

An increase in the applied field leads to a shift in mode energies without changing the shape of their zero-field dispersion, until the lowest mode becomes soft at $Q = (\pi,\pi,\pi)$. This determines the critical field as

$$h_{c1} = \Delta = \omega_0\sqrt{1 - \frac{yZ}{2}}, \tag{5}$$

where $y = t\bar{s}^2/\omega_0$ is a dimensionless parameter and Δ the energy spin gap. A simple understanding may be obtained by considering a single, isolated site with AF coupling J: at zero field the ground state is a singlet, and the threefold degenerate triplet excitations at energy gap $\Delta = J$ separate in an applied field due to the Zeeman interaction. At a critical field, given by $h_{c1} = \Delta$, the energy of the lowest triplet $|\downarrow\downarrow\rangle$ is reduced to zero, and the crossing of levels changes the ground state from singlet to triplet.

4. AF phase ($h_{c1} < h < h_{c2}$)

In the intermediate-field regime, the ground state of each site can be considered as a partially polarized ferromagnetic configuration. It is important to note that there is no explicit AF component in the singlet ground state, and that the ordering emerges only from closing of the gap to the lowest magnon branch at $k = Q$. In the bond-operator formulation, this ordered ground state is represented [6,7] by finite expectation values $\bar{s}$, $\bar{u}$, and $\bar{d}$ of these singlet and triplet operators. The component of the highest-lying triplet mode in the ground-state condensate may appear counterintuitive, and was neglected in a number of approximate treatments [5,8]. However, the presence of

terms of the form $u_k d_{-k}$ in the transformed Hamiltonian Eq. (3) makes clear that a finite component of this state is required in the consistent condensate. This process becomes important when the hopping t is comparable to the coupling exchange J and when h is not much larger than h_{c1}. So the ground state is of pure triplet nature and the lowest-lying excitation is a singlet. Although the conventional bond-operator treatment may lose consistency in the description of these excitations because higher-order interactions between triplets are contained in an uncontrolled manner we believe that it will give us a correct description. The coefficients of the ground-state singlet–triplet admixture change continuously with the applied field until the upper critical field or magnetic field of saturation h_{c2}, where all spins are aligned.

5. Saturated phase ($h > h_{c2}$)

In the strong field regime the spins are full parallel saturated. In bond operator notation the state with most probability is $|\uparrow\uparrow\rangle$ so we make assumption of $\langle u^\dagger\rangle = \langle u\rangle = \overline{u}$. Making approximations already used in the bond-operator formalism [5,9] and after performing a Fourier transformation of the boson operators, we get,

$$\begin{aligned} H_{mf} &= N((\omega_0 + h)\overline{u}^2 - \mu) \\ &\quad + \sum_{\mathbf{k}} [A_{\mathbf{k}} s^\dagger_{\mathbf{k}} s_{\mathbf{k}} + B_{\mathbf{k}} t^\dagger_{\mathbf{k},z} t_{\mathbf{k},z} + C_{\mathbf{k}} d^\dagger_{\mathbf{k}} d_{\mathbf{k}}] \\ &\quad + \sum_{\mathbf{k}} [D_{\mathbf{k}} (s_{\mathbf{k}} t^\dagger_{-\mathbf{k}z} + t_{\mathbf{k}z} s^\dagger_{-\mathbf{k}} + \text{h.c.})], \end{aligned} \tag{6}$$

where $A_{\mathbf{k}} = -\frac{3}{4}J + \mu + 2D_{\mathbf{k}}$, $B_{\mathbf{k}} = \omega_0 + 2D_{\mathbf{k}}$, $C_{\mathbf{k}} = \omega_0 - h$ and $D_{\mathbf{k}} = \frac{1}{4} t\overline{u}^2 \lambda(\mathbf{k})$. Using the Green's functions propagators method in Eq. (6) and solving the coupled equations of motion obtained we get,

$$\ll s_{\mathbf{k}}; s^\dagger_{\mathbf{k}} \gg_\omega = \frac{1}{2\pi} \frac{\omega - \Lambda_{\mathbf{k}}}{(\omega - \Lambda_{\mathbf{k}} + J/2)^2 - M^2_{\mathbf{k}}},$$

$$\ll t_{\mathbf{k},z}; t^\dagger_{\mathbf{k},z} \gg_\omega = \frac{1}{2\pi} \frac{\omega - \Lambda_{\mathbf{k}} + J}{(\omega - \Lambda_{\mathbf{k}} + J/2)^2 - M^2_{\mathbf{k}}},$$

$$\ll d_{\mathbf{k}}; d^\dagger_{\mathbf{k}} \gg_\omega = \frac{1}{2\pi(\omega - (\omega_0 - h))}, \tag{7}$$

where $M_{\mathbf{k}} = \sqrt{(J/2)^2 + (2D_{\mathbf{k}})^2}$, ω_0 and $\Lambda_{\mathbf{k}}$ as defined before. The poles of the Green's functions propagators Eq. (7) determine the excitation energies of the system in this phase as $\omega_{1,2}(\mathbf{k}) = \Lambda_{\mathbf{k}} - J/2 \mp M_{\mathbf{k}}$ and $\omega_3(\mathbf{k}) = \omega_0 - h$. Then one may deduce the upper critical field,

$$h_{c2} = \left(\frac{J}{4} + \mu\right). \tag{8}$$

This phase is characterized by a decoupling of the triplet modes and by a finite energy gap to the lowest mode, which corresponds to an excitation from the triplet ground state to a singlet.

In summary, we have investigated the effect of an applied magnetic field on the Kondo necklace ground state, using bond operators mean field calculations (in the thermodynamic limit) to characterize the phases of the KNM with field. From these analytical results, a consistent picture emerges: (i) In the $J/t > (J/t)_c$ the magnetic excitations at low fields are merely the Zeeman-split magnons of the zero-field case, whose dispersion is unaltered by any field up to the lower critical field h_{c1}, where the spin gap is closed. (ii) For $h_{c1} = \Delta$, the spin gap closes and the local singlet phase gives way to an AF phase. (iii) At larger fields, above the saturation field ($h \geqslant h_{c2}$), the ground state becomes a pure condensate of the lowest triplet and a saturation field h_{c2} is required to overcome all of the AF bonds.

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