

# Thermodynamic quantum critical behavior of the Kondo necklace model

Daniel Reyes\*

Centro Brasileiro de Pesquisas Físicas, Rua Dr. Xavier Sigaud, 150-Urca, Rio de Janeiro 22290-180, Brazil

Mucio A. Continentino<sup>†</sup>

Instituto de Física, Universidade Federal Fluminense, Campus da Praia Vermelha, Niterói, Rio de Janeiro 24.210-340, Brazil

(Received 23 July 2006; revised manuscript received 17 April 2007; published 15 August 2007)

We obtain the phase diagram and thermodynamic behavior of the Kondo necklace model for arbitrary dimensions  $d$  using a representation for the localized and conduction electrons in terms of local Kondo singlet and triplet operators. A decoupling scheme on the double time Green's functions yields the dispersion relation for the excitations of the system. We show that in  $d \geq 3$ , there is an antiferromagnetically ordered state at finite temperatures terminating at a quantum critical point (QCP). In two dimensions, long-range magnetic order occurs only at  $T=0$ . The line of Néel transitions for  $d > 2$  varies with the distance to the quantum critical point QCP  $|g|$  as  $T_N \propto |g|^\psi$ , where the shift exponent  $\psi = 1/(d-1)$ . In the paramagnetic side of the phase diagram, the spin gap behaves as  $\Delta \approx \sqrt{|g|}$  for  $d \geq 3$ , consistent with the value  $z=1$  found for the dynamical critical exponent. We also find in this region a power law temperature dependence in the specific heat for  $k_B T \gg \Delta$  and along the non-Fermi-liquid trajectory. For  $k_B T \ll \Delta$ , in the so-called Kondo spin liquid phase, the thermodynamic behavior is dominated by an exponential temperature dependence.

DOI: 10.1103/PhysRevB.76.075114

PACS number(s): 74.20.De, 74.70.Tx

## I. INTRODUCTION

Quantum phase transitions from an antiferromagnetic (AF) ordered state to a nonmagnetic Fermi liquid in heavy fermion systems have been the subject of intense research recently.<sup>1</sup> In contrast to classical phase transitions, driven by temperature, quantum phase transitions can be driven by magnetic field, external pressure, or doping. The physics of heavy fermion compounds is mainly due to the competition of two main effects: the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between the magnetic ions which favors long-range magnetic order and the Kondo effect which tends to screen the moments and produce a nonmagnetic ground state. These effects are contained in the Kondo lattice model (KLM) Hamiltonian,<sup>2</sup> which can be derived from the more fundamental Anderson lattice model in the case of well-developed local spin moments.<sup>3</sup> Although this model neglects charge fluctuations, since the relevant quantum critical point (QCP) in heavy fermion materials is associated with a magnetic transition, to consider only spin fluctuations<sup>4</sup> turns out to be an excellent approximation. The KLM has been studied by different techniques, and the general physical picture that arises is that at  $T=0$ , there is a quantum phase transition from a magnetic phase at small coupling strength  $J/t$  to a nonmagnetic dense Kondo phase at a critical value of  $J/t$ .

Here, we investigate a simplified version of this model, the so-called Kondo necklace model<sup>2</sup> (KNM), which for all purposes can be considered yield results similar to the original model. We use the bond-operator approach introduced by Sachdev and Bhatt<sup>5</sup> which was employed previously to both KLM<sup>6</sup> and KNM<sup>4</sup> models but always at zero temperature. We extend this approach to finite temperatures<sup>7</sup> and obtain the phase diagram of the KNM for arbitrary dimensions. We find that this method yields a critical Néel line in three dimensions but not in two dimensions as expected from general arguments.<sup>8</sup> This implies that fluctuations are taken into

account to an important extent in spite of the mean-field type of decoupling used to deal with the bond-operator Hamiltonian. We also calculate the thermodynamic properties along the non-Fermi-liquid (NFL) trajectory above the QCP.<sup>9-12</sup>

The KNM replaces the hopping term of the conduction electrons by an  $X$ - $Y$  interaction among the conduction electron spins.<sup>2</sup> It is given by

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

where  $\tau_i$  and  $\mathbf{S}_i$  are independent sets of spin-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 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  $J$ .

The paper is organized as follows: In Sec. II, we introduce the bond-operator treatment of the KNM. In Sec. III, we make and discuss the approximations required to solve the problem. The Green's function method is employed to attain this solution, as can be easily generalized to finite temperatures. We obtain a closed set of equations for the Green's functions that can be immediately solved without further approximations. The temperature dependence of the singlet and triplet order parameters is found in Sec. IV. In Sec. V, the finite-temperature phase diagram of the KNM is discussed. In Sec. VI, we study the paramagnetic phase and find the dependence of the spin gap with the distance to QCP. In Sec. VII, the behavior of the specific heat of the KNM is presented. The last section (Sec. VIII) offers the conclusions and discussions.

## II. BOND-OPERATOR REPRESENTATION

We use the method of bond operators, which has the advantage of making the connection to the lattice degrees of freedom most direct. For two  $S = \frac{1}{2}$  spins, Sachdev and Bhatt<sup>5</sup> 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. In terms of these triplet and singlet operators, the localized and conduction electron spin operators are given by

$$\begin{aligned} S_{i,\alpha} &= \frac{1}{2}(s_i^\dagger t_{i,\alpha} + t_{i,\alpha}^\dagger s_i - i\epsilon_{\alpha\beta\gamma} t_{i,\beta}^\dagger t_{i,\gamma}), \\ \tau_{i,\alpha} &= \frac{1}{2}(-s_i^\dagger t_{i,\alpha} - t_{i,\alpha}^\dagger s_i - i\epsilon_{\alpha\beta\gamma} t_{i,\beta}^\dagger t_{i,\gamma}), \end{aligned} \quad (2)$$

where  $\alpha, \beta$ , and  $\gamma$  take the values  $x, y$ , and  $z$ , repeated indices are summed over, and  $\epsilon$  is the totally antisymmetric Levi-Civita tensor. In particular, an important feature of the bond-operator mean-field approach is that the simplest mean-field theory to be used below already yields ground states and excitations with the correct quantum numbers, so a strong fluctuation analysis is not needed to capture the proper physics. The restriction that the physical states are either singlets or triplets leads to the constraint  $s_i^\dagger s_i + \sum_\alpha t_{i,\alpha}^\dagger t_{i,\alpha} = 1$ . Moreover, the singlet and triplet operators at each site satisfy bosonic commutation relations  $[s, s^\dagger] = 1, [t_\alpha, t_\beta^\dagger] = \delta_{\alpha,\beta}, [s, t_\alpha^\dagger] = 0$ . Substituting the operator representation of spins defined in Eq. (2) into the original Hamiltonian and considering the commutation relations, we obtain

$$H = H_0 + H_1 + H_2, \quad (3)$$

where

$$H_0 = \frac{J}{4} \sum_i \left( -3s_i^\dagger s_i + \sum_\alpha t_{i,\alpha}^\dagger t_{i,\alpha} \right) + \sum_i \mu_i \left( s_i^\dagger s_i + \sum_\alpha t_{i,\alpha}^\dagger t_{i,\alpha} - 1 \right),$$

$$H_1 = \frac{t}{4} \sum_{\langle ij \rangle, \alpha} [s_i^\dagger s_j^\dagger t_{i,\alpha} t_{j,\alpha} + s_i^\dagger s_j t_{i,\alpha} t_{j,\alpha}^\dagger + \text{H.c.}],$$

$$H_2 = -\frac{t}{4} \sum_{\langle ij \rangle, \alpha} [t_{i,z}^\dagger t_{j,z}^\dagger t_{i,\alpha} t_{j,\alpha} - t_{i,z}^\dagger t_{j,z} t_{i,\alpha} t_{j,\alpha}^\dagger + \text{H.c.}],$$

with  $\alpha = x, y$ .  $H_0$  represents the interaction between spins  $S$  and  $\tau$  in site  $i$  and the constraint  $s_i^\dagger s_i + \sum_\alpha t_{i,\alpha}^\dagger t_{i,\alpha} = 1$  is implemented through the local chemical potentials  $\mu_i$ .  $H_1$  and  $H_2$  are terms associated with the hopping. There is still another term in the Hamiltonian that consists of three triplets and one singlet operator. This is not taken into account since it vanishes in the approximation that we use below.<sup>4</sup>

## III. ANTIFERROMAGNETIC PHASE

The Hamiltonian above, at half filling, i.e., with one conduction electron per site, can be simplified using a mean-field decoupling of the quartic terms while still retaining the relevant physics. The resulting effective Hamiltonian  $H_{mf}$  with only quadratic operators is sufficient to describe exactly the quantum phase transition from the ordered AF state to the disordered Kondo spin liquid at least for  $d \geq 3$ , as discussed

below. Besides, it also yields sensible results in two dimensions, where no line of finite-temperature transitions is found. Relying on the nature of the strong coupling limit ( $t/J \rightarrow 0$ ), we take  $\langle s_i^\dagger \rangle = \langle s_i \rangle = \bar{s}$ , which corresponds to a *condensation of the local Kondo spin singlets on each site*. Next, to describe the condensation of one local Kondo spin triplet  $t_{k,x}$  on the AF reciprocal vector  $Q = (\pi/a, \pi/a, \pi/a)$ , we introduce  $t_{k,x} = \sqrt{N\bar{t}} \delta_{k,Q} + \eta_{k,x}$  corresponding to *fixing the orientation of the localized spins along the  $x$  direction*. The quantity  $\bar{t}$  is the mean value of the  $x$ -component spin triplet in the ground state and  $\eta_{k,x}$  represents the fluctuations. Finally, the translation invariance of the problem implies that we may assume the local chemical potential as a global one.

We will consider here only the terms  $H_0$  and  $H_1$ ; the  $H_2$  term has only small contributions to the results, therefore, it is neglected.<sup>13,14</sup>

After performing a Fourier transformation of the boson operators, the mean-field effective Hamiltonian is given by

$$\begin{aligned} H_{mf} &= N \left( -\frac{3}{4} J \bar{s}^2 + \mu \bar{s}^2 - \mu \right) \\ &+ \left( \frac{J}{4} + \mu \right) \sum_{\mathbf{k}} t_{k,z}^\dagger t_{k,z} + \left( \frac{J}{4} + \mu - \frac{1}{2} t Z \bar{s}^2 \right) N \bar{t}^2 \\ &+ \sum_{\mathbf{k}} [\Lambda_{\mathbf{k}} \eta_{k,x}^\dagger \eta_{k,x} + \Delta_{\mathbf{k}} (\eta_{k,x}^\dagger \eta_{-k,x}^\dagger + \eta_{k,x} \eta_{-k,x})] \\ &+ \sum_{\mathbf{k}} [\Lambda_{\mathbf{k}} t_{k,y}^\dagger t_{k,y} + \Delta_{\mathbf{k}} (t_{k,y}^\dagger t_{-k,y}^\dagger + t_{k,y} t_{-k,y})], \end{aligned} \quad (4)$$

with  $\Lambda_{\mathbf{k}} = \omega_0 + 2\Delta_{\mathbf{k}}$ ,  $\lambda(\mathbf{k}) = \sum_{s=1}^d \cos k_s$ ,  $\Delta_{\mathbf{k}} = \frac{1}{4} t \bar{s}^2 \lambda(\mathbf{k})$ ,  $N$  is the number of lattice sites, and  $Z$  is the total number of the nearest neighbors on the hypercubic lattice. The wave vectors  $k$  are taken in the first Brillouin zone, and the lattice spacing was assumed to be unity. This mean-field Hamiltonian can be solved using the Green's functions to obtain the thermal averages of the singlet and triplet correlation functions. These are given by

$$\langle\langle t_{k,\alpha}; t_{k,\alpha}^\dagger \rangle\rangle_\omega = \frac{1}{2\pi} \frac{\omega + \Lambda_{\mathbf{k}}}{\omega^2 - \omega_{\mathbf{k}}^2}, \quad (5)$$

$$\langle\langle t_{k,z}; t_{k,z}^\dagger \rangle\rangle_\omega = \frac{1}{2\pi} \frac{1}{\omega - \omega_{\mathbf{k}}}, \quad (6)$$

where  $\alpha = x, y$ . The poles of the Green's functions determine the excitation energies of the system as  $\omega_0 = (\frac{J}{4} + \mu)$ , which is the dispersionless spectrum of the longitudinal spin triplet states, and  $\omega_{\mathbf{k}} = \pm \sqrt{\Lambda_{\mathbf{k}}^2 - (2\Delta_{\mathbf{k}})^2}$  which corresponds to the excitation spectrum of the transverse spin triplet states for both branches  $\omega_x = \omega_y$ . From these modes and their bosonic character, an expression for the average energy at finite temperatures can be easily obtained as

$$U = \langle \mathcal{H}_{mf} \rangle = \varepsilon_0 + \frac{\omega_0}{2} \sum_{\mathbf{k}} \left( \coth \frac{\beta \omega_0}{2} - 1 \right) + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left( \coth \frac{\beta \omega_{\mathbf{k}}}{2} - 1 \right), \quad (7)$$

where

$$\varepsilon_0 = N \left[ -\frac{3}{4} J \bar{s}^2 + \mu \bar{s}^2 - \mu + \left( \frac{J}{4} + \mu - \frac{1}{2} t Z \bar{s}^2 \right) \bar{t}^2 \right] + \sum_{\mathbf{k}} (\omega_{\mathbf{k}} - \omega_0) \quad (8)$$

is the ground state energy of the system,  $\beta = 1/k_B T$ , and  $\bar{s}$  and  $\bar{t}$  are the singlet and triplet order parameters, respectively. Since the parameter  $\bar{s}$  is always nonzero<sup>4,6</sup> and  $\bar{t} \neq 0$  in the antiferromagnetic phase, we minimize the ground state energy with respect to  $\bar{t}$  to find  $\mu = (1/2) Z t \bar{s}^2 - J/4$  and, consequently,  $\omega_{\mathbf{k}} = (1/2) Z t \bar{s}^2 \sqrt{1 + 2\lambda(\mathbf{k})/Z}$ . The ground state energy  $\varepsilon_0$  corresponds to a magnetically long-range ordered state characterized by the momentum  $q = Q$ . The excitations over this ground state are given by two spin-wave branches associated with  $t_x$  and  $t_y$  that represent rotations or transverse oscillations of the order parameter  $\bar{t}$ . The third mode associated with  $t_z$  corresponds to fluctuations in the amplitude of this order parameter. In the next section, we consider low temperatures with the purpose of studying the behavior of the system near the magnetic instability.

#### IV. SINGLET AND TRIPLET ORDER PARAMETERS AT FINITE TEMPERATURES

The low temperature thermodynamic and transport properties of heavy fermions in the vicinity of the magnetic quantum critical point are far from being completely understood.<sup>15</sup> In order to study the KNM at finite temperatures, we calculate in this section the finite-temperature order parameters  $\bar{s}^2 = \bar{s}^2(T)$  and  $\bar{t}^2 = \bar{t}^2(T)$ . The free energy is given by  $F = U - TS$ , where  $U = \langle \mathcal{H}_{mf} \rangle$  is given by Eq. (7), and the entropy of free bosons is given by

$$S = k_B \sum_{\mathbf{k}} \left( [n(\omega_{\mathbf{k}}) + 1] \ln [n(\omega_{\mathbf{k}}) + 1] - n(\omega_{\mathbf{k}}) \ln [n(\omega_{\mathbf{k}})] \right). \quad (9)$$

After some straightforward algebra using Eqs. (7) and (9), one obtains

$$F = \varepsilon_0 - \frac{2}{\beta} \sum_{\mathbf{k}} \ln [1 + n(\omega_{\mathbf{k}})] - \frac{N}{\beta} \ln [1 + n(\omega_0)], \quad (10)$$

where

$$n(\omega) = \frac{1}{2} \left( \coth \frac{\beta \omega}{2} - 1 \right). \quad (11)$$

Minimizing the free energy of the KNM using  $(\partial \varepsilon / \partial \mu, \partial \varepsilon / \partial \bar{s}) = (0, 0)$ , we can easily get the following saddle-point equations:

$$\begin{aligned} \bar{s}^2 &= 1 + \frac{J}{Zt} - \frac{1}{2N} \sum_{\mathbf{k}} \sqrt{1 + \frac{2\lambda(\mathbf{k})}{Z}} \coth \frac{\beta \omega_{\mathbf{k}}}{2} - \xi, \\ \bar{t}^2 &= 1 - \frac{J}{Zt} - \frac{1}{2N} \sum_{\mathbf{k}} \frac{1}{\sqrt{1 + \frac{2\lambda(\mathbf{k})}{Z}}} \coth \frac{\beta \omega_{\mathbf{k}}}{2} - \xi, \end{aligned} \quad (12)$$

where  $\xi = \frac{1}{4} [\coth(\beta \omega_0/2) - 1]$ . Generally, the equations for  $\bar{s}$  and  $\bar{t}$  in Eq. (12) should be solved, and at  $T=0$ , the results of Ref. 4 are recovered. For  $J/t > (J/t)_c$ , triplet excitations remain gapped, and at  $J/t < (J/t)_c$ , the ground state has both condensation of singlets and triplets at the antiferromagnetic wave vector  $Q = (\pi, \pi, \pi)$ . Then, the quantum critical point at  $T=0$ ,  $(J/t)_c$  separates an antiferromagnetic long-range ordered phase from a gapped spin liquid phase. For finite temperatures, the condensation of singlets  $s$  occurs at a temperature scale which, to a first approximation, tracks the exchange  $J$ . The energy scale below which the triplet excitations condense is given by the Néel temperature ( $T_N$ ), which is calculated in the next section.

#### V. CRITICAL NÉEL LINE IN THE KONDO NECKLACE MODEL

In terms of the KNM, the condensation of triplets (singlets) follows from the RKKY interaction (Kondo effect). Thus, the fact that at the mean-field level both  $\bar{s}$  and  $\bar{t}$  do not vanish may be interpreted as the coexistence of Kondo screening and antiferromagnetism in the ordered phase<sup>4,6</sup> for all values of the ratio  $J/t < (J/t)_c$ . Notice that the bond-operator mean-field theory is appropriate in the strong coupling limit and near the QCP. However, it does not give an accurate description of the weak limit for  $(J/t) \rightarrow 0$ , where the ground state is macroscopically degenerate.

The Néel line giving the finite-temperature instability of the antiferromagnetic phase for  $J/t < (J/t)_c$  is obtained as the line in the  $T$  vs  $J/t$  plane at which  $\bar{t}$  vanishes ( $\bar{t}=0$ ). From Eq. (12), we can then obtain the boundary of the AF state. From this equation, we get

$$\frac{|g|}{Z} = \frac{1}{2N} \sum_{\mathbf{k}} \frac{1}{\sqrt{1 + \frac{2\lambda(\mathbf{k})}{Z}}} \left( \coth \frac{\beta \omega_{\mathbf{k}}}{2} - 1 \right) + \xi, \quad (13)$$

where  $g = |(J/t)_c - (J/t)|$  measures the distance to the QCP. The latter is given by  $(J/t)_c = Z \left[ 1 - \frac{1}{2N} \sum_{\mathbf{k}} \frac{1}{\sqrt{1 + 2\lambda(\mathbf{k})/Z}} \right]$ , where  $Z$  is the number of nearest neighbors. Expanding close to the wave vector  $\mathbf{Q} = (\pi, \pi, \pi)$  associated with the antiferromagnetic instability, we get

$$\lambda(\mathbf{k}) = -d + \frac{k^2}{2} + O(k^4). \quad (14)$$

This yields the spectrum of transverse spin triplet excitations as

$$\omega_{\mathbf{k}} = \omega_0 \sqrt{1 + \frac{2\lambda(\mathbf{k})}{Z}} \approx \sqrt{D}k, \quad (15)$$

where  $\sqrt{D} = \omega_0/\sqrt{2d}$ , with  $\omega_0$  the  $z$ -polarized dispersionless branch of excitations and  $d$  is the Euclidean dimension. Notice that the low temperature specific heat in the antiferromagnetic phase is dominated by the contribution of these modes. In three dimensions, this has a  $T^3$  temperature dependence due to the linear, phononlike, dispersion relation.

Substituting Eq. (15) to Eq. (13) and considering that for temperatures  $k_B T \ll \omega_0$ ,  $\xi$  goes to zero faster than the first term of Eq. (13), we obtain

$$\frac{|g|}{Z} = \frac{2^{d-2} S_d Z^{d/2}}{\pi^d} \left( \frac{k_B T}{\omega_0} \right)^{d-1} \int_0^{(\pi/2\sqrt{Z})(\omega_0/k_B T)} u^{d-2} (\coth u - 1) du, \quad (16)$$

where  $S_d$  is the solid angle and  $u = \beta\omega_0 k/2\sqrt{Z}$ . For temperatures  $k_B T \ll \omega_0$ , the integral in Eq. (16) can be calculated and we get

$$\frac{|g|}{Z} = \frac{2^{d-2} S_d Z^{d/2}}{\pi^d \omega_0^{d-1}} (k_B T_N)^{d-1} f(d), \quad (17)$$

where  $f(d) = \int_0^\infty u^{d-2} (\coth u - 1) du$ . The solution of this expression gives us the critical line of Néel transitions for any dimension and temperatures  $k_B T \ll \omega_0$ , where  $\omega_0 = (\frac{J}{4} + \mu)$  is the dispersionless spectrum of the longitudinal spin triplet states that track  $J$ . We notice that the integral  $f(d)$  diverges for  $d < 3$ , showing that there is no critical line in two dimensions at finite temperatures,<sup>7</sup> in agreement with the Mermin-Wagner theorem.<sup>8</sup> For  $d \geq 3$ ,  $f(d)$  is finite and the equation for the critical line is given by

$$T_N \propto |g|^{1/(d-1)}, \quad (18)$$

which defines a shift exponent  $\psi = 1/(d-1)$ . In particular, for three dimensions,  $f(3) = \pi^2/12$  and the critical line of Néel is given by  $k_B T_N = 0.13 \omega_0 |g|^{1/2}$ . In summary, in this section, we have obtained analytically the expression for the Néel line close to the QCP and we have shown that this line does not exist for  $d=2$  as expected.

## VI. PARAMAGNETIC PHASE

Our interest here is to obtain the thermodynamic properties near but above the QCP, i.e., for finite temperatures in the spin liquid phase for  $J/t \geq (J/t)_c$ . In this case, we have to consider only the condensation of singlets since  $\bar{t}=0$  in the paramagnetic phase. We find

$$\varepsilon' = \varepsilon'_0 + \frac{\omega_0}{2} \left( \coth \frac{\beta\omega_0}{2} - 1 \right) + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left( \coth \frac{\beta\omega_{\mathbf{k}}}{2} - 1 \right). \quad (19)$$

The ground state energy is now given by  $\varepsilon'_0 = N(-\frac{3}{4}J\bar{s}^2 + \mu\bar{s}^2 - \mu) + \sum_{\mathbf{k}} (\omega_{\mathbf{k}} - \omega_0)$  and the free energy by

$$F' = \varepsilon'_0 - \frac{2}{\beta} \sum_{\mathbf{k}} \ln[1 + n(\omega_{\mathbf{k}})] - \frac{N}{\beta} \ln[1 + n(\omega_0)]. \quad (20)$$

The transverse spin triplet excitation spectrum can be expressed in the general form  $\omega_{\mathbf{k}} = \sqrt{\Lambda_{\mathbf{k}}^2 - (2\Delta_{\mathbf{k}})^2}$ , where the excitations are triply degenerate *magnons* (triplons) with a spin gap that vanishes on approaching the QCP, as we show below.

We minimize the paramagnetic KNM free energy, deriving the following saddle-point equations:

$$2J \left( \frac{3}{4} - \frac{\mu}{J} \right) = \frac{t}{N} \sum_{\mathbf{k}} \frac{\omega_0}{\omega_{\mathbf{k}}} \lambda(\mathbf{k}) \coth \frac{\beta\omega_{\mathbf{k}}}{2}, \quad (21)$$

$$2 - \bar{s}^2 = \frac{1}{N} \sum_{\mathbf{k}} \frac{\Lambda_{\mathbf{k}}}{\omega_{\mathbf{k}}} \coth \frac{\beta\omega_{\mathbf{k}}}{2} + 2\xi.$$

At  $T=0$ , the self-consistent equations above are equivalent to those found in the Kondo spin liquid ground state.<sup>4</sup> Considering again the expansion close to the QCP of Eq. (14), we obtain the transverse spin triplet excitation spectrum in the paramagnetic phase as

$$\omega_{\mathbf{k}} = \sqrt{\Delta^2 + Dk^2}. \quad (22)$$

These quasiparticle excitations form a band whose bandwidth is a function of  $t$ . The band minimum is at  $k=\pi$ , and the triplet excitation spectrum has a spin gap given by

$$\Delta = \omega_0 \sqrt{1 - \frac{yZ}{2}}. \quad (23)$$

In Eq. (22),  $D = y\omega_0^2/2$  and  $y = t\bar{s}^2/\omega_0$  is a dimensionless parameter. The spin gap decreases as the hopping  $t$  (hence,  $y$ ) increases and vanishes when  $y \rightarrow 2/Z$ .

### Dependence of the spin gap on the distance to the quantum critical point

We now obtain the dependence of the spin gap  $\Delta$  with the distance to QCP, given by  $g = |(J/t) - (J/t)_c|$ , in the quantum disordered Kondo spin liquid state from Eq. (21) at  $T=0$ . This was done previously for the spin gap in spin ladder systems but always in one dimension.<sup>13,16</sup>

The first step is to express Eq. (21) as an equation for the parameter  $y$ ,

$$y = 2 \left( \frac{t}{J} \right) \left[ 1 - \frac{S_d}{2^{1-d} \pi^d} \frac{1}{\sqrt{1+yd}} K(\eta) \right], \quad (24)$$

with

$$K(\eta) = \int_0^{\pi/2} \frac{\theta^{d-1} d\theta}{\sqrt{1 - \eta^2 \sin^2 \theta}}, \quad (25)$$

where  $\eta = \sqrt{2yd/(yd+1)}$  and  $K(\eta)$  in one dimension is the complete elliptic integral of the first kind.<sup>13</sup> In Eq. (23), we see that when  $y = y_c = 2/Z$ , the spin gap vanishes, yielding

$$\left(\frac{J}{t}\right)_c = \frac{2}{y_c} \left[ 1 - \frac{S_d}{2^{1-d} \pi^d} \frac{1}{\sqrt{1+y_c d}} K(\eta_c) \right], \quad (26)$$

where  $\eta_c = \sqrt{2y_c d / (y_c d + 1)}$ . Since  $|g| = |J/t - (J/t)_c|$ , we obtain

$$\frac{2(y_c - y)}{y_c y} = |g| + \frac{S_d 2^d}{\pi^d} G(y), \quad (27)$$

where

$$G(y) = \frac{1}{y\sqrt{1+yd}} K(\eta) - \frac{1}{y_c\sqrt{1+y_c d}} K(\eta_c). \quad (28)$$

The above equation can be expanded in Taylor's series for  $y$  near  $y_c$ , yielding

$$G(y) \approx \frac{\partial}{\partial y} \frac{1}{y\sqrt{1+yd}} K(\eta) \Big|_{y=y_c} (y - y_c) + O(y - y_c)^2. \quad (29)$$

Now, considering Eq. (27), we can express the spin gap energy by

$$\Delta = J \left( \frac{1}{4} + \frac{\mu}{J} \right) \sqrt{\frac{yZ|g|}{2[Z + \zeta(y_c, d)]}}, \quad (30)$$

where  $\zeta(y_c, d) = \frac{S_d 2^d}{\pi^d} \frac{\partial}{\partial y} \frac{1}{y\sqrt{1+yd}} K(\eta) \Big|_{y=y_c}$ , with  $\zeta(y_c, 2) \approx 297.01$  and  $\zeta(y_c, 3) \approx 17.78$  in two and three dimensions, respectively.  $\mu/J$  and  $y$  are given by the self-consistent Eqs. (21) and (24), respectively, and are never critical. This relation between the spin gap and  $|g|$  shows that when  $J/t$  decreases from its strong coupling limit, the triplet gap at the wave vector  $k = (\pi, \pi, \pi)$  decreases and vanishes at  $|g| = 0$ . Since  $\Delta \propto |g|^{1/2}$ , when  $|g| \rightarrow 0$ , we can immediately identify the gap exponent  $\nu_z = 1/2$  at the quantum critical point of the Kondo lattice.

## VII. SPECIFIC HEAT IN THE PARAMAGNETIC PHASE

The purpose of this section is to consider the paramagnetic half-filled KNM energy given by Eq. (20) and discuss its finite-temperature properties near the QCP. Already the ground state and finite-temperature properties of the KLM have been intensively studied for one dimension using the density matrix renormalization group method.<sup>17-19</sup> For two dimensions, this has been accomplished using finite-temperature Lanczos technique,<sup>20</sup> perturbation theory,<sup>21</sup> and quantum Monte Carlo (QMC) simulation.<sup>22</sup> Lately, also for the KNM using QMC for two dimensions.<sup>23</sup> However, less analytical work has been carried out for higher-dimensional KNM and KLM. This way, motivated by the above, we are going to analyze the specific heat  $C/T \equiv \gamma$  using an analytical treatment valid for any dimension. We obtain  $\gamma$  in the paramagnetic disordered phase in two cases: First in the so-called non-Fermi-liquid trajectory ( $|g| = 0, T \neq 0$ ) and then below the spin gap for  $k_B T \ll \Delta \propto |g|^{1/2}$ . We consider the free energy in Eq. (20) with  $\omega_{\mathbf{k}} = \sqrt{\Delta^2 + Dk^2}$  and take into account only the contribution of the transverse spin triplet excitation spectrum  $\omega_{\mathbf{k}}$ , since the contribution of longitudinal triplet

excitation  $\omega_0$  tends to zero faster at low temperatures  $k_B T \ll \omega_0 \sim J$ .

### A. Specific heat along the non-Fermi-liquid trajectory

Non-Fermi-liquid behavior is often found near a magnetic QCP,<sup>24</sup> indicating that the NFL state in those systems may be linked to the magnetic instability at  $T=0$ . In this state, the coefficient of the linear term of the specific heat does not saturate as expected from the Landau scenario but shows a temperature dependence as the temperature is lowered. Exactly at the QCP, this may occur down to the lowest temperatures.<sup>25</sup> Next, we are going to find analytically  $C/T$  at the NFL trajectory. From Eq. (20) and using  $C/T = -\partial^2 F' / \partial T^2$ , we get

$$\frac{C}{T} = \frac{k_B^2 S_d}{D^{d/2} 2 \pi^d} \varsigma(d) (k_B T)^{d-1}, \quad (31)$$

where

$$\varsigma(d) = \int_{x_0}^{\sqrt{x_0^2 + D\beta^2 \pi^2}} u^3 (u^2 - x_0^2)^{(d-2)/2} \left( \coth^2 \frac{u}{2} - 1 \right) du,$$

with  $x_0 = \Delta / k_B T$ ,  $\Delta = \omega_0 \sqrt{yZ|g|} / (2[Z + \zeta(y_c, d)])$ ,  $u = \sqrt{x_0^2 + D\beta^2 \pi^2}$ , and  $g = |(J/T) - (J/T)_c|$  measures the distance to the QCP. Equation (31) yields the expression for the specific heat in the paramagnetic region and it is due, as we already pointed out, to the contribution of bosons  $t_x$  and  $t_y$ . At  $|g| = 0$  and low temperatures, such that  $J \gg k_B T \gg \Delta$  (NFL trajectory), we can rewrite Eq. (31) as follows:

$$\frac{C}{T} \Big|_{|g|=0} = \gamma_{|g|=0} = \frac{S_d k_B^2 \varsigma(|g|=0, d)}{D^{d/2} 2 \pi^d} (k_B T)^{d-1}, \quad (32)$$

where  $\varsigma(|g|=0, d) = \int_0^\infty u^{d+1} [\coth^2(u/2) - 1] du$  is  $24\zeta(3)$  and  $16\pi^4/15$  in two and three dimensions, respectively, and  $\zeta$  is the Riemann zeta function. Thereby,  $C/T \propto T^{d-1}$  at the QCP. Notice that this is consistent with the general scaling result  $C/T \propto T^{(d-z)/z}$ , with the dynamic exponent taking the value<sup>25</sup>  $z=1$ . Together with the previous result for the gap exponent  $\nu_z = 1/2$ , we find that  $\nu = 1/2$ , a result in agreement with the mean-field or Gaussian character of the approximations we have used to deal with the bond-operator Hamiltonian. Furthermore, since  $z=1$ , in three dimensions  $d_{eff} = d + z = d_c = 4$ , where  $d_c$  is the upper critical dimension for the magnetic transition.<sup>25</sup> Consequently, the present approach yields the correct description of the quantum critical point of the KNM for  $d \geq 3$ .

### B. Specific heat in the Kondo spin liquid state

In region II of Fig. 1, we have to consider the paramagnetic contribution to the specific heat given by Eq. (19) but now taking into account that  $k_B T \ll \Delta$ . Then for  $k_B T \ll \Delta \approx \sqrt{|g|}$ , we obtain

$$\frac{C}{T} = \frac{2S_d}{\pi^d D^{d/2}} \frac{\Delta^{d+2}}{k_B T^3} e^{\Delta/k_B T} \delta(d, T), \quad (33)$$

where  $\cosh u_f = 1 + x_0^{-1}$ ,  $x_0 = \Delta / k_B T$ , and  $\delta(d) = \int_0^{u_f} (\sinh u)^{d-1} \cosh^3 u du$ . This can be calculated, and

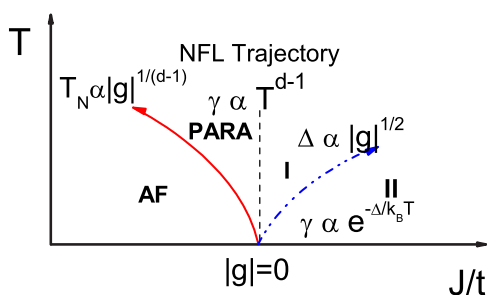


FIG. 1. (Color online) Schematic phase diagram of the Kondo necklace model at finite temperatures. The AF phase is located below the Néel line  $T_N$  (solid line), which vanishes at a critical value  $(J/t)_c$  (QCP). The spin gap energy (dashed line) is shown as a function of  $g$ . Below this line, there is a Kondo spin liquid state. The temperature dependence of the specific heat  $\gamma=C/T$  is given along the NFL trajectory and in the Kondo spin liquid state for any dimension. The phase diagram shows that at low temperatures, a small value of  $J/t$  supports the development of AF order via the RKKY interaction. If the value of  $J/t$  becomes too high, the local moments are quenched by the conduction electrons and the system has a dense Kondo ground state.

we obtain  $\delta(d=2, T) = \left[ \frac{k_B T}{\Delta} + \frac{3}{2} \left( \frac{k_B T}{\Delta} \right)^2 \right]$  and  $\delta(d=3, T) = \frac{\sqrt{2}}{3} \left[ 2 \left( \frac{k_B T}{\Delta} \right)^{3/2} + \frac{17}{5} \left( \frac{k_B T}{\Delta} \right)^{5/2} \right]$  in two and three dimensions, respectively. In this case, the specific heat is governed by the exponential term, and we can conclude that the dimensionality does not make much difference in thermodynamic properties. This point was also indicated using numerical methods for the two-dimensional KLM.<sup>20</sup>

Summarizing, we have

$$C/T \propto \begin{cases} T^{d-1}, & J \gg k_B T \gg \Delta \text{ (NFL trajectory)} \\ e^{-\Delta/k_B T}, & k_B T \ll \Delta, \end{cases} \quad (34)$$

where in the latter case only the dominant term has been written. Then, we have obtained the specific heat due to the

magnetic degrees of freedom in the paramagnetic phase of the half-filled KNM for any dimension and temperatures  $k_B T \ll J$ . We have investigated it in two cases: along the NFL trajectory and in the dense Kondo spin liquid phase, where an exponential temperature due to the spin gap dominates over the power law associated with different dimensionalities. Unfortunately, there are few existing results in higher dimension considering the approaches done; almost all results above were obtained for the strong coupling limit ( $t=0$ ). Our work should provide a valuable benchmark for other approaches. While we have not attempted a detailed comparison on or fit to experiment, this would be possible.

## VIII. CONCLUSIONS

In the present work, we have constructed analytical expressions to find the phase diagram of the Kondo necklace model for any dimension and at low temperatures such that  $k_B T \ll J$ . Although there were several approaches treating the Kondo lattice model with methods similar to the one we use, they were all restricted to zero temperature. The present finite-temperature treatment allowed us to determine the critical line for antiferromagnetic transitions as well as the thermodynamic behavior along the quantum critical trajectory and in the noncritical part of the phase diagram. We obtained the relevant critical exponents governing the critical line and the thermodynamic behavior due to the magnetic degrees of freedom. For three dimensions, these results turn out to be exact since  $d_{eff}=d+z=4$  is equal to the upper critical dimension for the Kondo lattice.

We also found that the spin gap in the Kondo singlet phase vanishes as  $\sqrt{|g|}$  at the QCP, consistent with  $z=1$  and a mean-field correlation length  $\nu=1/2$ .

## ACKNOWLEDGMENTS

The authors would like to thank A. Troper for helpful discussions and also the Brazilian Agencies FAPERJ and CNPq for financial support.

\*daniel@cbpf.br

†mucio@if.uff.br

<sup>1</sup>J. Larrea J., M. B. Fontes, E. M. Baggio-Saitovitch, J. Plessel, M. M. Abd-Elmeguid, J. Ferstl, C. Geibel, A. Pereira, A. Jornada, and M. A. Continentino, Phys. Rev. B **74**, 140406(R) (2006).

<sup>2</sup>S. Doniach, Physica B & C **91**, 231 (1977).

<sup>3</sup>J. R. Schrieffer and P. A. Wolff, Phys. Rev. **149**, 491 (1966).

<sup>4</sup>Guang-Ming Zhang, Qiang Gu, and Lu Yu, Phys. Rev. B **62**, 69 (2000).

<sup>5</sup>S. Sachdev and R. N. Bhatt, Phys. Rev. B **41**, 9323 (1990).

<sup>6</sup>C. Jurecka and W. Brenig, Phys. Rev. B **64**, 092406 (2001).

<sup>7</sup>D. Reyes, M. A. Continentino, A. Troper, and A. Saguia, Physica B **359**, 714 (2005).

<sup>8</sup>N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

<sup>9</sup>M. A. Continentino, Phys. Rev. B **47**, 11587 (1993).

<sup>10</sup>J. A. Hertz, Phys. Rev. B **14**, 1165 (1976).

<sup>11</sup>T. Moriya and T. Takimoto, J. Phys. Soc. Jpn. **64**, 960 (1995).

<sup>12</sup>A. J. Millis, Phys. Rev. B **48**, 7183 (1993).

<sup>13</sup>S. Gopalan, T. M. Rice, and M. Sigrist, Phys. Rev. B **49**, 8901 (1994).

<sup>14</sup>B. Normand and T. M. Rice, Phys. Rev. B **54**, 7180 (1996).

<sup>15</sup>M. A. Continentino, J. Phys. I **1**, 693 (1991).

<sup>16</sup>T. Barnes, E. Dagotto, J. Riera, and E. S. Swanson, Phys. Rev. B **47**, 3196 (1993).

<sup>17</sup>N. Shibata, B. Ammon, M. Troyer, M. Sigrist, and K. Ueda, J. Phys. Soc. Jpn. **67**, 1086 (1998).

<sup>18</sup>N. Shibata and H. Tsunetsugu, J. Phys. Soc. Jpn. **68**, 744 (1999).

<sup>19</sup>N. Shibata and K. Ueda, J. Phys.: Condens. Matter **11**, R1 (1999).

<sup>20</sup>K. Haule, J. Bonča, and P. Prelovšek, Phys. Rev. B **61**, 2482 (2000).

<sup>21</sup>Qiang Gu, Phys. Rev. B **66**, 052404 (2002).

<sup>22</sup>S. Capponi and F. F. Assaad, Phys. Rev. B **63**, 155114 (2001).

<sup>23</sup>C. Brünger and F. F. Assaad, Phys. Rev. B **74**, 205107 (2006).

<sup>24</sup>G. R. Stewart, Rev. Mod. Phys. **73**, 797 (2001).

<sup>25</sup>M. A. Continentino, *Quantum Scaling in Many-Body Systems* (World Scientific, Singapore, 2001).