Journal of Magnetism and Magnetic Materials 321 (2009) 348–353

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Thermodynamic quantum critical behavior of the anisotropic Kondo necklace model

D. Reyes [a,*,1], M.A. Continentino [b,2], Han-Ting Wang [c,3]

[a] Centro Brasileiro de Pesquisas Físicas, Rua Dr. Xavier Sigaud, 150-Urca, 22290-180 RJ, Brazil
[b] Instituto de Física, Universidade Federal Fluminense, Campus da Praia Vermelha, Niterói, RJ 24.210-340, Brazil
[c] Beijing National Laboratory of Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100080, People's Republic of China

ARTICLE INFO

Article history:
Received 29 May 2008
Received in revised form
26 August 2008
Available online 21 September 2008

PACS:
71.27.+a
75.30.Mb
75.10.Jm

Keywords:
Anisotropic Kondo necklace model
Quantum phase transition
Kondo insulator

ABSTRACT

The Ising-like anisotropy parameter δ in the Kondo necklace model is analyzed using the bond-operator method at zero and finite temperatures for arbitrary d dimensions. A decoupling scheme on the double time Green's functions is used to find the dispersion relation for the excitations of the system. At zero temperature and in the paramagnetic side of the phase diagram, we determine the spin gap exponent $\nu z \approx 0.5$ in three dimensions and anisotropy between $0 \leqslant \delta \leqslant 1$, a result consistent with the dynamic exponent $z = 1$ for the Gaussian character of the bond-operator treatment. On the other hand, in the antiferromagnetic phase at low but finite temperatures, the line of Neel transitions is calculated for $\delta \ll 1$. For $d > 2$ it is only re-normalized by the anisotropy parameter and varies with the distance to the quantum critical point (QCP) $|g|$ as, $T_N \propto |g|^{\psi}$ where the shift exponent $\psi = 1/(d-1)$. Nevertheless, in two dimensions, a long-range magnetic order occurs only at $T = 0$ for any $\delta \ll 1$. In the paramagnetic phase, we also find a power law temperature dependence on the specific heat at the *quantum critical trajectory* $J/t = (J/t)_c$, $T \to 0$. It behaves as $C_V \propto T^d$ for $\delta \leqslant 1$ and ≈ 1, in concordance with the scaling theory for $z = 1$.

1. Introduction

Quantum phase transitions (QPTs) from an antiferromagnetic (AF) ordered state to a nonmagnetic Fermi liquid (FL) in heavy fermion (HF) systems have received considerable attention from both theoretical [1] and experimental points of view [2]. In contrast to classical phase transitions (CPT), driven by temperature, QPT can be driven by tuning an independent-temperature control parameter (magnetic field, external pressure, or doping). The physics of HF is mainly due to the competition of two main effects: the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction between the magnetic ions which favors a long-range magnetic order, and the Kondo effect which tends to screen the local moments and to produce a nonmagnetic ground state. These effects are contained in the Kondo lattice model (KLM) Hamiltonian in which spin degrees of freedom of conduction electrons and localized moments, as well as charge degree of freedom of the conduction electrons, are considered. Here we investigated a simplified version of the KLM, the so-called Kondo necklace model [3] (KNM) which for all purposes can be considered to yield results similar to the KLM. While the ground state properties of this model have been investigated rather extensively by a variety of methods [4–14], the thermodynamic and finite temperature critical properties, close to a magnetic instability, remain an open issue. It was observed by us, and it was our first motivation for studying the quantum critical properties of this model, as a function of the distance to the QCP $|g|$, at zero and low temperatures [1,15]. Now we extend this treatment introducing a finite inter-site anisotropy δ in the y-spin operator component such that, $0 \leqslant \delta \leqslant 1$ since the $\delta = 1$ case is appropriate to describe compounds where the ordered magnetic phase has a strong Ising component. However, the main reason to consider the anisotropy δ in the KNM is to try to describe its effects in the neighborhood of a magnetic QCP in HF systems, rather than a symmetry problem [12]. This is a goal in HF systems, and already several theories were formulated to explain their unusual properties [16–18]. Besides, in a previous work we were successful in finding that the Neel line exists since turning on a geometric anisotropy [19], stressing thatanisotropy is an inherent ingredient in real HF systems. Henceforth, the model will be called anisotropic Kondo necklace model (AKNM). This model was already investigated

* Corresponding author.
E-mail address: daniel@cbpf.br (D. Reyes).
[1] Work supported by CNPq.
[2] Work supported by CNPq-Brasil(PRONEX 98/MCTCNPq-0364.00/00) and FAPERJ.
[3] Work supported by NKBRSF of China under Grant no. 2006CB921400.

0304-8853/$ - see front matter
doi:10.1016/j.jmmm.2008.09.010

using the real space renormalization group machinery [20] but just in one dimension (1d) and zero temperature. We use the bond-operator approach introduced by Sachdev and Bhatt [21] which was employed previously in both, KLM [22] and KNM [11] models but always at $(T,\delta)=(0,0)$. We find that this method yields a *shift exponent* that characterizes the shape of the critical line in the neighborhood of the QCP as well as the power law temperature dependence on the specific heat along the so-called *quantum critical trajectory* $J/t=(J/t)_c$, $T\to 0$. We consider the following AKNM:

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

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 which strength t and the second term is the magnetic interaction between conduction electrons and localized spins $\mathbf{S}_i$ by means of the Kondo exchange coupling J ($J>0$). The Ising-like anisotropy parameter δ varies from the full anisotropic case $\delta=1$ to the well established case $\delta=0$.

Considering the bond-operator representation for two spins $S=\frac{1}{2}$, $\tau_i(S_i)^\alpha=\mp\frac{1}{2}(s_i^\dagger t_{i,\alpha}+t_{i,\alpha}^\dagger s_i\pm \mathrm{i}\varepsilon_{\alpha\beta\gamma}t_{i,\beta}^\dagger t_{i,\gamma})$ $(\alpha=x,y,z)$ [21], the Hamiltonian above, at half-filling, i.e., with one conduction electron per site, can be simplified. The resulting effective Hamiltonian $\mathscr{H}_{\mathrm{mf}}$ with only quadratic operators is sufficient to describe exactly the QPT from the disordered Kondo spin liquid to the AF phase [12,23,24], as discussed below. By replacing the spin operator representation above in the Hamiltonian given by Eq. (1) we obtain the following mean-field Hamiltonian:

$$\begin{aligned}\mathscr{H}_{\mathrm{mf}}&=N(-\tfrac{3}{4}J\bar{s}^2+\mu\bar{s}^2-\mu)+\omega_0\sum_{\mathbf{k}}t_{\mathbf{k},z}^\dagger t_{\mathbf{k},z}\\&+\sum_{\mathbf{k}}[\Lambda_{\mathbf{k}}t_{\mathbf{k},x}^\dagger t_{\mathbf{k},x}+\Delta_{\mathbf{k}}(t_{\mathbf{k},x}^\dagger t_{-\mathbf{k},x}^\dagger+t_{\mathbf{k},x}t_{-\mathbf{k},x})]\\&+\sum_{\mathbf{k}}[\Lambda'_{\mathbf{k}}t_{\mathbf{k},y}^\dagger t_{\mathbf{k},y}+\Delta'_{\mathbf{k}}(t_{\mathbf{k},y}^\dagger t_{-\mathbf{k},y}^\dagger+t_{\mathbf{k},y}t_{-\mathbf{k},y})],\end{aligned}\tag{2}$$

where $\Lambda_{\mathbf{k}}=\omega_0+2\Delta_{\mathbf{k}}$, $\Lambda'_{\mathbf{k}}=\omega_0+2\Delta'_{\mathbf{k}}$, $\Delta_{\mathbf{k}}=\frac{1}{4}t\bar{s}^2\lambda(\mathbf{k})$, $\Delta'_{\mathbf{k}}=\frac{1}{4}t\bar{s}^2\lambda(\mathbf{k})(1-\delta)$, and the structure factor $\lambda(\mathbf{k})=\sum_{s=1}^d\cos k_s$. The singlet order parameter $\bar{s}$, is consistent with the strong coupling limit $J/t\to\infty$, where the model becomes trivial, since each $\mathbf{S}$ spin captures a conduction electron spin to form a singlet, and where the ground state corresponds to a direct product of those singlets. The chemical potential μ was introduced to impose the constraint condition of single occupancy, N is the number of lattice sites and Z is the total number of the nearest neighbors on the hyper-cubic 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

$$\begin{aligned}\langle\langle t_{\mathbf{k},x};t_{\mathbf{k},x}^\dagger\rangle\rangle&=\frac{(\omega^2-\omega_k'^2)(\omega+\Lambda_k)}{2\pi\xi},\\\langle\langle t_{\mathbf{k},y};t_{\mathbf{k},y}^\dagger\rangle\rangle&=\frac{(\omega^2-\omega_k^2)(\omega+\Lambda'_k)}{2\pi\xi},\\\langle\langle t_{\mathbf{k},z};t_{\mathbf{k},z}^\dagger\rangle\rangle&=\frac{1}{2\pi(\omega-\omega_0)},\end{aligned}\tag{3}$$

where $\xi=(\omega^2-\omega_k^2)(\omega^2-\omega_k'^2)$. The poles of the Green's functions determine the excitation energies of the system as $\omega_0=((J/4)+\mu)$, which is the dispersionless spectrum of the longitudinal spin triplet states, $\omega_k=\pm\sqrt{\Lambda_k^2-(2\Delta_k)^2}$ that corresponds to the excitation spectrum of the x-transverse spin triplet states, and $\omega'_k=\pm\sqrt{\Lambda_k'^2-(2\Delta'_k)^2}$ that corresponds to the y-transverse one. We can see that if $\delta=0$, $\Delta_k=\Delta'_k$, and $\Lambda_k=\Lambda'_k$. Thereby, the transverse excitation modes coincide $\omega_k=\omega'_k$, which corresponds to the isotropic Kondo lattice model [1].

2. Paramagnetic state

From these modes above and their Bosonic character an expression for the paramagnetic internal energy at finite temperatures can be easily obtained [1,15,19],

$$U=\varepsilon_0+\sum_{\mathbf{k}}(\omega_0 n(\omega_0)+\omega_{\mathbf{k}}n(\omega_{\mathbf{k}})+\omega'_{\mathbf{k}}n(\omega'_{\mathbf{k}})),\tag{4}$$

where

$$\begin{aligned}\varepsilon_0&=N(-\tfrac{3}{4}J\bar{s}^2+\mu\bar{s}^2-\mu)\\&+\tfrac{1}{2}\sum_{\mathbf{k}}(\omega_{\mathbf{k}}+\omega'_{\mathbf{k}}-\Lambda_{\mathbf{k}}-\Lambda'_{\mathbf{k}})\end{aligned}\tag{5}$$

is the paramagnetic ground state energy, $\beta=1/k_{\mathrm{B}}T$, k_B the Boltzman's constant, $n(\omega)=\frac{1}{2}(\coth(\beta\omega/2)-1)$ the Bose factor and T the temperature. After some straightforward algebra [1,19] using Eq. (4), the paramagnetic free energy renders

$$\begin{aligned}F&=\varepsilon_0-\frac{1}{\beta}\sum_{\mathbf{k}}\ln[1+n(\omega_{\mathbf{k}})]\\&-\frac{1}{\beta}\sum_{\mathbf{k}}\ln[1+n(\omega'_{\mathbf{k}})]-\frac{N}{\beta}\ln[1+n(\omega_0)].\end{aligned}\tag{6}$$

To obtain the parameters introduced $\bar{s}^2$ and μ we minimize the free energy by the saddle-point equations $(\partial\varepsilon/\partial\mu,\partial\varepsilon/\partial\bar{s})=(0,0)$, and we get

$$\begin{aligned}2(2-\bar{s}^2)&=f(\omega_0)+\frac{1}{2N}\sum_{\mathbf{k}}\frac{\Lambda_{\mathbf{k}}}{\omega_{\mathbf{k}}}\coth\frac{\beta\omega_{\mathbf{k}}}{2}\\&+\frac{1}{2N}\sum_{\mathbf{k}}\frac{\Lambda'_{\mathbf{k}}}{\omega'_{\mathbf{k}}}\coth\frac{\beta\omega'_{\mathbf{k}}}{2},\\\frac{2J}{t}\left(\frac{3}{4}-\frac{\mu}{J}\right)&=\frac{1}{2N}\sum_{\mathbf{k}}\frac{\omega_0}{\omega_{\mathbf{k}}}\lambda(\mathbf{k})\coth\frac{\beta\omega_{\mathbf{k}}}{2}\\&+\frac{1}{2N}\sum_{\mathbf{k}}\frac{\omega_0}{\omega'_{\mathbf{k}}}\lambda(\mathbf{k})(1-\delta)\coth\frac{\beta\omega'_{\mathbf{k}}}{2},\end{aligned}\tag{7}$$

where $f(\omega_0)=(N/2)(\coth(\beta\omega_0/2)-1)$.

2.1. Numerical results at $T=0$

We first studied the case $T=0$, i.e., without thermal fluctuations. At zero temperature the self-consistent equations given by Eqs. (7) can be simplified as

$$\begin{aligned}4(2-\bar{s}^2)&=I_1(y)+I_2(y)+I_3(y)+I_4(y),\\\frac{4Jy}{t}\left(\frac{3}{4}-\frac{\mu}{J}\right)&=I_2(y)-I_1(y)+I_4(y)-I_3(y),\end{aligned}\tag{8}$$

with

$$\begin{aligned}I_1(y)&=\frac{1}{\pi^d}\int_0^\pi\frac{d^dk}{\sqrt{1+y\lambda(\mathbf{k})}},\\I_3(y)&=\frac{1}{\pi^d}\int_0^\pi\frac{d^dk}{\sqrt{1+y(1-\delta)\lambda(\mathbf{k})}},\\I_2(y)&=\frac{1}{\pi^d}\int_0^\pi d^dk\sqrt{1+y\lambda(\mathbf{k})},\\I_4(y)&=\frac{1}{\pi^d}\int_0^\pi d^dk\sqrt{1+y(1-\delta)\lambda(\mathbf{k})},\end{aligned}\tag{9}$$

where we have introduced a dimensionless parameter $y = t\bar{s}^2/\omega_0$. An equation about y can then be obtained:

$$y = \frac{2t}{J}(1 - [I_1(y) + I_3(y)]/4). \tag{10}$$

We will now obtain the numerical solutions to the zero temperature self-consistent equations (8) using Eq. (10). In this case (paramagnetic phase), we have that the z-polarized branch of excitations has a dispersionless value $\omega_z(k) = \omega_0$ and the other two branches show a dispersion which has a minimum at the AF reciprocal vector $Q = (\pi, \pi, \pi)$ in three dimensions ($3d$). The minimum value of the excitations defines

$$\Delta^x = \omega_0\sqrt{1 - yd}, \quad \Delta^y = \omega_0\sqrt{1 - yd(1 - \delta)}. \tag{11}$$

The spin gap energies Δ^x and Δ^y define the energy scale for the Kondo singlet phase, for $0 \leqslant \delta \leqslant 1$ and $\delta < 0$, respectively. For $\delta = 0$, Δ^x and Δ^y are identical and we obtain the original spin gap in the KNM [11]. Although we are interested in the case where $0 < \delta \leqslant 1$, we considered $\delta < 0$ due to theoretical reasons. This case will only be consider at $T = 0$ and will not be sketched in this report. The analysis of the spin gap is important because the vanishing of gap and the appearance of soft modes define the transition from the disordered Kondo spin liquid to the AF phase at the QCP ($J/t = (J/t)_c, T = 0$). At this point, it is suitable to clarify that in Figs. 1, 2 and 3, we sketched the spin gap energy like Δ/J versus t/J by following the $\delta = 0$ case [11], despite that we have considered throughout this paper the control parameter as J/t. That will not yield any physical difference since it only will change the onset of the curves from the left to the right.

In the ($1d$) case, the energy gap falls linearly for small values of t/J, and deviates considerably from the linear behavior as t/J gets larger, as shown in Fig. 1. Thereby, it is always nonzero for any δ, supporting its disordered phase, characteristic of $1d$ Kondo lattices [11,25]. However, it was reported in the production of this report a study for the AKNM in $1d$ using spin wave approach [26], which gives a critical value δ_c that separates the disordered Kondo spin liquid state from the AF phase. In our case, using a bond-operator mean field approximation in $1d$, we did not find this critical value. We believe it is a consequence of the strong coupling limit where the ground state is always a Kondo spin liquid state.

The anisotropy dependence on the spin gap in two dimensions ($2d$) is sketched in Fig. 2. For $0 < \delta \leqslant 1$, the effect of anisotropy is still weak and it slightly changes the position of the QCP $(t/J)_c$, until $\delta = 0$, where both soft modes, Δ^x and Δ^y, contribute and we find the QCP for the $2d$ isotropic KNM $(t/J)_c \approx 0.69$ [11]. Then, the qualitative behavior of the spin gap is the *same* for this range and the gap exponent is approximately $\nu z \simeq 1$. It is plotted in the inset of Fig. 2. On the other hand, for $\delta < 0$, the QCP diminishes its value and the Kondo spin liquid phase is limited to a narrower region. It is not shown in Fig. 2.

In $3d$, the effect of anisotropy on the spin gap is similar as in the $2d$ case. It is sketched in Fig. 3. The spin gap has an exponent $\nu z \simeq 0.5$ for $0 \leqslant \delta \leqslant 1$ and changes its universality for $\delta < 0$, where the spin gap is found to vanish continuously around the QCP more faster. As in the $2d$ case, for $\delta = 0$ all soft modes coincide and we find the QCP for the $3d$ isotropic KNM $(t/J)_c \approx 0.375$ [11].

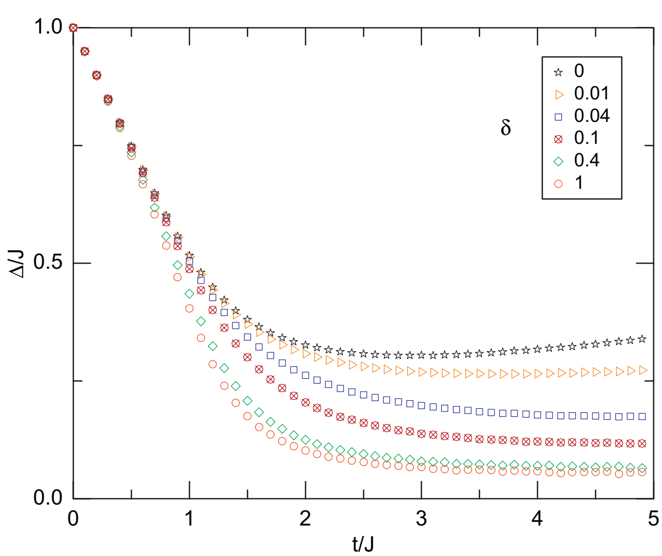

Fig. 1. (Color online) The spin gap Δ/J versus the control parameter t/J is sketched for different values of δ in one dimension and $T = 0$. It shows that spin gap is always nonzero for $0 \leqslant \delta \leqslant 1$.

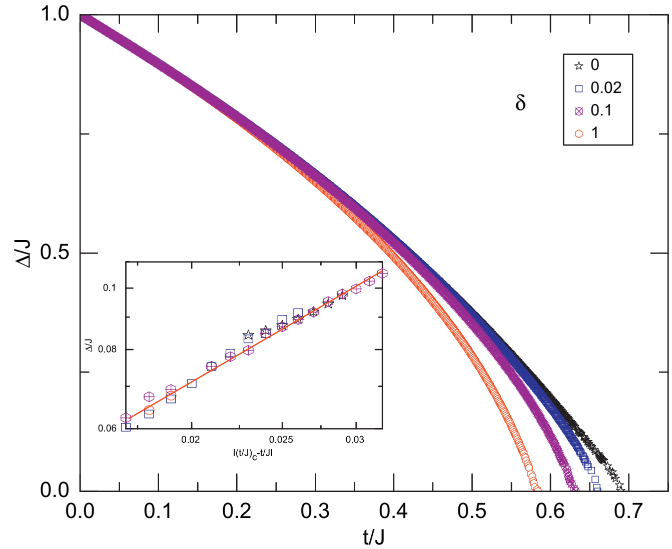

Fig. 2. (Color online) Sketch at zero temperature of the spin gap versus the strength t/J in two dimensions. The inset shows the log–log plot of the spin gap versus $|(t/J)_c - t/J|$ for $0 \leqslant \delta \leqslant 1$. It shows that Δ/J vanishes close to $(t/J)_c$ with a exponent $\nu z \approx 1$.

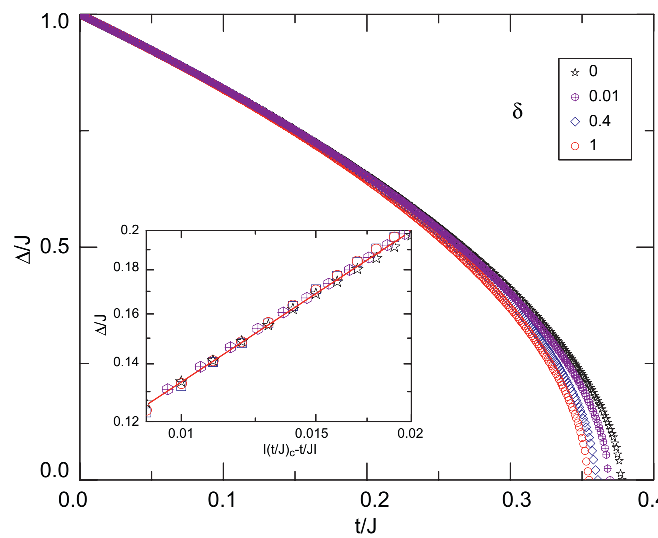

Fig. 3. (Color online) Anisotropy dependence on the spin gap versus the strength t/J in three dimensions at $T = 0$ and $0 \leqslant \delta \leqslant 1$. The scaling of gap close to the QCP is shown in the inset of the figure. It shows the log–log plot of Δ/J vs $|(t/J)_c - t/J|$ for $\delta = 0, 0.1, 0.4, 1$, and scales close to the QCP like $\Delta/J \sim |(t/J)_c - t/J|^{\nu z}$ with spin gap exponent $\nu z \approx 0.5$.

We conclude that, for all anisotropy between $0 \leqslant \delta \leqslant 1$, there exists a critical value $(t/J)_c$, where the spin gap vanishes as $\Delta/J \propto |(t/J)_c - t/J|^{\nu z}$, and a QPT to the ordered magnetic phase occurs in $2d$ and $3d$ whereas no transition happens in $1d$. This is similar to the results in Ref. [11] for $\delta = 0$, and it gives us a kind of universality similar as in the isotropic Kondo lattices [1,11,22]. Considering the relationship between the spin gap and the distance to the QCP, sketched in the onset of Fig. 3, it is shown that when t/J increases from its strong coupling limit, the triplet spin gap at the wave vector $Q = (\pi, \pi, \pi)$ decreases and vanishes at $t/J = (t/J)_c$. Since $\Delta/J \propto |(t/J)_c - t/J|^{0.5}$, close to the QPT, we can immediately identify the spin gap exponent $\nu z \approx 0.5$ at the QCP of the Kondo lattice, confirming our early theoretical results [1]. Finally, for $\delta < 0$ exists also a QPT in $d = 2, 3$ but no phase transition appears in $1d$.

2.2. Analytical results at the quantum critical trajectory

Since QPTs are generally associated with soft modes at the QCP, where the gap for excitation vanishes, then physical quantities have power law temperature dependencies determined by the quantum critical exponents [27]; one of them is the specific heat C_V, that we will calculate here. This strategy has been intensively explored in the study of HF materials, in the so-called *quantum critical trajectory* $J/t = (J/t)_c, T \to 0$, fixing the pressure (in our case the control parameter J/t) at its critical value for the disappearance of magnetic order [28]. Then, we calculate analytically the anisotropy dependence on the specific heat at $J/t = (J/t)_c$, $T \to 0$ for both cases, $\delta \ll 1$ and $\delta \approx 1$. All the calculations will be done considering two essential approximations: (i) The system is at the QCP $J/t = (J/t)_c$, and temperatures $T \to 0$. (ii) The temperature region where the specific heat will be found will be lower than the Kondo temperature (T_K). We will begin writing $k = Q + q$ and expanding for small q: $\lambda(q) = -d + q^2/2 + O(q^4)$, this yields the spectrum of transverse spin triplet excitations as

$$\begin{aligned} \omega_q &\approx \omega_0\sqrt{1 + y\lambda(q)} \\ &= \sqrt{\Delta^2 + Dq^2}, \\ \omega'_q &\approx \omega_0\sqrt{1 + y\lambda(q)(1-\delta)} \\ &= \sqrt{\Delta^2 + D(1-\delta)q^2 + \omega_0^2\delta}, \end{aligned} \tag{12}$$

where $\Delta = \Delta^x$ is the spin gap energy given by Eq. (11) since $0 \leqslant \delta \leqslant 1$, $D = \omega_0^2/2d$ the spin-wave stiffness at $T = 0$, and ω_0 is the z-polarized dispersionless branch of excitations. Considering $\Delta = 0$, at the QCP [27] in the excitations spectrum given by Eq. (12), and using $C_V = -T\partial^2 F/\partial T^2$ in Eq. (6) we get

$$\begin{aligned} C_V = &\frac{S_d}{4k_B T^2 \pi^d}\int_0^\pi \mathrm{d}q\, q^{d-1}(\omega_q^2 + {\omega'_q}^2) \\ &\times \left(\sinh^{-2}\frac{\beta\omega_q}{2} + \sinh^{-2}\frac{\beta\omega'_q}{2}\right), \end{aligned} \tag{13}$$

where S_d is the solid angle. Eq. (13) yields the expression for the anisotropic dependence on specific heat at the *quantum critical trajectory*, as a contribution of bosons t_x and t_y.

Case $0 \leqslant \delta \ll 1$—Having shown the relationship between the specific heat C_V and δ, we now discuss the case $\delta \ll 1$. Making a change of variables in Eq. (13), we obtain

$$\begin{aligned} C_V(\delta \ll 1) = &\frac{S_d k_B Z^{d/2}}{\pi^d}\left(\frac{k_B T}{\omega_0}\right)^d \\ &\times \left[\Upsilon_1(d) + \frac{\delta}{4}(\Upsilon_2(d) - 2\Upsilon_1(d))\right], \end{aligned} \tag{14}$$

where $x = \beta\omega_0 q/\sqrt{Z}$, $\Upsilon_1(d) = \int_0^\infty \mathrm{d}x\, x^{d+1}\sinh^{-2}(x/2)$ and $\Upsilon_2(d) = \int_0^\infty \mathrm{d}x\, x^{d+2}\coth(x/2)\sinh^{-2}(x/2)$. In $2d$ we found $\Upsilon_1(2) = 24\zeta(3)$ and $\Upsilon_2(2) = 96\zeta(3)$, where ζ is the Riemann zeta-function. In $3d$ $\Upsilon_1(3) = 16\pi^4/15$ and $\Upsilon_2(3) = 16\pi^4/3$. For $\delta = 0$, the excitations spectrum given by Eq. (12) coincide and we recover the exact value as obtained in an previous work for the isotropic KNM [1].

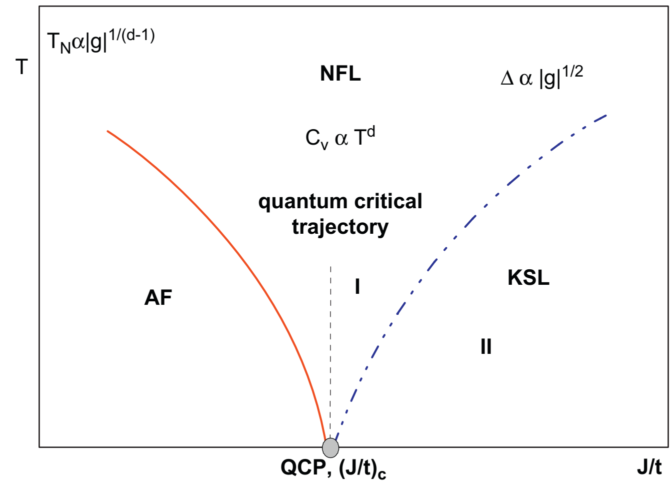

Fig. 4. (Color online) Schematic phase diagram of the anisotropic Kondo necklace model at finite temperatures. The AF phase is located below the Neel line T_N (solid line), which vanishes at a critical value $(J/t)_c$ (QCP) for any anisotropy $\delta \ll 1$. The spin gap energy (dashed line) is shown as a function of g. It was taken from Ref. [1]. Below this line, in the region II of the paramagnetic phase, there is a Kondo spin liquid state (KSL). The temperature dependence of the specific heat $C_V \propto T^d$ is given along the quantum critical trajectory, in the Non-Fermi liquid (NFL) regime, for any dimension and for any anisotropy $\delta \ll 1$ and $\delta \approx 1$. It is shown in the region I of the paramagnetic phase.

Case $\delta \approx 1$—Here, it is sufficient to consider, $\xi = 1 - \delta \ll 1$, where ξ is a dimensionless parameter that controls the Ising-like anisotropy in this case. Thereby, working in analogy with the preceding case, we obtain

$$C_V(\delta \approx 1) = \frac{S_d k_B Z^{d/2}}{4\pi^d}\left(\frac{k_B T}{\omega_0}\right)^d \Upsilon_1(d)(2 - \delta), \tag{15}$$

where we have already replaced the ξ expression. The results above show that the specific heat of the AKNM for $\delta \ll 1$ and $\delta \approx 1$ is only re-normalized by the anisotropy, concluding that $C_V \propto T^d$ at the *quantum critical trajectory* for $\delta \ll 1$ and $\delta \approx 1$. Notice that this is consistent with the general scaling result $C_V \propto T^{d/z}$ with the dynamic exponent z taking the value $z = 1$ [27]. Since $z = 1$, in $3d$ the effective dimension $d_{\text{eff}} = d + z = d_c = 4$ where d_c is the upper critical dimension for the magnetic transition [27]. Consequently, the present approach yields the correct description of the QCP of the Kondo lattices for $d \geqslant 3$, though this mean-field approximation does not reproduce the logarithmic corrections of the specific heat typical of systems with $d_{\text{eff}} = d_c$. Fig. 4 shows the temperature dependence of the specific heat $C_V \propto T^d$ along the quantum critical trajectory for any dimension and for any anisotropy $0 \leqslant \delta \ll 1$ and $\delta \approx 1$.

3. AF phase

The mean-field approach can be extended to the AF phase assuming the condensation in the x component of the spin triplet like: $t_{\mathbf{k},x} = \sqrt{N}\bar{t}\delta_{k,Q} + \boldsymbol{\eta}_{\mathbf{k},x}$, where $\bar{t}$ is its mean value in the ground state and $\boldsymbol{\eta}_{\mathbf{k},x}$ represents the fluctuations. Making the same steps as before, the internal energy renders

$$U' = \varepsilon'_0 + \sum_{\mathbf{k}}(\omega_0 n(\omega_0) + \omega_{\mathbf{k}} n(\omega_{\mathbf{k}}) + \omega'_{\mathbf{k}} n(\omega'_{\mathbf{k}})), \tag{16}$$

where

$$\varepsilon_0' = N\left[-\frac{3}{4}J\bar{s}^2 + \mu\bar{s}^2 - \mu + \left(\frac{J}{4} + \mu - \frac{1}{2}tZ\bar{s}^2\right)\bar{t}^2\right] + \frac{1}{2}\sum_{\mathbf{k}}(\omega_{\mathbf{k}} + \omega_{\mathbf{k}}' - \Lambda_{\mathbf{k}} - \Lambda_{\mathbf{k}}') \tag{17}$$

is the AF ground state. The free energy is now

$$F' = \varepsilon_0' - \frac{1}{\beta}\sum_{\mathbf{k}}\ln[1+n(\omega_{\mathbf{k}})] - \frac{1}{\beta}\sum_{\mathbf{k}}\ln[1+n(\omega_{\mathbf{k}}')] - \frac{N}{\beta}\ln[1+n(\omega_0)]. \tag{18}$$

Minimizing the free energy equation (18), as in the paramagnetic case, using $(\partial F'/\partial\mu, \partial F'/\partial\bar{s}, \partial F'/\partial\bar{t}) = (0,0,0)$, we can easily get the following saddle-point equations:

$$\begin{aligned}
\bar{s}^2 &= 1 + \frac{J}{Zt} - \frac{f(\omega_0)}{2} - \frac{1}{4N}\sum_{\mathbf{k}}\sqrt{1+\frac{2\lambda(\mathbf{k})}{Z}}(1+2n(\omega_{\mathbf{k}})) + \frac{1}{4N}\sum_{\mathbf{k}}\sqrt{1+\frac{2\lambda(\mathbf{k})(1-\delta)}{Z}}(1+2n(\omega_{\mathbf{k}}')),\\
\bar{t}^2 &= 1 - \frac{J}{Zt} - \frac{f(\omega_0)}{2} - \frac{1}{4N}\sum_{\mathbf{k}}\frac{(1+2n(\omega_{\mathbf{k}}))}{\sqrt{1+\frac{2\lambda(\mathbf{k})}{Z}}} + \frac{1}{4N}\sum_{\mathbf{k}}\frac{(1+2n(\omega_{\mathbf{k}}'))}{\sqrt{1+\frac{2\lambda(\mathbf{k})(1-\delta)}{Z}}},\\
\mu &= \tfrac{1}{2}Zt\bar{s}^2 - J/4,
\end{aligned} \tag{19}$$

with the excitation spectrum of the x-transverse and y-transverse spin triplet states given now by

$$\omega_{\mathbf{k}} = \tfrac{1}{2}Zt\bar{s}^2\sqrt{1+2\lambda(\mathbf{k})/Z}, \tag{20}$$

$$\omega_{\mathbf{k}}' = \tfrac{1}{2}Zt\bar{s}^2\sqrt{1+2\lambda(\mathbf{k})(1-\delta)/Z}, \tag{21}$$

respectively. Generally the equations for $\bar{s}$ and $\bar{t}$ in Eq. (19) should be solved and for $\delta = 0$ the results of Ref. [1] are recovered. Here, in the magnetic ordered state, the condensation of triplets (singlets) follows from the RKKY interaction (Kondo effect). At finite temperatures the condensation of singlets occurs at a temperature scale which, to a first approximation, tracks the exchange J while the energy scale below which the triplet excitations condense is given by the critical Neel temperature (T_{N}), which is calculated in the next section. 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 [1,11,22] for all values of the ratio $J/t < (J/t)_c$.

4. Critical line in the AKNM

Following the discussion above, the critical line giving the finite temperature instability of the AF phase for $J/t < (J/t)_c$ is obtained making $\bar{t} = 0$. Hence, from Eq. (19) we can obtain the boundary of the AF state as

$$\frac{|g|}{Z} = \frac{f(\omega_0)}{2} + \frac{1}{2N}\sum_{\mathbf{k}}\left(\frac{n(\omega_{\mathbf{k}})}{\sqrt{1+\frac{2\lambda(\mathbf{k})}{Z}}} + \frac{n(\omega_{\mathbf{k}}')}{\sqrt{1+\frac{2\lambda(\mathbf{k})(1-\delta)}{Z}}}\right), \tag{22}$$

where $g = |(J/t)_c - (J/t)|$ measures the distance to the QCP. The latter is given by

$$(J/t)_c = Z\left[1 - \frac{1}{4N}\sum_{\mathbf{k}}\left(\frac{1}{\sqrt{1+2\lambda(\mathbf{k})/Z}} + \frac{1}{\sqrt{1+2\lambda(\mathbf{k})(1-\delta)/Z}}\right)\right],$$

which separates an AF long-range ordered phase from a gapped spin liquid phase. Performing the same analysis as in Section 2.2, and expanding the excitations spectrum close to $\mathbf{Q} = (\pi,\pi,\pi)$, Eq. (22) becomes

$$\frac{|g|}{Z} = \frac{S_d\omega_0}{4\pi^d}\int_0^{\pi} \mathrm{d}q\, q^{d-1} \times \left(\frac{1}{\omega_q}\left(\coth\frac{\beta\omega_q}{2} - 1\right) + \frac{1}{\omega_q'}\left(\coth\frac{\beta\omega_q'}{2} - 1\right)\right), \tag{23}$$

where we have considered that for temperatures $k_B T \ll \omega_0$, $f(\omega_0)$ goes to zero faster than the first term of Eq. (22). This equation above allows us to obtain the critical line in the AKNM as a function of the anisotropy parameter δ.

4.1. Case $0 \leqslant \delta \ll 1$

We now demonstrate analytically the appearance of a finite Neel line when a small degree of anisotropy δ in y-component spin is turned on. Then, solving Eq. (23) for $0 \leqslant \delta \ll 1$, we get

$$\frac{|g|}{Z_{\delta\ll 1}} = \frac{S_d Z^{d/2}}{2\pi^d}\left(\frac{k_{\mathrm{B}}T}{\omega_0}\right)^{d-1} \times \left[\Phi_1(d) + \frac{\delta}{8}(\Phi_2(d) + 2\Phi_1(d))\right], \tag{24}$$

where $\Phi_1(d) = \int_0^\infty \mathrm{d}x\, x^{d-2}(\coth x/2 - 1)$ and $\Phi_2(d) = \int_0^\infty \mathrm{d}x\, x^{d+1} \sinh^{-2}(x/2)$. We noticed that the integrals $\Phi_1(d)$ and $\Phi_2(d)$ diverge for $d<3$, showing that there is no critical line in $2d$ at finite temperatures [1,15] for any anisotropy $\delta \ll 1$, in agreement with the Mermin–Wagner theorem [29] when $\delta = 0$. Nevertheless, for $d \geqslant 3$, the integrals are finite and the equation for the critical line shows $(T_{\mathrm{N}})_{\delta\ll 1} \propto |g|^{\phi}$, with $\phi = 1/(d-1)$. If we write the equation for the critical line, $f(g,T) = 0$, in the form, $(J/t)_c(T) - (J/t)_c(0) + v_0 T^{1/\psi} = 0$, with v_0 related to the spin-wave interaction, we can identify the *shift exponent*, $\psi = z/(d+z-2)$ [30], that comparing with ϕ gives us the dynamic exponent $z = 1$, a Gaussian result, since the critical line only exists for $d>2$. The temperature dependence of the function f arising from the spin-wave interactions can modify the temperature dependence of the physical properties, as the specific heat, at $J/t = (J/t)_c$. However, in the limit $T \to 0$ we can easily see that the purely Gaussian results for the specific heat calculated in Section 2.2 is dominant, in agreement with the mean-field treatment used here. For $\delta = 0$, we obtain the well established result for the critical line in the KNM [1], which is due to the fact that the spectrum energy of the two excitations coincide. In summary, we have obtained analytically the expression for the Neel line below which the triplet excitations condense, close to the QCP for $0 \leqslant \delta \ll 1$. We have shown that this line does not exist for $d = 2$ for any value of the anisotropy $\delta \ll 1$, as we expected, whereas for $d \geqslant 3$, the power dependence on $|g|$ of the critical line in the presence of the anisotropy is the *same* of the KNM original. Therefore, the criticality close the QCP is governed by the *same* critical exponents of the isotropic $\delta = 0$ case that we have calculated before [1]. Fig. 4 shows the phase diagram of the anisotropic KNM at finite temperatures. The AF phase is located below the Neel line T_{N} (solid line), which vanishes at a critical value $(J/t)_c$ (QCP) for any anisotropy $\delta \ll 1$.

5. Conclusions

In conclusion, we have examined the phase diagram of the Kondo necklace model in the presence of an Ising-like anisotropy at zero and low temperatures by means of analytical and numerical techniques. At zero temperature we have derived and solved the self-consistent equations on the Kondo spin liquid phase for any value of δ. This allowed us to calculate the anisotropy dependence on the spin gap for $d = 1, 2, 3$. In the 1d case, there is no indication at all suggesting a critical value for t/J, where the gap would vanish for any value of anisotropy δ. For $d = 2, 3$ we found that the anisotropy in the range $0 < \delta \leqslant 1$ dislocates slightly the QCP's position until $\delta = 0$, where the excitations spectrum coincide. In this range $0 \leqslant \delta \leqslant 1$ the spin gap exponent is approximately the *same*, while for $\delta < 0$ the QCP's value decreases and it belongs to other universality class. In particular, in three dimensions, the triplet spin gap for anisotropy $0 \leqslant \delta \leqslant 1$, close to the wave vector $Q = (\pi, \pi, \pi)$, decreases and vanishes at $t/J = (t/J)_c$ with spin gap exponent $\nu z \approx 0.5$. It is consistent with the dynamic exponent $z = 1$ and with the correlation length $\nu = \frac{1}{2}$, a result in agreement with the mean-field or Gaussian character of the approximations we have used to deal with the bond-operator Hamiltonian. On the other hand, at low but finite temperatures, we found that in general the dependence on $|g|$ of the critical line for the AKNM, in the presence of the anisotropy, is the *same* as on the original KNM. This implies that the critical exponents controlling the transition close to the QCP, for nonzero δ, are the same as those of the isotropic case. We have also obtained the thermodynamic behavior of the specific heat along the *quantum critical trajectory* $J/t = (J/t)_c, T \to 0$. It has a power law temperature dependence as $C_V \propto T^d$, a result consistent with the scaling theory with the dynamic exponent $z = 1$, though it does not reproduce the logarithmic correction of the specific heat characteristic of systems with $d_{\mathrm{eff}} = d_c$. It is alsoworth pointing out that the approximations used here are valid very close to the quantum phase transition in the QCP $(J/t)_c$. It was the reason for that we have expanded the excitation spectrum close to the antiferromagnetic wave vector $\mathbf{Q} = (\pi, \pi, \pi)$. Therefore, the most essential features of the Kondo lattices, i.e., the competition between a long-range-ordered state and a disordered state, is clearly retained in the model for $0 \leqslant \delta \leqslant 1$. The qualitative features regarding the stability of the AF phase are well displayed in the model and it allows a simple physical interpretation of the phase diagram in anisotropic Kondo lattices.

Acknowledgments

D. Reyes would like to thank professor Andre M.C. de Souza for useful computational help and professor A. Pérez-Gramatges for the careful reading of the manuscript. Han-Ting Wang would like to acknowledge the financial support from NKBRSF of China under Grant no. 2006CB921400. The authors D. Reyes and M.A. Continentino would like to thank also the Brazilian Agencies CNPq and FAPERJ for financial support.

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