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LETTER TO THE EDITOR

The fate of Kondo resonances in certain Kondo lattices: a 'poor woman's' scaling analysis

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Abstract
We present an effective field theory for the Kondo lattice, which can exhibit, in a certain range of parameters, a non-Fermi-liquid paramagnetic phase at the brink of a zero-temperature anti-ferromagnetic (AF) transition. The model is derived in a natural way from the bosonic Kondo–Heisenberg model, in which the Kondo resonances are seen as true (but damped) Grassmann fields in the field theory sense. One-loop renormalization group (RG) treatment of this model gives a phase diagram for the Kondo lattice as a function of J_K where for $J_K < J_c$ the system shows AF order, for $J_K > J_1$ one has the heavy electron phase and for $J_c < J_K < J_1$ the formation of the Kondo singlets is incomplete, leading to the breakdown of the Landau Fermi liquid theory.

In the last ten years, there has been an increasing body of experimental evidence showing striking deviations from conventional Landau Fermi liquid theory (LFL) at some heavy fermion quantum critical points (QCPs) [1–10]. The specific heat coefficient is seen to diverge at the QCPs, showing a logarithmic increase [2, 7, 9, 8] as the temperature is decreased, followed for two compounds ($YbRh_2Si_2$ and $CeCoIn_5$ tuned to criticality under magnetic field) by an upturn at lower temperature [9–11]. The resistivity is quasi-linear in temperature for most compounds [5, 10, 6], with perfectly linear dependence for $YbRh_2(Si_{0.95}Ge_{0.05})_2$ and $CeCu_{5.9}Au_{0.1}$ [1, 2, 9]. NMR and μ-SR studies show that, generically, the susceptibility acquires anomalous exponents [5, 10, 8]. For $CeCu_{6-x}Au_x$ [8] neutron scattering measurements reveal the presence of B/T and ω/T scaling in the dynamic spin susceptibility at the QCPs. Recent e-SR [12], thermal expansion [13] as well as Hall effect [14, 15], heat transport [16] and Nernst effect [17] studies show further deviation from the LFL predictions. Last, for both the compounds $CeCoIn_5$ [18] and $YbRh_2(Si_{0.95}Ge_{0.05})_2$ [19] driven to criticality by applying a magnetic field, there are indications that deviations from the LFL theory of metals might appear over a whole region—instead of a point—of the phase diagram, in the vicinity of the QCP.

These very striking results have inspired several theoretical descriptions. Some require fully anisotropic (2D) spin fluctuations [20, 21]. Recently the idea of a local mode at criticality [1, 8, 21] has emerged in relation to the compounds $CeCu_{6-x}Au_x$ [8] and $YbRh_2Si_2$ [9, 10]. There are also some approaches invoking deconfinement and 'fractionalization' in gauge theories [22], but none of the theoretical approaches so far can account for a non-Fermi-liquid paramagnetic phase, as well as fitting more than one or two experimental observations.

In this letter we present an effective model for the Kondo lattice, which exhibits a non-Fermi-liquid paramagnetic phase in the vicinity of a zero-temperature AF transition or QCP. The starting point is the Kondo–Heisenberg lattice model, where we use a Schwinger boson representation for the spins of the impurities. We call this model the bosonic Kondo–Heisenberg model (BKH). In this framework, the Kondo bound states are represented by spinless Grassmann fields ($\chi^\dagger$, χ), which have no expectation value at the mean field level. On the other hand, the bosonic representation of the impurity spins enables us to get a decent treatment of antiferromagnetism at the mean field level. We observe that, starting from high energy and going to the infra-red sector, the Kondo bound states ($\chi^\dagger$, χ) acquire dynamics, damping and dispersion, since they are coupled to 'itinerant' excitations. The key ingredient of our effective theory is thus to treat the Grassmann Kondo resonances as *true fields* in the field theory sense. We attribute to them some dynamics as well as some damping from the start, and couple them in a physical way to fields of the BKH model. A renormalization group (RG) treatment applied to this model has the remarkable property that both the formation of Kondo singlets and the AF fluctuations—which prevent Kondo singlets from being formed—appear at the one-loop level in the form of a logarithmic singularity. That the formation of Kondo singlets has a logarithmic signature at the one-loop level is a well known fact, in the context of the Kondo impurity, where it was observed a long time ago [23, 24]. The new feature, here, is the presence of a logarithm at the one loop, characteristic of the AF fluctuations. This is the direct consequence of treating the resonances as true fields, with some intrinsic dynamics as well as damping. We are then in a position to obtain a phase diagram for the Kondo lattice, which can exhibit non-Fermi-liquid properties over a finite region of the diagram.

The BKH lattice Hamiltonian

$$H = H_c + H_K + H_H, \qquad \text{where}$$
$$H_c = \sum_{k\sigma} \varepsilon_k f^\dagger_{k\sigma} f_{k\sigma}, \quad H_K = J_K \sum_{i\sigma\sigma'} b^\dagger_{i\sigma} b_{i\sigma'} f^\dagger_{i\sigma'} f_{i\sigma}, \quad H_H = J_H \sum_{(i,j)\sigma\sigma'} b^\dagger_{i\sigma} b_{i\sigma'} b^\dagger_{j\sigma'} b_{j\sigma} \tag{1}$$

describes the conduction band (H_c), the Kondo coupling between local moments and the conduction electrons at site i (H_K), and the super-exchange between neighbouring spins (H_H).

The physics of this model depends on the ratio $x = J_K/J_H$. In the Doniach scenario [25] for the Kondo lattice, when $x \ll 1$ the spins anti-ferromagnetically order, and as x is increased the AF state undergoes a transition towards a heavy electron paramagnet. It is the goal of this paper to take a closer look at the nature of this transition.

When we formulate the BKH model as a functional integral, we can decouple the fields as follows:

$$\begin{aligned} H_K \to H'_K &= \sum_{i\sigma} \left[b^\dagger_{i\sigma} \chi^\dagger_i f_{i\sigma} + \text{h.c.} \right] - \frac{\chi^\dagger_i \chi_i}{J_K} \\ H_H \to H'_H &= \sum_{(i,j)\sigma} \left[|\Delta_{ij}| e^{i\frac{\pi}{a}\mathbf{r_i}-\mathbf{r_j}} b^\dagger_{i\sigma} b^\dagger_{j-\sigma} + \text{h.c.} \right] - \frac{|\Delta_{ij}|^2}{J_H}, \end{aligned} \tag{2}$$

where the bond variable in the first term is a Grassmann field which does not carry a spin and the bond variable in the second term has been chosen following an SP(2N) decomposition of the interaction [26]. The mean field theory of this model requires an additional constraint term on the Schwinger boson [27, 28] representation of the impurity spin

$$H = H_{\mathrm{c}} + H_{\mathrm{K}} + H_{\mathrm{H}} + \sum_i \lambda \left(b^{\dagger}_{i\sigma} b_{i\sigma} - 2S \right),$$

where S is the spin of the impurity, taken to be $1/2$ in the case of our concern.

At the mean field level, the χ-fermions do not acquire any expectation value, while the bosonic bound state Δ can condense, leading to an AF phase. After diagonalizing the bosonic part of H in a mean field approximation, one gets the following propagator for the spinons:

$$\hat{G}(\omega, k) = \begin{bmatrix} \langle T b_{k\sigma} b^{\dagger}_{-k-\sigma} \rangle & \langle T b_{k\sigma} b_{-k-\sigma} \rangle \\ \langle T b^{\dagger}_{-k-\sigma} b^{\dagger}_{k\sigma} \rangle & \langle T b^{\dagger}_{-k-\sigma} b_{-k-\sigma} \rangle \end{bmatrix} = \frac{1}{(\mathrm{i}\omega)^2 - \omega_k^2} \begin{bmatrix} \mathrm{i}\omega - \lambda & \Delta_k \\ \Delta_k & -\mathrm{i}\omega - \lambda \end{bmatrix}, \qquad (3)$$

where ω is a bosonic Matsubara frequency, $\Delta_k = \Delta \left(\sin k_x + \sin k_y + \sin k_z \right)$ is an odd function of k and $\omega_k = \sqrt{\lambda^2 - \Delta_k^2}$. If $|\lambda| > \Delta$ the system is in the paramagnetic phase and spinons have a mass $\omega_0 = \sqrt{\lambda^2 - \Delta^2}$. When $|\lambda| = \Delta$ the system is at a second order phase transition towards an AF ground state and spinons become massless ($\omega_0 = 0$). In what follows we consider that the Kondo lattice undergoes an AF transition, such that part of the phase diagram is paramagnetic ($\omega_0 \neq 0$) and part is antiferromagnetic ($\omega_0 = 0$). ω_0 is the mass of the spinons and plays the role of a parameter in the effective theory.

Through coupling to the spinons ($b_{k\sigma}$) and the itinerant electrons ($f_{k\sigma}$) the χ-fermion Kondo resonances acquire some dynamics, damping and dispersion. It is natural to think that at some energy scale the dynamics will become linear in ω—actually a propagator linear in ω is needed to regulate the high energy dependence. We propose the following effective action, comprising three fields:

$$\begin{aligned} S &= S_f + S_b + S_\chi + S_{\mathrm{int}}, \\ S_f &= \int \mathrm{d}\omega\, \mathrm{d}^d k \sum_\sigma f^{\dagger}_{k\sigma} \left(\mathrm{i}\omega - \varepsilon_k \right) f_{k\sigma}, \\ S_b &= \int \mathrm{d}\nu\, \mathrm{d}^d q \sum_\sigma V_b^{\dagger} \hat{G}^{-1}(\nu, q) V_b, \\ S_\chi &= \int \mathrm{d}\omega\, \mathrm{d}^d p\, \chi^{\dagger}_p \left(\mathrm{i}\omega + \mathrm{i}\Gamma(\omega)\, \mathrm{sgn}(\omega) + g_0^2/J_{\mathrm{K}} \right) \chi_p, \\ S_{\mathrm{int}} &= g \int (\mathrm{d}\omega)^2\, \mathrm{d}^d k\, \mathrm{d}^d q\, \mathrm{d}^d p\, \delta_{\mathbf{p}+\mathbf{q}-\mathbf{k}} \sum_\sigma \left(b^{\dagger}_{q\sigma} \chi^{\dagger}_p f_{k\sigma} + \mathrm{h.c.} \right), \end{aligned} \qquad (4)$$

where $V_b = \binom{b_{q\sigma}}{b^{\dagger}_{-q-\sigma}}$ is the spinor basis for the mean field description (3) of the AF fluctuations, $\Gamma(\omega)$ is the damping associated with the χ-fermions, which we take constant in order to simplify computations, but which in all generality is taken to be relevant in the infrared sector (for example $\Gamma(\omega) = |\omega|^\alpha$ with $\alpha < 1$), and g is the interaction between the three fields. We have re-scaled the χ fields such that their inverse propagator has the dimension of energy. Now the χ-fermions are considered as true fields with a finite lifetime and a dispersion $\varepsilon_\chi(p) = -g_0^2/J_{\mathrm{K}}$. The dispersion becomes a tuning parameter of our theory. Generically, three cases are possible.

(1) The χ-'band' is full, or $J_{\mathrm{K}} > 0$. This case corresponds to AF Kondo coupling and is considered in this paper. The dispersion of the band is neglected as long as the band is full.

(2) The χ-'band' is empty, or $J_{\mathrm{K}} < 0$. This is the ferromagnetic Kondo coupling, where the interaction g is marginally irrelevant. This case is of no great interest for HF compounds, but can be of some relevance for the manganites.

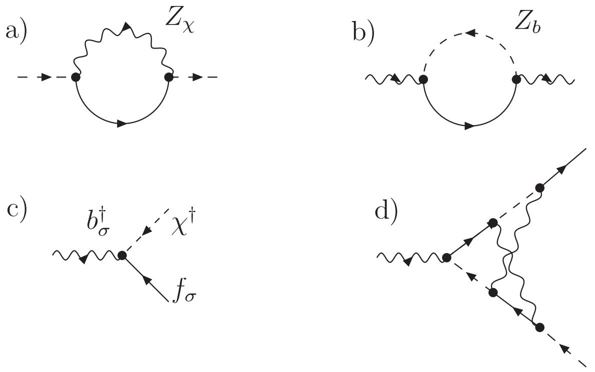

Figure 1. Diagrams associated with (a) the renormalization of the χ-fermion field, (b) the spinon field, (c) the vertex g and (d) two-loop renormalization of the vertex. Solid, dashed and wavy lines are respectively f-fermion, χ-fermion and boson propagators.

(3) The χ-'band' is so renormalized through its interaction with the spinons and the conduction electron that it acquires a 'Fermi' surface—or a surface in k-space where the dispersion changes sign. This is a very intriguing possibility, allowing the presence of *massless* χ-fermions. This case will be addressed in a future work.

We now turn to the study of the stability of the model with respect to the coupling g (diagram (c) in figure 1). One peculiarity of our model is that at one loop there is no renormalization of the vertex coming from irreducible diagrams. The logarithmic contribution comes from the renormalization of the spinon and χ-fermion propagators (diagrams (a) and (b) in figure 1).

We use an RG scheme, where the parameter g_0^2/J_{K} as well as λ are fixed, while the counter-terms are absorbed into the renormalization of the fields $\chi = Z_\chi^{1/2}\chi^{\mathrm{R}}$ and $b = Z_b^{1/2} b^{\mathrm{R}}$, where χ^{R} and b^{R} are the renormalized fields. The invariance of the propagators is ensured by introducing two new parameters, keeping track of the field's lifetime $G_\chi^{-1} = Z_{\chi\omega}\mathrm{i}\omega + g_0^2/J_{\mathrm{K}}$ and $G_b^{-1} = Z_{b\omega}\mathrm{i}\omega - \lambda$. The β-function for the local interaction g takes the form

$$\beta(g) = \frac{\mathrm{d}g}{\mathrm{d}\log D} = -\pi\rho g^3\left(J_{\mathrm{K}}/g_0^2 - 1/\lambda\right), \tag{5}$$

where D is the bandwidth of the conduction electrons, ρ is the density of states and λ is generically positive, such that for $J_{\mathrm{H}} = 0$ in (1) spinons have poles at positive energies. In the flow (5) the first term comes from the renormalization of the Kondo resonances (diagram (a) in figure 1) and is responsible for the usual Kondo behaviour of the model, leading g to strong coupling. The new feature is the presence of a logarithm at one loop, coming from the renormalization of the spinon propagator (diagram (b) in figure 1) and opposing the Kondo effect in the RG flow. Note that this term would not be present if we did not give *dynamics* to the χ-fields in (4). Two different possible flows are shown in figure 2. For $J_{\mathrm{K}} - g_0^2/\lambda > 0$, the flow goes to strong coupling. We identify the strong coupling fixed point with the heavy Fermi liquid phase, where Kondo singlets form. On the other hand, for $J_{\mathrm{K}} - g_0^2/\lambda < 0$ the flow goes to weak coupling and the model is stable. Note that the stability criterion does not depend on the sign of g.

Integrating (5) enables us to get the energy scales:

$$g^2 = \frac{g_0^2}{1 + 2\pi\rho J^* \log(T/D)}; \qquad T^* = D\exp[-1/(2\pi\rho J^*)],$$

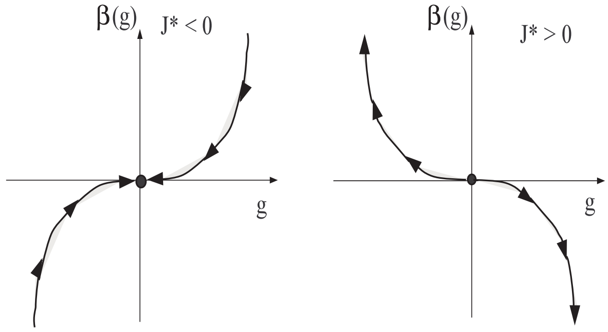

Figure 2. RG flows for the coupling constant g.

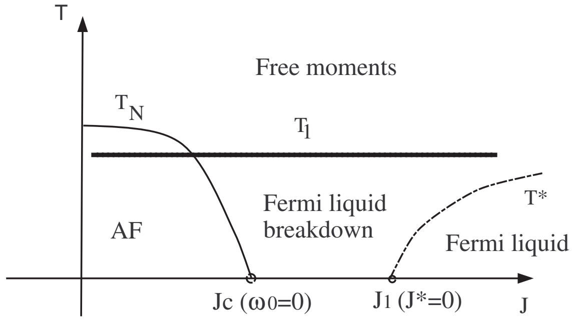

Figure 3. Phase diagram for $J_K < g_0^2/\Delta$.

where $J^* = J_K - g_0^2/\lambda$, and T^* is the temperature at which the Kondo singularity appears, or in other words the 'lattice' Kondo temperature. One notices that compared to the single impurity $T_K = D\exp[-1/(2\pi\rho J_K)]$, the lattice Kondo temperature T^* is reduced by the presence of AF fluctuations.

Examination of the field's lifetimes leads to

$$\frac{\mathrm{d}Z_{\chi\omega}}{\mathrm{d}\log D} = -2\pi\rho J_K g^2/g_0^2; \qquad \frac{\mathrm{d}Z_{b\omega}}{\mathrm{d}\log D} = 2\pi\rho g^2/\lambda. \tag{6}$$

The lifetime of the χ-fermion becomes infinitely small in the IR sector, which signals a breakdown of the Landau Fermi liquid theory, while at one loop the spinon lifetime is stable.

Three phase diagrams are possible, depending on the strength of the AF fluctuations. At large J_K we are, at zero temperature, in a heavy Fermi liquid phase, where our model flows to strong coupling. The first possibility is that J^* stays *positive* in the whole paramagnetic phase, reaching the AF QCP while the heavy quasi-particles are still well formed. In this scenario, conduction electrons are destabilized by a spin density wave (SDW) [29] connecting portions of the Fermi surface. The best candidate for this scenario is surely $CeNi_2Ge_2$, for which a study of the Grüneisen parameter has shown reasonable agreement with 3D Moriya theory [13].

The second possibility is that J^* stays positive in the whole paramagnetic phase, but vanishes at the AF QCP, where the fluctuations are the strongest. This happens for $J_K = g_0^2/\lambda_{\min} = g_0^2/\Delta = g_0^2/(SJ_H)$, in a large S expansion of the Heisenberg model.

Last, it might happen that the AF fluctuations close to the QCP are so strong that the Kondo effect is already broken in the paramagnetic phase, when J^* changes sign *before* reaching the AF transition (see figure 3). This happens for $J_K < g_0^2/\Delta$. In this case, the Landau Fermi liquid theory is broken in a whole *region* of the phase diagram for which our model (4) is stable. Recently, measurements on $CeCoIn_5$ [17, 18] and $YbRh_2(Si_{9.95}Ge_{0.05})_2$ [19] have indicated the presence of such a phase.

In order to further justify our identification of the strong coupling with the heavy Fermi liquid phase, we derived the RG flow at two loops. The diagram (d) in figure 1 is the sole contributor, and we find

$$\beta(g) = -2\pi\rho g^3 \left(J^* + 2\pi\rho g^2 A \log(g^2/J_{\mathrm{K}})\right), \tag{7}$$

where $A = 8\pi\lambda\,((\omega_{\mathrm{m}} - \omega_0)/v_{\mathrm{s}})^2$ in $D = 3$, with ω_{m} and ω_0 the upper and lower energies of the spinons and v_{s} the spinon dispersion $\omega_q = v_{\mathrm{s}} q$ taken linear over the whole spectrum. Since at high energy the starting parameters of our model are $g_0^2/J_{\mathrm{K}}^0 > 1$, the correction to scaling has the sign of the AF Kondo coupling J_{K}. When $J^* > 0$, the two-loop flow reinforces the tendency to flow to strong coupling, and comforts our identification of the strong coupling fixed point with the heavy Fermi liquid. When $J^* < 0$ two-loop corrections have opposite sign, revealing the presence of an intermediate energy scale T_1, where the β-function changes sign. When one renormalizes from high energy, the system first wants to form Kondo singlets, until we reach T_1. Further down in energy, for $J > J_1$ the formation of the Kondo heavy quasi-particles continues, while for $J < J_1$ it stops and the model (4) is stable, where the three fields corresponding to damped spinless χ-fermions, conduction electrons and spinons interact weakly with each other. The energy scale T_1 is seen in most of the heavy fermion compounds. It can be identified as the scale above which Curie susceptibilities are observed, or the scale at which the resistivity and the specific heat coefficient have a maximum.

The precise determination of the nature of the non-Fermi-liquid (NFL) phase deserves more intensive work. The reason why so many compounds—with low disorder—show linear resistivity over a wide temperature range may lie in the conjecture that a damping $\Gamma(\omega) = |\omega| \log(\omega)$ stabilizes our model at an intermediate energy scale.

It has been advanced recently [22] that deconfinement of spinons and the emergence of a 'fractionalized' state might be the clue for understanding the heavy fermion phase diagram. We believe, however, that the key most probably lies in the idea of a competition between the formation of Kondo singlets and AF fluctuations, which are maximal close to a QCP. Our study of model (4) shows that de-confinenent of spinons [30–32] is a separate issue from Kondo singlet formation. Even though our mean field treatment of the Heisenberg part assumes spinon deconfinement, previous work [33] incites us to believe that in $D = 3$, gauge theories being deconfining, spinons are de-confined in the NFL phase. The question is less clear in $D = 2$.

Since in our treatment we have assumed that the χ-band is full, we have not addressed the question of the variation of the Fermi surface volume. In all generality, though, the chemical potential of the χ-fermion can be renormalized to zero, leading to a reconfiguration of the charge carriers close to the QCP.

In conclusion, we have introduced an effective theory for Kondo lattices where the Kondo bound states are considered as true fields, with the statistics of spinless fermions. RG analysis of this model signals both the formation of Kondo singlets and AF fluctuations as logarithmic singularities at the one-loop level. This leads to a phase diagram where direct competition between Kondo and AF is apparent, resulting in the possibility of an NFL phase separating the AF phase from the heavy Fermi liquid. We believe the nature of the elementary excitations at the QCP in heavy fermion compounds is essentially captured by (4).

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