Critical Kondo destruction and the violation of the quantum-to-classical mapping of quantum criticality

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Abstract

Antiferromagnetic heavy fermion metals close to their quantum critical points display a richness in their physical properties unanticipated by the traditional approach to quantum criticality, which describes the critical properties solely in terms of fluctuations of the order parameter. This has led to the question as to how the Kondo effect gets destroyed as the system undergoes a phase change. In one approach to the problem, Kondo lattice systems are studied through a self-consistent Bose-Fermi Kondo model within the Extended Dynamical Mean Field Theory. The quantum phase transition of the Kondo lattice is thus mapped onto that of a sub-Ohmic Bose-Fermi Kondo model. In the present article we address some aspects of the failure of the standard order-parameter functional for the the Kondo-destroying quantum critical point of the Bose-Fermi Kondo model.

Key words: Heavy fermion compounds, Extended Dynamical Mean Field Theory, Bose-Fermi Kondo models; quantum phase transitions; quantum-to-classical mapping

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1. Introduction

Heavy fermion systems have attracted considerable interest ever since the initial studies [1] in the 1970s. While the early interest was fueled by the unusual Fermi liquid properties and superconductivity in these naturally magnetic materials, recent focus has been on their quantum critical behavior. In the following, we will focus on antiferromagnetic heavy fermion metals, in which a zero-temperature phase transition between a paramagnet and an itinerant antiferromagnet occurs when an external tuning parameter, e.g. external pressure, magnetic field, or compound composition, is varied [28]. This is made possible in part by the fact that the magnetic energy scales in these systems are small enough so that a moderate change of the tuning parameter corresponds to a sizeable perturbation. Because they are metallic, these materials allow for systematically addressing the interplay between quantum critical fluctuations and unusual electronic excitations.

The traditional approach to an itinerant antiferromagnetic quantum critical point (QCP) describes its universal properties in terms of a Ginzburg-Landau-Wilson functional of the order parameter and its fluctuations – the $\phi^4$ theory – in $d + z$ dimensions [19], where $d$ is the spatial dimension (typically 3 or 2) and $z$ corresponds to the dynamic exponent. Because the effective dimensionality is at or above the upper critical dimension of the $\phi^4$ theory, one is led to expect Gaussian behavior for such a Hertz-Millis or $T=0$ spin-density wave (SDW) QCP. The anticipated behavior of the spin relaxation rate $\Gamma_Q$ at the ordering wave vector is (for $d = 3$) $\Gamma_Q \sim T^{3/2}$, which has indeed been observed in one heavy fermion system [6]. There are however a number of observations that cannot be explained within the SDW approach [78910]. In $\text{CeCu}_6-x\text{Au}_x$, at its critical concentration $x_c \approx 0.1$, the spin relaxation rate is linear in temperature, and the order-parameter susceptibility singularly depends on temperature and frequency with a fractional exponent [7]. In $\text{YbRh}_2\text{Si}_2$, multiple energy scales collapse at its field-tuned QCP and, moreover, the Fermi surface has been implicated to transition from large to small when the QCP is crossed from the paramagnetic side. These rich behaviors have led to the question as to whether and how the Kondo screening is affected as the system undergoes a magnetic phase change [1112].

An alternative to the traditional approach that is able to explain the aforementioned experiments is the local quantum critical scenario, in which a destruction of Kondo screening of the f-moments coincides with the magnetic...
transition of the Kondo lattice [11]. The name local quantum criticality refers to the localization of the electronic excitations associated with the f-moments. It also stresses the importance of long-range correlations along imaginary time, when the spatial correlations remain mean-field like as in the SDW scenario. Both types of QCP have been described with the extended dynamical mean field theory (EDMFT) approach to the Kondo lattice model, see Fig. 1.

### 2. Extended DMFT, quantum critical Bose-Fermi Kondo models and the quantum-to-classical mapping

The quantum critical point in the heavy fermion compounds arises out of the competition between Kondo screening and the RKKY interaction [13]. A minimal model for these systems is the Kondo lattice model,

$$H = \sum_{k,\sigma} \epsilon_k d_{k,\sigma}^\dagger d_{k,\sigma} + J_K \sum_i s_{i} \cdot \mathbf{s}_i + \sum_{ij} \frac{I_{ij}}{2} \mathbf{s}_i \cdot \mathbf{s}_j$$  

where $s_{i} \cdot \mathbf{r}_i$ denotes the conduction $d$-electron spin density at the location of the local moment $\mathbf{s}_i$. The EDMFT approach captures not only the Kondo screened Fermi liquid phase and the itinerant magnetic phase but also the dynamical competition between the two underlying interactions. It maps the Kondo lattice onto the Bose-Fermi Kondo (BFK) model,

$$\mathcal{H}_{\text{bfkm}} = J_K \mathbf{S} \cdot \mathbf{s} + \sum_{p\sigma} E_p c_{p\sigma}^\dagger c_{p\sigma} + g \sum_p \mathbf{S} \cdot (\phi_p + \phi_p^\dagger) + \sum_p w_p \phi_p^\dagger \phi_p$$  

augmented by a self-consistency constraint, see Fig. 1. Here $\mathbf{S}$ is a spin-1/2 local moment, $J_K$ and $g$ are the Kondo coupling and the coupling constant to the bosonic bath respectively, $c_{p\sigma}$ describes a fermionic bath with a constant density of states, $\sum_p \delta(\omega - E_p) = N_0$, and $\phi_p^\dagger$ is the bosonic bath with the self-consistently determined spectral density.

Numerical evaluations of the EDMFT scheme for the easy-axis Kondo lattice at finite temperature [14,15] and at zero temperature [16,17] indicate that the general phase diagram of the Kondo lattice contains both the Hertz-Millis and the local quantum critical point. Within EDMFT, the local quantum critical point of the lattice problem is related to the quantum critical point (QCP) of a dissipative BFK model [18,19,20]. If the self-consistency condition leads to a spectral density for the bosonic bath that behaves as

$$\text{Im} \chi_0^{-1}(\omega) \equiv \sum_p [\delta(\omega - w_p) - \delta(\omega + w_p)]$$  

$$\sim |\omega|^{1-\epsilon} \Theta(\omega_c - |\omega|)$$  

below some dynamically generated scale $\omega_c$ with a bath exponent $0 < \epsilon < 1$, the lattice QCP is mapped on the QCP of the sub-Ohmic BFKM.

When arguments related to the ones that lead to the Ginzburg-Landau-Wilson functional of order-parameter fluctuations are applied, the sub-Ohmic BFK model would be mapped to a one-dimensional classical spin chain with long-ranged interaction [21] and, by extension, a local-$\phi^4$ theory in 0 + 1 dimension [23,24]. We will refer to this as the quantum-to-classical mapping of the QCP in the BFK model. In general, the quantum-to-classical mapping relates the quantum criticality to the classical criticality of order-parameter fluctuations in elevated dimensions [22]. For the local $\phi^4$ theory [23,24], $\epsilon = 1/2$ effectively acts as an upper critical dimension and a Gaussian fixed point is expected for $1/2 < \epsilon < 1$. Correspondingly, there will be a violation of $\omega/T$ scaling due to the dangerously irrelevant quartic coupling of the $\phi^4$ theory. For $\epsilon = 0$, the bosonic bath of the BFK model is Ohmic and the corresponding classical spin chain is placed at its lower critical dimension. The transition at $\epsilon = 0$ is thus Kosterlitz-Thouless like [25,26].

This raises the question as to how EDMFT manages to yield critical properties that differ from those of a local $\phi^4$-theory, especially the $\omega/T$-scaling of the order parameter susceptibility [14,15]. One possibility is that the self-consistency requirement leads effectively to a different quantum impurity problem for every temperature, i.e. $\text{Im} \chi_0^{-1} = \text{Im} \chi_0^{-1}(\omega,T)$ is explicitly $T$-dependent in contrast to Eq. 3. Another possibility is that already the quantum critical point of the BFK model cannot be described by a local $\phi^4$-theory and that the quantum-to-classical mapping relating the two fails for the BFK model. This possibility has been recently discussed for the totally spin-isotropic BFK model as well as the easy-axis BFK model [27,28,29,30,31]. As already mentioned, the QCP arises out of the competition between the Kondo effect and magnetic fluctuations. It therefore seems a prerequisite to choose an approach that correctly captures Kondo screening, including the restoration of SU(2) invariance at the Kondo-screened fixed point. For this reason the easy-axis BFK model is delicate [30,31]. In the following, we will focus on the spin-isotropic BFK model where the restoration
Comparing Eqs. (4,5) shows the absence of the SU(2) invariance in the Kondo-screened phase is not an issue.

The starting point for the quantum-to-classical mapping is the coherent state path integral representation of the quantum problem, which leads to the most classical formulation of the problem [27]. In the case of the BFK model, the effective functional integral is formulated in terms of spin coherent states to take into account the finite size of the Hilbert space for the local moment [24,33]. As a consequence, the order parameter manifold is the unit sphere in three dimensions and possesses rotational invariance. The usual canonical term of the bosonic coherent state path integral has to be replaced by a term, the Berry phase term has been studied in a dynamical large-$N$ limit [27]. The Hamiltonian of the SU(N) $\times$ SU($\kappa N$) BFK model is

$$H_{\text{MBFK}} = (J_K/N) \sum_{\alpha} S \cdot s_{\alpha} + \sum_{p,\sigma,\sigma'} E_p c_{p\alpha}^\dagger c_{p\sigma}$$

$$+ (g/\sqrt{N}) S \cdot \Phi + \sum_{p} w_p \Phi_{p\sigma}^\dagger \Phi_p,$$

where $\sigma = 1, \ldots, N$ and $\alpha = 1, \ldots, \kappa N$ (with $\kappa N$ integer) are the spin and channel indices respectively, and $\Phi \equiv \sum_{p}(\Phi_p + \Phi_p^\dagger)$ contains $N^2 - 1$ components. The local moment is expressed in terms of pseudo-fermions $S_{\sigma,\sigma'} = f_{\sigma}^\dagger f_{\sigma'} - \delta_{\sigma,\sigma'} Q/N$, where $Q$ is related to the chosen irreducible representation of SU($N$) [24,33]. At the QCP, the order parameter susceptibility behaves as

$$\chi_{\text{loc}}(\omega, T = 0) \sim 1/\omega^{1-\epsilon}; \quad \chi_{\text{loc}}(\omega, 0, T) \sim 1/T^{1-\epsilon}$$

(7)

for all $0 < \epsilon < 1$. The $\omega/T$-scaling of $\chi_{\text{loc}}(\omega, T)$ for $1/2 \leq \epsilon < 1$ is determined by the mapped classical critical point which has $\chi_{\text{loc}}(\omega = 0, T) \sim 1/T^{1/2}$ for $1/2 < \epsilon < 1$. That this large-$N$ result is stable against dangerously irrelevant couplings that may occur at finite $N$ has been demonstrated in [32] for the particular value $\epsilon = 2/3$. This issue is addressed by introducing a self-energy for the order parameter susceptibility,

$$M(\omega, T) \equiv g_0^2 \chi_0^{-1}(\omega) - 1/\chi_{\text{loc}}(\omega, T),$$

(8)

where $\chi_0^{-1}(\omega)$ follows from Eq. (3) and $g_0^2(J_K)$ is the value of the coupling constant $g_0^2$ at which the system becomes critical for a given $J_K$. The $\omega$-independent part of $M(\omega, T = 0)$, $M(\omega = 0, T = 0)$, vanishes at $g_0^2(J_K)$ by definition.

This self-energy has a temperature dependent part, formally defined as

$$\Delta M(\omega, T) = M(\omega, T) - M(\omega = 0, T = 0),$$

(9)

with the important property

$$\Delta M(\omega = 0, T) \sim T^{1-\epsilon}.$$  

(10)

It was shown in Ref. [32] that the temperature dependence implies that no dangerously irrelevant coupling can alter $\chi_{\text{loc}}(\omega = 0, T) \sim 1/T^{1-\epsilon}$ for $\epsilon > 1/2$.

We will now demonstrate that a similar spin self-energy can be obtained for the region with $\epsilon < 1/2$. Numerical details can be found in Ref. [27,32]. The dynamical spin susceptibility obeys the scaling form

$$\chi_{\text{loc}}(\omega, T) = T^{\epsilon-1} \Phi(\omega/T),$$

(11)

as demonstrated in Fig.2 for the particular value $\epsilon = 0.3$ and consistent with Eq. (7). The imaginary part of the spin susceptibility is therefore $\omega$-dependent with a power-law consistent with that for $\text{Im} \chi^{-1}_0(\omega)$ from
Eq. (3). This is shown in Fig. 3 for a particular temperature $T = 5 \times 10^{-4} T_K$ (where $T$ is the bandwidth). The spin self-energy at the critical coupling $g_c$, is shown in Fig. 3. It behaves as $\Delta M(\omega = 0, T) \sim T^\alpha$, $\alpha = 0.69 \approx 1 - \epsilon$. This demonstrates again that the critical properties of the spin-isotropic BFK model (i.e. with the Berry phase) have the same characteristics for both $0 < \epsilon < 1$ and $1/2 < \epsilon < 1$. Finally, we note in passing that the critical point of the $\epsilon = 1/2$ case does not appear to be special compared to that of the $0 < \epsilon < 1/2$ and $1/2 < \epsilon < 1$ cases, in particular, we do not observe the emergence at $\epsilon = 1/2$ of any logarithmic corrections to the power laws in the dynamical local susceptibility and related quantities.

3. Summary

In summary, the current interest in quantum critical heavy fermion systems has led to the question as to whether the Kondo effect itself may become critical concomitant with the magnetic quantum transition. The effect of a critical Kondo destruction can already be studied in a sub-Ohmic Bose-Fermi Kondo impurity model. We have reexamined the evidence that the Berry phase term cannot be neglected at the quantum critical point and that its presence changes the critical properties. Without the Berry phase term the quantum criticality is in the universality class of the classical local $\phi^4$-theory. With the Berry phase term the quantum critical point is interacting in the whole parameter region $0 < \epsilon < 1$ and, therefore, not equivalent to that of a local $\phi^4$-theory. We demonstrated that the temperature dependence of the spin self-energy has the same characteristics between $0 < \epsilon < 1/2$ and $1/2 < \epsilon < 1$. Since the standard quantum-to-classical mapping links the critical properties of sub-Ohmic impurity models to those of one-dimensional classical spin-chains with long-ranged interaction, one is led to the conclusion that this mapping fails for the sub-Ohmic Bose-Fermi Kondo model.

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