Dynamical Scaling of Charge and Spin Responses at a Kondo Destruction Quantum Critical Point

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Quantum critical points often arise in metals perched at the border of an antiferromagnetic order. The recent observation of singular and dynamically scaling charge conductivity in an antiferromagnetic quantum critical heavy fermion metal implicates beyond-Landau quantum criticality. Here we study the charge and spin dynamics of a Kondo destruction quantum critical point (QCP), as realized in an SU(2)-symmetric Bose-Fermi Kondo model. We find that the critical exponents and scaling functions of the spin and single-particle responses of the QCP in the SU(2) case are essentially the same as those of the large-N limit, showing that $1/N$ corrections are subleading. Building on this insight, we demonstrate that the charge responses at the Kondo destruction QCP are singular and obey ω/T scaling. This property persists at the Kondo destruction QCP of the SU(2)-symmetric Kondo lattice model.

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Introduction.—Quantum criticality is of extensive current interest to a variety of strongly correlated systems [1–4]. Within the Landau framework, phases of matter are differentiated by the spontaneous breaking of global symmetry and its associated order parameter, and quantum criticality is described by the fluctuations of the order parameter. For a continuous transition between antiferromagnetic to paramagnetic phases at $T = 0$, the corresponding singularity is associated with the slow fluctuations of the staggered magnetization [5].

Antiferromagnetic (AF) heavy fermion metals provide a prototype setting to elucidate the quantum critical properties and the associated strange-metal physics. In these systems, strong correlations manifest themselves through the development of local moments out of their f electrons. The local moments interplay with a band of conduction electrons by an AF Kondo coupling, and interact with each other via an RKKY coupling. In the process of understanding heavy fermion quantum criticality, it has been emphasized that the Landau framework, in the form of a spin-density wave (SDW) quantum critical point (QCP) [5–7], can break down in a fundamental way. The beyond-Landau physics has been characterized in terms of the notion of Kondo destruction [8–10]. The distinction of the Kondo destruction quantum criticality from its SDW counterpart reflects the amplitude of the Kondo singlet going to zero as the system approaches the AF QCP from the paramagnetic phase. Correspondingly, the quasiparticle weight vanishes at the QCP and the Fermi surface jumps across the transition.

In the context of critical phenomena, the Kondo destruction QCP epitomizes the effect of quantum entanglement on criticality singularity. From the perspective of strongly correlated electrons, it corresponds to a partial Mott transition, i.e., the localization of the $4f$ electrons. Such an electronic localization-delocalization transition links quantum critical heavy fermion metals to other strongly correlated systems. For instance, in the cuprate superconductors near optimal hole doping, Hall measurements implicate an electron localization-delocalization transition [11]. In an organic superconductor, such measurements have suggested a similarly rapid change in the carrier density [12]. Finally, in the twisted bilayer graphene, quantum oscillation measurements indicate a small Fermi surface when the system is doped away from the half-filled correlated insulator [13].

In quantum critical heavy fermion metals, there is extensive experimental evidence for the Fermi surface jump [14–16] as well as the emerging Kondo destruction energy scale [14,17]. One of the early experimental clues for anomalous heavy fermion quantum criticality came from the observation of ω/T scaling together with an anomalous value for the critical exponent in the spin dynamics [18]. The Kondo destruction quantum criticality has provided a natural understanding of such singular dynamical scaling in the critical spin response [8,19].

Recently, terahertz spectroscopy measurements in a quantum critical heavy fermion metal have discovered a charge response that is singular and satisfies ω/T scaling [20]. This is inconsistent with an SDW QCP, where only the response of antiferromagnetic order parameter should be singular and the charge correlations are expected to be smooth. A critical destruction of the Kondo effect, however, involves the localization delocalization of the f electrons at the QCP. Thus, the charge degrees of freedom (d.o.f.) are an integral part of the quantum criticality leading to the suggestion of a singular response in the charge channel. Indications of a singular charge response have appeared in a dynamical large-N study (see below for the definition of N) for a Kondo destruction QCP of the Bose-Fermi Kondo model (BFKM) and in related settings [21–24], with the BFKM being associated with the Kondo lattice model within the approach of extended dynamical mean field theory (EDMFT). In light of the recent experimental development, theoretical studies at the physical $N = 2$ case are called for.

In this Letter, we demonstrate for the first time that the charge response of the Kondo destruction QCP is singular and has dynamical ω/T scaling in the physical $N = 2$ case. Our result is facilitated by analyzing the BFKM at both $N = 2$ and a dynamical large-N limit, which shows that $1/N$ corrections to the scaling quantities are subleading but not dangerously irrelevant. Based on this insight, we carry out calculations on both the BFKM and the Kondo lattice model. Our results provide the theoretical basis to understand the striking recent measurement of singular charge response at an antiferromagnetic heavy fermion QCP [20].

BFKM with SU(2) symmetry.—We will study the quantum critical properties of the spin rotationally invariant BFKM [25–28] and related Bose-Fermi Anderson model (BFAM), compare the results determined for the SU(2)-invariant case ($N = 2$) with those obtained in the dynamical large-N limit. For the SU(2) case, we will study the BFAM defined by the following Hamiltonian:

$$\begin{aligned}\mathcal{H}_{\mathrm{BFA}} = &\sum_{\sigma}\epsilon_d d_\sigma^\dagger d_\sigma + U n_\uparrow n_\downarrow \\ &+ \sum_{p\sigma}(V d_\sigma^\dagger c_{p\sigma} + \mathrm{H.c.}) + \sum_{p\sigma}\epsilon_p c_{p\sigma}^\dagger c_{p\sigma} \\ &+ g\sum_p \mathbf{S}_d\cdot\mathbf{\Phi} + \sum_p w_p \mathit{\Phi}_p^\dagger\cdot\mathbf{\Phi}_p. \end{aligned} \quad (1)$$

Here, strongly correlated d electrons, with the Hubbard interaction U defined in terms of $n_\sigma = d_\sigma^\dagger d_\sigma$ and in the presence of a particle-hole symmetry, $\epsilon_d = -U/2$, hybridize with the conduction c electrons with an amplitude V. For the interactions we consider, the hybridization amounts to a Kondo coupling of the d electron spin, $\mathbf{S}_d = d_\sigma^\dagger \boldsymbol{\tau}_{\sigma\sigma'} d_{\sigma'}$, with $\boldsymbol{\tau}_{\sigma\sigma'}$ being the three component Pauli matrices, to the fermionic c bath. Simultaneously, the d-electron spin is coupled to a vector $\mathit{\Phi}$-bosonic bath; we have defined $\mathit{\Phi} = \sum_p(\mathbf{\Phi}_p + \mathbf{\Phi}_{-p}^\dagger)$. We assume a flat fermionic density of states

$$\rho_f(\epsilon) = \sum_p \delta(\epsilon - \epsilon_p) = \rho_0\Theta(D-\epsilon)\Theta(D+\epsilon), \quad (2)$$

where Θ is the Heaviside function. This defines a hybridization function $\Gamma(\epsilon) = \Gamma = \pi\rho_0 V^2$ for $\epsilon \in [-D, D]$. We choose $D = 1$ as the energy unit. For the bosonic bath, we consider a subohmic spectrum ($s < 1$)

$$\rho_b(\omega) = \sum_p \delta(\omega - \omega_p) = K_0 \omega^s e^{-\omega/\Lambda}\Theta(\omega), \quad (3)$$

where Λ is a cutoff frequency. The model is studied using a continuous-time quantum Monte Carlo (CT-QMC) method developed in Ref. [29] (see also Refs. [30–34]).

BFKM in dynamical large-N limit.—The BFKM in the dynamical large-N limit is defined in terms of the Hamiltonian:

$$\begin{aligned}\mathcal{H}_{\mathrm{BFK}} = &(J/N)\sum_\alpha \mathbf{S}\cdot\mathbf{s}_\alpha + \sum_{p,\alpha,\sigma}\epsilon_p c_{p\alpha\sigma}^\dagger c_{p\alpha\sigma} \\ &+ (g/\sqrt{N})\mathbf{S}\cdot\mathbf{\Phi} + \sum_p w_p \mathit{\Phi}_p^\dagger\cdot\mathbf{\Phi}_p. \end{aligned} \quad (4)$$

As in the SU(2) case, a local moment $\mathbf{S}$ is coupled to a fermionic and a vector bosonic bath, $c_{p\alpha\sigma}$ and $\mathit{\Phi}_p$, respectively. The spin symmetry is SU(N), with $\sigma = 1, \ldots, N$, and the channel symmetry is SU(κN), with $\alpha = 1, \ldots, \kappa N$ (Ref. [35,36]). Here, $\mathit{\Phi}$ has $N^2 - 1$ components. The density of states is likewise given by Eqs. (2) and (3). The bare bath Green's functions are $\mathcal{G}_0 = -\langle T_\tau c_{\sigma\alpha}(\tau) c_{\sigma\alpha}^\dagger(0)\rangle_0$ and $\mathcal{G}_\Phi = \langle T_\tau \Phi(\tau)\Phi^\dagger(0)\rangle_0$.

We use a fermionic spinon representation, $S_{\sigma\sigma'} = f_\sigma^\dagger f_{\sigma'} - \delta_{\sigma,\sigma'}/2$, enforcing the constraint of the Hilbert space $\sum_{\sigma=1}^N f_\sigma^\dagger f_\sigma = N/2$ by a Lagrange multiplier $i\mu$. The conduction electrons are in the fundamental representation of the SU(N) $\times$ SU(κN) group. A dynamical field $B_\alpha(\tau)$ is used to decouple the Kondo coupling, $(J/N)\sum_{\sigma\sigma'}(f_\sigma^\dagger f_{\sigma'} - \delta_{\sigma,\sigma'}/2)c_{\alpha\sigma'}^\dagger c_{\alpha\sigma}$, leading to a $B_\alpha^\dagger \sum_\sigma c_{\alpha\sigma}^\dagger f_\sigma/\sqrt{N}$ interaction. The B field is charge carrying, given that the spinon field f is charge neutral.

Taking the large-N limit with κ being kept fixed leads to the following saddle point equations:

$$\begin{aligned} &G_B^{-1}(i\omega_n) = 1/J - \Sigma_B(i\omega_n), \qquad \Sigma_B(\tau) = -\mathcal{G}_0(\tau)G_f(-\tau), \\ &G_f^{-1}(i\omega_n) = i\omega_n - \lambda - \Sigma_f(i\omega_n), \\ &\quad \Sigma_f(\tau) = \kappa\mathcal{G}_0(\tau)G_B(\tau) + g^2 G_f(\tau)\mathcal{G}_\Phi(\tau), \end{aligned} \quad (5)$$

which are supplemented by the following constraint:

$$G_f(\tau = 0^-) = (1/\beta)\sum_{i\omega_n} G_f(i\omega_n)e^{i\omega_n 0^+} = 1/2. \quad (6)$$

These equations are solved on the real frequency axis. For definiteness, we will fix $\kappa = 1/2$.

Critical properties—large-N limit vs SU(2).—In the large-N limit, a QCP separates the strong-coupling Kondo phase from a Kondo destruction critical phase. In the SU(2) model, for the value of s we focus on, the Kondo

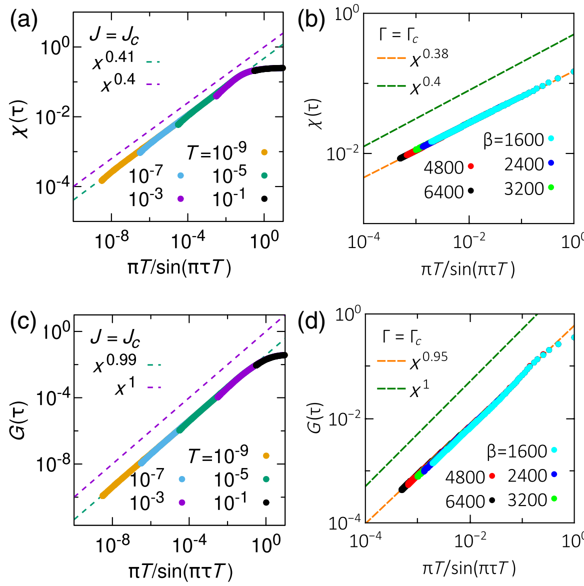

FIG. 1. Local spin susceptibility $\chi(\tau)$ at the QCP of (a) the dynamical large-N limit (purple dashed line represents the analytically obtained leading $T = 0$ behavior) and (b) the SU(2) case; and electron Green's function $G(\tau)$ at the QCP of (c) the dynamical large-N limit and (d) the SU(2) case. In (a), (c), the temperature T is measured in D. In (b), (d), $\beta = 1/T$.

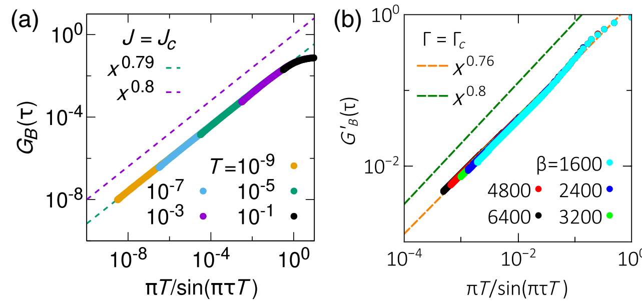

FIG. 2. Singular charge response of the B field calculated in the dynamical large-N limit (a) and extracted in the SU(2) case (b) obtained at the QCP. In (a), the temperature T is in units of D. In (b), $\beta = 1/T$.

destruction phase also corresponds to a critical phase [29]. Comparing the critical properties of the dynamical large-N limit with the SU(2) model allows us to assess the degree to which $1/N$ corrections modify the leading quantum critical singularities.

We first consider the local spin susceptibility, χ, at the QCP and in the Kondo destruction phase. In the dynamical large-N limit,

$$\chi(\tau) = -G_f(\tau)G_f(-\tau). \tag{7}$$

In the SU(2) case, $\chi(\tau)$ is directly calculated from the CT-QMC procedure. The result for the dynamical large-N calculations for $s = 0.6$ (i.e., $\epsilon = 1 - s = 0.4$) is shown in Fig. 1(a). We find that χ as a function of the imaginary time, τ, collapses in terms of $\pi T/\sin(\pi\tau T)$, where T is the temperature, with a power-law exponent η that is less than 1. This implies a singular spin response: The static local spin susceptibility diverges in the $T \to 0$ limit, and so does the $T = 0$ local spin susceptibility as $\omega \to 0$; both divergencies have the power-law exponent of $1 - \eta$. The exponent η is numerically fit to be 0.41. This value is in excellent agreement with the analytical result, $\eta = \epsilon = 0.4$, that can be extracted from the saddle point Eqs. (5) and (6) in the zero-temperature limit [21].

As a comparison, we show in Fig. 1(b) the CT-QMC result for $\chi(\tau)$ at the QCP of the SU(2) BFAM, again for $s = 0.6$. Unlike the large-N limit where the real-frequency analysis is carried out over many (more than ten) decades, here the dynamical range is more limited. Still, by using the algorithm recently developed in Ref. [29], we are able to reach low-enough temperatures and a sufficiently large dynamical range in τ to determine the scaling properties in the quantum critical regime. We see from Fig. 1(b) that the scaling function is also a power-law of $\pi T/\sin(\pi\tau T)$. The fitted exponent is 0.38, which is quite close to the large-N result (0.41 as calculated and 0.4 as expected). We attribute the difference to the subleading corrections that are amplified in the CT-QMC calculation, given the narrower scaling range being accessed.

We now turn to a parallel study of the d-electron Green's function $G(\tau)$. In the large-N limit, it is determined as follows:

$$G(\tau) = G_f(\tau)G_B(-\tau). \tag{8}$$

For the SU(2) case, $G(\tau)$ is again directly calculated from the CT-QMC procedure. The results for the QCP is shown for the large-N limit in Fig. 1(c), with the exponent being 0.99, very close to the value analytically expected, which is 1. In addition, for the SU(2) case shown in Fig. 1(d), within numerical accuracy, both the critical exponent and the scaling functions are essentially the same as the large-N limit.

Critical charge and spin responses and ω/T scaling.— The above calculations and comparisons lead to an important new insight. For the Kondo destruction QCP, the leading critical singularities determined in the dynamical large-N limit apply to finite N including $N = 2$. This implies that, while the $1/N$ corrections modify the location of the quantum critical point, they preserve its Kondo-destruction nature and, equally important, make only subleading contributions to the critical singularities. Analyzing the Feynman diagrams shows that the processes at the $1/N$ and higher orders are irrelevant [35]. In addition, the $1/N$ corrections cannot be dangerously irrelevant: given that the susceptibilities at the large-N limit satisfy ω/T scaling (see below), the subleading corrections will preserve the leading singularities as a function of not only the frequency but also the temperature. This insight leads to a

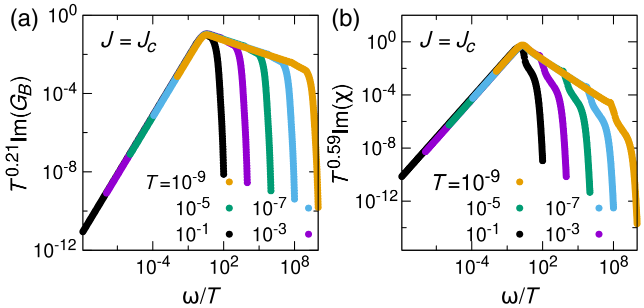

FIG. 3. ω/T scaling at the QCP. (a) The charge response, showing the spectral function of the B field and (b) the spin response, showing the spectral function of **S**, both in the dynamical large-N limit. The temperature T and ω are in units of D.

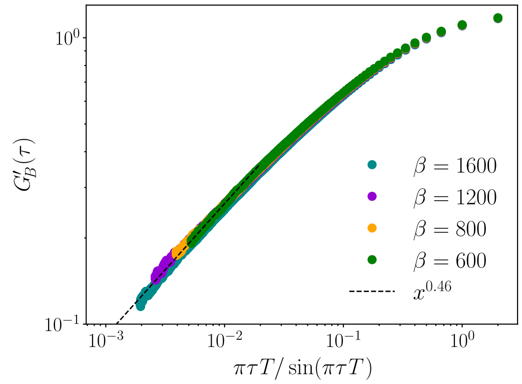

FIG. 4. Singular charge response of the B field calculated in the lattice model at the Kondo destruction QCP.

remarkable simplification, because it implies that we can use the results determined in the dynamical large-N limit to gain an understanding about the critical properties at realistic Kondo destruction QCPs at finite N.

We start from the response of the charge-carrying B field, which is expected to be singular [21]. In Fig. 2(a), we show that it too is a power law of $\pi T/\sin(\pi\tau T)$, with a critical exponent being very close to the value determined analytically for the leading singularity, i.e., 0.8 (which corresponds to $1-\epsilon/2$).

The lack of $1/N$ corrections to the leading critical singularities at the Kondo destruction QCP suggests that the structure of Eqs. (7) and (8) is still valid at finite N. The form of the scaling functions simplifies these equations into $\chi(\tau) = [G_f(\tau)]^2$ and $G(\tau) = G_f(\tau)G_B(\tau)$ [for $\tau \in (0,\beta)$]. We therefore define

$$G'_B(\tau) = \frac{G(\tau)}{\sqrt{\chi(\tau)}} \tag{9}$$

as a measure of the singular correlator of the charge-carrying B field. The τ-dependence of G'_B from our CT-QMC calculation of the SU(2) BFAM is presented in Fig. 2(b). Both the critical exponent and the scaling function are, within the numerical uncertainty, the same as for the large-N result. This particular form of scaling function in the τ dependence, with its power-law exponent being less than 1, implies a singular dependence on ω and T with an ω/T scaling.

Thus, we have established that the Kondo destruction QCP displays a singular response in both charge and spin channels. The real-frequency dependences of the spectral functions of both the charge-carrying B field and the spin **S** are shown to collapse in ω/T in Figs. 3(a) and 3(b). Each quantity satisfies ω/T scaling over a dynamical range of more than 15 decades.

Kondo lattice model.—Since the lattice model is more relevant to the real materials, we study the SU(2)-symmetric Kondo lattice model. The model itself is standard, as is the EDMFT approach [19]. However, systematic calculations for the SU(2)-symmetric case has only become possible recently with the advent of the SU(2) CT-QMC method [29]. Within EDMFT the lattice model is described by the BFKM involving self-consistently determined bath.

In the lattice model, we numerically identity a Kondo destruction QCP, which separates a paramagnetic Kondo screened phase from an antiferromagnetic Kondo destruction phase [37]. We then investigate the charge response G'_B at the QCP. As shown in Fig. 4, we find G'_B to collapse as a function of $\pi T/\sin(\pi\tau T)$. The critical exponent is about 0.5 which corresponds to the $s \sim 0$ case in the BFKM. This form of charge response is critical and satisfies ω/T scaling.

Discussion and conclusion.—Importantly, in both the Bose-Fermi Kondo model and Kondo lattice model, only spin appears in the (strongly correlated) local d.o.f. At the corresponding Kondo destruction QCP, we find that the charge response not only is singular but also satisfies ω/T scaling. The development of a singular charge response in such a model is surprising, because the only microscopic charge d.o.f. in the Hamiltonian are associated with the noninteracting conduction electrons; only spins are involved in any of the interaction terms. It demonstrates the power of quantum (Kondo) entanglement in strongly correlated metallic settings. More generally, our results capture the aspects of quantum criticality that are unique to strongly correlated metals, namely the quantum entwining of the charge and spin d.o.f.

Our work provides the theoretical basis for the understanding of the surprising experimental observation in Ref. [20], where a singular charge response with ω/T scaling is found at an antiferromagnetic QCP. Finally, because Kondo destruction represents a partial-Mott transition, our work suggests that probing the singularities of both charge and spin responses represents a fruitful means of elucidating strange metals near an electronic localization, such as the cuprate high temperature superconductors and organic charge transfer salts.

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