Critical Kondo Destruction in a Pseudogap Anderson Model: Scaling and Relaxational Dynamics

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Critical Kondo destruction in a pseudogap Anderson model: scaling and relaxational dynamics

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We study the pseudogap Anderson model as a prototype system for critical Kondo destruction. We obtain finite-temperature (T) scaling functions near its quantum critical point, using a continuous-time quantum Monte Carlo method and also considering a dynamical large-N limit. We are able to determine the behavior of the scaling functions in the typically-difficult-to-access quantum-relaxational regime ($\hbar\omega < k_BT$), and conclude that the relaxation rates for both the spin and single-particle excitations are linear in temperature. We discuss the implications of these results for the quantum critical phenomena in heavy fermion metals.

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Continuous zero temperature phase transitions in strongly correlated electronic and atomic models have attracted considerable attention as a new paradigm for addressing the universal features of correlated quantum systems [1]. Quantum criticality links two nearby phases and determines the physical properties in a large range of temperature and control parameter, the quantum critical region, that fans out from the quantum critical point (QCP). This paradigm is especially pertinent to the understanding of intermetallic rare earth compounds. The phase diagram of these heavy fermion metals close to the border of antiferromagnetism features a QCP, but the associated quantum critical properties are highly unusual when viewed from the standard description based on Landau's notion of order-parameter fluctuations [2]. Especially, inelastic neutron-scattering measurements have shown that the dynamical spin susceptibility in the quantum critical regime features a linear-in-T spin relaxation rate and satisfies a frequency over temperature (ω/T) scaling [3]. Very recently, Hall-effect measurements have indicated that the single-particle relaxation rate in the quantum critical regime is also linear in T [4].

These dynamical scaling and relaxational properties provide important clues to the nature of the heavy-fermion QCP. Yet, theoretically, such real-frequency behavior is difficult to study. At finite temperatures, two regimes need to be distinguished: the quantum coherent ($\hbar\omega > k_BT$) and quantum relaxational ($\hbar\omega < k_BT$) regimes [5]. Calculation methods (such as Monte Carlo) typically work in the imaginary time domain, and the non-zero Matsubara frequencies (ω_n) are necessarily in the $|\omega_n|/T > 1$ regime. Extracting the behavior at real frequencies requires an analytical continuation, which is in general a numerically ill-conditioned procedure. The numerical renormalization group (NRG) operates on the real frequency axis, but it is not reliable for the quantum relaxational regime at nonzero temperatures.

In this Letter, we address the dynamical and relaxational properties of the particle-hole symmetric pseudogap Anderson model in both frequency regimes. Our motivations to study this model are multi-fold. In local quantum criticality for heavy-fermion metals, the critical destruction of the Kondo effect [6–9] is local in space, and the resulting interacting critical modes are manifested in local correlators which can be studied in quantum-impurity problems. The pseudogap Anderson model is the simplest impurity problem that contains the physics of critical Kondo destruction; it is well known that varying the Kondo coupling yields a QCP [10–16], which separates a Kondo-screened Fermi-liquid phase from a Kondo-destroyed local-moment phase. However, a proper understanding of the dynamical scaling at finite temperatures and the associated relaxational behavior is not yet available even in this simplest model. Furthermore, the pseudogap Anderson/Kondo model is relevant in a number of realistic physical settings. It has been invoked in the context of non magnetic impurities in cuprate superconductors [17]. It has also been shown that a judicious tuning of a double quantum-dot system can produce a pseudogap in the effective density of states [18]. In disordered metals, a novel phase has been attributed to the occurrence of local pseudogaps near the Fermi energy at local moment sites [19]. Finally, the pseudogap Kondo model is the appropriate model to describe point defects in graphene [20].

We study the model using a continuous-time quantum Monte Carlo approach (CT-QMC) [21]. We determine the full scaling functions at real frequencies and finite temperatures for both the dynamical spin susceptibility and single-electron Green's function. We achieve this by taking advantage of insights gained from exact calculations at real frequencies and finite temperatures in a dynamical large-N limit of the model. The results in the large-N limit motivate us to analyze the imaginary-time correlators in the physical $N = 2$ model in a way that uncovers the form of a boundary conformally-invariant fixed point. The latter, in turn, can readily be analytically-continued to real frequency at finite temperatures. We establish that both the dynamical spin susceptibility and single-electron Green's function display an ω/T-scaling and contain a linear-in-T relaxation rate. As a by-product, we show that the CT-QMC approach, which is based on a high-temperature expansion, can reach low-enough temperatures with enough accuracy to resolve quantum critical features.

Pseudogap Kondo model in a dynamical large-N limit: To set the stage for the CT-QMC study, we start with the SU(N)×SU(M) Kondo model [22] in the presence of a pseudogap in the limit of large N and M. In what follows, we set $\hbar = k_B = 1$. The Hamiltonian is

$$\mathcal{H}_{\rm PKM} \;=\; (J_K/N)\sum_{\alpha}\mathbf{S}\cdot\mathbf{s}_\alpha + \sum_{p,\alpha,\sigma} E_p\, c^\dagger_{p\alpha\sigma}c_{p\alpha\sigma}. \quad (1)$$

Here, the spin and channel indices are $\sigma = 1, \ldots, N$ and $\alpha = 1, \ldots, M$. The conduction electron density of states takes the form:

$$\rho(\omega) = \sum_p \delta(E_p - \omega) = \rho_0|\omega/D|^r\Theta(D - |\omega|), \qquad (2)$$

with $2D$ being the bandwidth. That this limit has a non-trivial QCP can be seen through the particular form of the perturbative (in r) RG equation [10]. In the limit of large N and M, the RG beta function becomes $\beta(j) = -j(r - j + \kappa j^2)$, with $j = J_K/D$ and $\kappa = M/N$ [23]. This establishes that the QCP survives the large-N limit and can be accessed perturbatively. To order r, the large-N beta function is identical to its N= 2 counterpart [10, 12] suggesting that the universal critical scaling properties of the $N = 2$ QCP are preserved by taking the large-N limit. In this limit, the local degrees of freedom are expressed in terms of pseudo-fermions f_σ and a bosonic decoupling field B_α, where $S_{\sigma,\sigma'} = f^\dagger_\sigma f_{\sigma'} - \delta_{\sigma,\sigma'}Q/N$, and Q is related to the chosen irreducible representation of SU(N) [22, 24]. The large-N equations are

$$\begin{aligned}\Sigma_B(\tau) &= -\mathcal{G}_0(\tau)G_f(-\tau);\ \Sigma_f(\tau) = \kappa\mathcal{G}_0(\tau)G_B(\tau);\\ G_B^{-1}(i\nu_n) &= 1/J_K - \Sigma_B(i\nu_n);\\ G_f^{-1}(i\omega_n) &= i\omega_n - \lambda - \Sigma_f(i\omega_n); \qquad (3)\end{aligned}$$

together with a constraint $G_f(\tau \to 0^-) = Q/N$ [22]. Here, λ is a Lagrangian multiplier enforcing the constraint and $\mathcal{G}_0 = -\langle T_\tau c_{\sigma\alpha}(\tau)c^\dagger_{\sigma\alpha}(0)\rangle_0$ is the non-interacting Green's function [13].

Solving the large-N equations in real frequencies for arbitrary ω and T [23], the full scaling functions in both, the quantum coherent ($\omega > T$) and relaxational ($T > \omega$) regimes are obtained. At the critical coupling $J_c(r)$, we find that all the correlators display an ω/T-scaling. This is demonstrated in Fig. 1(a) for the local single-particle Green's function [*i.e.*, the T-matrix, $\mathcal{G}(\omega, T)$, associated with $\mathcal{G}(\tau) = G_f(\tau)G_B(\tau)$], and in Fig. 1(b) the local spin susceptibility $\chi(\omega, T)$, which corresponds to $\chi(\tau) = -G_f(\tau)G_f(-\tau)$.

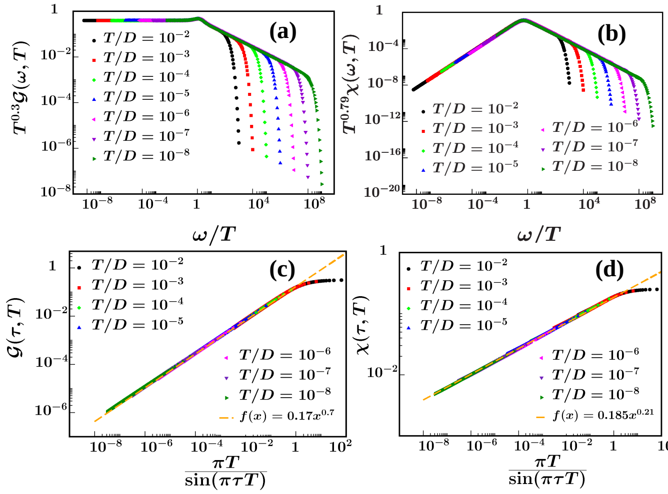

FIG. 1: Scaling functions for the imaginary part of (a) Green's function $\mathcal{G}(\omega, T)$ and (b) susceptibility $\chi(\omega, T)$ for $r = 0.3$ and $\kappa = 0.5$ at the critical $J_c \approx 1.54$ (with $T_K^0 \approx 0.3D$ for $r = 0$). Both functions display ω/T-scaling with scaling functions Φ obeying $\Phi(\omega/T \longrightarrow 0) \longrightarrow c$ or 0 for $\mathcal{G}$ or χ, where $c \neq 0$ is a constant. (c),(d) the scaling functions in imaginary time.

A key insight from the large-N result is that the scaling functions contain more information beyond ω/T scaling *per se*. They have the particular form associated with a boundary conformally-invariant fixed point, depending on τ as a power law in $\pi T/\sin(\pi\tau T)$ [25]. To see this, we obtain the imaginary-time dependence from the real-frequency results via

$$\Phi(\tau) \;=\; -\eta\int_{-\infty}^{\infty} d\omega\, \frac{\exp(-\tau\omega)}{\exp(-\beta\omega) - \eta}{\rm Im}(\Phi(\omega + i0^+)), \quad (4)$$

for $0 < \tau \leq \beta$. Here, $\eta = \pm$ for bosonic/fermionc Φ. Fig. 1 shows the (c) Green's function $\mathcal{G}(\tau, T)$ and (d) susceptibility $\chi(\tau, T)$ versus the combination $\pi T/\sin(\pi\tau T)$. Both collapse on a single scaling curve in terms of $\pi T/(\sin(\pi\tau T))$ for all (low-enough) T. A power-law behavior for $\tau \to 1/(2T)$ is seen over about 7 decades, and the exponents are compatible with those for the frequency dependence.

Pseudogap Anderson model at $N = 2$: Guided by the large-N results, we turn to the scaling functions for $\mathcal{G}(\tau, T)$ and $\chi(\tau, T)$ of the particle-hole symmetric pseudogap Anderson model at $N = 2$; the low-energy properties of this model are identical to its pseudogap Kondo counterpart. To this end, we bring to bear the recently developed hybridization-expansion Monte Carlo method [21, 26] on a quantum critical model. This CT-QMC approach involves a stochastic sampling of a perturbation expansion in the host-impurity hybridization or a weak coupling expansion [21, 26–28]. The results are free of any finite-size effects [29].

The Anderson impurity model is defined by $\hat{H} = \hat{H}_0 +$

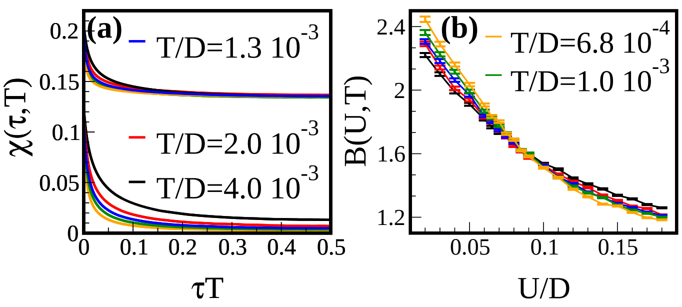

FIG. 2: Dynamical local susceptibility $\chi(\tau, T)$ versus τT for $r = 0.4$, $\Gamma_0 = 0.1D$ with $U = 0$ and $U = 0.3D$ (a). Finite temperature scaling of the Binder cumulant $B(U,T)$ as a function of U at various temperatures (b), error bars are obtained from a jackknife error analysis. From the intersection of the curves we determine the critical point to be $U_c(r = 0.4)/D = 0.085 \pm 0.002$.

$\sum_\sigma \hat{H}_1^{(\sigma)}$ where

$$\hat{H}_0 = \hat{H}_c + \hat{H}_{\rm loc} = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} \hat{n}_{\boldsymbol{k}\sigma} + \sum_\sigma (\epsilon_d + \tfrac{1}{2} U \hat{n}_{d,-\sigma}) \hat{n}_{d\sigma}$$
$$\hat{H}_1^{(\sigma)} = \sum_{\boldsymbol{k}} \left(V_{d\boldsymbol{k}} d_\sigma^\dagger c_{\boldsymbol{k}\sigma} + \text{H. c.} \right) \qquad (5)$$

with $\hat{n}_{\boldsymbol{k}\sigma} = c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma}$, $\hat{n}_{d\sigma} = d_\sigma^\dagger d_\sigma$, $\epsilon_{\boldsymbol{k}}$ being the host dispersion, $V_{d\boldsymbol{k}}$ the hybridization, and ϵ_d the impurity level energy. We consider the particle-hole symmetric case where $\epsilon_d = -\frac{1}{2}U$, with U being the onsite Coulomb repulsion. The host-impurity coupling is specified by the imaginary part of the hybridization function $\Gamma(\omega) = \pi \sum_{\boldsymbol{k}} |V_{d\boldsymbol{k}}|^2 \delta(\omega - \epsilon_{\boldsymbol{k}})$. As in Eq. (2), we choose $\Gamma(\omega) = \Gamma_0 \left|\frac{\omega}{D}\right|^r \Theta(D - |\omega|)$. The critical point exists only for $0 < r < \frac{1}{2}$ [11].

Central to the CT-QMC approach adopted here is the expansion of the partition function $Z = \text{Tr}\{\hat{T}_\tau e^{-\beta \hat{H}_0} \prod_\sigma \exp[-\int_0^\beta \mathrm{d}\tau \; \hat{H}_1^{(\sigma)}(\tau)]\}$ in the hybridization term [21].

We measure the single particle Green's function $\mathcal{G}_\sigma(\tau) = \langle T_\tau d_\sigma(\tau) d_\sigma^\dagger \rangle$, the local spin susceptibility $\chi(\tau) = \langle T_\tau S_z(\tau) S_z(0) \rangle$ and powers of the local magnetization $\langle M_z^n \rangle = \langle \left(\frac{1}{\beta} \int_0^\beta d\tau S_z(\tau) \right)^n \rangle$ where $S_z(\tau) = \frac{1}{2}[\hat{n}_\uparrow(\tau) - \hat{n}_\downarrow(\tau)]$. The static susceptibility is obtained from $\chi(\omega = 0) = (g\mu_B)^2 \int_0^\beta \mathrm{d}\tau \; \chi(\tau)$. Thermalization can be traced by $\langle n_d \rangle$ which obeys $\langle n_d \rangle = 1$ in the particle-hole symmetric model. We also performed a binning analysis and obtained the integrated autocorrelation time which increases with decreasing temperature but turned out to be small (compared to the number of measurements) at all temperatures. For the lowest temperature considered ($\beta D = 9,000$) we performed $800,000$ Monte Carlo steps (MCS) for thermalization, $1,500$ MCS between each measurement and $18,750$ measurements. A MCS consists of an attempt to remove, insert and shift a segment as described in reference [21].

By varying U we can tune the model through a QCP. Correspondingly, Fig. 2(a) shows that the large-β limit of $\chi(\tau = \beta/2, \beta)$ vanishes for small U (Kondo-screened phase) and is equal to the Curie constant for large U (Kondo-destroyed local-moment phase). To accurately determine $U_c(r)$ we apply finite temperature scaling to the Binder cumulant, $B(U,T) = \frac{\langle M_z^4 \rangle}{\langle M_z^2 \rangle^2}$, where $1/T = \beta$ plays the role of the system size. We find swap moves between up and down spin segments [30] are necessary to accurately measure the Binder cumulant; for the results in Fig. 2(b) we performed a swap move every 100 measurements. The nature of the intersection of the data in Fig. 2(b) implies the phase transition is continuous, from the location of the intersection we obtain the critical value of U. For $r = 0.4$ we obtain $U_c/D = 0.085 \pm 0.002$. In the quantum critical regime the static local susceptibility displays an anomalous r-dependent exponent; we find

$$\chi(T, U_c, r = 0.4) \sim T^{-x}, \qquad (6)$$

with $x = 0.68(3)$ in good agreement with NRG results [12].

We now discuss the finite-temperature dynamical scaling properties of $\mathcal{G}(\tau, T)$ and $\chi(\tau, T)$. Guided by the large-N results, we plot them as functions of $(\pi T)/\sin(\pi \tau T)$ in Fig. 3. Excellent scaling collapse is observed over about two decades, for all temperatures in the scaling regime. We reach an important conclusion:

$$\chi_{crit}(\tau, T) = \Phi\Big(\frac{\pi \tau_0 T}{\sin(\pi \tau T)}\Big) \overset{T \ll T_K^0}{\sim} \Big(\frac{\pi \tau_0 T}{\sin(\pi \tau T)}\Big)^{1-x}, \qquad (7)$$

for $\tau^{-1} \ll T_K^0$, Fig. 3(b). Since $0 < 1 - x < 1$, the results for $\chi(\tau, T)$ imply that the order parameter susceptibility shows ω/T-scaling. A similar conclusion applies to $\mathcal{G}(\tau, T)$, as seen in Fig.3(a). Our results yield $\mathcal{G}(\tau, T \to 0) \sim \tau^{-\delta}$, with the exponent $\delta = 1 - r$, which is believed to be exact [16]. The fact that $2\delta \neq 1 - x$ signifies the importance of vertex corrections and in part reflects the interacting nature of the QCP (see below).

The boundary conformally-invariant form of χ and $\mathcal{G}$ immediately imply that their dependence on real frequency satisfies ω/T scaling and that their relaxation rates, defined in the quantum relaxational regime, is linear in T. Expressed in terms of $\Gamma_M = i(\partial \ln M(\omega, T)/\partial \omega|_{\omega=0})^{-1}$ for a correlator M, the relaxation rates $\Gamma_\chi = aT$ and $\Gamma_{\mathcal{G}} = bT$, where a and b are universal dimensionless constants. Such a linear-in-T form is consistent with what has been observed in quantum critical heavy fermion compounds, for both the single-particle Green function [4] and order parameter susceptibility [3]. A linear-in-T relaxation rate signifies that the QCP is interacting, *i.e.*, containing a nonzero nonlinear coupling among the critical modes. By contrast, at a Gaussian QCP (whose critical modes do not interact at

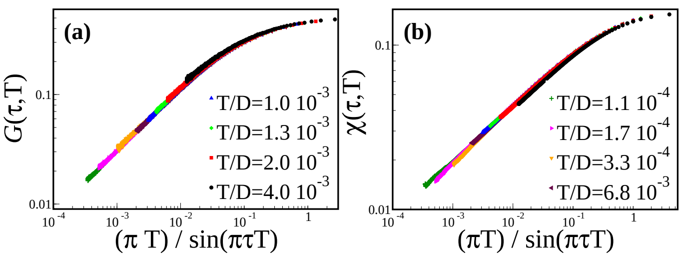

FIG. 3: Scaling of (a) Green's function $\mathcal{G}(\tau,T)$ and (b) susceptibility $\chi(\tau,T)$ at the QCP for $r=0.4$, $\Gamma_0=0.1D$ and $U_c(r=0.4)=0.085D$. The Kondo temperature in this case is $T_K^0\approx 0.029D$ (for $r=0$). For $T/D<5\cdot 10^{-3}$, we observe collapse of the data over several decades for more than two decades of the parameter $(\pi T)/\sin(\pi\tau T)$, i.e., $\mathcal{G}_c(\tau,T)=\Psi(\pi T/\sin(\pi\tau T))$ and $\chi_c(\tau,T)=\Phi(\pi T/\sin(\pi\tau T))$. $\Psi(y\to 0)\propto y^{\delta}$ with $\delta=0.57(5)$, and $\Phi(y\to 0)\propto y^{1-x}$ with $x=0.68(3)$.

the fixed point), the relaxation rate will be super-linear-in-T because the nonlinear coupling itself vanishes as T approaches zero [5].

It is instructive to compare our study with previous theoretical treatments of the finite-temperature scaling behavior of the pseudogap Anderson/Kondo model. One study [12] is perturbative in r, which not only becomes unreliable for finite r but also does not allow the study of the single-particle Green's function. Another study carries out calculations in real frequency at finite temperatures, but relies on the resummation of a perturbation series whose validity for the quantum critical regime is not clear [15]. Yet another study utilizes a Callan-Symanzik approach which requires analytic continuation that is problematic as reflected in the non-commutativity of the resummation and analytic continuation [16]; it will be important to check whether that procedure yields a $\mathcal{G}'(\omega,T)$ that is compatible in analyticity with $\mathcal{G}''(\omega,T)$. As a more specific illustration of our results, we note that $T^r\mathcal{G}''(\omega/T\to 0)$ is a nonzero constant, which is contrary to both the perturbative results of Ref. [15] and the results of the real-frequency Callan-Symanzik resummation for $\mathcal{G}''(\omega,T)$ [16].

The scaling of the local correlators in terms of $\pi T/\sin(\pi\tau T)$ suggests that the boundary critical state and the associated boundary operators may be described by their counterparts in an effective model with conformal invariance. This is so in spite of the fact that, for our problem, the pseudogap form of the DOS means that the bulk fermionic component of the Hamiltonian lacks conformal invariance. Hence, our results suggest an enhanced conformal symmetry that characterizes the QCP.

Summary. We have obtained the full finite-temperature scaling functions at the local quantum critical point of the pseudogap Anderson and Kondo models. Using the results directly obtained in real frequency (ω) in the large-N limit, and by showing that the imaginary-time local correlators of the physical $N=2$ model have the form of a boundary conformally-invariant fixed point, we succeeded in determining the full scaling function in both the quantum coherent and relaxational regimes without using numerically ill-conditioned analytical-continuation schemes. We demonstrated that the Kondo-breakdown QCP features a linear-in-T relaxation rate for both spin and single-electron dynamics, which is consistent with the experimental observations in the quantum-critical heavy fermion metals.

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