Magnetic Quantum Phase Transition in an Anisotropic Kondo Lattice

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The quantum phase transition between paramagnetic and antiferromagnetic phases of the Kondo lattice model with Ising anisotropy in the intersite exchange is studied within extended dynamical mean-field theory. Nonperturbative numerical solutions at zero temperature point to a continuous transition for both two- and three-dimensional magnetism. In the former case, the transition is associated with critical local physics, characterized by a vanishing Kondo scale and by an anomalous exponent in the dynamics close in value to that measured in heavy-fermion $CeCu_{5.9}Au_{0.1}$.

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Heavy-fermion materials close to a zero-temperature antiferromagnetic (AFM) instability manifest a rich variety of non-Fermi-liquid behaviors [1]. By tuning a control parameter (doping, pressure, or magnetic field), the Néel temperature can be suppressed to $T = 0$. The resulting quantum phase transition (QPT) separates an AFM metal from a paramagnetic (PM) metal in which local moments are Kondo-screened by conduction electrons. In the standard spin-density wave (SDW) theory [2] for such QPTs, the important critical modes are long-wavelength order-parameter fluctuations; non-Fermi-liquid physics arises from scattering of quasiparticles by SDWs. However, data for a number of heavy fermions are at odds with this picture. In particular, neutron scattering for $CeCu_{5.9}Au_{0.1}$ [3,4] points to a strongly interacting quantum critical point involving novel local physics [5].

Many of the deviations from the SDW theory can be explained if criticality in the magnetic ordering renders Kondo physics simultaneously critical, producing a "locally critical QPT" [6–8]. Here work has focused on the Kondo lattice model, mapped within extended dynamical mean-field theory (EDMFT) [9] onto a self-consistently determined Bose-Fermi Kondo (BFK) model for a magnetic impurity coupled both to a fermionic band and to a dissipative bosonic bath representing nonlocal fluctuations arising from Ruderman-Kittel-Kasuya-Yoshida (RKKY) interactions between local moments.

The central question we set out to answer is whether the EDMFT captures a *continuous* QPT. Such a transition is expected to be of SDW type for three-dimensional (3D) magnetic spin fluctuations, with local moments that are Kondo-screened below a finite low-temperature scale T_K^* and hence play no role at the QPT. By contrast, if the fluctuations are two-dimensional (2D)—for which there is some evidence in $CeCu_{5.9}Au_{0.1}$ [10]—the scale T_K^* is claimed [6] to vanish precisely at the QPT with coexisting long-wavelength and local critical modes. To confirm the scenarios described above, it must be demonstrated that the PM and AFM phases terminate at a common value of the control parameter. Numerical studies employing quantum Monte Carlo impurity solvers have addressed the particular case of Ising anisotropy believed to be relevant to $CeCu_{5.9}Au_{0.1}$ [7,11]. The character of the QPT remains contentious [7,8,11], in part due to the limitations of quantum Monte Carlo methods in accessing the lowest temperature scales. Solutions of the Kondo lattice model, found via a mapping of the effective BFK model onto the spin-boson model, have pointed to a continuous, locally critical QPT for the 2D case [7]. By contrast, studies of the related periodic Anderson model have predicted a strongly first-order QPT, casting doubt on the ability of EDMFT to capture the key physics [11].

This Letter presents *zero-temperature* EDMFT solutions, obtained by using a numerical renormalization-group (NRG) technique [12] to solve the underlying BFK model. Results for both 2D and 3D spin fluctuations point to a continuous QPT, at which the magnetic order parameter vanishes continuously as the static susceptibility at the AFM ordering wave vector diverges, and the terminus of PM solutions coincides with the onset of magnetic ordering. For the topical 2D case, a concomitant divergence of the static local susceptibility signals that Kondo physics is driven critical at the QPT, and we are able to extract an anomalous exponent in good agreement with experiments on $CeCu_{5.9}Au_{0.1}$ [4]. These results provide important support for the notion of local quantum criticality [6–8], both as a description of specific heavy-fermion systems and, more generally, as a paradigm for novel phase transitions in other areas of physics.

Model.—We focus on the Kondo lattice model with Ising RKKY anisotropy, specified by the Hamiltonian

$$\hat{H} = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i J \boldsymbol{S}_i \cdot \boldsymbol{s}_{c,i} + \frac{1}{2}\sum_{i,j} I_{ij} S_i^z S_j^z. \quad (1)$$

A spin-$\frac{1}{2}$ local moment $\boldsymbol{S}_i$ at site i is coupled to the on-site conduction-electron spin $\boldsymbol{s}_{c,i}$ via an exchange $J > 0$, favoring quenching of local moments. The competing tendency towards magnetism enters through the RKKY interaction I_{ij} between the z components of the localized spins on different sites i and j. The tight-binding parameters t_{ij} determine the conduction-band dispersion $\epsilon_{\boldsymbol{k}}$ and hence the density of states $\rho(\epsilon) = \sum_{\boldsymbol{k}} \delta(\epsilon - \epsilon_{\boldsymbol{k}})$.

EDMFT formulation.—We study the Kondo lattice (1) using EDMFT [9], which amounts to considering a single lattice site, described by the impurity Hamiltonian

$$\hat{H}_{\mathrm{BFK}} = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} \phi^{\dagger}_{\boldsymbol{q}} \phi_{\boldsymbol{q}} + J\boldsymbol{S}\cdot\boldsymbol{s}_c + S_z \sum_{\boldsymbol{q}} g_{\boldsymbol{q}} (\phi_{\boldsymbol{q}} + \phi^{\dagger}_{-\boldsymbol{q}}) + h_{\mathrm{loc}} S_z, \tag{2}$$

at which a single spin $\boldsymbol{S}$ interacts with the on-site spin $\boldsymbol{s}_c$ of a conduction band and, via S_z, with both a dissipative bosonic bath (representing magnetic fluctuations due to spins at all other lattice sites) and a local magnetic field h_{loc}. The coupling of the impurity to the nonlocal degrees of freedom is fully specified by $J\rho(\epsilon)$ and the bosonic spectral function $B(\omega) = \pi \sum_{\boldsymbol{q}} g^2_{\boldsymbol{q}} \delta(\omega - \omega_{\boldsymbol{q}})$.

Within EDMFT, the dynamical spin susceptibility is written $\chi(\boldsymbol{q},\omega) = [M(\omega) + I_{\boldsymbol{q}}]^{-1}$ in terms of a "spin self-energy" $M(\omega)$ and $I_{\boldsymbol{q}}$, the spatial Fourier transform of I_{ij}. The key approximation in EDMFT is neglect of the momentum dependence of both M and the self-energy Σ_σ entering the conduction-electron Green's function $G_\sigma(\boldsymbol{k},\epsilon) = [\epsilon - \epsilon_{\boldsymbol{k}} - \Sigma_\sigma(\epsilon)]^{-1}$. M and Σ_σ are determined self-consistently by requiring that the wave-vector average of the lattice correlation function equals the corresponding *local* correlation function of the impurity problem (2). Thus, the local susceptibility must satisfy

$$\chi_{\mathrm{loc}}(\omega) \equiv i \int_0^\infty dt\, e^{i\omega t} \langle [S_z(t), S_z(0)] \rangle = \int \frac{\rho_I(\epsilon) d\epsilon}{M(\omega) + \epsilon}, \tag{3}$$

$\rho_I(\epsilon) = \sum_{\boldsymbol{q}} \delta(\epsilon - I_{\boldsymbol{q}})$ being the RKKY density of states. The Weiss field $\chi_0^{-1}(\omega) = M(\omega) - \chi^{-1}_{\mathrm{loc}}(\omega)$ determines the bosonic bath density of states through $\mathrm{Im}\chi_0^{-1}(\omega) = \mathrm{sgn}(\omega) B(|\omega|)$. Analogously, $G^{-1}_{0,\sigma}(\epsilon) = G^{-1}_{\mathrm{loc},\sigma}(\epsilon) - \Sigma_\sigma(\epsilon)$ determines the band density of states $\rho(\epsilon)$. However, to study critical properties, it is not necessary to enforce self-consistency on $G_\sigma(\boldsymbol{k},\epsilon)$. Following Ref. [7], we instead take $\rho(\epsilon) = \rho_0 \Theta(D - |\epsilon|)$ and work with fixed $\rho_0 J$, taking $D = 1$ as the energy unit. This choice of a featureless conduction band avoids double counting of RKKY interactions, discussed [8] as the source of discrepancies between previous $T > 0$ studies [7,8,11].

For PM solutions, $h_{\mathrm{loc}} \equiv 0$, and we follow solutions upon increasing the control parameter $\delta = I/T_K^0$; here $-I \equiv I_{\boldsymbol{Q}}$ is the most negative value of $I_{\boldsymbol{q}}$, found at the AFM ordering wave vector $\boldsymbol{q} = \boldsymbol{Q}$, and $T_K^0 \equiv \chi^{-1}_{\mathrm{loc}}(\omega = 0; \delta = 0)$ is the bare Kondo scale of the pure-fermionic impurity problem. Instability of the PM phase is signaled by a divergence of $\chi(\boldsymbol{Q}, 0)$ for some $\delta = \delta_{c,P}$. For AFM solutions, h_{loc} is related self-consistently to a nonzero staggered magnetization $m_{\mathrm{AFM}} \equiv \langle S_z \rangle$ by

$$h_{\mathrm{loc}} = -[I - \chi_0^{-1}(\omega = 0)] m_{\mathrm{AFM}}. \tag{4}$$

We follow AFM solutions from large δ down to $\delta = \delta_{c,A}$, below which the only solution is $m_{\mathrm{AFM}} = 0$.

Examination of the self-consistency condition (3) at $\omega = 0$ reveals that the nature of the QPT depends crucially on the dimensionality of the spin fluctuations: In 3D, $\rho_I(\epsilon)$ has a square-root onset at its lower edge $\epsilon = -I$. We take $\rho_I(\epsilon) = 2\sqrt{I^2 - \epsilon^2}/(\pi I^2)\Theta(I - |\epsilon|)$, for which Eq. (3) gives $\chi_{\mathrm{loc}}(\omega) = 4\chi_0^{-1}(\omega)/I^2$, and the local static susceptibility $\chi_{\mathrm{loc}}(0)$ remains finite when the peak susceptibility $\chi(\boldsymbol{Q}, 0)$ diverges (dashed line in Fig. 1). For 2D magnetism, $\rho_I(\epsilon)$ instead has a jump onset, caricatured as $\rho_I(\epsilon) = (2I)^{-1}\Theta(I - |\epsilon|)$, for which Eq. (3) yields $\chi_{\mathrm{loc}}(\omega) = (2I)^{-1} \ln[1 + 2I\chi(\boldsymbol{Q}, \omega)]$. In this case, any divergence of $\chi(\boldsymbol{Q}, 0)$ is necessarily accompanied by a divergence (albeit weaker) of $\chi_{\mathrm{loc}}(0)$ (solid line in Fig. 1).

To determine where on the parametric curves shown in Fig. 1 the EDMFT solution lies for a given δ, it is necessary to solve the full set of EDMFT equations at all frequencies. The key issue is whether, for 2D magnetism, EDMFT yields a locally critical QPT, i.e., whether $\delta_{c,A} = \delta_{c,P} = \delta_c$ with $\chi^{-1}_{\mathrm{loc}}(\omega = 0; \delta = \delta_c) = 0$.

Solution method.—We solve Eq. (2) by using an extension [12] of the NRG [13]. After logarithmic discretization of the energy axis ($|\epsilon|$, $\omega = D\Lambda^{-n}$ for $n = 0, 1, 2, \ldots$, with $\Lambda > 1$), $\hat{H}_{\mathrm{BFK}}$ is recast in terms of a fermionic and a bosonic chain, each coupled to the impurity at the first site only. An exponential decay of tight-binding coefficients along each chain allows iterative diagonalization of chains of increasing length. The Fock space must be truncated, allowing a maximum of N_b bosons per site and retaining only the lowest N_s many-body eigenstates from one iteration to construct the basis for the next.

The NRG method gives an excellent account of the universal critical properties of the BFK model, which converge rapidly with increasing N_b and N_s and are insensitive to Λ [12]. However, obtaining a satisfactory description of the Kondo lattice places more stringent demands on the impurity solver. The NRG gives the imaginary part of $\chi_{\mathrm{loc}}(\omega)$ as a set of delta functions that are broadened to recover a continuous $\chi''_{\mathrm{loc}}(\omega)$ [13]; the real

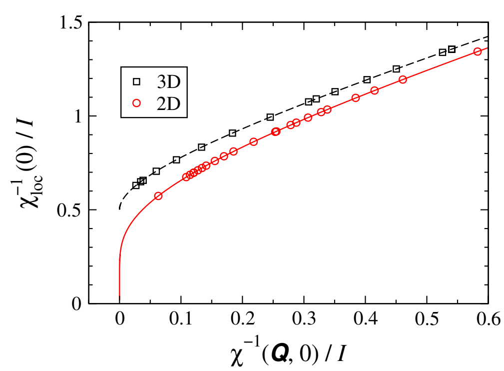

FIG. 1 (color online). Converged values of $y \equiv [I\chi_{\mathrm{loc}}(0)]^{-1}$ vs $x \equiv [I\chi(\boldsymbol{Q}, 0)]^{-1}$. In 3D (squares), Eq. (3) forces $y = \frac{1}{2} \times (1 + x) + \frac{1}{2}\sqrt{x(x + 2)}$ (dashed line) to approach $\frac{1}{2}$ as x vanishes. In 2D (circles), both quantities vanish together according to $y = 2/\ln(1 + 2/x)$ (solid line), signaling critical Kondo physics.

part $\chi'_{\rm loc}(\omega)$ follows by Hilbert transformation. When $h_{\rm loc} \to 0$, $\chi_{\rm loc}(0)$ so obtained should coincide with $-\langle S_z \rangle / h_{\rm loc}$, but in practice there is a mismatch between these two values. If the self-consistently determined $m_{\rm AFM}$, and hence $h_{\rm loc}$, vanish continuously at $\delta_{c,A}$, then, by rewriting Eq. (3) in the equivalent form $h_{\rm loc}/m_{\rm AFM} + \chi^{-1}_{\rm loc}(0) = \chi^{-1}(\boldsymbol{Q}, 0)$, one sees that any such mismatch prevents divergence of $\chi(\boldsymbol{Q}, 0)$, which in turn leads to coexistence of PM and AFM solutions. It is this previously neglected mismatch that underlies the unconventional scenarios presented in Refs. [14,15] and not truncation error or a failure of EDMFT as suggested there.

We ensure internal consistency of the NRG by applying a multiplicative correction $1 + c$ to $\chi_{\rm loc}(\omega, h_{\rm loc})$, such that $\chi_{\rm loc}(0, \eta) = -\langle S_z \rangle / \eta$, where $\eta \approx 10^{-6}$ is the smallest field used in our calculations. For $\Lambda = 3$, $c \approx 0.15$ for the BFK model, very similar to the value for the pure-fermionic Kondo model. Within the EDMFT, the static lattice susceptibility $\chi(\boldsymbol{Q}, 0)$ now diverges by construction if $h_{\rm loc} \to \eta$ self-consistently, i.e., if the order parameter vanishes continuously—a scenario that we emphasize is in no way imposed by the correction scheme.

Self-consistent EDMFT solutions are obtained as follows: For given I, Eq. (2) is solved by using the NRG with a trial $B(\omega)$ and an initial field $h_{\rm loc} > \eta$ [$h_{\rm loc} = \eta$] for AFM [PM] solutions. At this point, the numerical mismatch is corrected. For AFM solutions, finding c requires an additional NRG calculation performed at $h_{\rm loc} = \eta$. Then $B(\omega)$ [and for AFM solutions, $h_{\rm loc} > \eta$] is updated for use in the next loop via Eq. (3) [and Eq. (4)]. Typically, 10–50 EDMFT loops suffice to converge $B(\omega)$ to within 0.0001% for all ω, though convergence is considerably slower around the critical couplings. The solution reached is independent of the details of the trial $B(\omega)$ and, for AFM solutions, of the initial $h_{\rm loc}$.

Results are presented for $\Lambda = 3$, $N_b = 8$, and $N_s = 300$ (requiring up to 1 h per EDMFT loop on a 2.2-GHz AMD Opteron CPU). All data shown are for $\rho_0 J = 0.2$, corresponding to a bare Kondo scale $T_K^0 \approx 0.014$, but we find near-perfect scaling with T_K^0 for $T_K^0 \lesssim 0.1$. We have established in representative cases that the numerics are converged with respect to N_b and N_s and that the essential physical picture is independent of Λ.

Results for 3D magnetism.—In this case, EDMFT has been supposed (but not explicitly shown) to exhibit a continuous QPT of the SDW type [6]. This picture is confirmed in Fig. 2(a), which shows the variation of three $T = 0$ static quantities with $\delta \equiv I/T_K^0$. The inverse peak susceptibility $\chi^{-1}(\boldsymbol{Q}, 0)$ of the PM solutions decreases with increasing δ and vanishes linearly at $\delta_{c,P} = 1.33(2)$ [see Fig. 3(a)], beyond which no PM solutions are found. The local susceptibility $\chi_{\rm loc}(0)$ approaches $T_K^0 \chi_{\rm loc}(0) = 2/\delta_{c,P}$ at $\delta_{c,P}$, as follows from the self-consistency (see Fig. 1). For large δ, AFM solutions converge with nonzero $h_{\rm loc}$ and $m_{\rm AFM}$. Our data are consistent with a continuous vanishing of $m_{\rm AFM}$ upon decreasing δ and, provided the

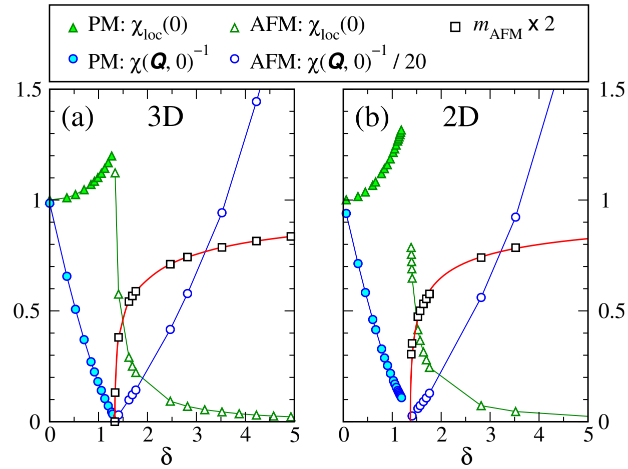

FIG. 2 (color online). Peak and local static susceptibilities (in units of T_K^0) of PM and AFM solutions, along with the order parameter $m_{\rm AFM}$, for (a) 3D and (b) 2D magnetic fluctuations. AFM solutions for $\delta \equiv I/T_K^0 \le \delta_{c,A}$ (where $m_{\rm AFM} = 0$ self-consistently) coincide with PM solutions (with $m_{\rm AFM} \equiv 0$). Lines are guides to the eye.

internal consistency of the NRG is enforced (see the solution method), a concomitant divergence of $\chi(\boldsymbol{Q}, 0)$. Extrapolation of the lowest $\chi^{-1}(\boldsymbol{Q}, 0)$ values to zero yields $\delta_{c,A} = 1.31(2)$. For $\delta < \delta_{c,A}$, AFM and PM solutions coincide.

The large (around 30% of $\delta_{c,A}$) region of coexisting PM and AFM solutions reported in Ref. [14] is sharply suppressed by enforcing the internal consistency of the NRG. The reduced coexistence range of 0%–5% likely stems from residual errors (due to discretization, truncation, Hilbert transformation, numerical rounding, etc.) that will tend to destabilize the fine balance inherent to any continuous transition. We conclude that, within numerical accu-

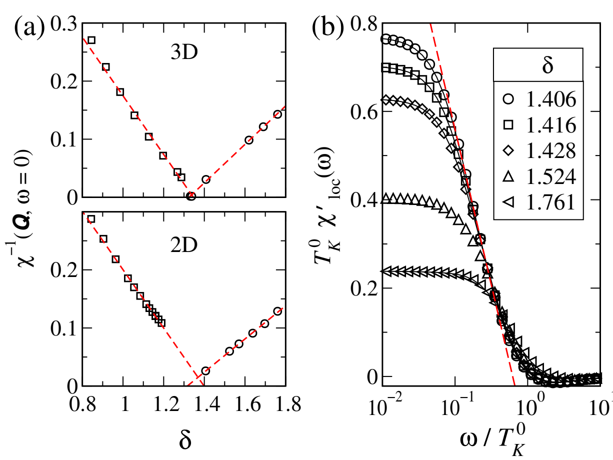

FIG. 3 (color online). (a) Extrapolation to zero of PM $\chi^{-1}(\boldsymbol{Q}, 0)$ (squares) and AFM $\chi^{-1}(\boldsymbol{Q}, 0)/20$ (circles) for 3D and 2D magnetism. (b) Real part of $\chi_{\rm loc}(\omega)$ for five δ values approaching δ_c in the 2D AFM phase. The dashed line is a fit to the logarithmically singular form that develops for $\delta \to \delta_c$.

racy, the EDMFT description of the QPT for 3D magnetism is continuous and of conventional SDW type [2].

Results for 2D magnetism.—Static quantities for the 2D case are shown in Fig. 2(b). Convergence slows markedly in the vicinity of the transition due to the logarithmic form of the self-consistency, making it exceedingly difficult to obtain solutions having very small $\chi^{-1}(\boldsymbol{Q}, 0)$. PM-phase calculations also require a careful choice of starting parameters to avoid flowing towards an unphysical solution [16]. Nonetheless, linear extrapolation of $\chi^{-1}(\boldsymbol{Q}, 0)$ to zero for each phase [Fig. 3(a)] yields $\delta_{c,P} = 1.40(2)$ close to $\delta_{c,A} = 1.34(2)$. The ground-state energy (not shown) provides another handle on the position of the transition. Extrapolations of the PM and AFM energies indicate a crossing at $\delta_c = 1.36(1)$, consistent with $\delta_{c,A}$ deduced from $\chi^{-1}(\boldsymbol{Q}, 0)$.

The slower convergence in 2D has prevented us from approaching the transition as closely as in 3D or from converging AFM solutions below $m_{\mathrm{AFM}} \approx 0.14$ (after more than 300 EDMFT loops). However, the narrow coexistence region (1%–8% of $\delta_{c,A}$) is comparable with that in 3D and to within our numerical accuracy is consistent with a continuous transition. Such a QPT is necessarily of the locally critical type [6], with $\chi_{\mathrm{loc}}(0)$ and $\chi(\boldsymbol{Q}, 0)$ diverging together at δ_c (see Fig. 1), where the self-consistently determined BFK model lies at its critical point [17]. We cannot rule out a very weakly first-order transition either in 2D or 3D, but physically this scenario is virtually indistinguishable from the continuous case.

Support for critical local physics is provided by $\chi'_{\mathrm{loc}}(\omega)$ [Fig. 3(b)], which develops a logarithmically singular form [6] $T_K^0 \chi'_{\mathrm{loc}}(\omega) \sim (\alpha/2\delta_c) \ln|\omega|^{-1}$ in the vicinity of the critical coupling for $T_K^* \ll |\omega| \ll T_K^0$, where the effective Kondo scale T_K^* vanishes logarithmically slowly as $\delta \to \delta_c$. We find $\alpha/2\delta_c = 0.29(1)$ or $\alpha = 0.78(4)$, consistent with the value measured in $CeCu_{5.9}Au_{0.1}$ ($\alpha = 0.75$) and with that obtained in one $T > 0$ study [7]. No such anomalous exponent was found in connection with the strong first-order behavior reported in Ref. [11].

A separate EDMFT study of the Kondo lattice has reached similar conclusions about the nature of the QPT. In Ref. [18], the fermionic degrees of freedom are eliminated by mapping the BFK model onto a spin-boson model. While this mapping introduces another level of approximation and rules out direct comparison of the ground-state energy in the PM and AFM phases, the spin-boson model can be solved via a purely bosonic NRG method requiring less computational effort per EDMFT iteration, allowing investigation closer to the critical points where convergence slows markedly. That two complementary approaches yield essentially the same physical picture is an important confirmation of the key results.

Summary.—We have obtained nonperturbative, zero-temperature solutions of the Kondo lattice model, of great present interest in connection with heavy-fermion quantum criticality. For magnetic fluctuations in both two and three dimensions, our results point to a continuous transition. In the 2D case, critical local-moment fluctuations are observed with an anomalous exponent $\alpha \simeq 0.8$ in the dynamics that is in good agreement with the experimentally determined value for $CeCu_{5.9}Au_{0.1}$. This provides significant new evidence for local quantum criticality in strongly correlated systems.

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