Locally critical quantum phase transitions in strongly correlated metals

Qimiao Si*, Silvio Rabello*, Kevin Ingersent† & J. Lleweilun Smith*

- * Department of Physics & Astronomy, Rice University, Houston, Texas 77251-1892, USA
- † Department of Physics, University of Florida, Gainesville, Florida 32611-8440, USA

When a metal undergoes a continuous quantum phase transition, non-Fermi-liquid behaviour arises near the critical point. All the low-energy degrees of freedom induced by quantum criticality are usually assumed to be spatially extended, corresponding to long-wavelength fluctuations of the order parameter. But this picture has been contradicted by the results of recent experiments on a prototype system: heavy fermion metals at a zero-temperature magnetic transition. In particular, neutron scattering from $CeCu_{6-x}Au_x$ has revealed anomalous dynamics at atomic length scales, leading to much debate as to the fate of the local moments in the quantum-critical regime. Here we report our theoretical finding of a locally critical quantum phase transition in a model of heavy fermions. The dynamics at the critical point are in agreement with experiment. We propose local criticality to be a phenomenon of general relevance to strongly correlated metals.

Quantum (zero-temperature) phase transitions are ubiquitous in strongly correlated metals (for a recent review, see ref. 1). The extensive present interest in metals close to a second-order quantum phase transition has stemmed largely from studies of high-temperature superconductors. In these systems, however, it has been hard to locate the putative quantum critical points (QCPs). The situation seems to be simpler in some related families of strongly correlated metals. In particular, there are many heavy-fermion metals that can be tuned between an antiferromagnetic metal and a paramagnetic metal. In recent years, QCPs have been explicitly identified in a number of stoichiometric or nearly stoichiometric systems. Non-Fermi-liquid behaviour² is observed, usually through transport and thermodynamic measurements, in the quantum-critical regime. Examples^{3–11} include CePd₂Si₂, CeCu_{6-x}Au_x, CeNi₂Ge₂ and YbRh₂Si₂.

The most fundamental question regarding any condensed matter system concerns the nature of its low-energy excitations. The traditional theory for metals close to a QCP assumes that the only important degrees of freedom are long-wavelength fluctuations of the order parameter. For a magnetic QCP, such long-wavelength fluctuations are usually called paramagnons. This theory has its origins back in the 1960s in the description of liquid ³He (for a historical perspective, see ref. 12), and was subsequently formulated in the modern language of critical phenomena^{13,14}. The assumption that the long-wavelength paramagnons are the only critical degrees of freedom, adopted from the theory of classical (finite-temperature) phase transitions, turns out to have three important consequences. First, the dynamical spin susceptibility at generic wavevectors (wavevectors far from the antiferromagnetic ordering wavevector) has the usual Fermi-liquid form, that is, it is linear in frequency. Second, even close to the ordering wavevector, the dynamical spin susceptibility is also linear in frequency. Third, there is a violation of the so-called ω/T scaling (defined in the next section).

This picture has been subjected to experimental testing in recent years. Heavy-fermion metals have undergone by far the most systematic study. A major puzzle has been raised by neutron-scattering experiments⁹⁻¹¹ on $\text{CeCu}_{6-x}\text{Au}_{x0}$ which goes from a paramagnetic metal to an antiferromagnetic metal as x increases through a critical value, $x_c \approx 0.1$ (ref. 4). Close to the antiferromagnetic ordering wavevector, a fractional exponent ($\alpha < 1$) appears in the frequency and temperature dependences of the dynamical spin susceptibility. The same exponent α describes the frequency and temperature dependences at generic wavevectors,

over essentially the entire Brillouin zone. Finally, the dynamical spin susceptibility exhibits ω/T scaling. These experiments have led to much debate as to the nature of the QCPs in heavy-fermion metals, especially concerning the fate of the local magnetic moments in the quantum-critical regime $^{9-11,15-18}$.

Here we show that a dynamical spin susceptibility of the form observed experimentally may arise at a locally critical quantum phase transition, where local critical degrees of freedom coexist with spatially extended ones. Although we reach this conclusion by solving a microscopic model appropriate for heavy-fermion metals, the possibility of such a QCP can be seen on general grounds. The universality class of a classical phase transition is entirely determined by statics¹. The critical degrees of freedom must be spatially extended, as only long-wavelength fluctuations of the order parameter are energetically favourable. At a quantum phase transition, by contrast, both the statics and dynamics (that is, quantum fluctuations) are important¹. The effect of quantum fluctuations on local degrees of freedom is to introduce a coupling to certain dissipative baths. When this coupling is sufficiently strong, the local degrees of freedom can become critical. (A similar situation—local degrees of freedom driven critical by a dissipative bath—arises in macroscopic quantum tunnelling problems¹⁹.)

Locally critical quantum phase transition

The microscopic model that we consider here is the Kondo lattice model²⁰ (Fig. 1a). At each lattice site, a local moment²¹ interacts via an exchange coupling J_K with the spin of any conduction electron sitting at the site. There are two important energy scales in the problem^{22,23}: the Kondo temperature T_K sets the scale below which an isolated local moment would be screened by the spins of the conduction electrons, while the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction characterizes the induced coupling between two local moments. We will assume an average occupancy of less than one conduction electron per lattice site; as a result, all phases considered here are metallic. To systematically analyse the behaviour of the local degrees of freedom in this model, we apply the extended dynamical mean-field theory (EDMFT) developed in refs 24-26. As in the standard dynamical mean-field theory²⁷, the correlation functions of the lattice problem in the EDMFT are calculated through a self-consistent impurity Kondo problem. The latter (Fig. 1b) describes a local moment simultaneously coupled to two dissipative baths¹⁹. A fermionic bath accounts for all temporal fluctuations arising from hopping of electrons between the local site and the rest of the lattice, while a bosonic bath represents the fluctuating magnetic field generated by the local moments at all other sites. The couplings to the two baths are J_K and g, respectively. Further details are given in the next section.

We find two types of QCP, illustrated by the phase diagrams in Figs 2 and 3. In each case, the tuning parameter δ is the ratio of the RKKY interaction to the Kondo temperature. Increasing δ has two effects. First, the magnetic correlations become more pronounced. The dynamical spin susceptibility $\chi(\mathbf{Q}, \omega)$ —where **Q** is the peak wavevector—diverges at some threshold value $\delta = \delta_c$, which defines a QCP separating a paramagnetic metal ($\delta < \delta_c$) from an antiferromagnetic metal ($\delta > \delta_c$). Second, the local Kondo physics governed by the effective impurity problem is also changed^{28–30}. Through self-consistency, an increase in δ causes an increase in the coupling g between the local moment and the fluctuating magnetic field. At some value $\delta = \delta_{loc}^{c}$, the corresponding ratio g/T_{K} reaches a threshold value where the local Kondo problem becomes critical. The existence of such a critical point reflects two competing processes in the local problem (Fig. 1b): quenching of the local moment through its Kondo coupling to the spins of the fermionic bath, and the tendency of the coupling g to polarize the local moment along the direction of the fluctuating magnetic field. At $\delta = \delta_{loc}^{c}$, the fluctuating magnetic field just succeeds in preventing the spins of the fermionic bath from completely quenching the local moment, yielding a singular local susceptibility. This critical point is also marked by the vanishing of a local energy scale E_{loc}^* , reflecting a critical slowing down. E_{loc}^{\star} serves as an effective Fermi energy scale, in the sense that the local susceptibility has the usual Fermi-liquid form (that is, an imaginary part that is linear in the frequency ω) only at energies below E_{loc}^* .

At the first type of QCP (Fig. 2), the lattice system orders before the effective local problem has a chance to become critical, that is, $\delta_{\rm c} < \delta_{\rm loc}^{\rm c}$, so $E_{\rm loc}^{\star}$ remains finite at the transition. The local moments are completely quenched at zero temperature over the entire paramagnetic region and also at the QCP. Their only vestiges are

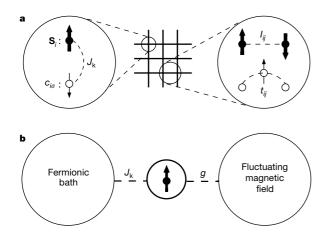


Figure 1 A theoretical model of heavy fermions. a, The Kondo lattice model. At each lattice site i, a spin-1/2 local moment \mathbf{S}_i interacts with a local conduction electron orbital $c_{i\sigma}$ through an antiferromagnetic Kondo coupling of strength J_K . The hopping amplitude between the conduction electron orbitals at sites i and j is t_{ij} . The Fourier transform of t_{ij} gives the band dispersion $\epsilon_{\mathbf{k}}$, corresponding to which is a density of states $\rho_0(\epsilon)$. The Kondo temperature T_K is the characteristic scale for the screening of an isolated local moment by the spins of the conduction electrons. For sufficiently small J_K , $T_{\rm K} \approx [\rho_0(\mu)]^{-1} \exp[-1/\rho_0(\mu)J_{\rm K}]$, where μ is the chemical potential. The RKKY interaction between two local moments at sites i and j is I_{ij} , the Fourier transform of which is l_a . **b**, The effective impurity Kondo model to which the Kondo lattice model is mapped in the EDMFT^{24–26}. The local moment is coupled to two dissipative baths, one fermionic and the other bosonic. The bosonic bath describes a fluctuating magnetic field. The couplings to the two baths are J_K and g, respectively. The energy dispersions of the two baths are determined self-consistently.

the Kondo resonances, which hybridize with the conduction electrons to form Landau quasiparticles^{20,22,23,31}. The RKKY interaction manifests itself as an interaction between these quasiparticles, leading to a spin-density-wave instability which drives the transition²². As a result, the dynamical spin susceptibility has the form as in the traditional theory^{13,14}. We find this type of QCP when the spin fluctuations are three-dimensional.

The second type of QCP is illustrated in Fig. 3. Here, $\delta_c = \delta_{loc}^c$, so the lattice system reaches its ordering transition precisely at the point where the local problem also becomes critical. Thus, E_{loc}^{\star} vanishes at the QCP, and two kinds of critical degrees of freedom coexist: long-wavelength fluctuations of the order parameter, and local fluctuations originating from the local moments. The transition is locally critical. We find this type of QCP when spin fluctuations are two-dimensional. (In order for the ordering temperature T_N shown in Fig. 3 to be nonzero for $\delta > \delta_c$, it is necessary to have an infinitesimal RKKY coupling in the third dimension.)

At the locally critical point, the zero-temperature dynamical spin susceptibility has an anomalous frequency dependence at wavevectors **q** not only close to the ordering wavevector **Q** but everywhere else in the Brillouin zone as well:

$$\chi(\mathbf{q},\omega) = \frac{1}{f(\mathbf{q}) + A\omega^{\alpha}} \tag{1}$$

Here α is an anomalous exponent (an expression for which is given in equation (13) below). For any wavevector \mathbf{q} far away from \mathbf{Q} , $f(\mathbf{q})$ is non-zero and varies smoothly with \mathbf{q} ; for \mathbf{q} close to \mathbf{Q} , $f(\mathbf{q})$ is proportional to $(\mathbf{q} - \mathbf{Q})^2$.

At finite temperatures, ω^{α} in equation (1) is replaced by $T^{\alpha}W(\omega/T)$, where $W(\omega/T)$ is a scaling function whose form depends only on α . This has two experimentally testable consequences. First, the dynamical spin susceptibility at $\mathbf{q} = \mathbf{Q}$ satisfies an ω/T scaling:

$$\chi(\mathbf{Q}, \omega, T) = \frac{1}{AT^{\alpha}W(\omega/T)}$$
 (2)

Second, the static uniform spin susceptibility has a modified Curie-Weiss form

$$\chi(T) = \frac{1}{\Theta + BT^{\alpha}} \tag{3}$$

where Θ is a positive constant.

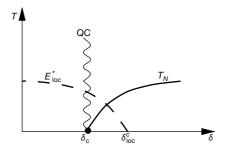


Figure 2 Diagram of a conventional quantum phase transition in Kondo lattices. The tuning parameter δ is the ratio of the RKKY interaction to the Kondo energy scale T_K . When δ is small the local moments are completely screened by the spins of the conduction electrons, and the system is a paramagnetic metal. Increasing δ strengthens the coupling between each local moment and the fluctuating magnetic field produced by all other local moments, as measured by the ratio g/T_K , where g parametrizes the effective local problem defined in Fig. 1b and equation (6). At δ^c_{loc} , the corresponding g/T_K would reach the critical value for a phase transition in the local dissipative problem (see main text); at this point, a local energy scale E^\star_{loc} (dashed line) would vanish. Increasing δ also increases the spin susceptibility at the peak wavevector, $\chi(\mathbf{Q})$, which diverges at a quantum critical point at $\delta = \delta_c$. Beyond δ_c , there exists a finite transition temperature T_N (solid line) below which the system is an antiferromagnetic metal. In this conventional case, $\delta_c < \delta_{loc}^c$, that is, E_{loc}^{\star} is finite at the critical point. The quantum-critical (QC) regime, denoted by the wavy line, is described by the traditional theory.

articles

Our results can be directly compared to neutron-scattering experiments on Au-doped CeCu_{6-x}Au_x at the critical concentration $x_c \approx 0.1$. (1) The experimental data have been fitted^{9,11} to the form of equation (1), with an exponent $\alpha \approx 0.75$. (2) Within experimental resolution, $f(\mathbf{q})$ goes to zero along lines in the threedimensional Brillouin zone, implying that the magnetic fluctuations are two-dimensional in real space 10,11,32 . (3) An ω/T scaling has been extensively reported^{9,11} (see also ref. 33).

In addition, the modified Curie-Weiss form (equation (3)) is known^{9,11} to fit the magnetization data in CeCu_{6-x}Au_x. This form also appears to describe the magnetization of some other heavyfermion metals near quantum criticality8. One example (F. Steglich, personal communication) is YbRh₂Si₂, which is already very close to being critical at ambient pressure and without any doping. The thermodynamic and transport properties⁵ of this compound are very similar to those of $CeCu_{6-x}Au_x$ at $x = x_c$.

From the local susceptibility we can also determine the NMR spin-lattice relaxation rate $1/T_1$. Barring subtle form-factor cancellations, the relaxation rate is expected to be temperature-independent in the relevant temperature range:

$$\frac{1}{T_1} \approx \text{constant}$$
 (4)

This prediction could be tested, for instance, through NMR measurements on the Cu sites in CeCu_{6-x}Au_x or the Si sites in YbRh₂Si₂.

Extended dynamical mean-field theory

We now outline the EDMFT analysis leading to the above conclusions. The Kondo lattice model illustrated in Fig. 1a is specified by the hamiltonian

$$H = \sum_{ii,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} J_{K} \mathbf{S}_{i} \cdot \mathbf{s}_{c,i} + \sum_{ii} I_{ij} \mathbf{S}_{i} \cdot \mathbf{S}_{j}$$
 (5)

where $\mathbf{s}_{c,i}$ is the conduction electron spin at site i. Within the EDMFT²⁴⁻²⁶, equation (5) is mapped onto an effective single-site problem, illustrated in Fig. 1b and represented by the hamiltonian

$$H_{\text{loc}} = J_{\text{K}} \mathbf{S} \cdot \mathbf{s}_{\text{c}} + \sum_{p,\sigma} E_{p} c_{p\sigma}^{\dagger} c_{p\sigma} + g \sum_{p} \mathbf{S} \cdot (\mathbf{\phi}_{p} + \mathbf{\phi}_{-p}^{\dagger}) + \sum_{p} w_{p} \mathbf{\phi}_{p}^{\dagger} \cdot \mathbf{\phi}_{p}$$

$$\tag{6}$$

where $c_{p\sigma}$ and ϕ_p describe the fermionic and bosonic dissipative baths, respectively. The self-consistent procedure is as follows. We put in trial forms for E_p , w_p and g, and solve the impurity Kondo problem to determine the electron self-energy $\Sigma(\omega)$, the 'spin selfenergy' $M(\omega)$, the local Green's function $G_{loc}(\omega)$, and the local susceptibility $\chi_{loc}(\omega)$. (For definitions of these functions and further details of the calculational procedure, see Methods. We note here that the key approximation of the EDMFT is the assumption that the electron and spin self-energies are momentum-independent.)

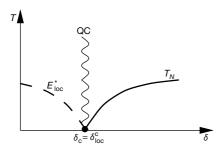


Figure 3 Diagram of a locally critical quantum phase transition in Kondo lattices. The notation is the same as in Fig. 2. The crucial new feature here is that $\delta_c = \delta_{loc}^c$, that is, E_{loc}^{\star} vanishes at the quantum critical point. Local and spatially-extended critical degrees of freedom coexist in the quantum-critical (QC) regime.

Self-consistency is imposed by demanding that G_{loc} and χ_{loc} are equal to the wavevector averages, respectively, of the lattice Green's function $G(\mathbf{k}, \omega)$ and the lattice susceptibility

$$\chi(\mathbf{q},\omega) = \frac{1}{M(\omega) + I_{\mathbf{q}}} \tag{7}$$

where $I_{\mathbf{q}}$ is the Fourier transform of I_{ij} . For the purpose of determining the universal low-energy behaviour, we take the density of states of the fermionic bath near the Fermi energy to be a non-zero constant, and the spectral function of the fluctuating magnetic field to have a power-law dependence on frequency, with an exponent γ , for ω below some cut-off scale Λ . The effective impurity Kondo problem is solved using a $1 - \gamma$ expansion^{28,29,34}. Two types of self-consistent solution are obtained for different forms of the 'RKKY density of states':

$$\rho_l(\epsilon) = \sum_{\mathbf{q}} \delta(\epsilon - I_{\mathbf{q}}) \tag{8}$$

The first type of solution (Fig. 2) arises when the RKKY density of states $\rho_l(\epsilon)$ increases from the lower band edge (at $\epsilon=I_Q$) in a square-root fashion (that is, as $\sqrt{\epsilon - I_Q}$). At the QCP, the spin selfenergy takes the form

$$M(\omega) = -I_0 - ia\omega \tag{9}$$

where a is a positive, real constant. Through equation (7), this yields a $\chi(\mathbf{q},\omega)$ of the form given in the traditional theory^{13,14}. The linear frequency dependence of $M(\omega)$ reflects the fact that the spin fluctuations describe quasiparticle-quasihole pairs.

The second type of solution (Fig. 3) arises when $\rho_l(\epsilon)$ increases from zero at the lower band edge with a jump. The self-consistent local dynamical spin susceptibility at the QCP is singular, and is given by

$$\chi_{\rm loc}(\omega) = \frac{1}{2\Lambda} \ln \frac{\Lambda}{-i\omega} \tag{10}$$

where

$$\Lambda = \frac{2}{\pi \rho_0(\mu)} \exp\left[-\frac{1}{\rho_0(\mu)J_K}\right]$$
 (11)

 $\rho_0(\mu)$ being the bare conduction electron density of states at the chemical potential μ . The corresponding spin self-energy has the form:

$$M(\omega) \approx -I_0 + A\omega^{\alpha}$$
 (12)

Here, $A = (-i)^{\alpha} \Lambda_0 \Lambda^{-\alpha}$, where Λ_0 is defined by the condition that, for $\epsilon \in (I_Q, I_Q + \Lambda_0)$, $\rho_l(\epsilon)$ is approximately equal to its value at the lower edge, $\rho_l(I_Q)$. The exponent α depends on both Λ and $\rho_l(I_Q)$: $\alpha = \frac{1}{2\Lambda\rho_l(I_Q)} \tag{13}$

$$\alpha = \frac{1}{2\Lambda \rho_l(I_Q)} \tag{13}$$

The spin self-energy acquires this anomalous frequency dependence because spin fluctuations can not only decay into particle-hole pairs, but can also couple to critical local modes. The dynamical spin susceptibility at zero temperature is then given by equation (1), with $f(\mathbf{q}) = I_{\mathbf{q}} - I_{\mathbf{Q}}$. At finite temperatures, the self-consistent solution gives a spin self-energy:

$$M(\omega, T) \approx -I_0 + AT^{\alpha}W(\omega/T)$$
 (14)

The scaling function is $W(\omega/T) = (i2\pi)^{\alpha} \exp[\alpha \psi(1/2 - i\omega/2\pi T)]$, where ψ is the digamma function. This directly leads to equations (2) and (3), with $\Theta = I_{q=0} - I_Q$ and $B \approx \Lambda_0 \Lambda^{-\alpha} (2\pi)^{\alpha} \exp[\alpha \psi(1/2)]$. A square-root onset and a jump at the lower edge of the RKKY

density of states are characteristic of magnetic fluctuations in three and two dimensions, respectively. These behaviours are exemplified by the RKKY density of states associated with nearest-neighbour coupling in a (three-dimensional) cubic lattice and its counterpart in a (two-dimensional) square lattice. Although the details depend

on the lattice type and the range of interactions, the square-root and jump onsets in the two cases are robust provided that I_q approaches $I_{\mathbf{Q}}$ in a $(\mathbf{q} - \mathbf{Q})^2$ fashion.

Beyond the microscopic theory

So far we have presented the results of a specific microscopic approach: the EDMFT for the Kondo lattice model. We now turn to more general considerations concerning the existence and properties of locally critical quantum phase transitions. There are four main points that we wish to discuss.

First, even in the traditional theory there are hints, albeit very subtle, that two-dimensionality facilitates the realization of a locally critical point. In this theory 13,14, the zero-temperature spin fluctuations are given by the harmonic, or gaussian, fluctuations of the order parameter. As a result, the zero-temperature, zero-frequency spin susceptibility is proportional to $(\mathbf{q} - \mathbf{Q})^{-2}$. In two dimensions, the corresponding local—that is, wavevector-averaged—susceptibility is in fact logarithmically singular. (For two-dimensional fermions coupled to two-dimensional commensurate spin fluctuations, there are other kinds of singularities in the spin-density-wave description; see ref. 35.) This singularity can cause important nonlinear effects in the dynamics of any non-trivial local degrees of freedom—such as local moments in heavy-fermion metals—and can ultimately drive them critical. Our EDMFT analysis amounts to a microscopic prescription for these nonlinear effects. We note that the situation is very different for QCPs in insulators^{1,36}. There, the effective field theory is usually below its upper critical dimension, implying that the spin susceptibility is $(\mathbf{q} - \mathbf{Q})^{-2+\eta}$, where the anomalous exponent η takes a positive value. The corresponding local susceptibility is no longer singular in two dimensions.

Second, the contrast between a locally critical transition and a spin-density-wave transition can also be seen at the level of a Ginzburg-Landau-like description. For a spin-density-wave transition, there is only one type of critical degrees of freedom, namely the long-wavelength fluctuations of the order parameter. The Ginzburg-Landau action is then written purely in terms of the frequency-dependent magnetization at wavevectors close to the ordering wavevector:

$$S_{\text{SDW}} = S_{\text{lw}}[\mathbf{m}(\mathbf{q} \approx \mathbf{Q}, \omega)] \tag{15}$$

This generalizes the standard ϕ^4 theory for a classical phase transition in that the fluctuations take place not only in the D spatial dimensions, but also in time. The temporal fluctuations can be thought of as adding z dimensions, where z is the dynamical exponent: S_{lw} is a ϕ^4 theory with an effective dimensionality $D_{\text{eff}} = D + z$ (see refs 1, 13, 14).

For a locally critical point, on the other hand, the Ginzburg-Landau action is no longer just a ϕ^4 theory. There are extra critical modes that characterize the continuous disappearance of the Kondo resonance as the critical point is approached from the paramagnetic side. These modes are independent of the fluctuations of the order parameter. They are spatially local because the destruction of the Kondo resonance is a local phenomenon. The Ginzburg-Landau action will now contain, in addition to the ϕ^4 component S_{lw} parts describing these new local critical degrees of freedom and their nonlinear coupling to the long-wavelength modes. The explicit construction of these additional parts of the Ginzburg-Landau action is left for future work.

Third, consideration of a Ginzburg-Landau description makes it likely that the locally critical point is stable beyond our EDMFT approximation, provided that $\alpha < 1$ (as is the case in CeCu_{6-x}Au_x and YbRh₂Si₂). The crucial question is what happens when we allow an explicit q dependence in the spin self-energy. The dynamical exponent entering S_{lw} will be $z = 2/\alpha$. When $\alpha < 1$, the effective dimension $D_{\text{eff}} = D + z = 2 + 2/\alpha$ will be above the upper critical dimension of 4, so that all the nonlinear couplings within S_{lw} will be irrelevant in the renormalization-group sense¹. As a result, the **q**-dependence of the spin self-energy from S_{lw} will be at most $(\mathbf{q} - \mathbf{Q})^2$. We also expect that the spin self-energy due to the coupling of the order-parameter field with the local modes will have a smooth **q**-dependence. As a result, the zero-temperature spin susceptibility should be proportional to $(\mathbf{q} - \mathbf{Q})^{-2}$ (that is, the anomalous exponent $\eta = 0$). This implies that the singular local susceptibility and the concomitant destruction of the Kondo resonance at the critical point are robust in two dimensions. We note that a rigorous proof of this stability awaits the explicit construction of the Ginzburg-Landau action for the locally critical point.

Fourth, Ginzburg-Landau considerations also provide a way to understand the ω/T scaling (equation (2)) at the locally critical point. At a spin-density-wave transition, the field theory, equation (15), is a ϕ^4 theory with an effective dimensionality $D_{\text{eff}} = D + z$. Whereas at QCPs in insulators^{1,36} the dynamical exponent is usually 1, in a metallic environment z = 2, raising D_{eff} above the upper critical dimension of 4 for the ϕ^4 theory. All the nonlinear couplings are then irrelevant, and ω/T scaling is absent^{1,14}. (A violation of ω/T scaling has been reported³⁷ near a QCP in $Ce_{1-x}La_xRu_2Si_2$.)

At a locally critical point, the nonlinear couplings among the long-wavelength modes remain irrelevant. However, the Ginzburg-Landau action also contains nonlinear couplings that involve the additional local critical modes. These couplings are relevant, making the field theory an interacting one, thereby³⁸ allowing the ω/T scaling given in equation (2). In terms of a suitably defined spin relaxation rate, the contribution from the ϕ^4 component depends on temperature with a power greater than 1. On the other hand, the contribution from the coupling to the local modes is linear in temperature due to the 'relevant' nonlinear couplings. The total relaxation rate is then linear in temperature, as required³⁹ for ω/T scaling. Again, the EDMFT analysis of the previous section amounts to a microscopic prescription for determining the relaxation rate and, more generally, the entire scaling function.

Broader implications

In addition to explaining the salient features of experiments on heavy-fermion metals close to a QCP, our results may have broader implications for other strongly correlated metals. The emergence of critical local modes in the case that we have studied depends crucially on the formation of local moments. A local moment is nothing other than a strongly interacting f-electron orbital that cannot be doubly occupied owing to a strong on-site Coulomb interaction²¹. It is formed at energies intermediate between the bare Coulomb interaction scale and the asymptotic low-energy limit. The existence of non-trivial local physics at such intermediate energy scales is in fact ubiquitous in strongly correlated metals, including metals close to being a Mott insulator. This suggests the possibility of a locally critical point occurring in a doped Mott insulator.

We adopt the EDMFT as a conserving resummation of diagrams for finite dimensional systems (Fig. 7b of ref. 24). The spatial dimensionality enters, among other ways, via the form of the RKKY density of states defined in equation (8). For any finite-dimensional system, the support to $\rho_l(\epsilon)$ is bounded and a stable paramagnetic solution exists.

The EDMFT provides a self-consistent procedure. In the Bose-Fermi Kondo hamiltonian, equation (6), we insert trial forms for the spectra of both the vector-bosonic bath and fermionic bath, which can be parametrized in terms of the Weiss fields χ_0^{-1} and G_0^{-1}

$$g^2 \sum_{p} \frac{2w_p}{\omega^2 - w_p^2} = -\chi_0^{-1}(\omega), \quad \sum_{p} \frac{1}{\omega - E_p} = G_0(\omega)$$
 (16)

The trial forms for the QCP are taken to be

$$\operatorname{Im} G_0(\omega + i0^+) = -\pi N_0,$$

$$\operatorname{Im} \chi_0^{-1}(\omega + i0^+) = C|\omega|^{\gamma} \operatorname{sgn} \omega \text{ for } |\omega| < \Lambda$$
(17)

where N_0 , γ , C, and Λ are parameters to be determined and 'sgn' refers to the sign function. Next, we solve the Bose-Fermi Kondo problem using a $(1 - \gamma)$ expansion. This step

articles

determines the local spin susceptibility and the local conduction electron Green's

$$\chi_{loc}(\tau) = -\langle T_{\tau}S_{x}(\tau)S_{x}(0)\rangle_{H_{loc}}$$

$$G_{loc}(\tau) = -\langle T_{\tau}c_{\sigma}(\tau)c_{\pi}^{\dagger}(0)\rangle_{H_{\tau}}$$
(18)

where τ is the imaginary time. This step also specifies²⁴ the spin self-energy $M(\omega)$, and the conduction electron self-energy $\Sigma(\omega)$:

$$M(\omega) = \chi_0^{-1}(\omega) + \frac{1}{\chi_{loc}(\omega)}$$

$$\Sigma(\omega) = G_0^{-1}(\omega) - \frac{1}{G_{loc}(\omega)}$$
(19)

(The spin self-energy is defined in terms of an effective spin cumulant that is

The $(1 - \gamma)$ expansion we use follows refs 28, 29, 34. To linear order in $1 - \gamma$, there is a renormalization-group fixed point located at $J_{\rm K}=C=(1-\gamma)/2$. In analogy to the standard application of the ϵ expansion⁴⁰, we assume that the local spin susceptibility $\chi_{loc}(\tau)$ takes a power-law form at the critical point. By setting J_K and C to their fixed point values, we can determine the exponent by matching the leading $ln(\tau)$ term in the expansion of the assumed power-law form for $\chi_{\text{loc}}(au)$ with the leading $\ln(au)$ term of the perturbative expression for $\chi_{loc}(\tau)$, calculated from the Bose–Fermi Kondo hamiltonian, equation (6), to linear order in $1 - \gamma$. This gives, for $0 < \gamma < 1$,

$$\chi_{\text{loc}}(\omega) = \frac{1}{2\Lambda^{1-\gamma}} \Gamma(\gamma) \sin \frac{\pi (1-\gamma)}{2} (-i\omega)^{-\gamma}$$
 (20)

where Γ is the gamma function, and for $\gamma = 0$, equation (10).

In addition, to linear order in $1 - \gamma$, the conduction electron self-energy vanishes:

$$\Sigma = O((1 - \gamma)^2) \tag{21}$$

Finally, we demand self-consistency, which amounts to the requirement that a local correlation function is equal to the wavevector average of the corresponding lattice correlation function. In terms of the RKKY density of states, $\rho_l(\epsilon)$ defined in equation (8), and the usual conduction electron density of states, $\rho_0(\epsilon)$, the self-consistency condition can be written as

$$\chi_{loc}(\omega) = \int d\epsilon \frac{\rho_{l}(\epsilon)}{M(\omega) + \epsilon}$$

$$G_{loc}(\omega) = \int d\epsilon \frac{\rho_{0}(\epsilon)}{\omega - \epsilon - \Sigma(\omega)}$$
(22)

When $\rho_I(\epsilon)$ is proportional to $\sqrt{\epsilon - I_Q}$ near its lower band edge $(\epsilon \to I_Q^+)$, χ_{loc} is finite at the QCP. The local moments are not critical.

The locally critical point arises when $\rho_{\rm I}(\epsilon)$ has a jump at the lower band edge. $\chi_{\rm loc}$ is now singular at the QCP. The self-consistent solution for the parameters introduced in equations (17) is

$$N_0 = \rho_0(\mu), \quad \gamma = 0^+, \quad C = \pi \Lambda \tag{23}$$

with the expression for Λ being given in the main text, as are those for χ_{loc} and M. We also note that the relationship between γ and α is indirect: it is specified by the self-consistency equation (22) along with equations (17)-(19).

The local susceptibility, given in equation (10), is universal. The exponent α for the spin self-energy depends on the product $\Lambda \rho_l(I_Q)$ (see equation (13)). It can be seen from equation (11) that Λ is of the order of the Kondo energy. As the QCP is reached through a competition between the RKKY and Kondo interactions, we expect that this product is close to unity, resulting in an α that is not too far from 1/2. The precise value of α , however, is interaction-dependent: it depends on which point of the phase boundary in the RKKY interaction-Kondo energy parameter space is crossed as the system is tuned through the quantum phase transition.

At finite temperatures, the self-consistent procedure outlined above can also be carried through, leading to the spin self-energy quoted in the main text.

Received 8 December 2000; accepted 29 August 2001.

- 1. Sachdev, S. Quantum Phase Transitions (Cambridge Univ. Press, Cambridge, 1999).
- Maple, M. B. et al. Non-Fermi-liquid behavior in strongly correlated f-electron materials. J. Low Temp Phys. 95, 225-243 (1994).
- 3. Mathur, N. D. et al. Magnetically mediated superconductivity in heavy fermion compounds. Nature **394,** 39-43 (1998).

- 4. von Löhneysen, H. et al. Non-Fermi-liquid behavior in a heavy-fermion alloy at a magnetic instability. Phys. Rev. Lett. 72, 3262-3265 (1994).
- Trovarelli, O. et al. YbRb₂Si₂: Pronounced non-Fermi-liquid effects above a low-lying magnetic phase transition. Phys. Rev. Lett. 85, 626-629 (2000)
- 6. Heuser, K. et al. Inducement of non-Fermi-liquid behavior with a magnetic field. Phys. Rev. B 57, R4198-R4201 (1998).
- 7. Estrela, P., de Visser, A., Naka, T., de Boer, F. R. & Pereira, L. C. J. High-pressure study of the non-Fermi liquid material U2Pt2In. Preprint cond-mat/0009324 at (http://xxx.lanl.gov) (2000).
- Steward, G. Non-Fermi liquid behavior in d- and f- electron metals. Rev. Mod. Phys. 73, in the press (2001).
- Schröder, A., Aeppli, G., Bucher, E., Ramazashvili, R. & Coleman, P. Scaling of magnetic fluctuations near a quantum phase transition. Phys. Rev. Lett. 80, 5623-5626 (1998).
- 10. Stockert, O., von Löhneysen, H., Rosch, A., Pyka, N. & Loewenhaupt, M. Two dimensional fluctuations at the quantum critical point of $CeCu_{6-x}Au_{x}$. Phys. Rev. Lett. 80, 5627–5630 (1998).
- 11. Schröder, A. et al. Onset of antiferromagnetism in heavy-fermion metals, Nature 407, 351-355 (2000).
- 12. Lonzarich, G. G. in Electron (ed. Springford, M.) 109-147 (Cambridge Univ. Press, Cambridge, 1997). 13. Hertz, J. A. Quantum critical phenomena. Phys. Rev. B 14, 1165-1184 (1976).
- 14. Millis, A. J. Effect of a nonzero temperature on quantum critical points in itinerant fermion systems. Phys. Rev. B 48, 7183-7196 (1993).
- 15. Coleman, P. Theories of non-Fermi liquid behavior in heavy fermions. Physica B 259-261, 353-358 (1999).
- 16. Si, Q., Smith, J. L. & Ingersent, K. Quantum critical behavior in Kondo systems. Int. J. Mod. Phys. B 13, 2331-2342 (1999)
- 17. Rosch, A. Interplay of disorder and spin fluctuations in the resistivity near a quantum critical point. Phys. Rev. Lett. 82, 4280-4283 (1999)
- 18. Coleman, P., Pépin, C. & Tsvelik, A. M. Supersymmetric spin operators. Phys. Rev. B 62, 3852-3868
- 19. Leggett, A. J. et al. Dynamics of the dissipative two-state system. Rev. Mod. Phys. 59, 1-86 (1987).
- 20. Hewson, A. C. The Kondo Problem to Heavy Fermions (Cambridge Univ. Press, Cambridge, 1993).
- 21. Anderson, P. W. Localized magnetic states in metals. Phys. Rev. 124, 41-53 (1961)
- 22. Doniach, S. The Kondo lattice and weak antiferromagnetism. Physica B 91, 231-234 (1977).
- 23. Varma, C. M. Mixed-valence compounds. Rev. Mod. Phys. 48, 219-238 (1976).
- 24. Smith, J. L. & Si, Q. Spatial correlations in dynamical mean-field theory. Phys. Rev. B 61, 5184-5192 (2000).
- 25. Si, Q. & Smith, J. L. Kosterlitz-Thouless transition and short range spatial correlations in an extended Hubbard model. Phys. Rev. Lett. 77, 3391-3394 (1996).
- 26. Chitra, R. & Kotliar, G. Effect of Coulomb long-range interactions on the Mott transition. Phys. Rev. Lett. 84, 3678-3681 (2000).
- 27. Georges, A., Kotliar, G., Krauth, W. & Rozenberg, M. J. Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions, Rev. Mod. Phys. 68, 13-125 (1996).
- 28. Smith, J. L. & Si, Q. Non-Fermi liquids in the two-band extended Hubbard model. Europhys. Lett. 45, 228-234 (1999).
- 29. Sengupta, A. M. Spin in a fluctuating field: the Bose (+Fermi) Kondo models. Phys. Rev. B 61, 4041-4043 (2000).
- 30. Sachdev, S. & Ye, J. Gapless spin-fluid ground state in a random quantum Heisenberg magnet. Phys. Rev. Lett. 70, 3339-3342 (1993).
- 31. Continentino, M. A. Universal behavior in heavy fermions. Phys. Rev. B 47, 11587-11590 (1993).
- 32. Rosch, A., Schröder, A., Stockert, O. & von Löhneysen, H. Mechanism for the non-Fermi-liquid behavior in CeCu_{6-x}Au_x. Phys. Rev. Lett. 79, 159-162 (1997).
- 33. Aronson, M. C. et al. Non-Fermi-liquid scaling of the magnetic response in $UCu_{5-x}Pd_x$ (x = 1, 1.5). Phys. Rev. Lett. 75, 725-728 (1995).
- 34. Vojta, M., Buragohain, C. & Sachdev, S. Quantum impurity dynamics in two-dimensional antiferromagnets and superconductors. Phys. Rev. B 61, 15152-15184 (2000).
- 35. Abanov, Ar. & Chubukov, A. V. Spin-fermion model near the quantum critical point: one-loop renormalization group results. Phys. Rev. Lett. 84, 5608-5611 (2000).
- 36. Chakravarty, S., Halperin, B. I. & Nelson, D. R. Two-dimensional quantum Heisenberg antiferromagnet at low temperatures. Phys. Rev. B 39, 2344-2371 (1989).
- 37. Raymond, S., Regnault, L. P., Flouquet, J., Wildes, A. & Lejay, P. Pressure dependence of the spin dynamics around a quantum critical point: an inelastic neutron scattering study of Ce_{0.87}La_{0.13}Ru₂Si₂. Preprint cond-mat/0102427 at (http://xxx.lanl.gov) (2001).
- 38. Sachdey, S. Theory of finite-temperature crossovers near quantum critical points close to, or above, their upper-critical dimensions. Phys. Rev. B 55, 142-163 (1997).
- 39. Varma, C. M., Littlewood, P. B., Schmitt-Rink, S., Abrahams, E. & Ruckenstein, A. E. Phenomenology of the normal state of Cu-O high temperature superconductors. Phys. Rev. Lett. 63, 1996-1999 (1989).
- 40. Wilson, K. G. & Kogut, J. The renormalization group and the ϵ expansion. Phys. Rep. C 12, 75–200 (1974).

Acknowledgements

We thank G. Aeppli, A. Chubukov, P. Coleman, A. J. Millis, A. Schröder, A. M. Sengupta, C. M. Varma and P. Wölfle for discussions. This work was supported by the NSF, TCSUH and the A. P. Sloan Foundation.

Correspondence and requests for materials should be addressed to Q.S. (e-mail: qmsi@rice.edu).