Quantum Criticality in Heavy Fermions: New Physics Near $T = 0$

Kevin Ingersent (U. of Florida)

Principal collaborators: Qimao Si & Matt Glossop (Rice U.)

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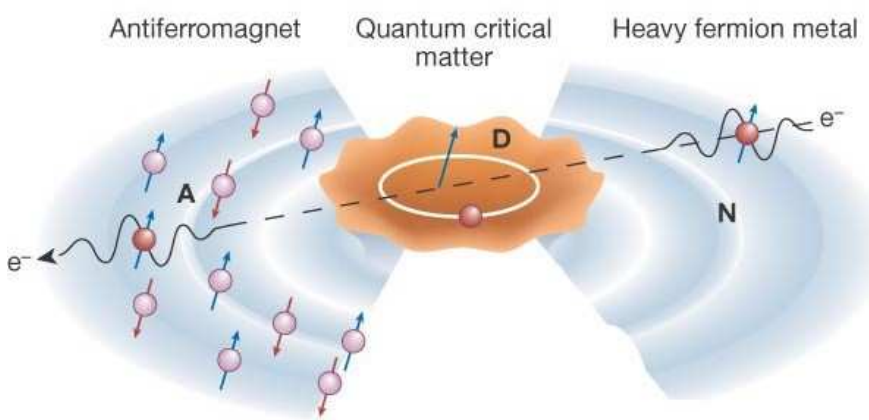
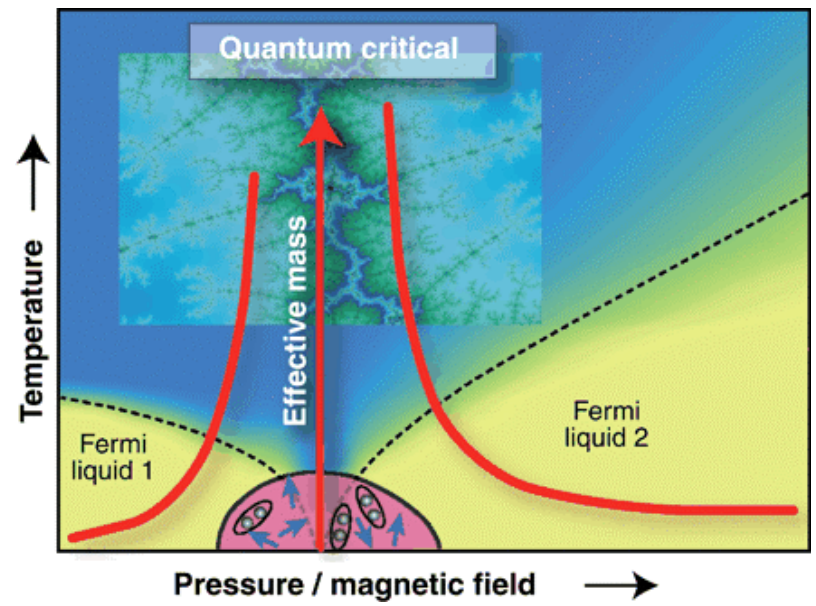


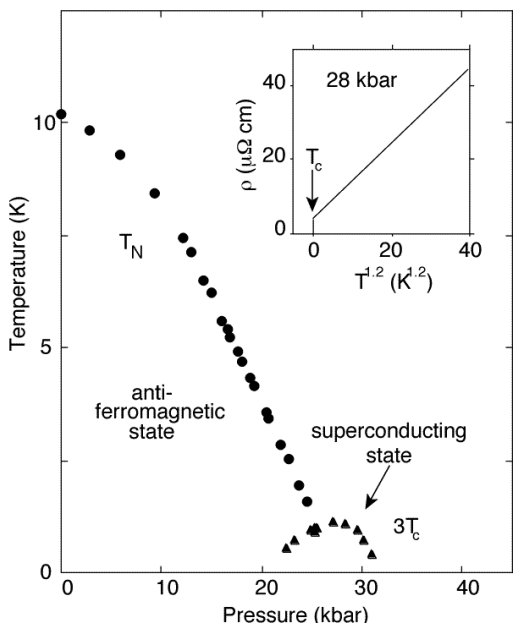
Coleman and Schofield, Nature (2005)



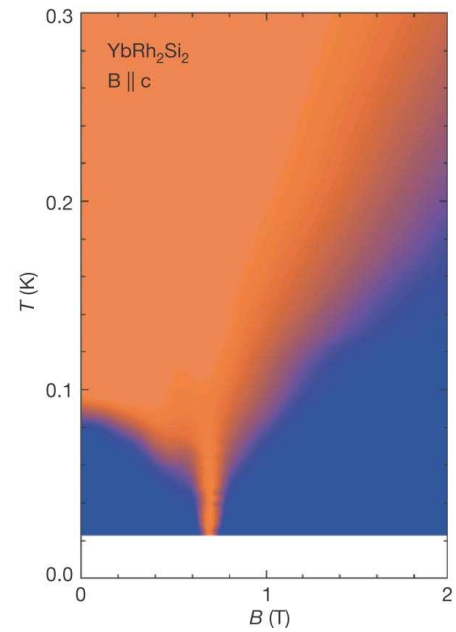
Zaanen, Science (2008)

Outline

1. Low-temperature metals: Fermi liquids vs non-Fermi liquids
2. Phase transitions: classical ($T > 0$) vs quantum ($T = 0$)
3. Heavy-fermion QPTs: The conventional picture
4. Heavy-fermion QPTs: Experimental puzzles and new ideas



$CePd_2Si_2$ (Mathur et al., 1998)



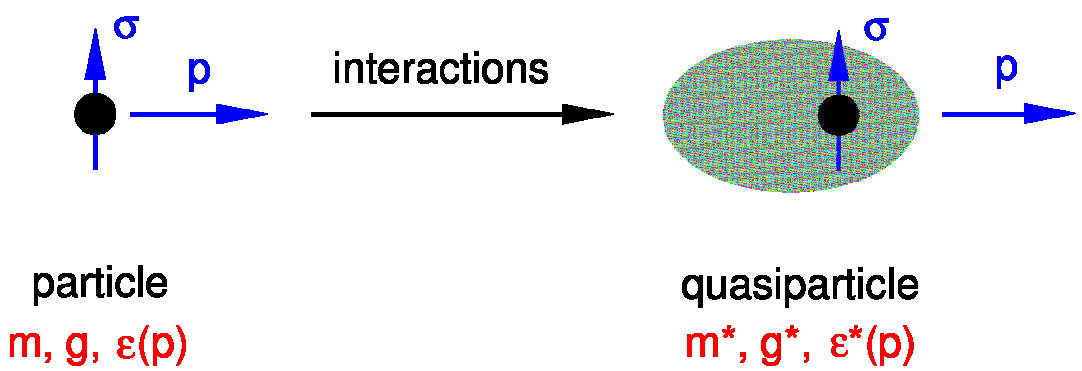
$YbRh_2Si_2$ (Custers et al., 2003)

1. Fermi Liquids and Non-Fermi Liquids

Fermi-Liquid Theory

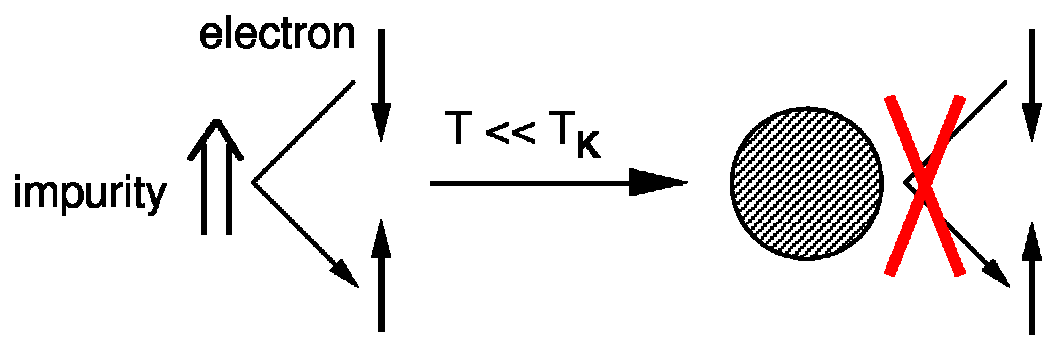
Key assumptions (Landau, 1956):

- Start with noninteracting fermions labeled by (p, σ).
- Adiabatically turn on (possibly strong) interactions.
- Particles close to ε_F evolve into long-lived quasiparticles.
- Quasiparticles are fermions, also labeled by (p, σ), but with renormalized parameters (mass, g-factor, energy, …)



Heavy-Fermion Systems

- Metals containing 4f or 5f local moments.
- Local moments induce strong correlations between conduction electrons—a lattice version of the Kondo effect:



- For $T \ll T_K$, find Fermi-liquid behavior.
- Example: $CeAl_3$ (Andres et al., 1975)
  - Remains a normal metal down to 10 mK.
  - $\gamma = \lim_{T\to 0} C/T \approx$ 1600 mJ/(mol Ce K^2) [γ(Cu,Ag,Au) ~ 0.7].
  - For $T <$ 0.1K, $\rho = \rho_0 + AT^2$.

Non-Fermi Liquids

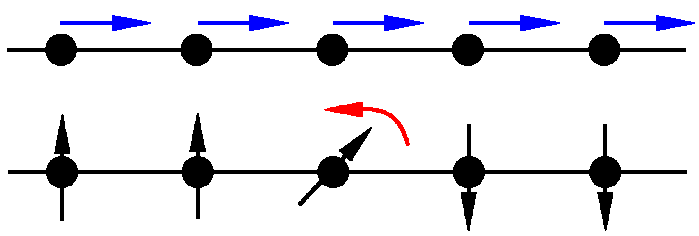
- The Fermi liquid was long thought to be the generic low-temp. state of metals (barring the opening of a gap at ε_F).
- However, several classes of materials exhibit gapless charge excitations but properties inconsistent with a Fermi liquid.
- These materials realize fundamental new states of electronic matter.

1D fermion systems

- The quasiparticle concept is untenable in 1D.
- Low-energy excitations are bosonic density waves:

charge wave

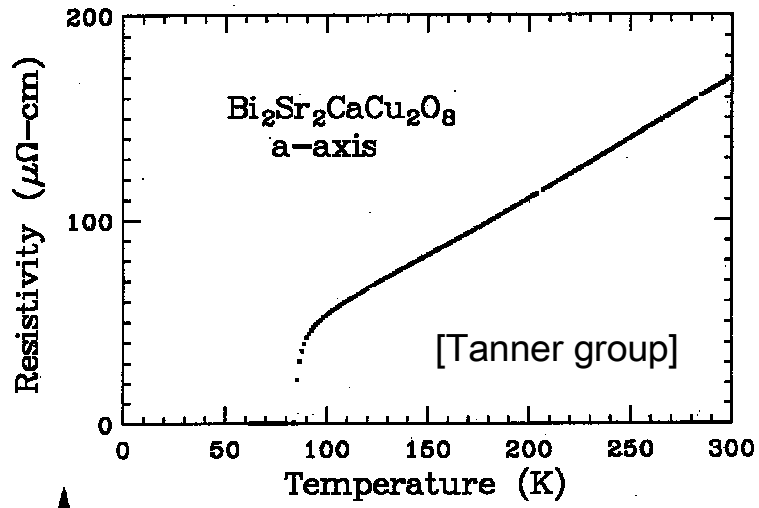
spin wave



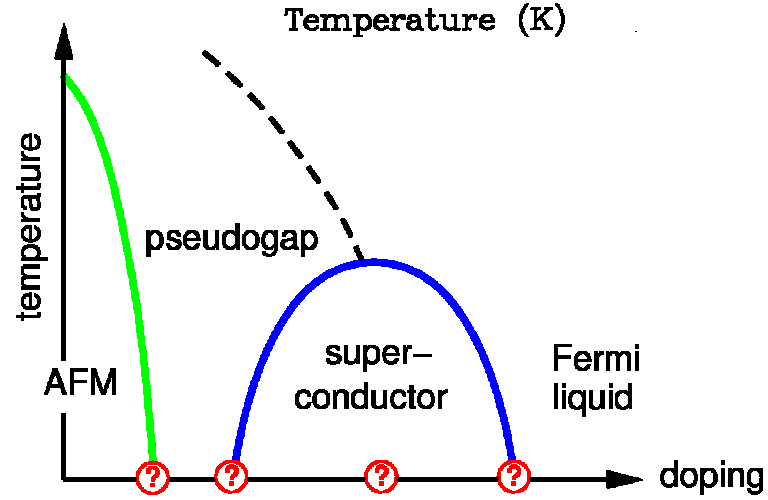
Non-Fermi Liquids (cont.)

Normal state of cuprate superconductors

- NFL signatures include a linear-in-T resistivity:



- The source of NFL behavior is still under debate:
  - Two-dimensionality (or even quasi-one-dimensionality)?
  - Proximity to a quantum phase transition? If so, which QPT?



Non-Fermi Liquids (cont.)

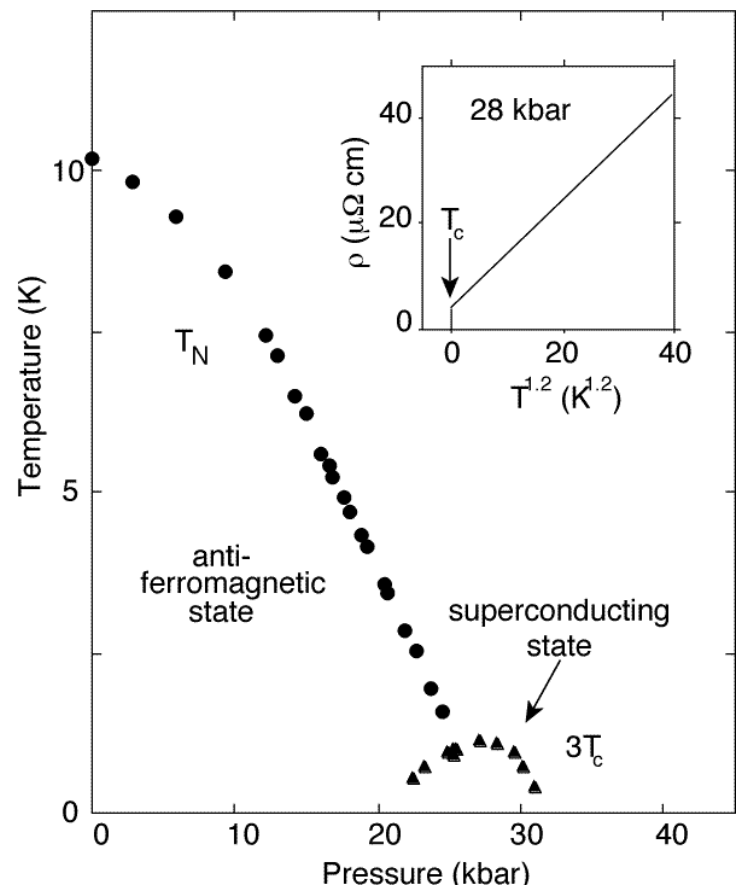
Heavy non-Fermi liquids

- A rich zoology of f-electron NFLs has emerged since 1991.
- For a review, see G. R.Stewart, Rev. Mod. Phys (2001, 2006).
- Typical properties:
  - specific heat $C/T \propto \log(T_0/T)$ c.f. Fermi liquid: $C/T = \gamma \propto m^*$.
  - resistivity $\rho(T) - \rho(0) \propto AT^{\alpha}, \quad 1 \le \alpha \le 1.5.$
- May arise from different sources in different materials:
  - Disorder: broad distribution of energy scales, or fluctuations of rare regions (Griffiths phases).
  - Local frustration (e.g., two-channel Kondo effect).
  - Proximity to a quantum phase transition.

Heavy-Fermion Quantum Phase Transitions

- Antiferromagnetic QPT likely in
  - $CeIn_3$
  - $CePd_2Si_2$
  - $CeCu_2R_2$, R = Si, Ge
  - $CeCu_{6-x}M_x$, M = Au, Ag, Pd, Pt
  - $YbRu_2Si_2$
- Ferromagnetic QPT likely in
  - UGe_2
  - $ZrZn_2$
  - $Sr_3Ru_2O_7$
  - MnSi

$CePd_2Si_2$ (Mathur et al., 1998)



2. Quantum Phase Transitions

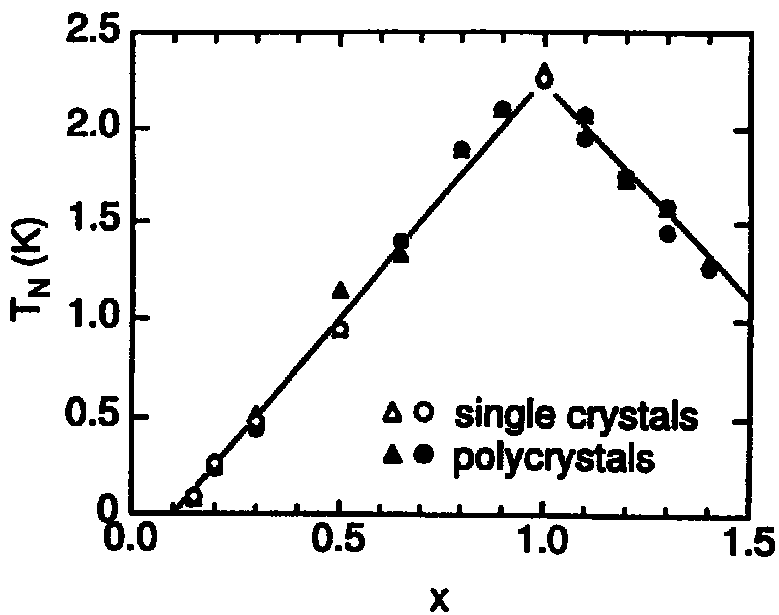
- A QPT separates quantum-mechanical ground states (A and B) distinguished by an order parameter ϕ such that $\phi_A \neq 0, \phi_B = 0$.
- The QPT is accessed via a nonthermal control parameter g.

  We will focus on continuous QPTs, where $\Delta\phi = 0$ at $g = g_c$.
- Examples:

  heavy fermions

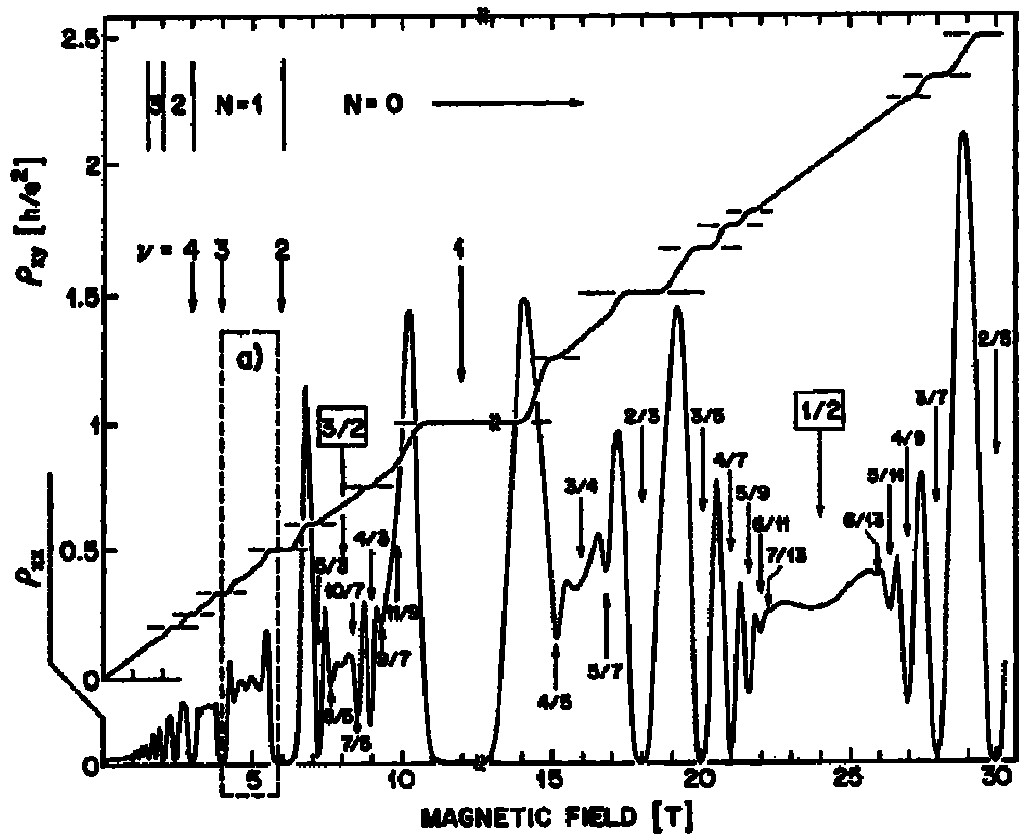
$CeCu_{6-x}Au_x$

(von Löhneysen, 1996)



Quantum Phase Transitions (cont.)

fractional quantum
Hall effect



(Tsui et al., 1990)

Note: Experiments were performed at finite T!

Classical ($T > 0$) vs Quantum ($T = 0$) Phase Transitions

- A classical phase transition between phases A and B occurs at the temperature T_c at which $F_A = F_B$ or $E_A - T_c S_A = E_B - T_c S_B$.

  The free energy F comes from a trace over configuration space:

$$Z_{CM} = \exp(-\beta F) = \mathrm{Tr}\,\exp(-\beta \mathrm{H}), \quad \beta = 1/\mathrm{k_B} T.$$

  $\Rightarrow$ Don't need to know the dynamics (equations of motion).

- The quantum-mechanical free energy is a trace over a basis:

$$Z_{QM} = \exp(-\beta F) = \sum_n \langle n | \exp(-\beta H) | n \rangle, \quad \beta = 1/k_B T.$$

  Since $\exp(-iHt/\hbar)$ is the quantum-mechanical propagator,

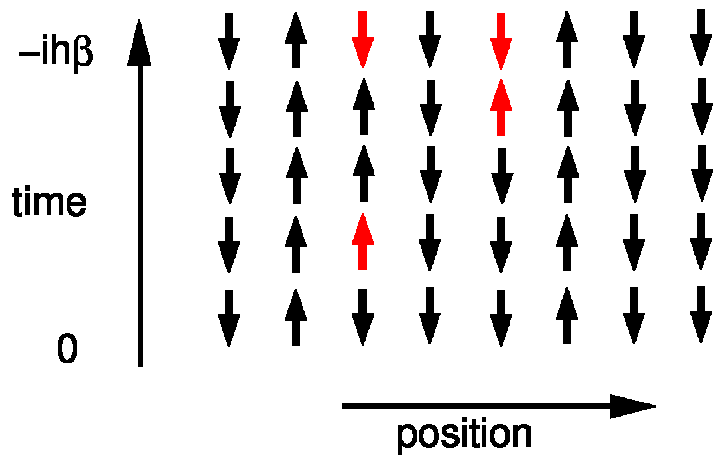
  $\Rightarrow \exp(-\beta H)$ propagates the system in imaginary time;

  $\Rightarrow Z_{QM}$ is the sum over all transition amplitudes for the system to return to its initial state after an imaginary time $\tau = -i\hbar\beta$.

"Statics and dynamics are inextricably connected" (J. Hertz, 1976).

Quantum to Classical Mapping

- Z_{QM} in d dimensions $\sim Z_{CM}$ for a system in $D = d + 1$ dimensions, with finite extent $L_\tau = \hbar / k_B T$ along the imaginary-time direction.



- As $T \to 0, \quad L_\tau \to \infty$.
- The mapping of a ***d***-dimensional quantum system to a **(*d*+1)**-dimensional classical system becomes rigorous in the limit of long length scales, where can use a continuum (field theory) description.
- The control parameter g controls the strength of fluctuation—plays the role of temperature in the effective classical model.

Role of Dimensionality: Classical Transitions

- Spatial fluctuations $\phi(\mathbf{r}) \to \phi + \delta\phi(\mathbf{r})$

  become less important with increasing D.
- The upper critical dimension D_u plays a key role.
- For $D > D_u$,
  - fluctuations $\delta\phi$ are relatively unimportant;
  - they can be taken to be independent (Gaussian) as $T \to T_c$.
  - mean-field theory ($\delta\phi = 0$) gives the correct exponents.
- For $D < D_u$,
  - interactions between fluctuations grow as $T \to T_c$.
  - need numerics or more sophisticated theory (e.g., RG).
  - exponents can take anomalous (non-mean-field) values.

Role of Dimensionality: Quantum Transitions

- At a continuous QPT, the spatial and temporal correlation lengths diverge, but not necessarily at the same rate:

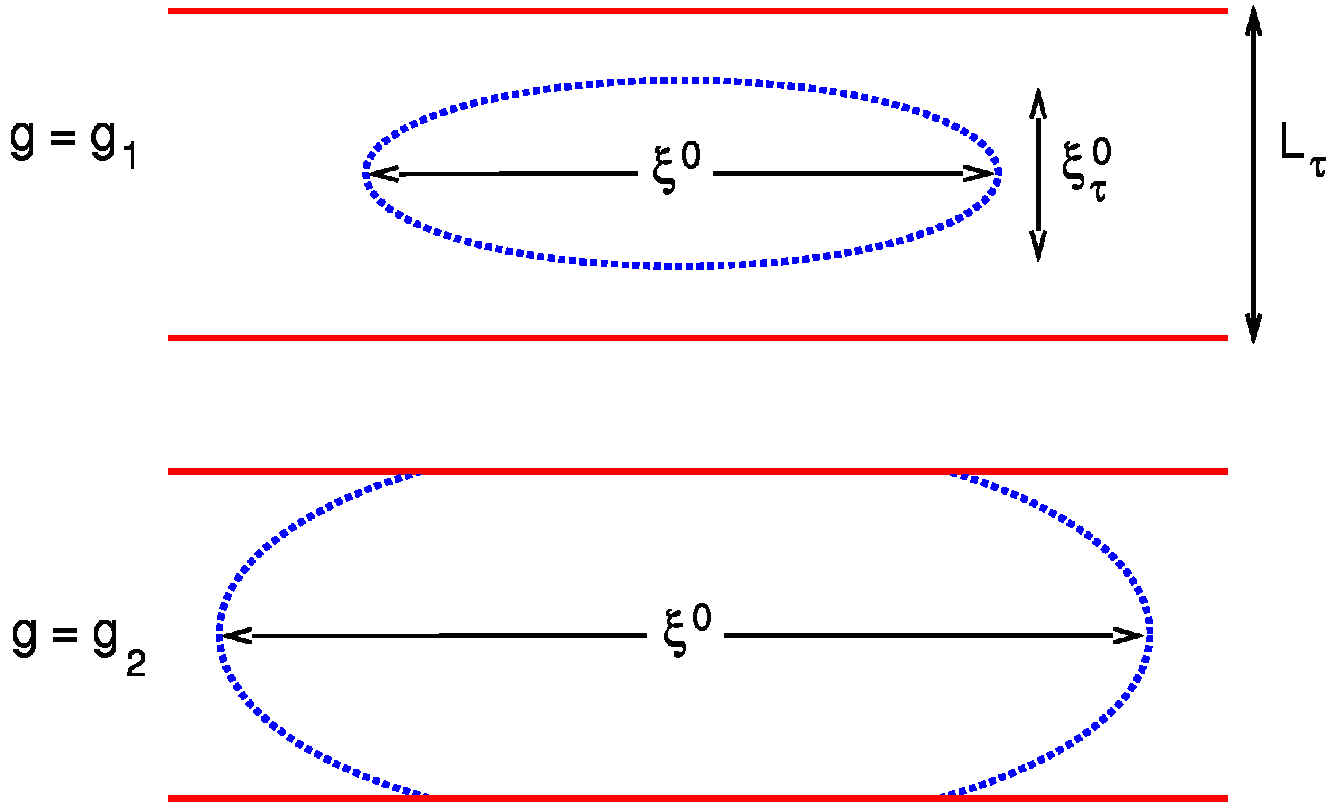
$$\xi^0 \sim |g - g_c|^{-\nu}, \qquad \xi_\tau^0 \sim |g - g_c|^{-z\nu}$$

  where z is the dynamical exponent.

- If $z = 1$ (e.g., the Ising ferromagnet)
  - the effective $(d+1)$-dimensional classical model is isotropic;
  - the quantum and classical critical points belong to the same universality class;
  - the upper critical dimension for the quantum model is $d_u = D_u - 1.$
- If $z > 1$ (e.g., $z = 2$ for heavy-fermion antiferromagnets)
  - the effective classical model is anisotropic;
  - the critical exponents differ from those for the isotropic case;
  - the upper critical dimension for the quantum model is $d_u = D_u - z.$

Finite-Temperature Manifestations of a QPT

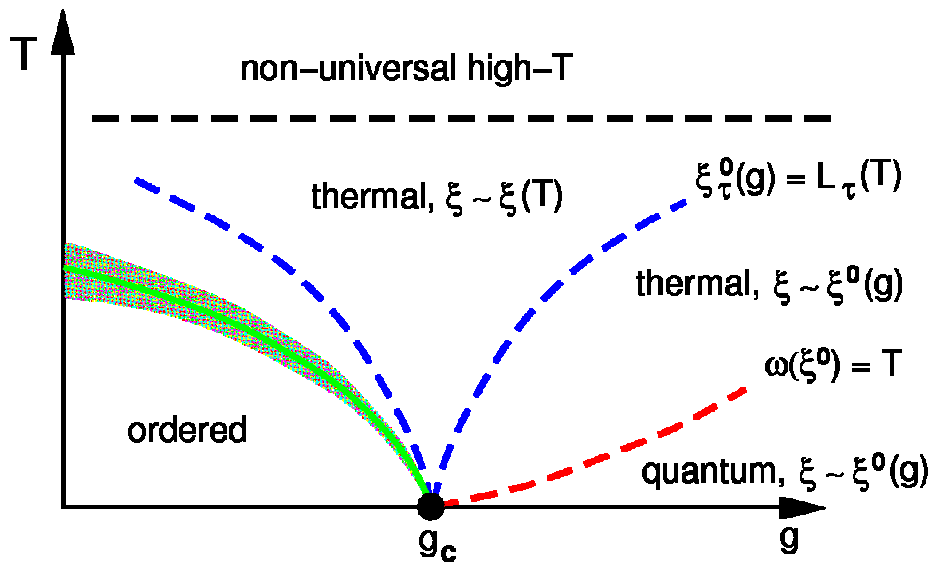
- At $T > 0$, the finite $L_\tau = \hbar / k_B T$ cuts off the divergence of ξ_τ^0:



- This may kill the phase transition (low d) or convert it to a CPT.

Finite-Temperature Manifestations of a QPT (cont.)

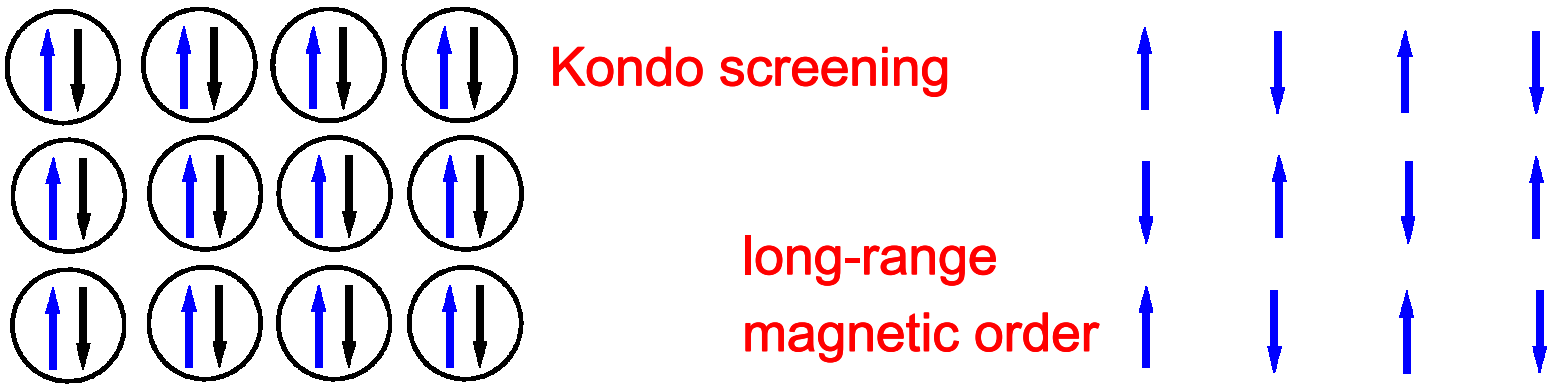
- Physical properties cross over as functions of L_τ / ξ_τ^0 and $T / \omega(\xi^0)$ from quantum to thermal behavior, e.g., for $d > \max(2, 4 - z)$,



- The thermal ("quantum critical") regimes at $T > 0$ provide a signature of the QPT located at $T = 0$.
- For more on QPTs, see: S. L. Sondhi, Rev. Mod. Phys. (1997); S. Sachdev, *Quantum Phase Transitions* (Cambridge, 1999).

3. Heavy-Fermion QPTs: The Conventional Picture

- Metals containing 4f or 5f moments exhibit conflicting tendencies:



- The competition is captured by the Kondo lattice model

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J \sum_{i} c^{\dagger}_{i\sigma} \tfrac{1}{2} \boldsymbol{\tau}_{\sigma\sigma'} c_{i\sigma'} \cdot \mathbf{S}_i + \tfrac{1}{2} \sum_{i,j} I_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

- In the paramagnetic phase, the Kondo effect wins.

  Residual interactions among quasiparticles can lead to …

  - Cooper instability (e.g., $CeCu_2Si_2$, UPt_3, UBe_{13}, $CeCoIn_5$).
  - spin-density-wave (SDW) instability (examples will follow).

SDW Theory for Antiferromagnetic QPTs

- The QPT corresponds to an SDW instability of the Fermi liquid.
- The effective Landau-Ginzburg-Wilson functional involves only the magnetic order parameter (integrate out fermions):

$$\Phi[\Psi] = \tfrac{1}{2} \sum_{\mathbf{q}, i\omega_n} \left[\delta(g) + |\mathbf{q} - \mathbf{Q}|^2 + |\omega_n| \tau \right] \left| \Psi(\mathbf{q}, i\omega_n) \right|^2 + \tfrac{1}{4} u \Psi \Psi \Psi \Psi$$

- The particle-hole continuum strongly damps the modes around the ordering wave vector $\mathbf{q} = \mathbf{Q}$. The dynamical exponent is $z = 2$.
- Since $D_u = 4$ for the effective classical theory, $d_u = 4 - z = 2.$

  $\Rightarrow$ For $d = 2$ [$d = 3$], system is at [above] its upper critical dimension.
- Renormalization-group analysis (Moriya, 1973; Hertz, 1976, Millis, 1993) gives as quantum critical behaviors at $g = g_c$

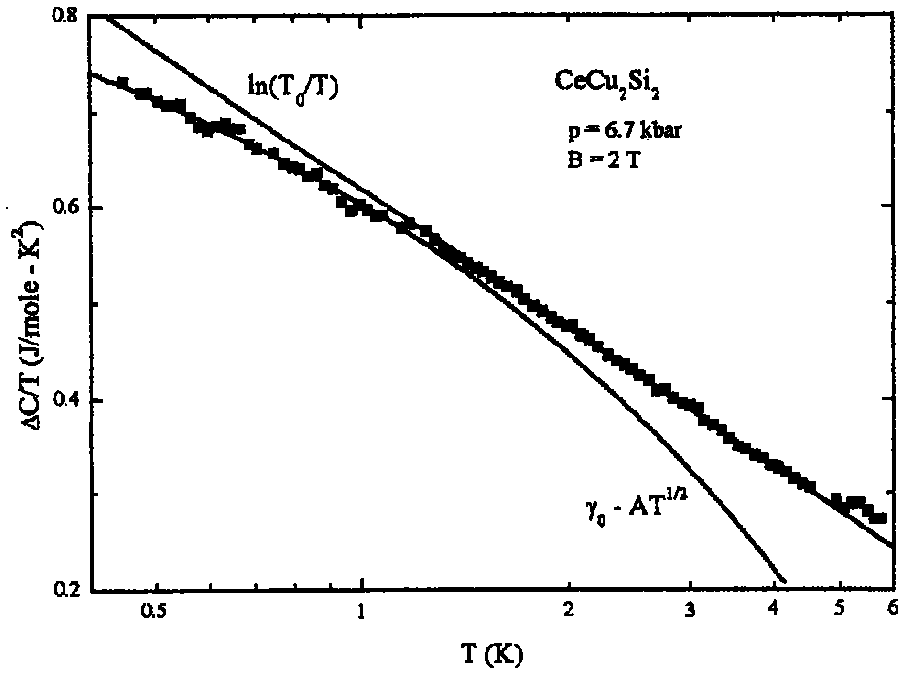
$$d = 2: \qquad \Delta C / T \sim \ln(T_0 / T), \qquad \Delta\rho \sim T.$$

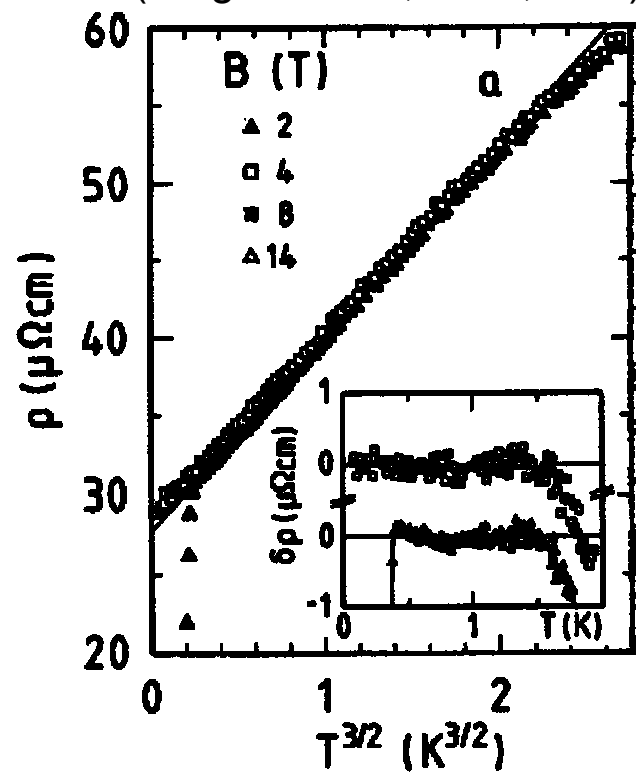
$$d = 3: \qquad \Delta C / T \sim \gamma - a\sqrt{T}, \qquad \Delta\rho \sim T^{3/2}.$$

SDW Antiferromagnetic QPTs: Candidate Materials

- $CeCu_2Si_2$:

(Steglich et al., 1996,1998)



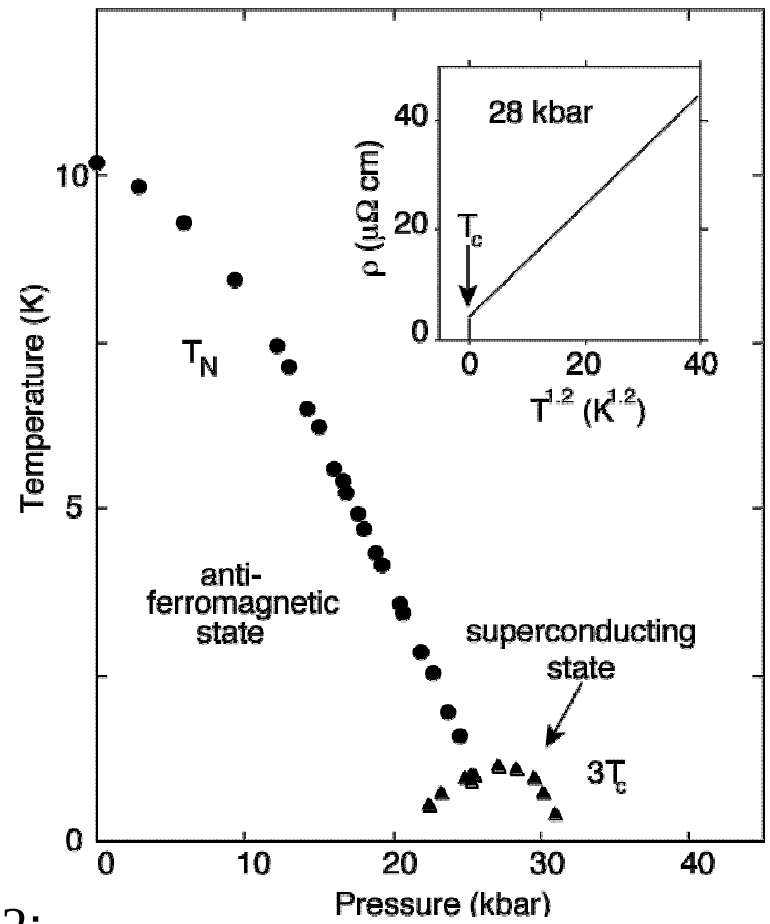


- Fits the SDW theory for $d = 3$: $\Delta C/T \sim \gamma - a\sqrt{T}, \quad \Delta\rho \sim T^{3/2}$.
- Same $\rho(T)$ is seen in $CeIn_3$.

SDW Antiferromagnetic QPTs: Candidate Materials

- $CePd_2Si_2$:

  - At $p = p_c, \quad \Delta\rho \sim T^{1.2}$.



(Mathur et al., 1998)

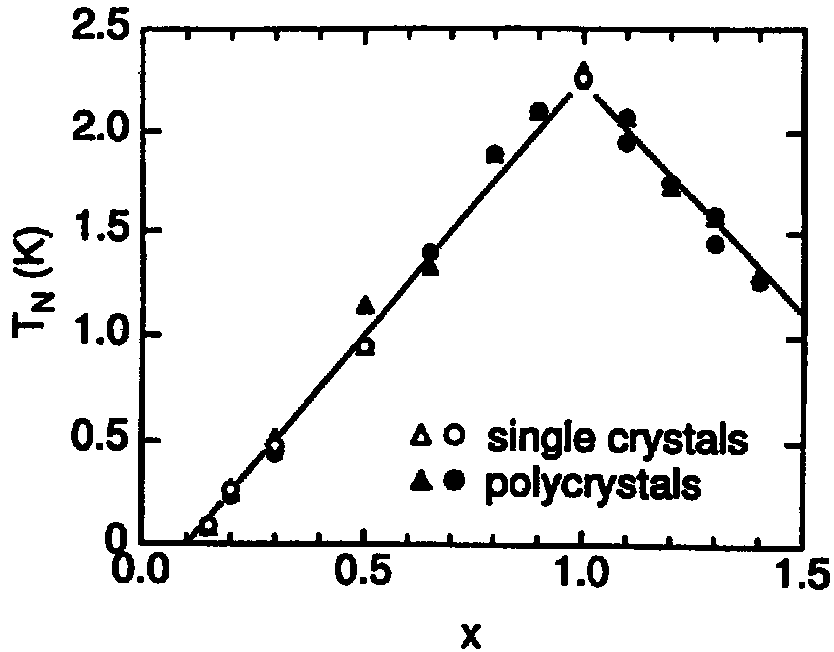
  - Close to the SDW theory for $d = 2$:

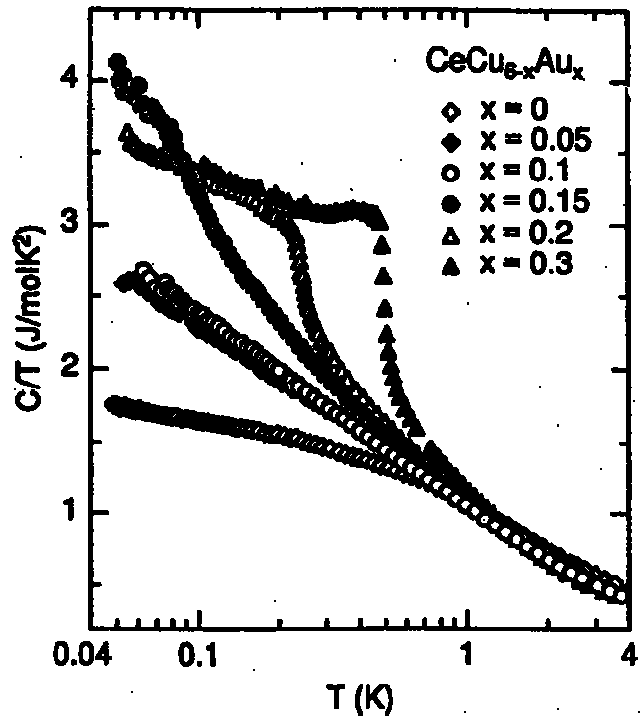
$$\Delta C / T \sim \ln(T_0 / T), \quad \Delta\rho \sim T.$$

4. Heavy-Fermion QPTs: Experimental Puzzles & New Ideas

The Curious Case of $CeCu_{6-x}Au_x$

- Neel temperature vanishes at $x_c \approx 0.1$.





(von Löhneysen, 1996)

- At $x = x_c$, $C/T \sim \log(T_0/T)$.

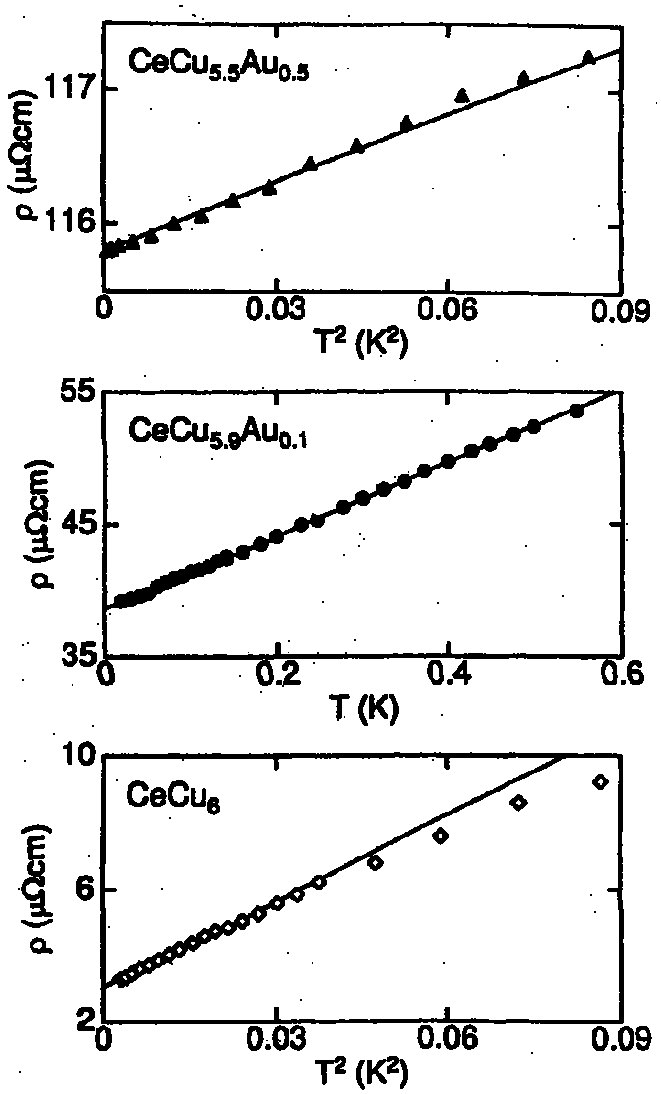
$CeCu_{6-x}Au_x$ (cont.)

- Also at $x = x_c$,

$$\rho(T) \approx \rho(0) + AT.$$

- For $x < x_c$ and $x > x_c$, recover the Fermi-liquid form

$$\rho(T) \approx \rho(0) + AT^2.$$



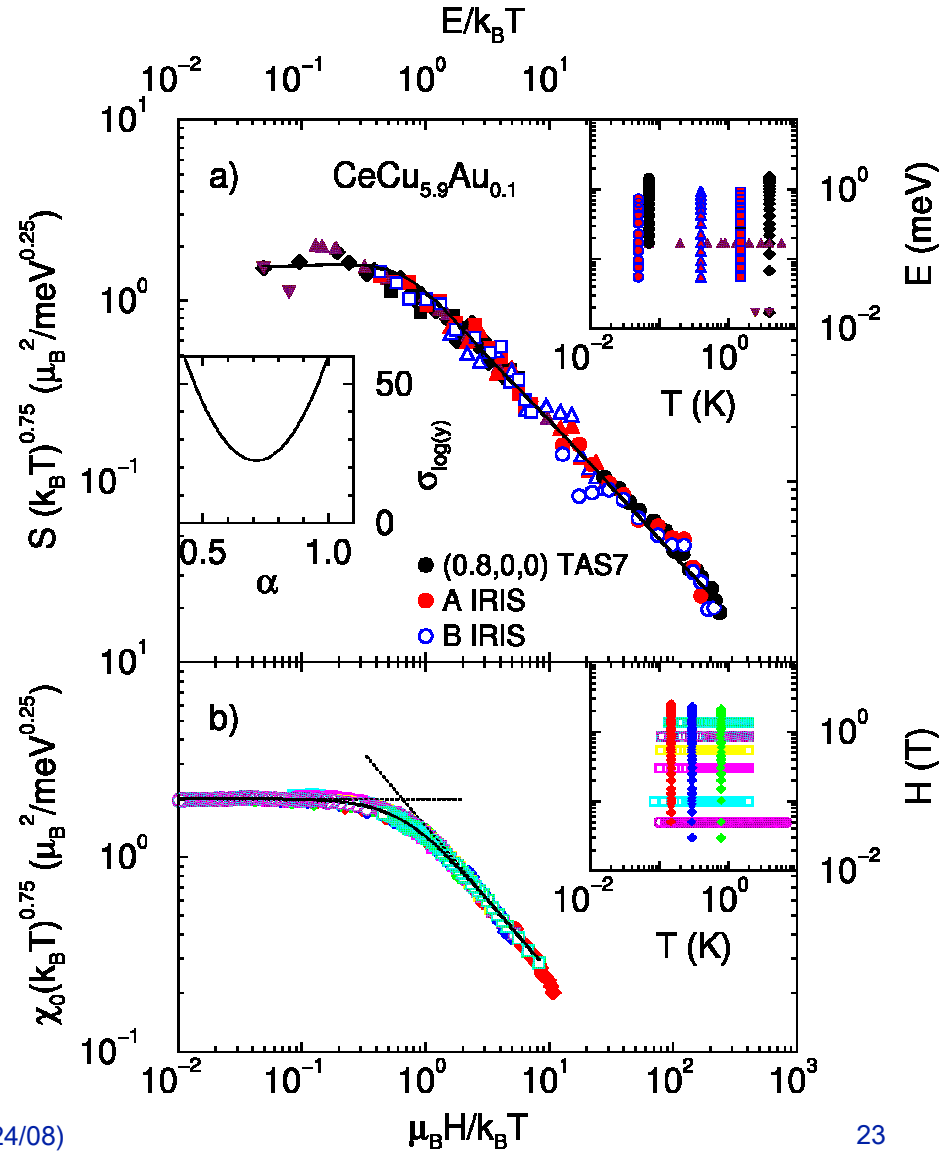
(von Löhneysen, 1996)

$CeCu_{6-x}Au_x$ (cont.)

- Neutron-scattering and magnetization data can be collapsed onto the form

$$\chi = \frac{C}{f(\mathbf{q}) + \left(\sqrt{T^2 + H^2} - ia\omega\right)^{\alpha}},$$

where $\alpha = 0.75 \pm 0.05$.



(Schröder et al., 2001)

The Puzzle of $CeCu_{6-x}Au_x$

- The form $C\chi^{-1} = f(\mathbf{q}) + \left(\sqrt{T^2 + H^2} - ia\omega\right)^{\alpha}, \quad \alpha = 0.75 \pm 0.05$

  is fundamentally incompatible with the standard SDW theory, which should be at or above its upper critical dimension:
  - The ω dependence exhibits a critical exponent $\alpha < 1$:
    - For $d \geq d_u$, expect $\alpha = 1$.
    - Expect anomalous exponents only for $d < d_u$.
  - ω and T enter with the same exponent α:
    - For $d \geq d_u$, expect $\omega \sim T^{d/z}$.
    - Expect "ω/T" scaling only for $d \leq d_u$.
- Suspicion falls on the validity of integrating out the fermions from

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J \sum_i c^{\dagger}_{i\sigma} \tfrac{1}{2} \boldsymbol{\tau}_{\sigma\sigma'} c_{i\sigma'} \cdot \mathbf{S}_i + \tfrac{1}{2} \sum_{i,j} I_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

  to get

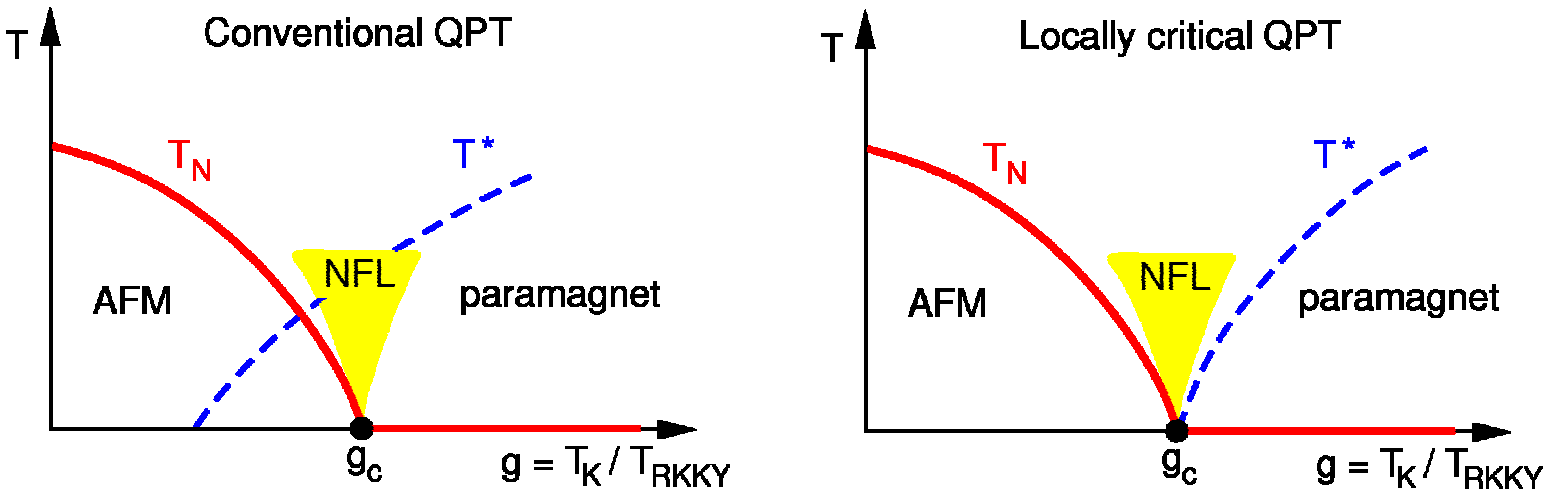
$$\Phi[\Psi] = \tfrac{1}{2} \sum_{\mathbf{q}, i\omega_n} \left[\delta(g) + |\mathbf{q} - \mathbf{Q}|^2 + |\omega_n| \tau\right] \left|\Psi(\mathbf{q}, i\omega_n)\right|^2 + \tfrac{1}{4} u \Psi\Psi\Psi\Psi$$

  (e.g., Abanov and Chubukov, 2004).

Proposals to Explain the $CeCu_{6-x}Au_x$ Puzzle

- Reduced dimensionality ($d = 2$) (Rosch et al.)
  - Spin fluctuations in $CeCu_{6-x}Au_x$ are quasi-two-dimensional.
  - Can account for ω/T scaling but not for $\alpha < 1$.
- Breakdown of quasiparticles at the QPT (Coleman; Si and K.I.)
  - Builds on fact that the local susceptibility $\chi_{\mathrm{loc}}(\omega) = \sum_{\mathbf{q}\neq\mathbf{Q}} \chi(\mathbf{q},\omega)$ diverges with the same exponent α.
  - Suggests that local moments are becoming unscreened as approach the QPT from the paramagnetic side—bicriticality.
  - May involve novel phase transitions and/or supersymmetry.
- Fractionalization (Senthil et al., Pépin et al.)
  - Quasiparticles break into spinons and gauge excitations.
  - Magnetism is incidental to the destruction of the quasiparticles.
  - Appears not to fit experiments in $CeCu_{6-x}Au_x$.

One Scenario: "Local Criticality"



- Fermi-liquid temperature T^* vanishes just at the SDW instability
  $\Rightarrow$ local moments reappear, and $\chi_{\rm loc}$ diverges.
- Critical local fluctuations couple to extended critical modes
  $\Rightarrow$ the critical point is interacting, can have anomalous exponents.
- This would constitute a new type of phase transition.

Microscopic Approach: EDMFT

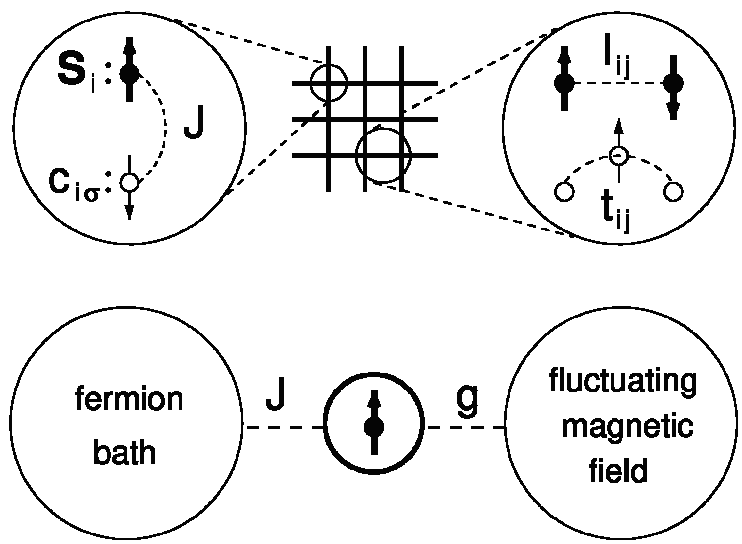
- Extended dynamical mean-field theory includes some spatial fluctuations [Si and Smith (1996), Chitra & Kotliar (2000)].
- Maps the Kondo lattice model

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J \sum_{i} c^{\dagger}_{i\sigma} \tfrac{1}{2} \boldsymbol{\tau}_{\sigma\sigma'} c_{i\sigma'} \cdot \mathbf{S}_i + \tfrac{1}{2} \sum_{i,j} I_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

to a Bose-Fermi Kondo impurity model:

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J\, c^{\dagger}_{0\sigma} \tfrac{1}{2} \boldsymbol{\tau}_{\sigma\sigma'} c_{0\sigma'} \cdot \mathbf{S} + \sum_{q} \omega_q \phi^{\dagger}_q \cdot \phi_q + g\left(\phi_0 + \phi^{\dagger}_0\right) \cdot \mathbf{S}$$

  - Fermionic band accounts for local dynamical correlations.
  - Dissipative baths represent a fluctuating magnetic field due to other local moments.
  - Band and bath densities of states must be found self-consistently.



EDMFT for the Ising-Anisotropic Kondo Model

- For easy-axis systems, use the Ising-anisotropic BFK model:

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J\, c^{\dagger}_{0\sigma} \tfrac{1}{2} \boldsymbol{\tau}_{\sigma\sigma'} c_{0\sigma'} \cdot \mathbf{S} + \sum_{q} \omega_q \phi^{\dagger}_q \phi_q + g\left(\phi_0 + \phi^{\dagger}_0\right) S^z + h_{\mathrm{loc}} S^z$$

- In EDMFT, the self-energies entering the lattice functions

$$G(\mathbf{k},\omega) = \left[\omega - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)\right]^{-1}$$

$$\chi(\mathbf{q},\omega) = \left[M(\mathbf{q},\omega) + I_{\mathbf{q}}\right]^{-1}$$

where the "RKKY density of states,"

$$\rho_I(\varepsilon) = \sum_{\mathbf{q}} \delta\left(\varepsilon - I_{\mathbf{q}}\right),$$

are approximated by $\Sigma(\omega)$ and $M(\omega)$ for the impurity problem.

- Self consistency requires

$$\chi_{\mathrm{loc}}(\omega) \equiv \sum_{\mathbf{q}} \chi(\mathbf{q},\omega) = \int d\varepsilon \frac{\rho_I(\varepsilon)}{M(\omega) + \varepsilon}.$$

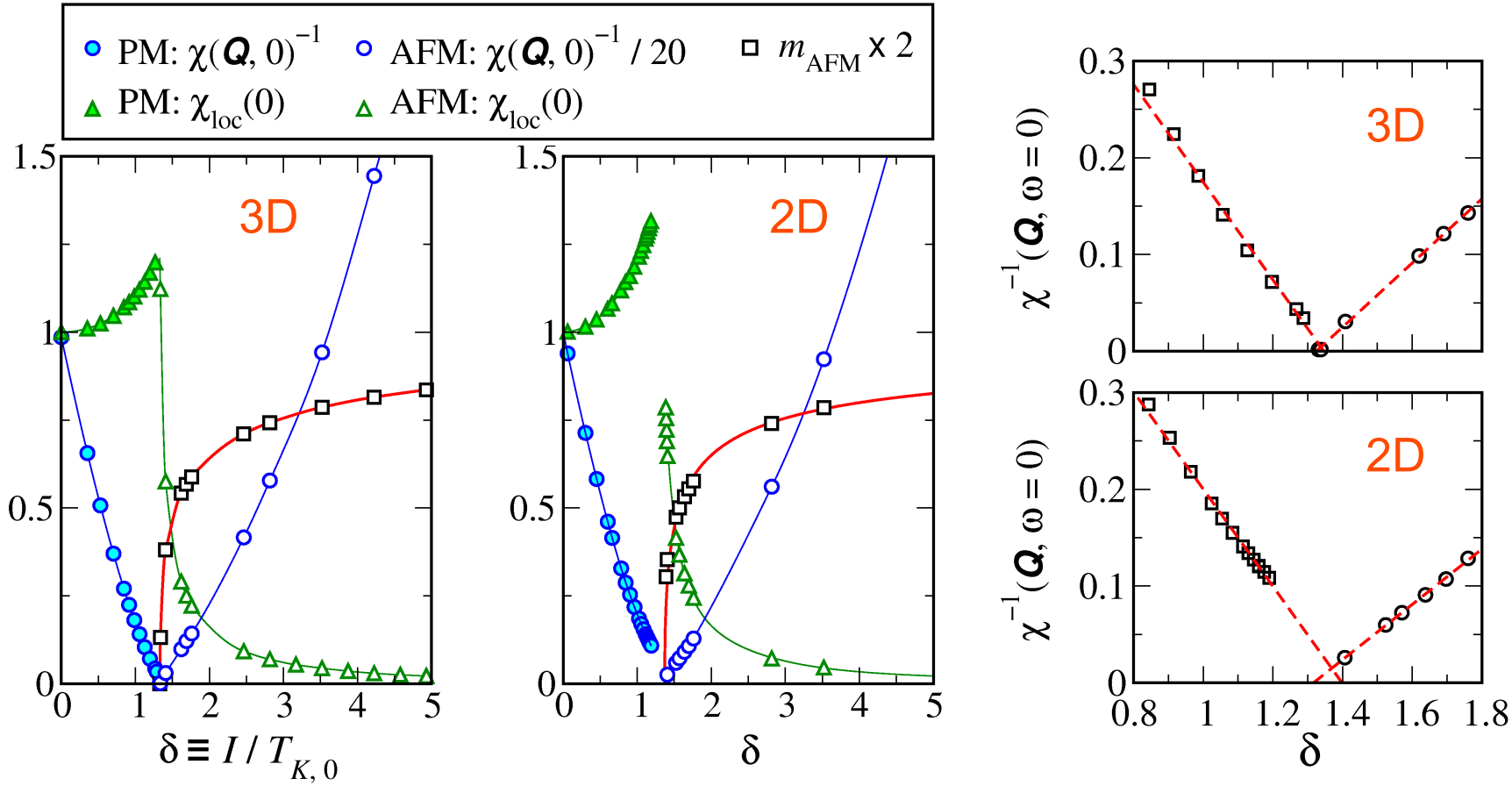
The form of $\rho_I(\varepsilon)$ near $\varepsilon = I_{\mathbf{Q}}$ turns out to be crucial.

What is the Nature of the QPT in EDMFT?

- EDMFT equations have been solved using various impurity solvers.
- ϵ-expansion finds two types of QPT (Si et al., 2001, 2003):
  - conventional spin-density-wave type for 3D spin fluctuations;
  - locally critical QPT for 2D spin fluctuations—reproduces some features of $CeCu_{6-x}Au_x$ and $YbRh_2Si_2$, **but** corresponds to $\epsilon = 1^-$.
- Quantum Monte Carlo yields conflicting results:
  - Anderson lattice has no locally critical QPT; transition is 1st order (Sun & Kotliar, 2003).
  - Kondo lattice has 1st order transition at $T > 0$, but a locally critical QPT at $T = 0$ (Grempel & Si, 2003; Zhu et al., 2004).
- To resolve the discrepancy, we have extended Wilson's numerical RG method to get nonperturbative $T = 0$ solutions (Glossop & KI, 2007).

Self-Consistent EDMFT Solutions at $T = 0$

- At the gross level, 3D and 2D spin fluctuations yield similar results:

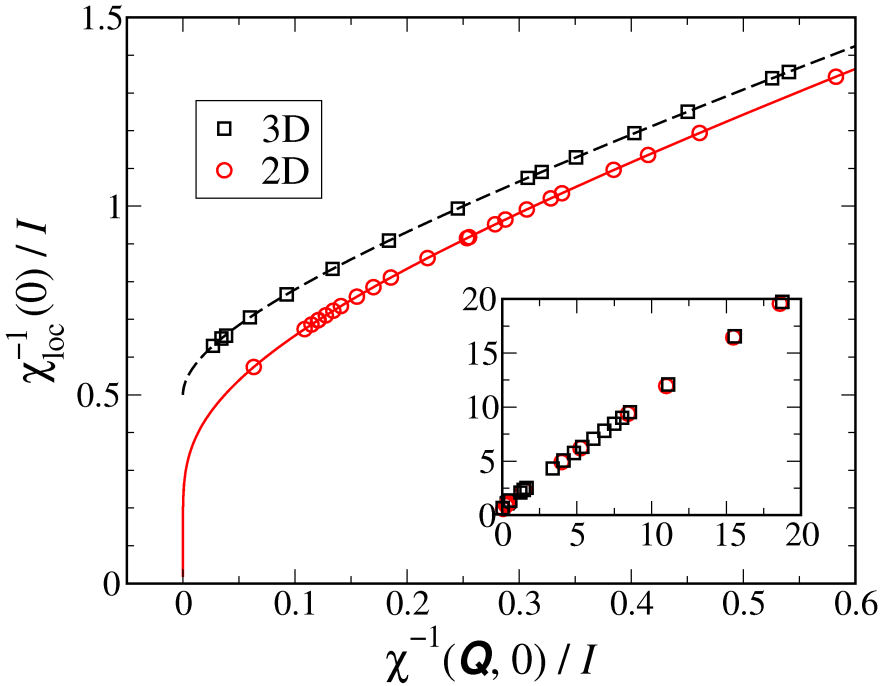


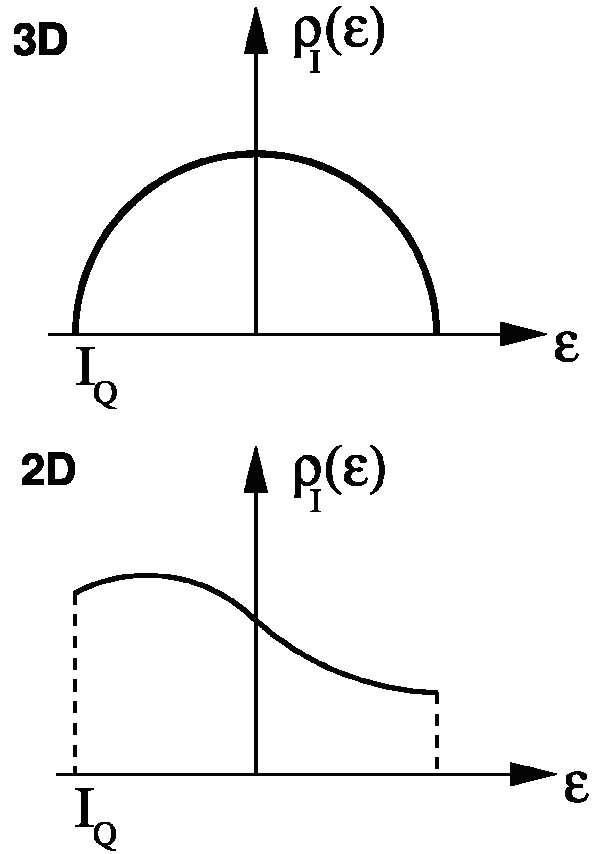
- To within numerical resolution, the QPT is continuous in both cases.

EDMFT: Static Self-Consistency

- Differences between 3D and 2D show up only very near the QPT: self-consistency requires

$$\chi_{\mathrm{loc}}(0) = \int d\varepsilon \frac{\rho_I(\varepsilon)}{\chi^{-1}(\mathbf{Q},0) - I_{\mathbf{Q}} + \varepsilon}$$





- Bosonic NRG can get closer to the QPT (Zhu et al., 2007).

EDMFT: Anomalous Exponent in the Dynamics

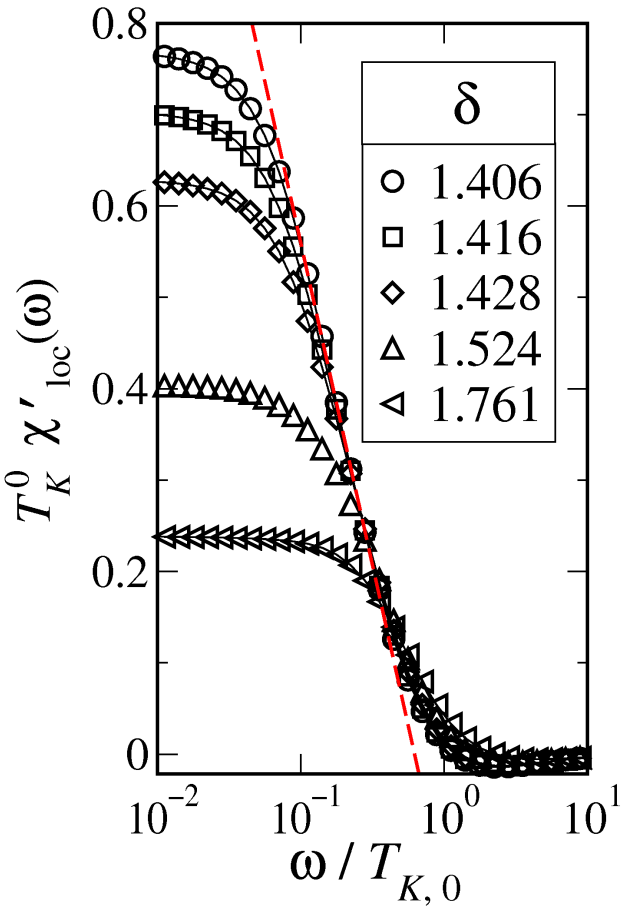
- Logarithmic divergence in $\chi'_{\mathrm{loc}}(\omega \to 0)$ implies an anomalous exponent

$$\alpha = 0.78(4)$$

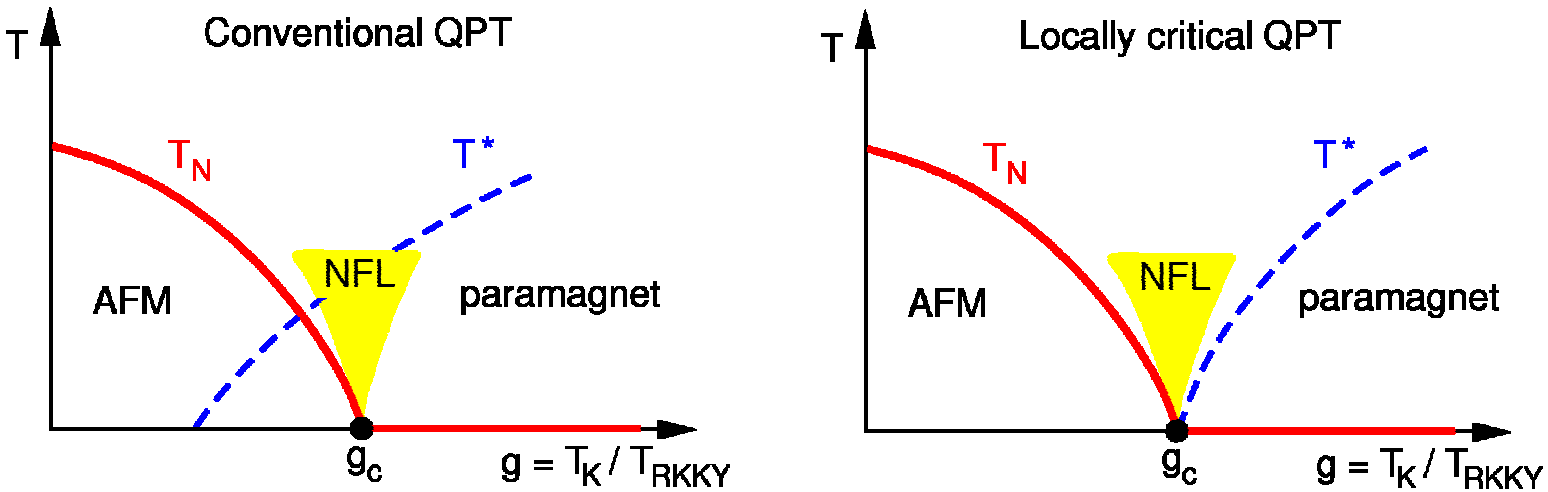
in the lattice susceptibility.

- Compares well with the experimental value in $CeCu_{6-x}Au_x$:

$$\alpha \approx 0.75.$$

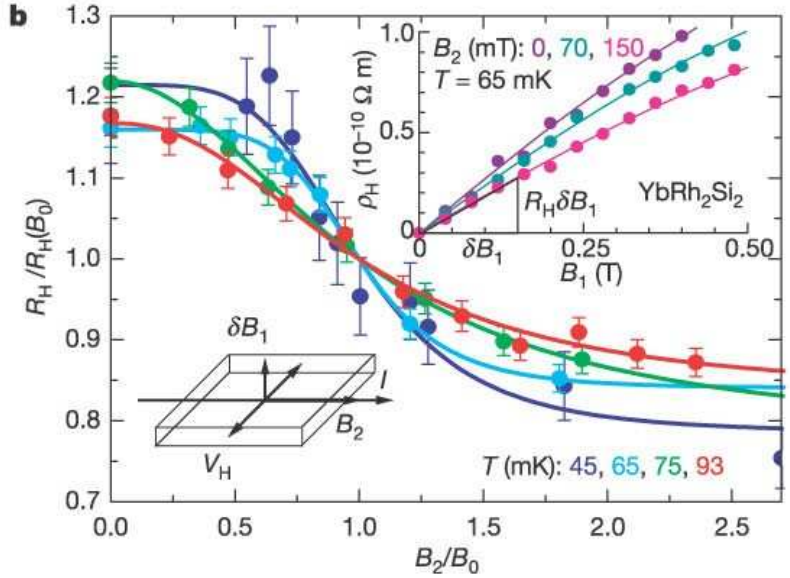


Local Criticality: Experimental Predictions



- Sensitivity to the dimensionality of the spin fluctuations.
- A jump in the Fermi-surface volume at the QPT (dHvA).
- A jump in the carrier concentration at the QPT (Hall coefficient).
- A divergence of the Gruneisen ratio β / C_p ($\beta =$ thermal exp.).
- T-independent (non-Korringa) spin-lattice relaxation (NMR, μSR).

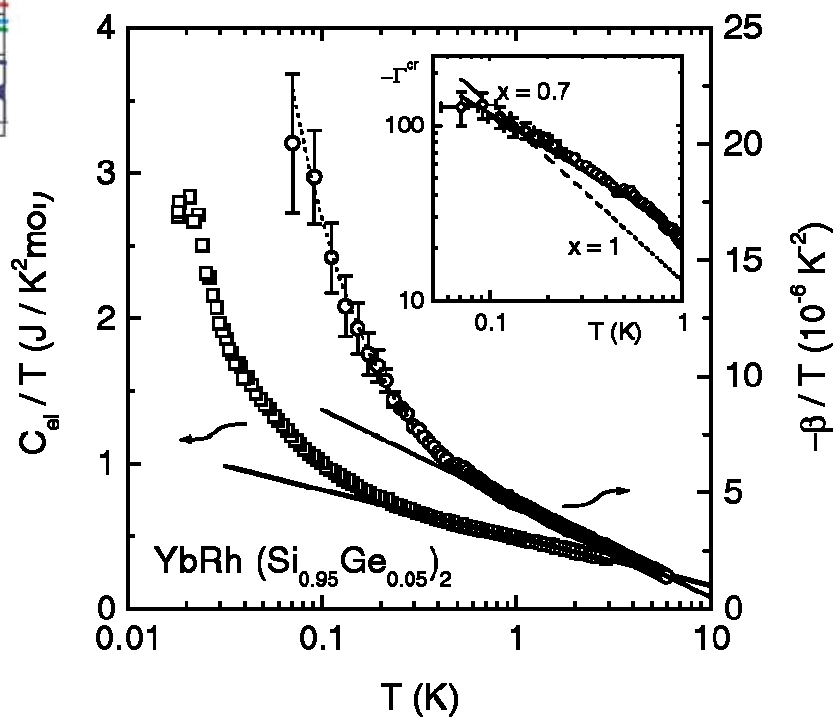
Local Criticality: Evidence from $YbRh_2Si_2$



(Paschen et al., 2004)

Does R_H jump at the QPT?

(Kuchler et al., 2003)



Gruneisen ratio diverges in a way consistent with local criticality.

Summary

- Many examples are now known of systems that deviate from the Fermi-liquid paradigm for low-temperature metals.
- Among the diverse sources of non-Fermi-liquid physics, quantum phase transitions (QPTs) form an interesting sub-class.
- Heavy-fermion systems allow systematic investigation of QPTs.
- Evidence is emerging for novel physics in certain materials.
- Possible theoretical explanations include
  - local criticality: a new universality class of phase transition;
  - supersymmetry: bosonic & fermionic spin character at the QPT;
  - fractionalization: spin-charge separation due to topological order.
- Much work remains to sort out these possibilities! There is a "complete lack of theoretical understanding of the quantum critical states found in the heavy fermion metals" (Krüger & Zaanen, 4/14).