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

Kevin Ingersent (U. of Florida)

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

Supported by NSF DMR-0312939


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$_2$Si$_2$ (Mathur et al., 1998)  
YbRh$_2$Si$_2$ (Custers et al., 2003)
1. Fermi Liquids and Non-Fermi Liquids
Fermi-Liquid Theory

Key assumptions (Landau, 1956):

• Start with noninteracting fermions labeled by \((p, \sigma)\).
• Adiabatically turn on (possibly strong) interactions.
• Particles close to \(\epsilon_F\) evolve into long-lived quasiparticles.
• Quasiparticles are fermions, also labeled by \((p, \sigma)\), 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:

  [Diagram of electron and impurity with temperature T \ll T_K]

• 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$^2$) \quad [\gamma(Cu,Ag,Au) \sim 0.7].
  ▶ For $T < 0.1$K, $\rho = \rho_0 + AT^2$. 
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 $\epsilon_F$).
- 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?

![Graph showing resistivity vs. temperature for Bi$_2$Sr$_2$CaCu$_2$O$_8$]
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 \( C/T \propto \log(T_0/T) \quad \text{c.f. Fermi liquid: } C/T = \gamma \propto m^*. \)
  ‣ resistivity \( \rho(T) - \rho(0) \propto AT^\alpha, \quad 1 \leq \alpha \leq 1.5. \)
• 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$_2$Si$_2$
  - CeCu$_2$R$_2$, R = Si, Ge
  - CeCu$_{6-x}$M$_x$, M = Au, Ag, Pd, Pt
  - YbRu$_2$Si$_2$

• **Ferromagnetic** QPT likely in
  - UGe$_2$
  - ZrZn$_2$
  - Sr$_3$Ru$_2$O$_7$
  - MnSi

CePd$_2$Si$_2$ (Mathur et al., 1998)
2. Quantum Phase Transitions

- A QPT separates quantum-mechanical ground states (A and B) distinguished by an order parameter $\phi$ 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**

  $\text{CeCu}_{6-x}\text{Au}_x$

  (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:

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

  ⇒ **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,

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

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

  “**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.

- The control parameter $g$ controls the strength of fluctuation—plays the role of temperature in the effective classical model.

- As $T \to 0$, $L_\tau \to \infty$.

- 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:
  \[ \xi^0 \sim |g - g_c|^{-\nu}, \quad \xi_x^0 \sim |g - g_c|^{-z\nu} \]
  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 $\xi_\tau^0$:

$$g = g_1$$

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

$$g = g_2$$
Finite-Temperature Manifestations of a QPT (cont.)

- Physical properties cross over as functions of $L_t / \xi_t^0$ 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:

  \[ H = \sum_{k, \sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J \sum_i c_{i\sigma}^\dagger \frac{1}{2} \tau_{\sigma\sigma'} c_{i\sigma'} \cdot S_i + \frac{1}{2} \sum_{i,j} I_{ij} S_i \cdot S_j \]

- The competition is captured by the Kondo lattice model

  - In the paramagnetic phase, the Kondo effect wins. Residual interactions among quasiparticles can lead to …
    - Cooper instability (e.g., CeCu$_2$Si$_2$, 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):
  \[ \Phi[\Psi] = \frac{1}{2} \sum_{\mathbf{q}, \omega_n} \left[ \delta(g) + |\mathbf{q} - \mathbf{Q}|^2 + |\omega_n| \tau \right]|\Psi(\mathbf{q}, i\omega_n)|^2 + \frac{1}{4} \mu \Psi \Psi \Psi \Psi \]
- 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, \( d_u = 4 - z = 2 \).
  \[ \Rightarrow \text{For } d = 2 \ [d = 3], \text{ system is at [above] its upper critical dimension.} \]
- Renormalization-group analysis (Moriya, 1973; Hertz, 1976, Millis, 1993) gives as quantum critical behaviors at \( g = g_c \)
  \[ d = 2 : \quad \Delta C / T \sim \ln(T_0 / T), \quad \Delta \rho \sim T. \]
  \[ d = 3 : \quad \Delta C / T \sim \gamma - a\sqrt{T}, \quad \Delta \rho \sim T^{3/2}. \]
SDW Antiferromagnetic QPTs: Candidate Materials

- **CeCu$_2$Si$_2$:**

  - Fits the SDW theory for $d = 3$: $\Delta C / T \sim \gamma - a\sqrt{T}$, $\Delta \rho \sim T^{3/2}$.
  - Same $\rho(T)$ is seen in CeIn$_3$.

(Steglich et al., 1996, 1998)
SDW Antiferromagnetic QPTs: Candidate Materials

- **CePd$_2$Si$_2$:**

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

  - Close to the SDW theory for $d = 2$:
    \[
    \Delta C / T \sim \ln\left( T_0 / T \right), \quad \Delta \rho \sim T.
    \]

  (Mathur et al., 1998)
4. Heavy-Fermion QPTs: Experimental Puzzles & New Ideas

The Curious Case of CeCu$_{6-x}$Au$_x$

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

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

(von Löhneysen, 1996)
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)
Neutron-scattering and magnetization data can be collapsed onto the form

\[ \chi = \frac{C}{f(q) + (\sqrt{T^2 + H^2} - i\omega)^\alpha}, \]

where \( \alpha = 0.75 \pm 0.05 \).

(Schröder et al., 2001)
The Puzzle of $\text{CeCu}_{6-x}\text{Au}_x$

- The form $C\chi^{-1} = f(q) + \left(\sqrt{T^2 + H^2} - ia\omega\right)^\alpha$, $\alpha = 0.75 \pm 0.05$
  is fundamentally incompatible with the standard SDW theory, which should be at or above its upper critical dimension:
  - The $\omega$ dependence exhibits a critical exponent $\alpha < 1$:
    - For $d \geq d_u$, expect $\alpha = 1$.
    - Expect anomalous exponents only for $d < d_u$.
  - $\omega$ and $T$ enter with the same exponent $\alpha$:
    - For $d \geq d_u$, expect $\omega \sim T^{d/z}$.
    - Expect “$\omega/T$” scaling only for $d \leq d_u$.
- Suspicion falls on the validity of integrating out the fermions from
  $$H = \sum_{k,\sigma} \epsilon_k c_k^{\dagger} c_{k\sigma} + J \sum_i c_i^{\dagger} \frac{1}{2} \tau_{\sigma\sigma'} c_{i\sigma'} \cdot S_i + \frac{1}{2} \sum_{i,j} I_{ij} S_i \cdot S_j$$
  to get
  $$\Phi[\Psi] = \frac{1}{2} \sum_{q,i\omega_n} \left[ \delta(g) + |q - Q|^2 + |\omega_n| \tau \right] |\Psi(q,i\omega_n)|^2 + \frac{1}{4} u \Psi \Psi \Psi \Psi$$
  (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 $\omega/ T$ scaling but not for $\alpha < 1$.

- **Breakdown of quasiparticles** at the QPT (Coleman; Si and K.I.)
  - Builds on fact that the **local** susceptibility $\chi_{\text{loc}}(\omega) = \sum_{q=Q} \chi(q, \omega)$ diverges with the same exponent $\alpha$.
  - 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.
One Scenario: “Local Criticality”

- Fermi-liquid temperature $T^*$ vanishes just at the SDW instability ⇒ local moments reappear, and $\chi_{\text{loc}}$ diverges.
- Critical local fluctuations couple to extended critical modes ⇒ 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**

  \[
  H = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J \sum_i c_{i\sigma}^\dagger \frac{1}{2} \tau_{\sigma\sigma'} c_{i\sigma'} \cdot S_i + \frac{1}{2} \sum_{i,j} I_{ij} S_i \cdot S_j
  \]

  to a Bose-Fermi Kondo **impurity model**:

  \[
  H = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J c_{0\sigma}^\dagger \frac{1}{2} \tau_{\sigma\sigma'} c_{0\sigma'} \cdot S + \sum_q \omega_q \phi_q^\dagger \cdot \phi_q + g \left( \phi_0 + \phi_0^\dagger \right) \cdot S
  \]

  - 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:

$$H = \sum_{k, \sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J c_{0\sigma}^\dagger \frac{1}{2} \tau_{\sigma\sigma'} c_{0\sigma'} \cdot S + \sum_q \omega_{q} \phi_q^\dagger \phi_q + g(\phi_0 + \phi_0^\dagger)S^z + h_{\text{loc}} S^z$$

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

$$G(k, \omega) = [\omega - \varepsilon_k - \Sigma(k, \omega)]^{-1}$$

$$\chi(q, \omega) = [M(q, \omega) + I_q]^{-1}$$

where the “RKKY density of states,”

$$\rho_I(\varepsilon) = \sum_q \delta(\varepsilon - I_q),$$

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

- Self consistency requires

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

The form of $\rho_I(\varepsilon)$ near $\varepsilon = I_Q$ turns out to be crucial.
What is the Nature of the QPT in EDMFT?

• EDMFT equations have been solved using various impurity solvers.
• $\epsilon$-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$_2$Si$_2$, but corresponds to $\epsilon = 1^{-}$.
• Quantum Monte Carlo yields conflicting results:
  ‣ Anderson lattice has no locally critical QPT; transition is 1$^{st}$ order (Sun & Kotliar, 2003).
  ‣ Kondo lattice has 1$^{st}$ 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 & Kl, 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.

- 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

\[ \chi_{\text{loc}}(0) = \int d\varepsilon \frac{\rho_1(\varepsilon)}{\chi^{-1}(Q,0) - I_Q + \varepsilon} \]

- Bosonic NRG can get closer to the QPT (Zhu et al., 2007).
EDMFT: Anomalous Exponent in the Dynamics

- Logarithmic divergence in $\chi'_{\text{loc}}(\omega \rightarrow 0)$ implies an anomalous exponent
  $$\alpha = 0.78(4)$$
  in the lattice susceptibility.
- Compares well with the experimental value in $\text{CeCu}_{6-x}\text{Au}_x$:
  $$\alpha \approx 0.75.$$
• 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 \( \beta / C_p \) (\( \beta \) = thermal exp.).
• \( T \)-independent (non-Korringa) spin-lattice relaxation (NMR, \( \mu \)SR).
Local Criticality: Evidence from YbRh$_2$Si$_2$

Does $R_H$ jump at the QPT?

(Kuchler et al., 2003)

Gruneisen ratio diverges in a way consistent with local criticality.

(Paschcn et al., 2004)
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).