Kondo Problem to Heavy Fermions and Local Quantum Criticality

Qimiao Si

Rice University

Advanced School – Developments and Prospects in Quantum Impurity Physics, MPI-PKS, Dresden, May 30, 2011

- **Introduction to quantum critical point**
- **Kondo problem to heavy Fermi liquid**
- **Heavy fermion quantum criticality**
- **Perspective and outlook**

Q. Si, arXiv:1012.5440, a chapter in the book "Understanding Quantum Phase Transitions", ed. L. D. Carr (2010).

Pallab Goswami, Jed Pixley, Jianda Wu (Rice University)

Stefan Kirchner (MPI-PKS, CPfS)

Seiji Yamamoto (NHMFL, FSU)

Jian-Xin Zhu, Lijun Zhu (Los Alamos)

Kevin Ingersent (Univ. of Florida)

Jianhui Dai (Zhejiang U.)

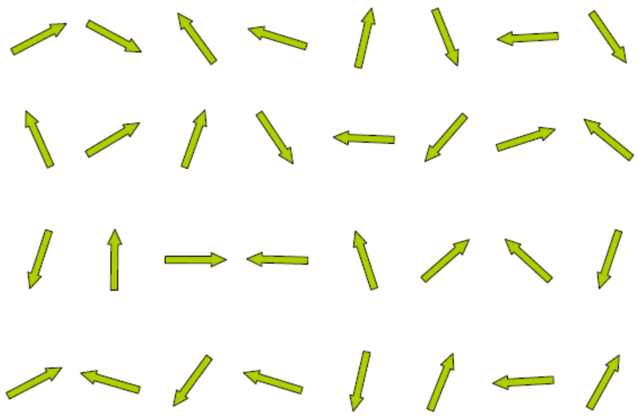
Daniel Grempel (CEA-Saclay)

Ralf Bulla (U. Cologne)

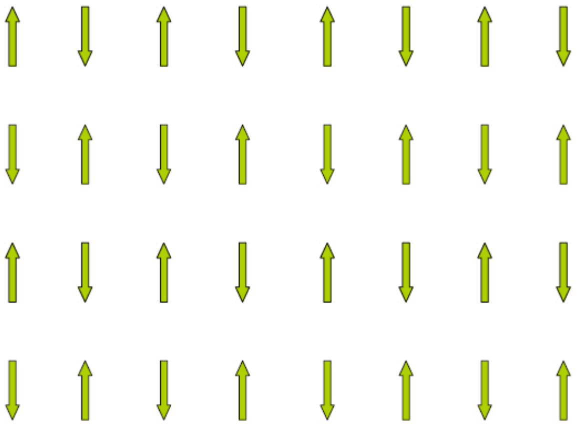
S. Friedemann	C. Krellner	Y. Tokiwa
P. Gegenwart	S. Paschen	S. Wirth
N. Oeschler	T. Westerkamp	R. Küchler
T. Lühmann	T. Cichorek	K. Neumaier
O. Tegus	O. Trovarelli	C. Geibel
F. Steglich	P. Coleman	E. Abrahams

Phases and Phase Transitions

Disorder
($T>T_{order}$)

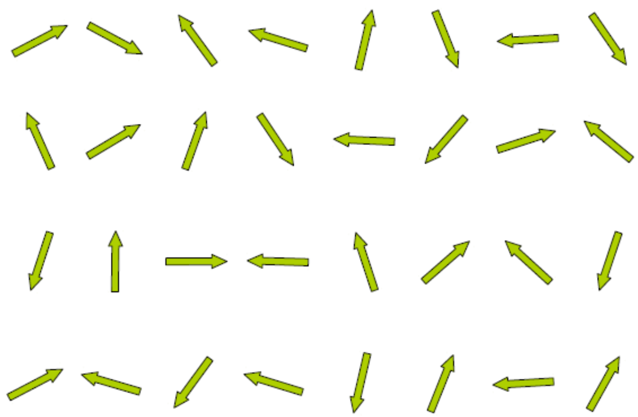


Order
($T<T_{order}$)

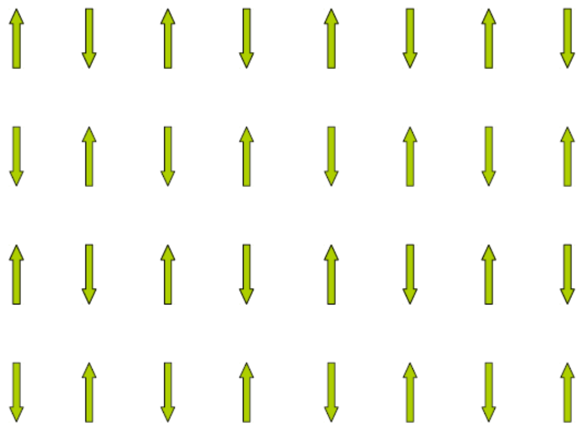


Continuous Phase Transitions: Criticality

Disorder
($T>T_{order}$)

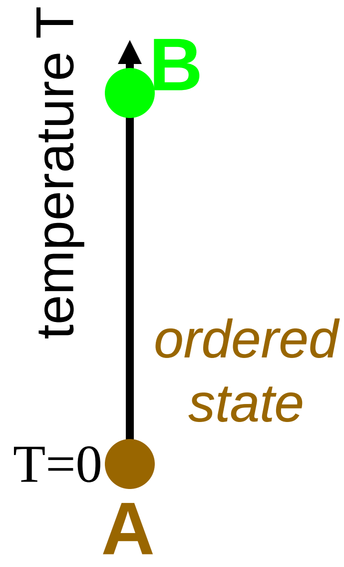


Order
($T<T_{order}$)



Criticality -- fluctuations of order parameter in d dimensions

$$H = -I \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z$$

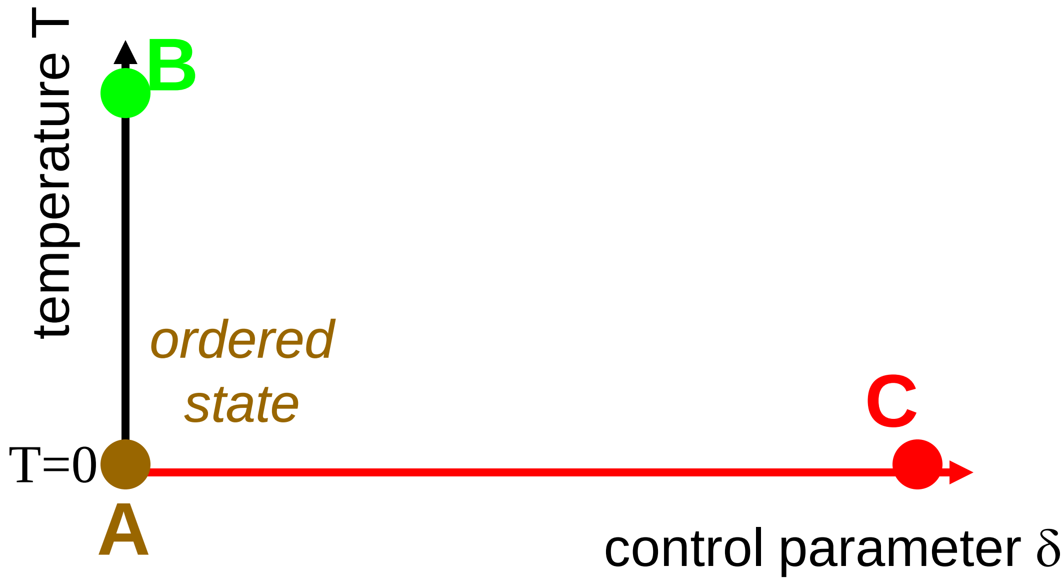


- **A: every spin (spontaneously) points up**

Order parameter: $m = \lim_{h \to 0^+} \lim_{N_{site} \to \infty} M / N_{site} = 1$

- **B: every microstate equally probable: m=0**

$$H = -I \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - (I\delta)\sum_i \sigma_i^x$$



- **A: every spin (spontaneously) points up**

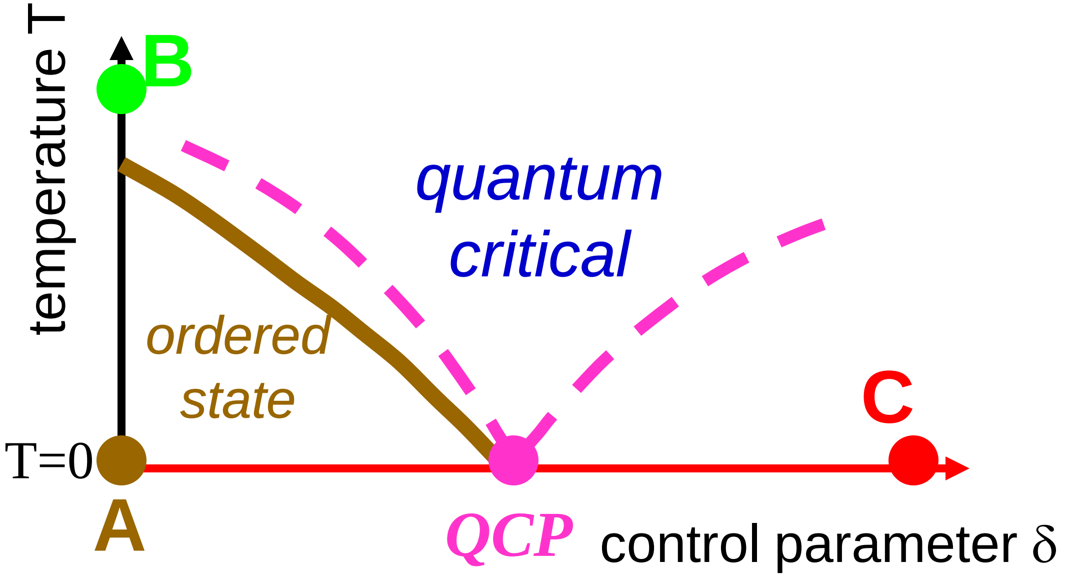
Order parameter: $m = \lim_{h \to 0^+} \lim_{N_{site} \to \infty} M / N_{site} = 1$

- **B: every microstate equally probable: m=0**

- **C: every spin points along the transverse field: m=0**

Quantum Phase Transition

$$H = -I \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - (I\delta) \sum_i \sigma_i^x$$



- **A: every spin (spontaneously) points up**

Order parameter: $m = \lim_{h \to 0^+} \lim_{N_{site} \to \infty} M / N_{site} = 1$

- **B: every microstate equally probable: m=0**

- **C: every spin points along the transverse field: m=0**

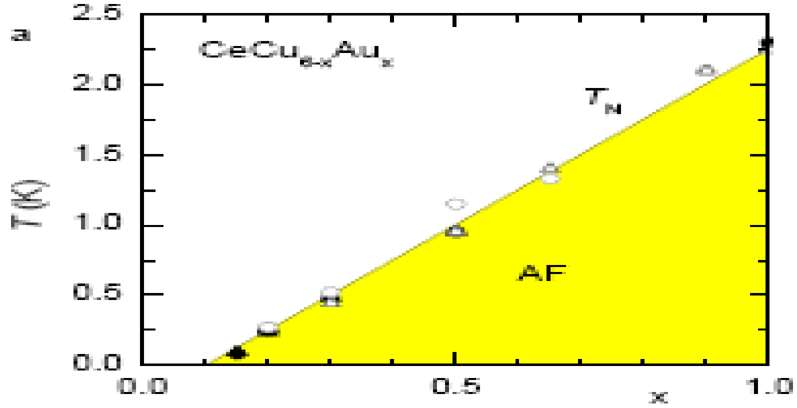
Materials (possibly) showing Quantum Phase Transitions

- Heavy fermion metals
- Iron pnictides
- Cuprates
- Organic charge-transfer salts
- Weak magnets (eg Cr-V, MnSi, Ruthenates)
- Mott transition (eg V2O3)
- Insulating Ising magnet (eg LiHoF4)
- Field-driven BEC of magnons
- MIT/SIT/QH-QH in disordered electron systems
- Tunable systems (eg quantum dots, cold atoms)

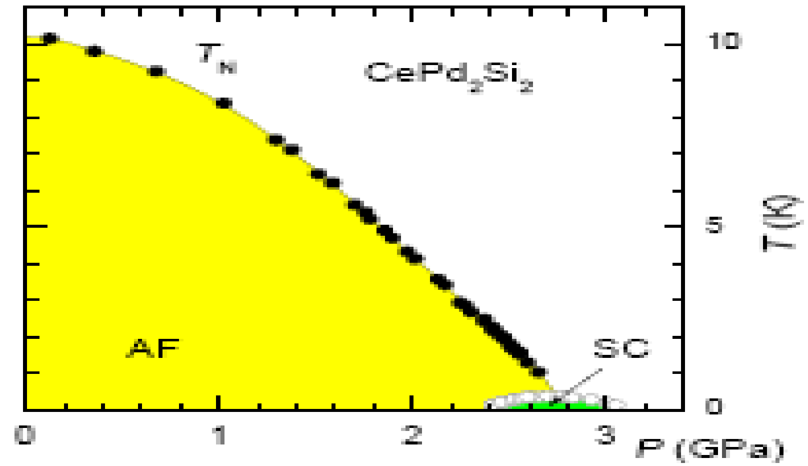
Heavy fermion metals as prototype quantum critical points

$CeCu_{6-x}Au_x$

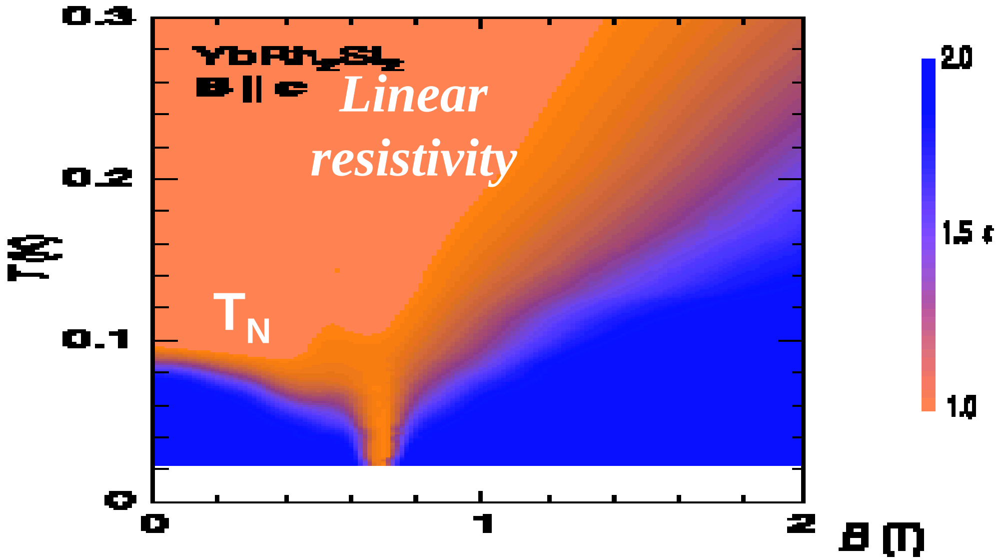
H. v. Löhneysen et al



$CePd_2Si_2$



N. Mathur et al



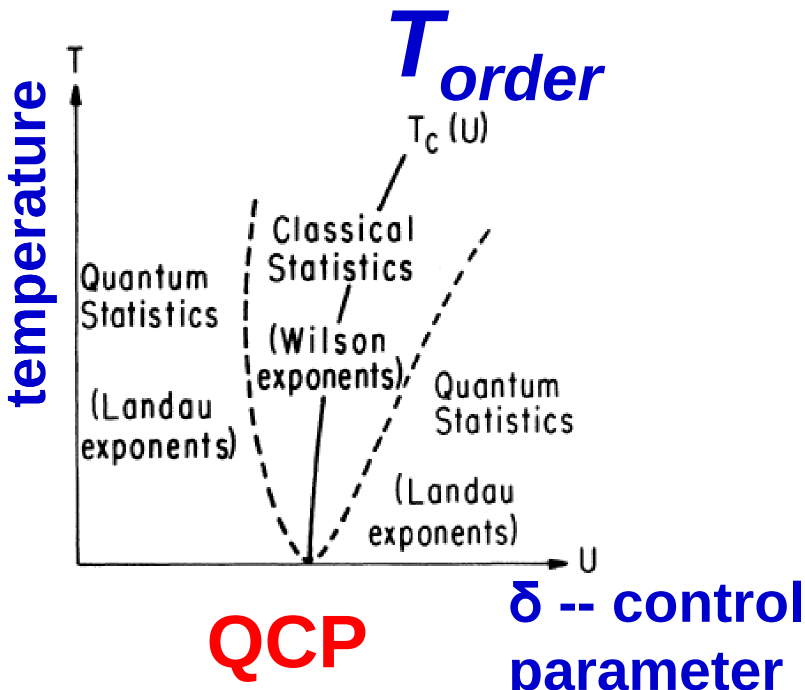
$YbRh_2Si_2$

J. Custers et al

PHYSICAL REVIEW B VOLUME 14, NUMBER 3 1 AUGUST 1976

Quantum critical phenomena*

John A. Hertz
The James Franck Institute and The Department of Physics, The University of Chicago, Chicago, Illinois 60637



PHYSICAL REVIEW B VOLUME 14, NUMBER 3 1 AUGUST 1976

Quantum critical phenomena*

John A. Hertz
The James Franck Institute and The Department of Physics, The University of Chicago, Chicago, Illinois 60637

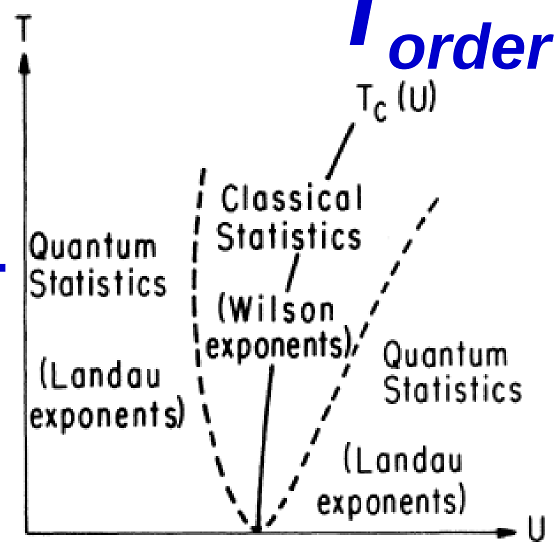
$\mathbf{Tr}\ e^{-(\hbar/kT)H/\hbar}$

$\tau \sim \hbar / kT_{\mathrm{order}}$

→ ∞ @QCP

temperature

T_{order}



QCP

δ -- control parameter

Following Landau -- fluctuations of order parameter, $m(\mathbf{x}, \tau)$, but in d+z dimensions

T=0 spin-density-wave transition

$$\mathcal{S} = \int d\mathbf{q} \frac{1}{\beta} \sum_{i\omega_n} \left(r + c\mathbf{q}^2 + |\omega_n| / \Gamma_{\mathbf{q}} \right) \phi^2 + \int u\, \phi^4 + \ldots$$

$d_{eff} = d + z > 4,$

Gaussian

no $\frac{\omega}{T}$ *scaling*

MF exponent

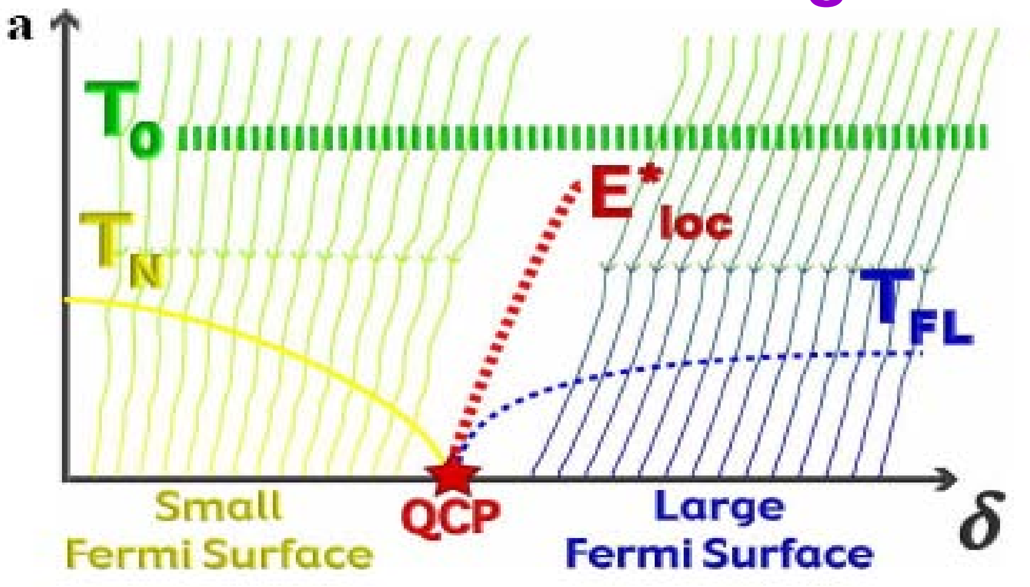
Beyond the Order-parameter Fluctuations

Inherent quantum modes may be important
-- need to identify the additional critical modes before constructing the critical field theory.

Critical Kondo Destruction
-- Local Quntum Critical Point

Kondo Destruction (f-electron Mott localization)

at the T=0 onset of antiferromagnetism



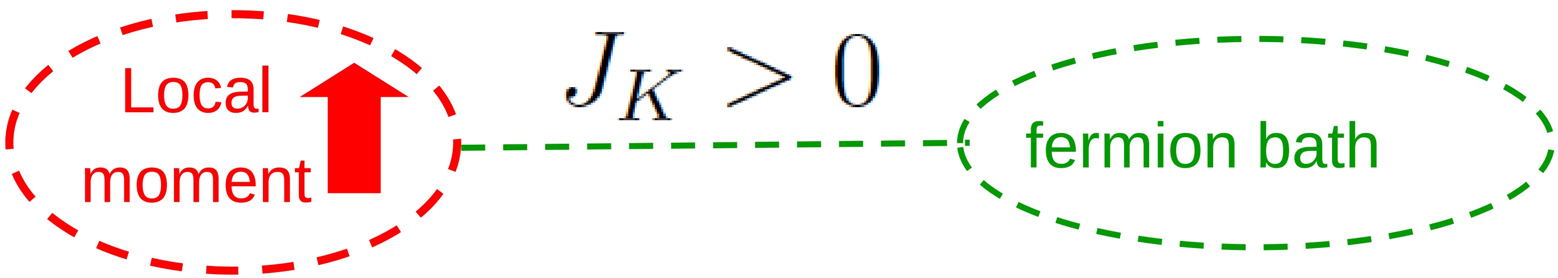
QS, S. Rabello, K. Ingersent, & J. L. Smith, Nature 413, 804 (2001);
Phys. Rev. B68, 115103 (2003)

P. Coleman et al, JPCM 13, R723 (2001)

- **Introduction to quantum critical point**
- **Kondo problem to heavy Fermi liquid**
- **Heavy fermion quantum criticality**
- **Perspective and outlook**

Single-impurity Kondo Model:

$$H_{\text{Kondo}} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \;+\; J_K \mathbf{S} \cdot \mathbf{s}_{c,0}$$



S: spin-1/2
moment at site 0

$$\mathbf{s}_{c,0} = (1/2) c_0^{\dagger} \vec{\sigma} c_0$$

Single-impurity Kondo Model:

$$\frac{dJ_K}{dl} \equiv \beta(J_K) = J_K^2$$

– resistivity minimum (scattering increases as T is lowered!)

– asymptotic freedom

– Kondo screening (process of developing Kondo singlet correlations as T is lowered)

Single impurity Kondo model

- Kondo temperature: $T_K^0 \approx \rho_0^{-1} \exp(-1/\rho_0 J_K)$

Single impurity Kondo model

- Kondo temperature: $T_K^0 \approx \rho_0^{-1} \exp(-1/\rho_0 J_K)$

- Kondo entanglement: singlet ground state

$$\frac{1}{\sqrt{2}}(|\uparrow>_f|\downarrow>_c - |\downarrow>_f|\uparrow>_c)$$

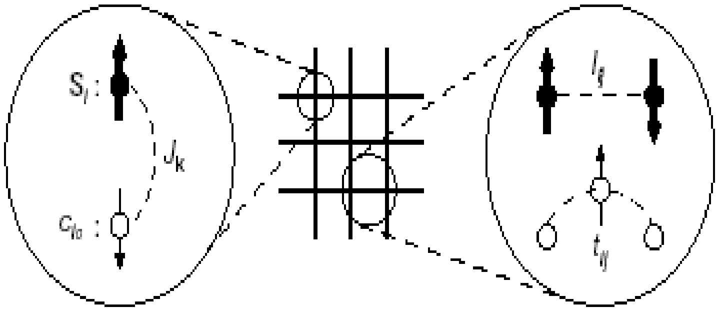
Single impurity Kondo model

- Kondo temperature: $T_K^0 \approx \rho_0^{-1} \exp(-1/\rho_0 J_K)$
- Kondo entanglement: singlet ground state

$$\frac{1}{\sqrt{2}}(|\uparrow>_f |\downarrow>_c - |\downarrow>_f |\uparrow>_c)$$

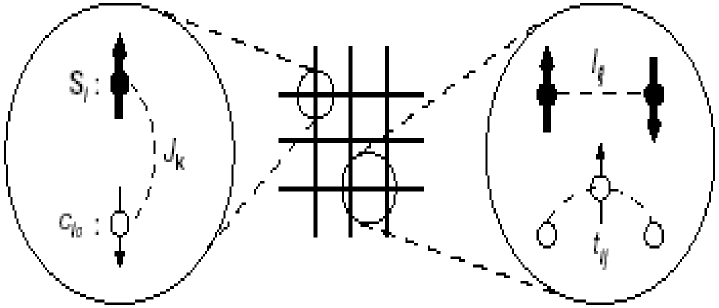
- Kondo effect (emergence of Kondo resonance):
  – Kondo-singlet ground state yields an electronic resonance
  – local moment acquires electron quantum number due to Kondo entanglement

Kondo lattices:



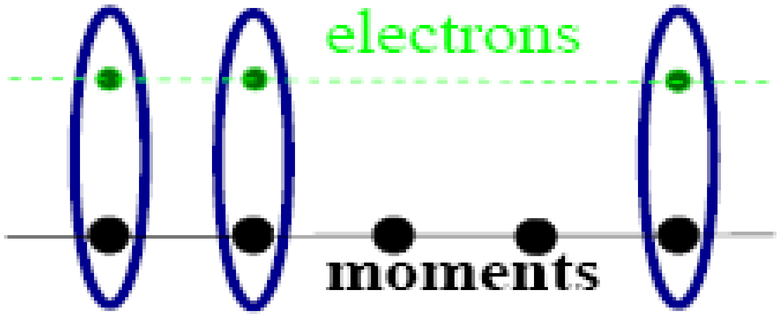
$$\mathcal{H} = \sum_{ij,a} I^a_{ij} \, S^a_i \, S^a_j + \sum_{ij,\sigma} t_{ij} \, \mathbf{c}^\dagger_{i\sigma} \, \mathbf{c}_{j\sigma} + \sum_{i,a} J^a_K \, S^a_i \, s^a_{c,i}$$

Kondo lattices:



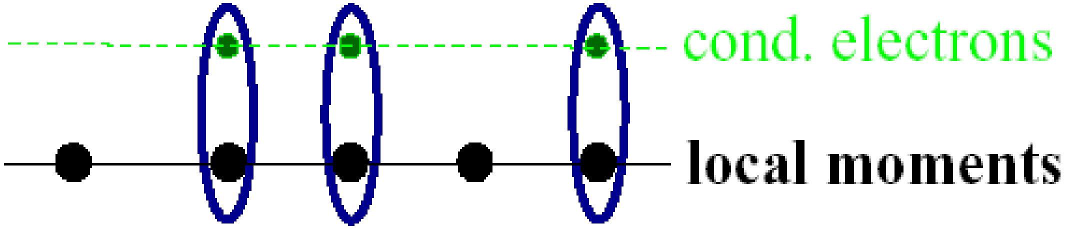
$$\mathcal{H} = \sum_{ij,a} I^a_{ij}\, S^a_i\, S^a_j + \sum_{ij,\sigma} t_{ij}\, \mathbf{c}^\dagger_{i\sigma}\, \mathbf{c}_{j\sigma} + \sum_{i,a} J^a_K\, S^a_i\, s^a_{c,i}$$

heavy Fermi liquid:



- Kondo singlet
- Kondo resonance

$J_K >> W >> I$



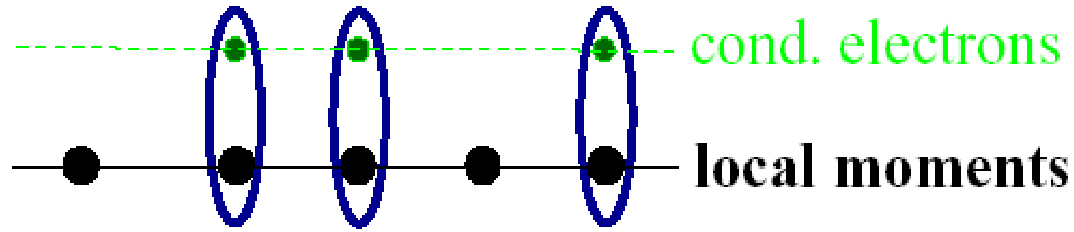
- xN_{site} **tightly bound local singlets**

$$|s>_i = \frac{1}{\sqrt{2}}\left(|\uparrow>_f|\downarrow>_c - |\downarrow>_f|\uparrow>_c\right)_i$$

(cf. If x were =1, Kondo insulator)

- $(1\text{-}x)N_{site}$ **lone moments:**

$J_K >> W >> I$



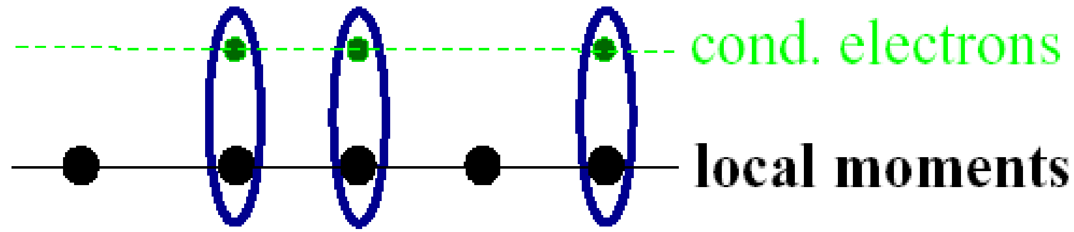
- ***xN_{site}* tightly bound local singlets**

$$|s>_i = \frac{1}{\sqrt{2}} \left(|\uparrow>_f |\downarrow>_c - |\downarrow>_f |\uparrow>_c \right)_i$$

(cf. If x were =1, Kondo insulator)

- ***$(1\text{-}x)N_{site}$* lone moments:** (C. Lacroix, Solid State Comm. ’85)
  - **projection:** $$|\text{lone moment} >_{i,\sigma} = (-\sqrt{2}\sigma)\, c_{i,\bar{\sigma}}\, |s>_i$$
  - **$(1\text{-}x)N_{site}$ holes with $U=\infty$**

$J_K >> W >> I$



- ***xN*$_{site}$ tightly bound local singlets**

$$|s>_i = \frac{1}{\sqrt{2}}\left(|\uparrow>_f |\downarrow>_c - |\downarrow>_f |\uparrow>_c\right)_i$$

(cf. If x were =1, Kondo insulator)

- ***(1-x)N*$_{site}$ lone moments:** (C. Lacroix, Solid State Comm. ’85)
  - **projection:** $$|\text{lone moment}>_{i,\sigma} = \left(-\sqrt{2}\sigma\right) c_{i,\bar{\sigma}}\, |s>_i$$
  - **(1-x)N$_{site}$ holes with U=∞**

- **Luttinger’s theorem:**

(1-x) holes/site in the Fermi surface

⟺ **(1+x) electrons/site ---- Large Fermi surface!**

Heavy Fermi Liquid
(Kondo Lattice)

- The large Fermi surface applies to the paramagnetic phase, when the ground state is a Kondo singlet.

- This can be seen through adiabatic continuity of a Fermi liquid.

- It can also be seen, microscopically, through eg slave-boson MFT (Auerbach & Levin, Millis & Lee, Coleman, Read & Newns)

Heavy Fermi Liquid
(Kondo Lattice)

- **Kondo resonance**

  …

$$G_c(k,\omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(k,\omega)}$$

$$\Sigma(\mathbf{k},\omega) = \frac{(b^*)^2}{\omega - \epsilon_f^*}$$

pole in Σ

- … ⇨ heavy electron bands

$$G_c(\mathbf{k},\omega) = \frac{u_k^2}{\omega - E_{1,\mathbf{k}}} + \frac{v_k^2}{\omega - E_{2,\mathbf{k}}}$$

Heavy Fermi Liquid
(Kondo Lattice)

- **Kondo resonance ...**

$$G_c(k,\omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(k,\omega)}$$

$$\Sigma(\mathbf{k},\omega) = \frac{(b^*)^2}{\omega - \epsilon_f^*}$$

k-independent

pole in Σ

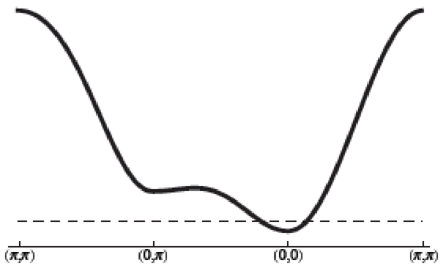
- … ⇨ heavy electron bands

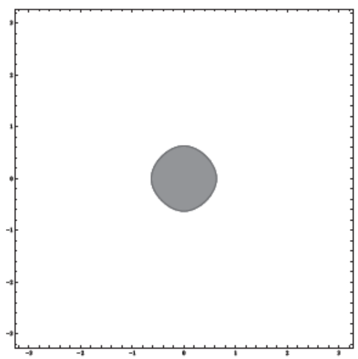
$$G_c(\mathbf{k},\omega) = \frac{u_k^2}{\omega - E_{1,\mathbf{k}}} + \frac{v_k^2}{\omega - E_{2,\mathbf{k}}}$$

Heavy Fermi Liquid

Cond. electron band

$\varepsilon(k)$

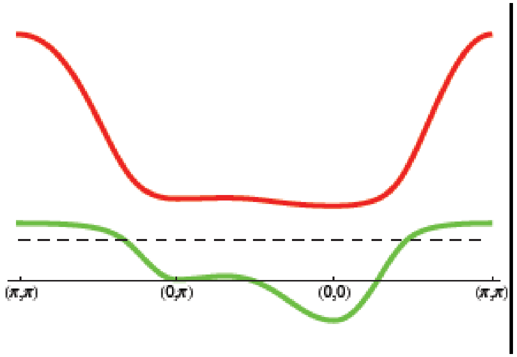


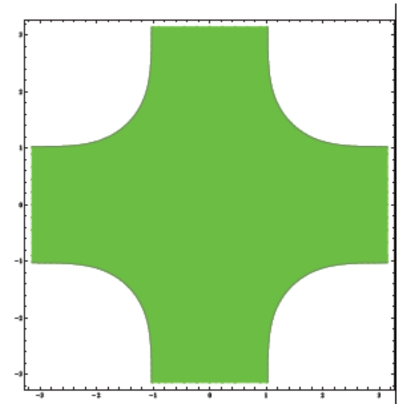


Kondo resonance

Heavy electron bands

$E_{1,2}(k)$

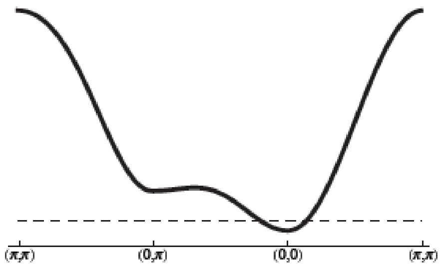


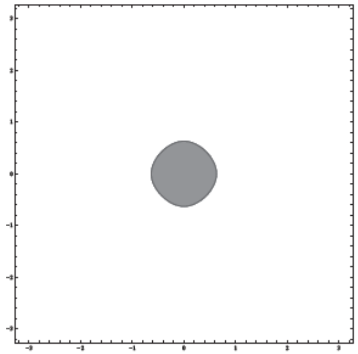


Heavy Fermi Liquid

Cond. electron band

$\varepsilon(k)$

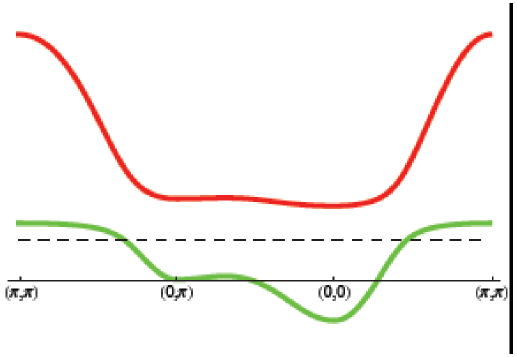


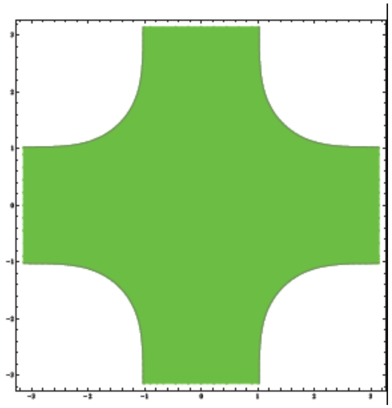


Kondo resonance

Heavy electron bands

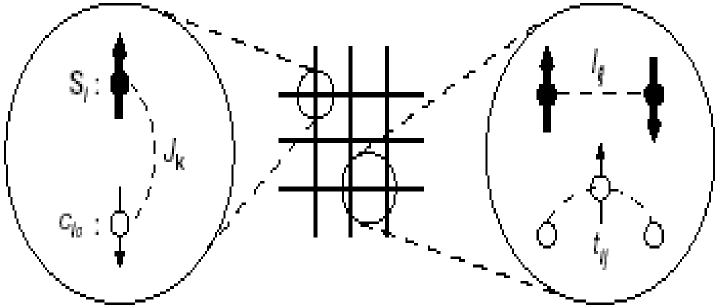
$E_{1,2}(k)$



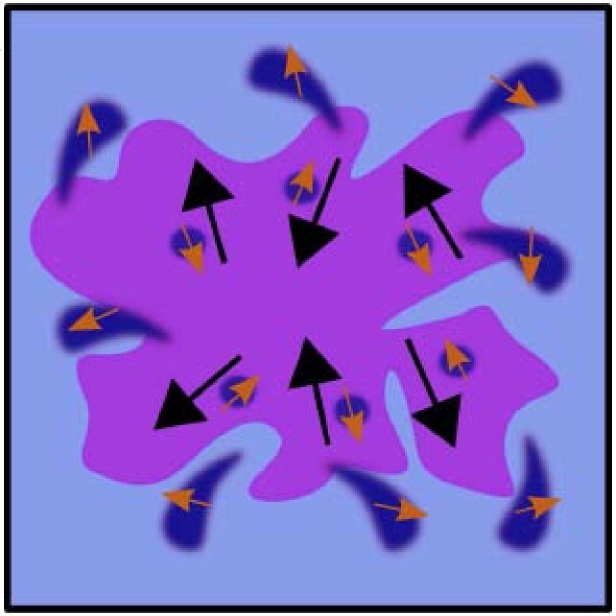


Large Fermi surface

• Kondo lattices:



$$\mathcal{H} = \sum_{ij,a} I_{ij}^a\, S_i^a\, S_j^a + \sum_{ij,\sigma} t_{ij}\, \mathbf{c}_{i\sigma}^\dagger\, \mathbf{c}_{j\sigma} + \sum_{i,a} J_K^a\, S_i^a\, s_{c,i}^a$$



heavy Fermi liquid:

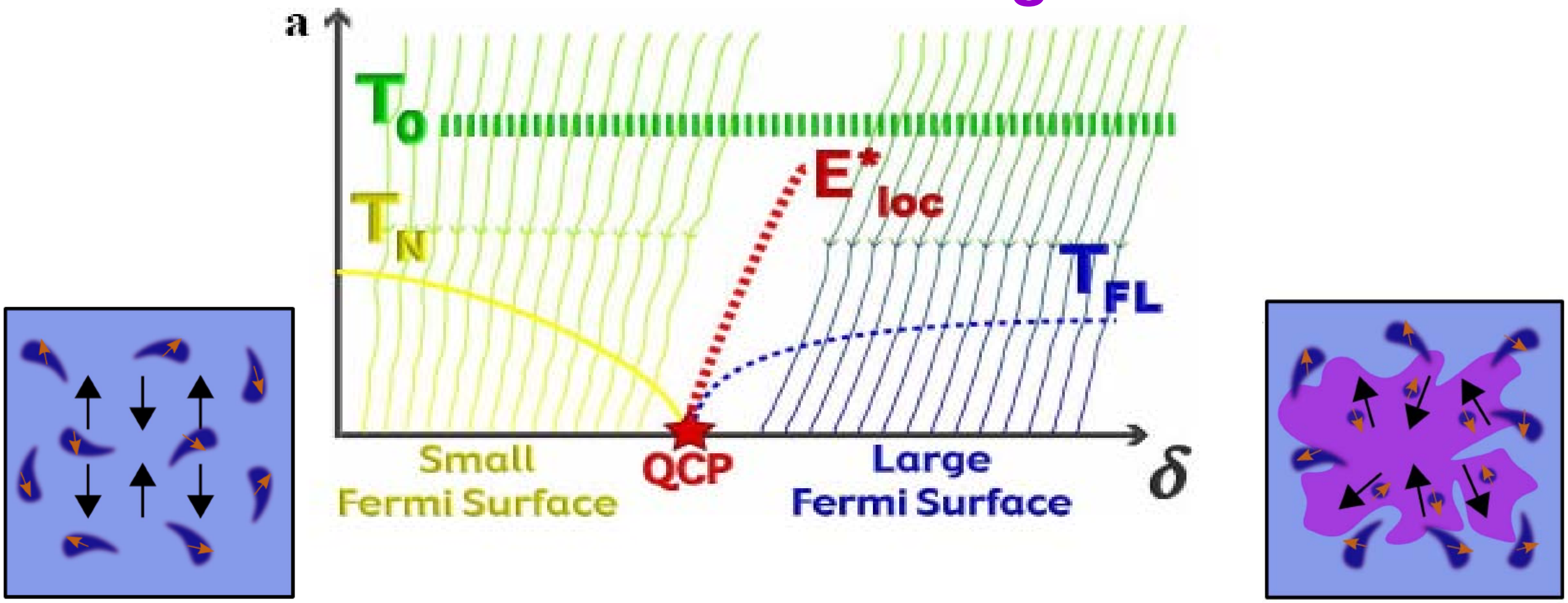
- Kondo singlet
- Kondo resonance

No symmetry breaking, but macroscopic order

Critical Kondo Destruction
-- Local Quantum Critical Point

Kondo Destruction (f-electron Mott localization)

at the T=0 onset of antiferromagnetism



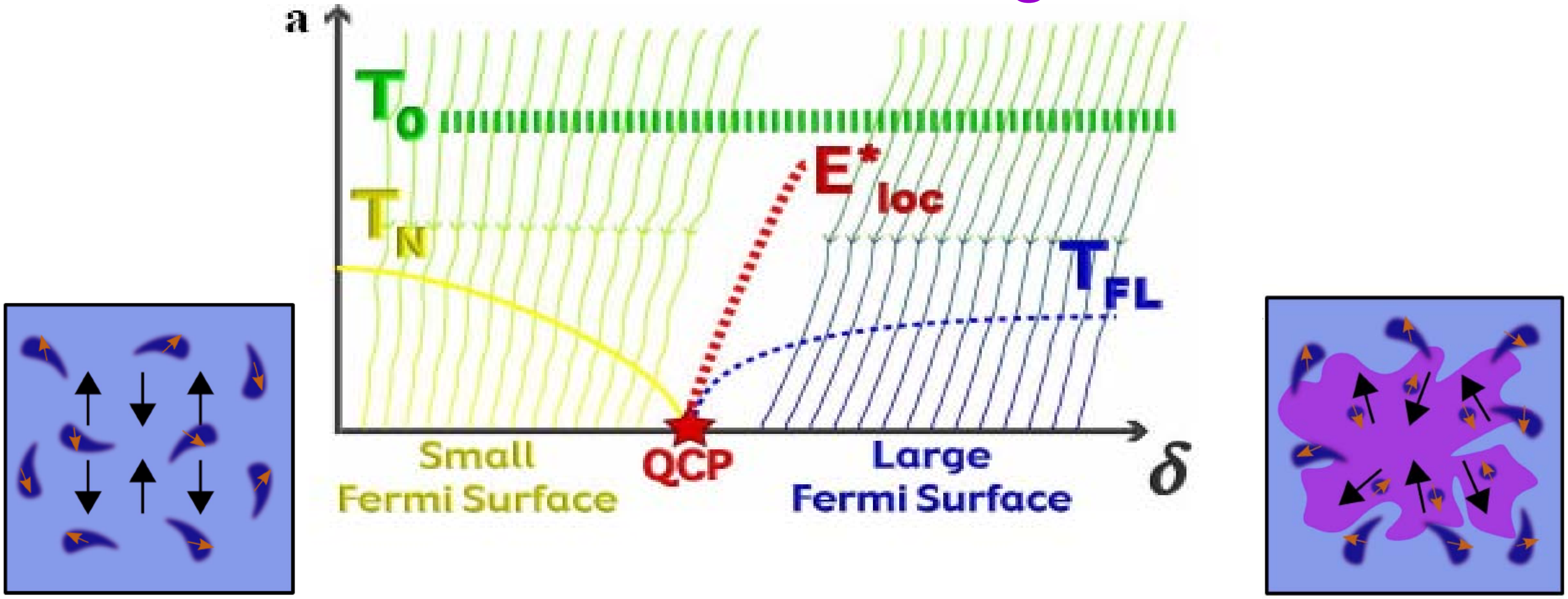
Q. Si, arXiv:1012.5440, a chapter in the book “Understanding Quantum Phase Transitions”, ed. L. D. Carr (2010).

- **Introduction to quantum critical point**
- **Kondo problem to heavy Fermi liquid**
- **Heavy fermion quantum criticality**
- **Perspective and outlook**

Critical Kondo Destruction
-- Local Quantum Critical Point

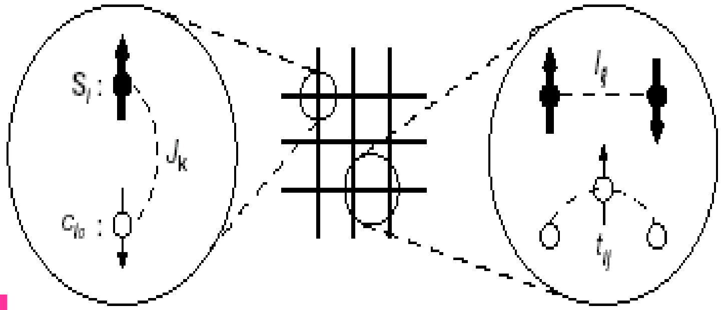
Kondo Destruction (f-electron Mott localization)

at the T=0 onset of antiferromagnetism



Q. Si, arXiv:1012.5440, a chapter in the book "Understanding Quantum Phase Transitions", ed. L. D. Carr (2010).

Kondo lattices:



$$\mathcal{H} = \sum_{ij,a} I_{ij}^{a} S_i^{a} S_j^{a} + \sum_{ij,\sigma} t_{ij} \mathbf{c}_{i\sigma}^{\dagger} \mathbf{c}_{j\sigma} + \sum_{i,a} J_K^{a} S_i^{a} s_{c,i}^{a}$$

$$\delta = T_K^0 / I$$

Kondo Effect at the AF QCP

- In the paramagnetic phase, E_{loc}^{*} is finite:
  - Ground state is a Kondo singlet
  - Fermi surface is large
  - Call this "P_L" phase
- Increasing RKKY interaction, I/T_K^0, leads to AF order, yielding AF QCP
- What happens to the E_{loc}* scale as the AF QCP is approached from the P_L side?

T=0 spin-density-wave transition

$$\mathcal{S} = \int d\mathbf{q} \frac{1}{\beta} \sum_{i\omega_n} (r + c\mathbf{q}^2 + |\omega_n|/\Gamma_{\mathbf{q}})\, \phi^2 + \int u\, \phi^4 + \ldots$$

smooth q-independence

Extended-DMFT* of Kondo Lattice

(* Smith & QS; Chitra & Kotliar)

Mapping to a Bose-Fermi Kondo model:

$$\mathcal{H}_{\rm eff} = J_K\, \mathbf{S}\cdot\mathbf{s}_c + \sum_{p,\sigma} E_p\, c_{p\sigma}^{\dagger}\, c_{p\sigma} + g\, \mathbf{S}\cdot\sum_p \left(\vec{\phi}_p + \vec{\phi}_{-p}^{\,\dagger}\right) + \sum_p w_p\, \vec{\phi}_p^{\,\dagger}\cdot\vec{\phi}_p$$

+ self-consistency conditions

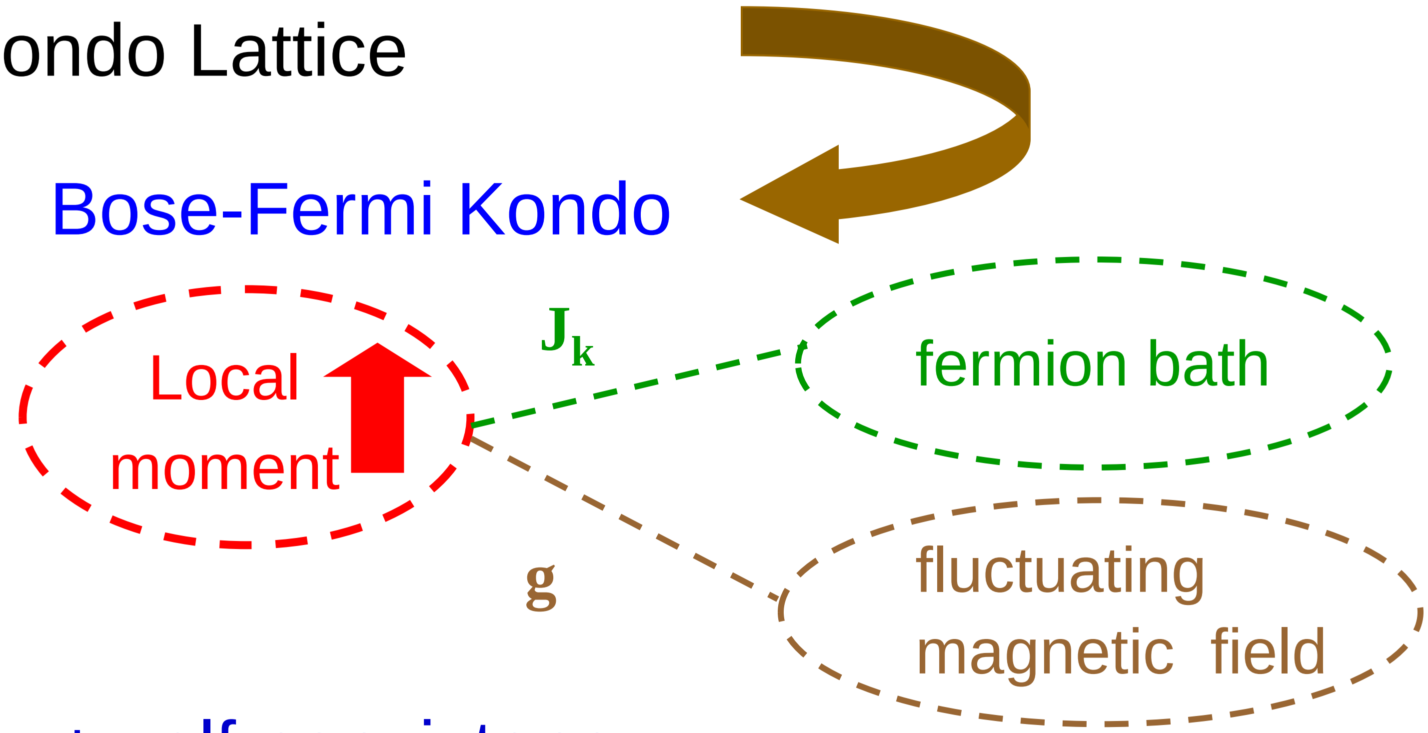
– **Electron self-energy** $\Sigma(\omega)$ ⟺ $G(k,\omega)=1/[\omega - \varepsilon_k - \Sigma(\omega)]$

– **"spin self-energy"** $M(\omega)$ ⟺ $\chi(q,\omega)=1/[I_q + M(\omega)]$

Extended-DMFT of Kondo Lattice

Kondo Lattice

Bose-Fermi Kondo



+ self-consistency

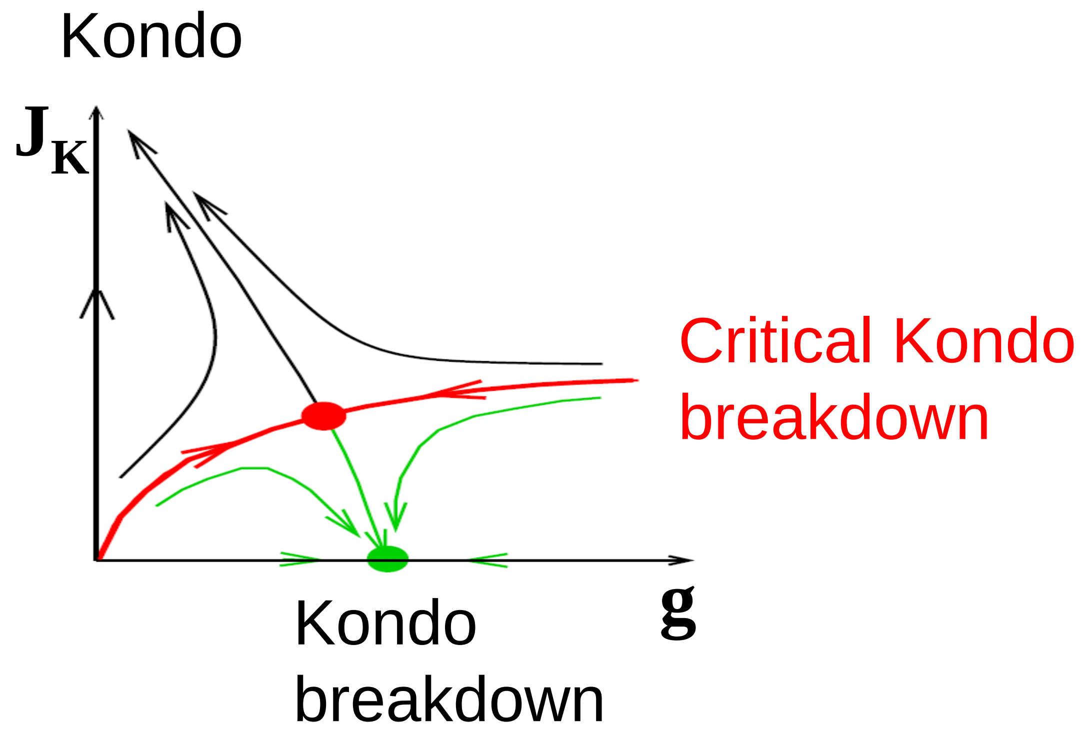
ε-expansion of Bose-Fermi Kondo Model

$$\sum_p \delta(\omega - w_p) \sim \omega^{1-\varepsilon}$$

0<ε<1:

sub-ohmic

dissipation

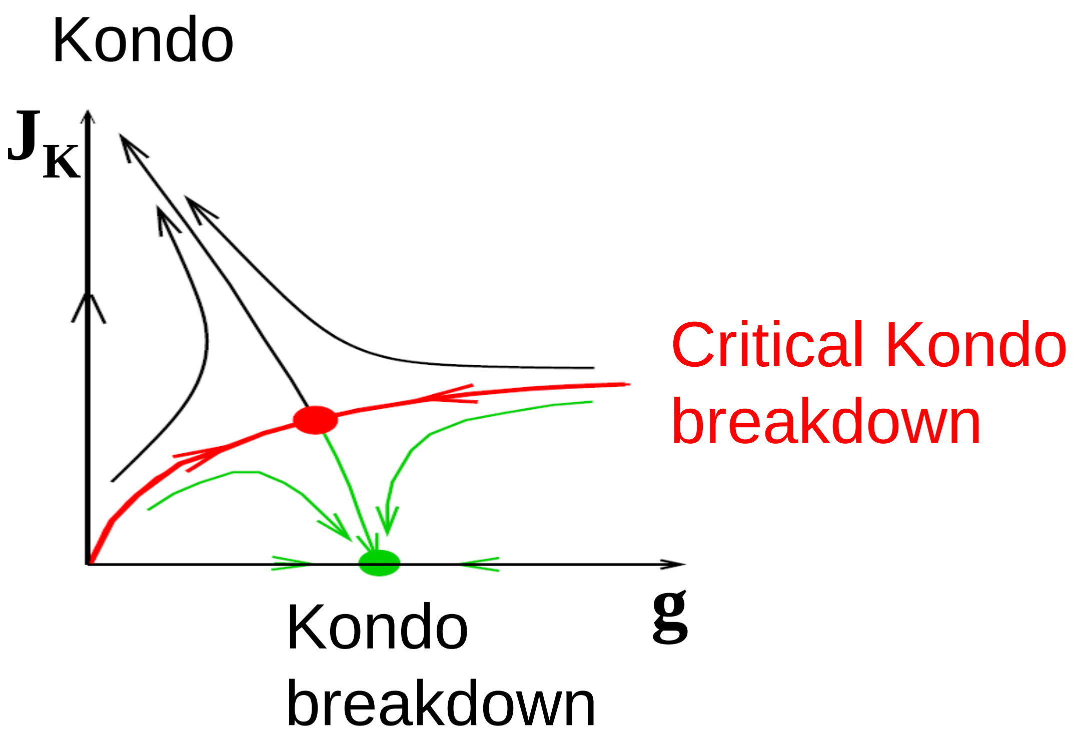


QS, Rabello, Ingersent, Smith, Nature ' 01; PRB ' 03;
L. Zhu & QS, PRB '02

ε-expansion of Bose-Fermi Kondo Model

$$\sum_p \delta(\omega - w_p) \sim \omega^{1-\varepsilon}$$

0<ε<1:
sub-ohmic
dissipation



Critical: $\chi_{\rm loc}(\tau) \sim 1/\tau^{\epsilon}$

Crucial for LQCP solution

QS, Rabello, Ingersent, Smith, Nature '01; PRB '03;
L. Zhu & QS, PRB '02

Role of Berry phase

$$\mathcal{H}_{\rm eff} = J_K\, \mathbf{S}\cdot \mathbf{s}_c + \sum_{p,\sigma} E_p\, c^{\dagger}_{p\sigma}\, c_{p\sigma} + g\, \mathbf{S}\cdot \sum_p \left(\vec{\phi}_p + \vec{\phi}^{\dagger}_{-p}\right) + \sum_p w_p\, \vec{\phi}^{\dagger}_p \cdot \vec{\phi}_p$$

S. Kirchner & QS, arXiv:0808.2647

$$\mathcal{Z} = \int \mathcal{D}[\vec{n}]\, e^{is\omega(\vec{n}) - \int_0^\beta H(s\vec{n})}$$

$is\omega(\vec{n})$ is a geometrical phase and equals the area on the unit sphere enclosed by $\vec{n}(\tau)$

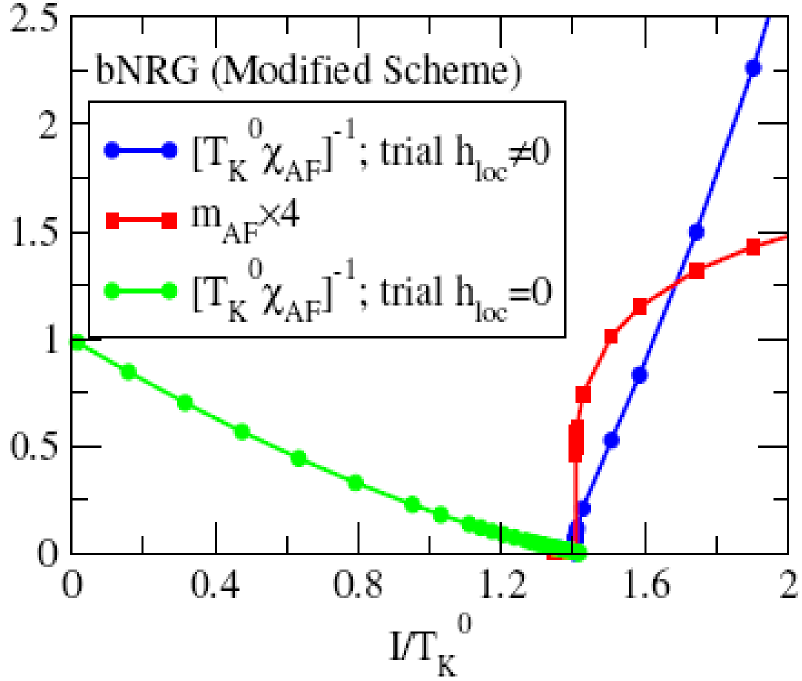
For ½<ε<1:

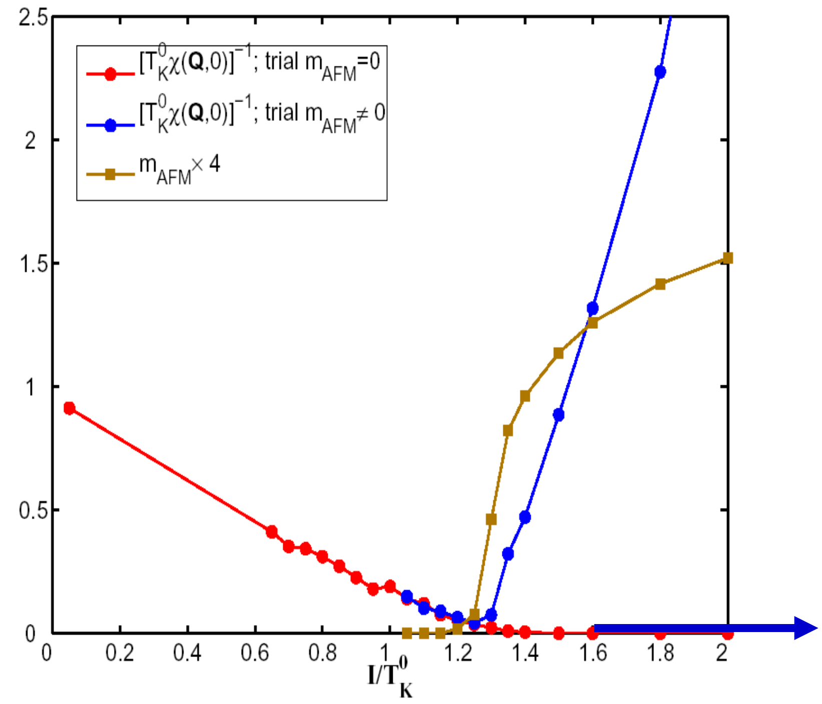
- Retaining Berry phase yields ω/T scaling
- Dropping Berry phase violates ω/T scaling

Dynamical Scaling
of Local Quantum Critical Point

$$\chi(\mathbf{q},\omega) = \frac{1}{\left(I_{\mathbf{q}} - I_{\mathbf{Q}}\right) + A\left(-i\omega\right)^{\alpha} \mathcal{M}(\omega/T)}$$

Continuous phase transition





$\delta \equiv I_{RKKY} / T_K^0$

J.-X. Zhu, S. Kirchner, R. Bulla & QS, PRL 99, 227204 (2007);
M. Glossop & K. Ingersent, PRL 99, 227203 (2007)

J.-X. Zhu, D. Grempel, and QS, Phys. Rev. Lett. (2003)

Dynamical Scaling of Local Quantum Critical Point

$$\chi(\mathrm{q},\omega) = \frac{1}{\left(I_{\mathrm{q}} - I_{\mathrm{Q}}\right) + A\left(-i\omega\right)^{\alpha}\mathcal{M}(\omega/T)}$$

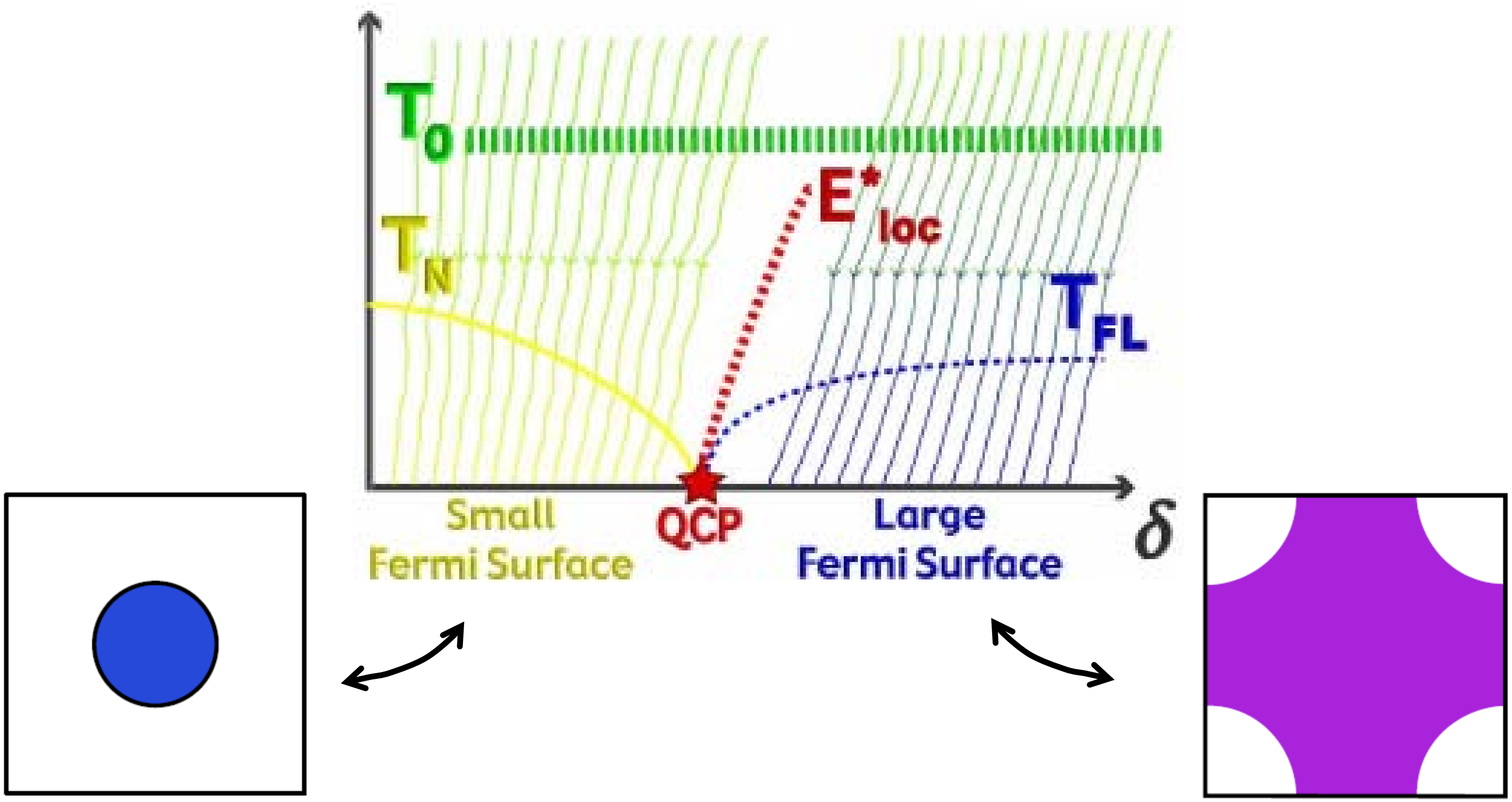
$\alpha = 0.72$ — J-X Zhu, D. Grempel and QS, PRL (2003)

$\alpha = 0.83$ — J-X Zhu, S. Kirchner, R. Bulla, and QS, PRL (2007)

$\alpha = 0.78$ — M. Glossop & K. Ingersent, PRL (2007)

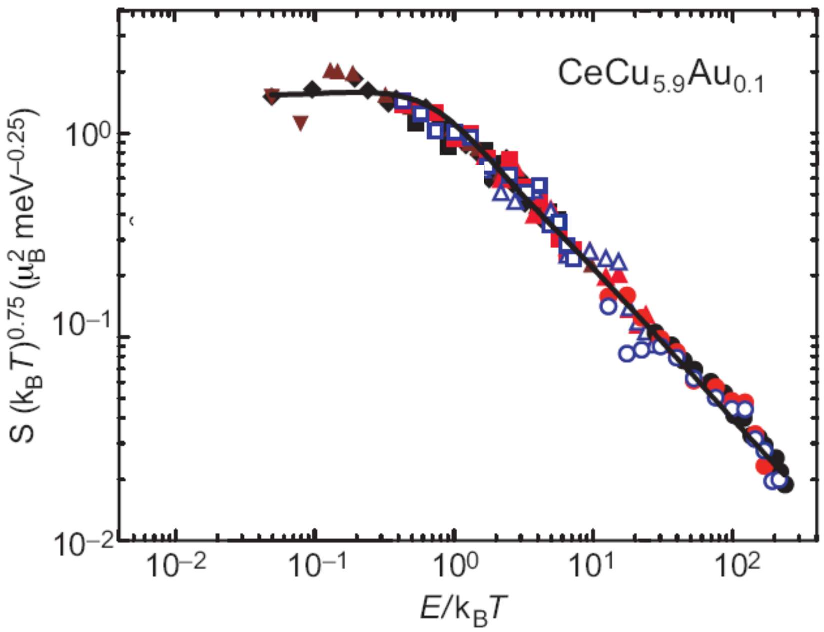
Local Quantum Critical Point

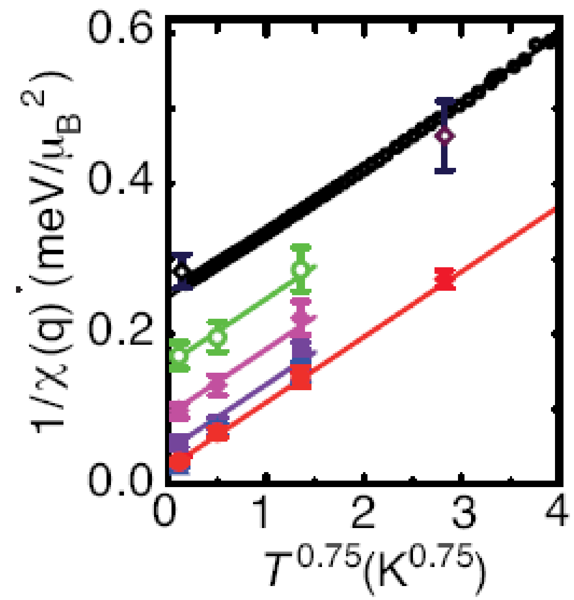
- ω/T scaling in $\chi(\omega,T)$ and $G(\omega,T)$
- Collapse of a large Fermi surface
- Multiple energy scales



- **Introduction to quantum critical point**
- **Kondo problem to heavy Fermi liquid**
- **Heavy fermion quantum criticality**
- **Perspective and outlook**

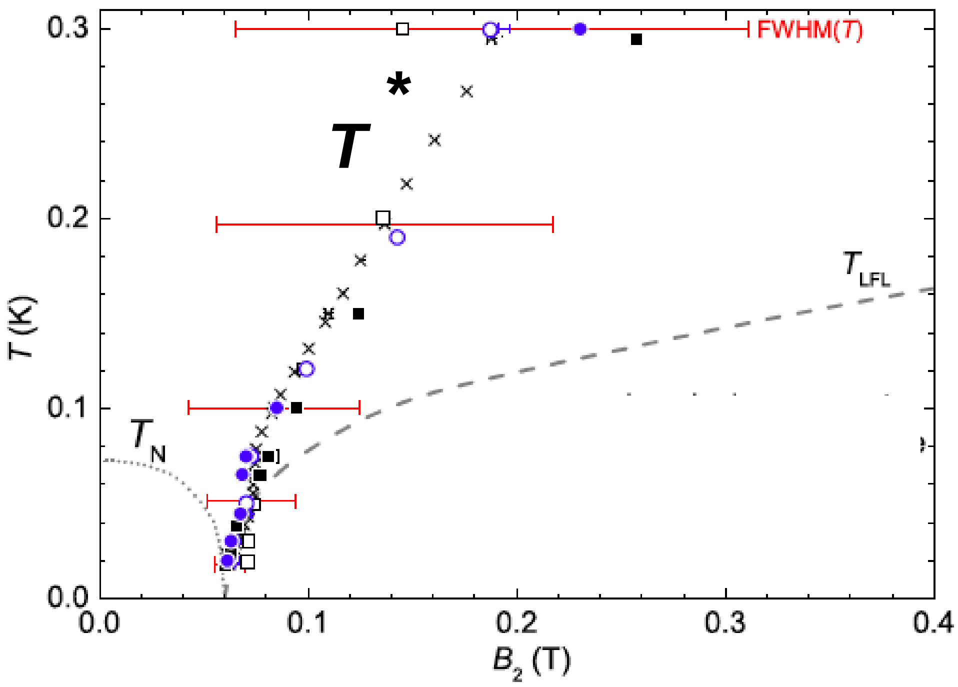
Experiments in $CeCu_{6-x}Au_x$





A. Schröder et al., Nature (’00);
O. Stockert et al; M. Aronson et al.

Experiments in $YbRh_2Si_2$

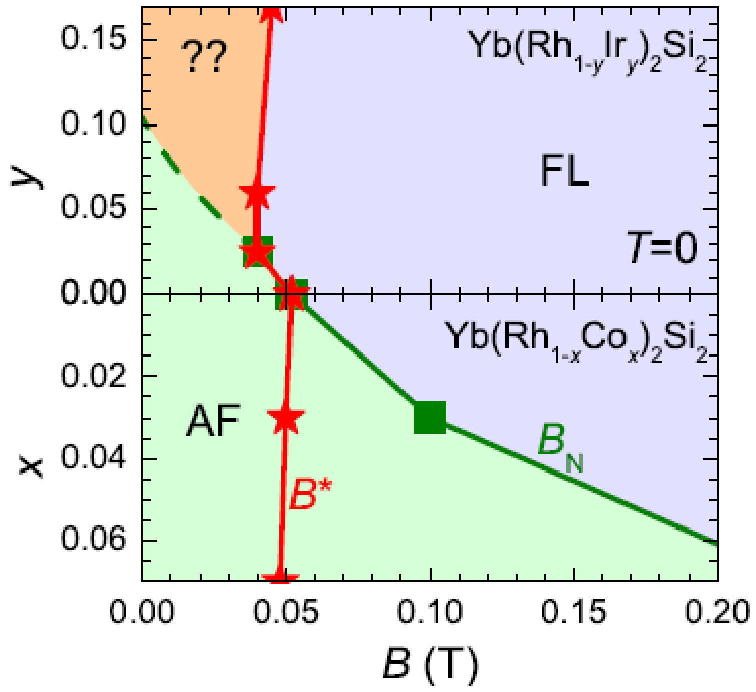


S. Friedemann, N. Oeschler, S. Wirth, C. Krellner, C. Geibel, F. Steglich, S. Paschen, S. Kirchner, and QS, PNAS 107, 14547 (2010)

S. Paschen et al, Nature (2004); P. Gegenwart et al, Science (2007)

Global Phase Diagram

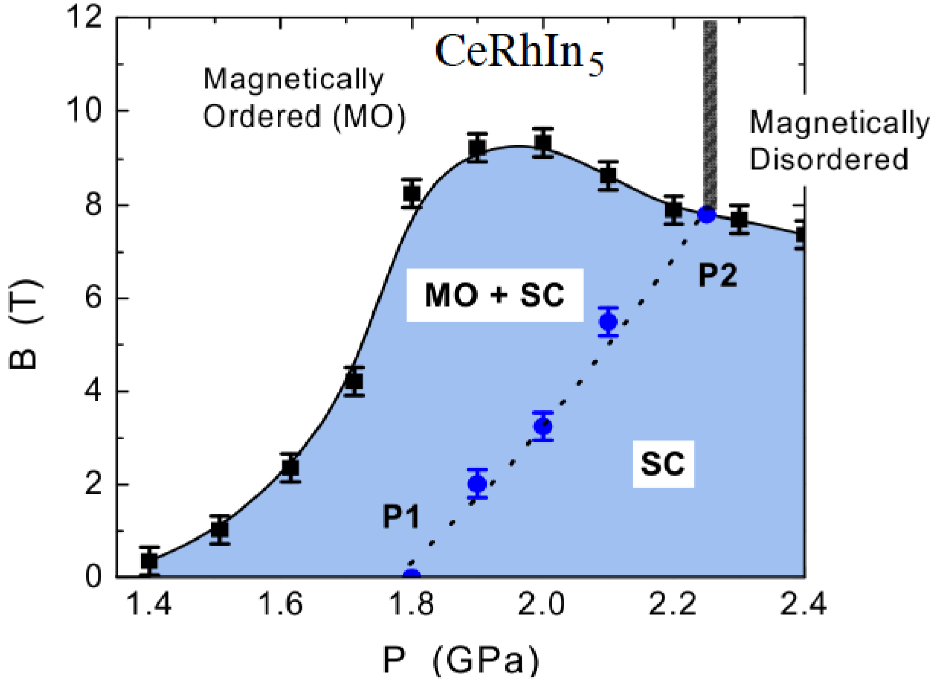
Pure and doped YbRh2Si2

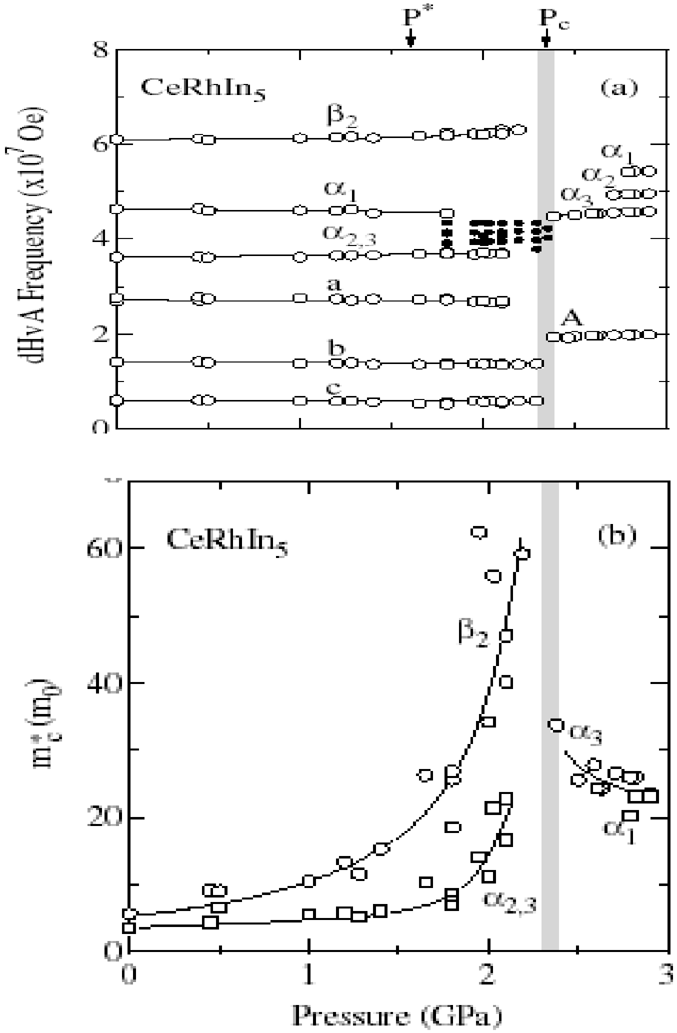


S. Friedemann et al, Nat. Phys. 5, 465 (2009)

also J. Custers et al, PRL 104, 186402 (2010)

Superconductivity near Kondo-destroying AF QCP in CeRhIn5

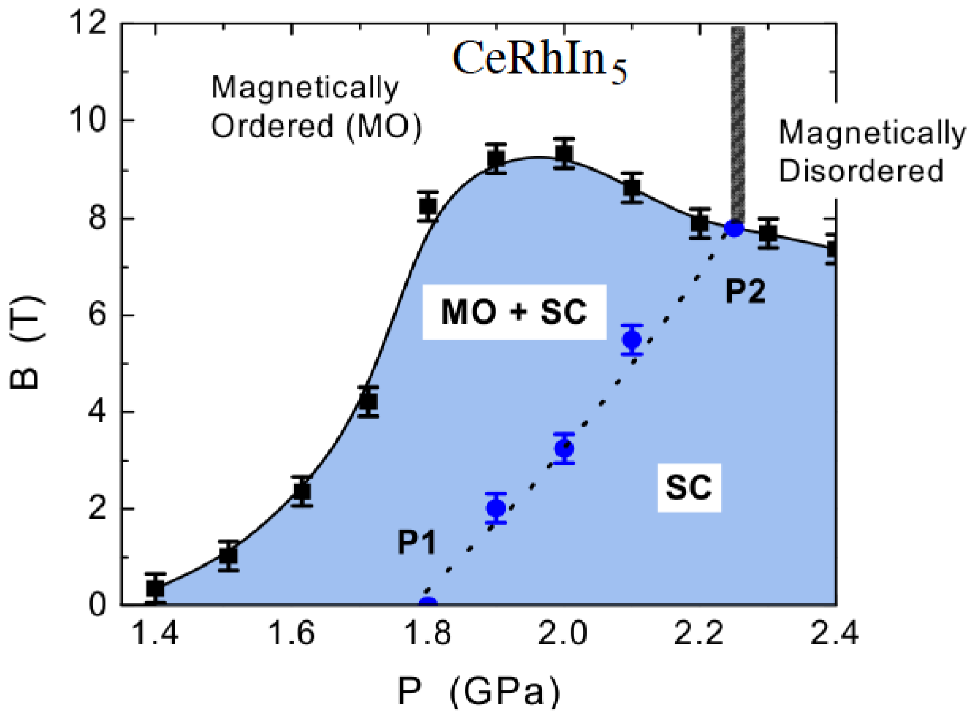


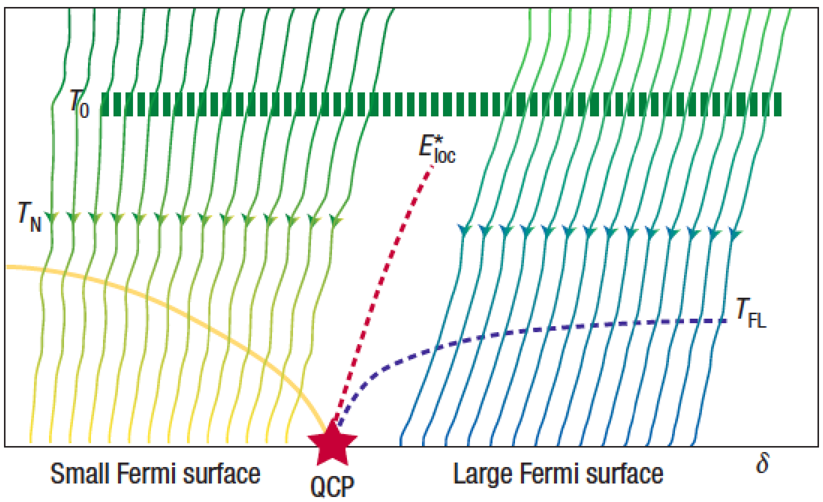


T. Park et al., Nature 440, 65 ('06);
G. Knebel et al., PRB74, 020501 ('06)

H. Shishido, R. Settai, H. Harima, & Y. Onuki, JPSJ 74, 1103 ('05)

Quantum Criticality vs Superconductivity





T. Park et al., Nature 440, 65 ('06);

G. Knebel et al., PRB74, 020501 ('06)

Dynamical Scaling of Local Quantum Critical Point

$$\chi(\mathrm{q},\omega) = \frac{1}{(I_{\mathrm{q}} - I_{\mathrm{Q}}) + A\,(-i\omega)^{\alpha} M(\omega/T)}$$

AdS/CMT:

N. Iqbal, H. Liu, M. Mezei and QS, PRD 82, 045002 ('10)

T. Faulkner, G. T. Horowitz and M. M. Roberts, arXiv:1008.1581

SUMMARY

- Heavy fermions -- prototype quantum critical points

- Heavy Fermi liquid
  - Kondo entaglement in the ground state
  - quantum order without broken symmetry, supports Kondo resonances

- Local quantum critical point: Kondo destruction at antiferromagnetic QCP