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XII WORKSHOP ON
STRONGLY CORRELATED ELECTRON SYSTEMS

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THEORETICAL STUDIES OF QUANTUM CRITICAL BEHAVIOR IN HEAVY FERMIONS

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QUANTUM CRITICAL BEHAVIOR IN HEAVY FERMION METALS

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Outline:

- Brief overview
  - Standard picture
  - Questions raised by recent experiments
- Dynamical competition between Kondo and RKKY
- Two types of quantum critical behavior

Collaborators:

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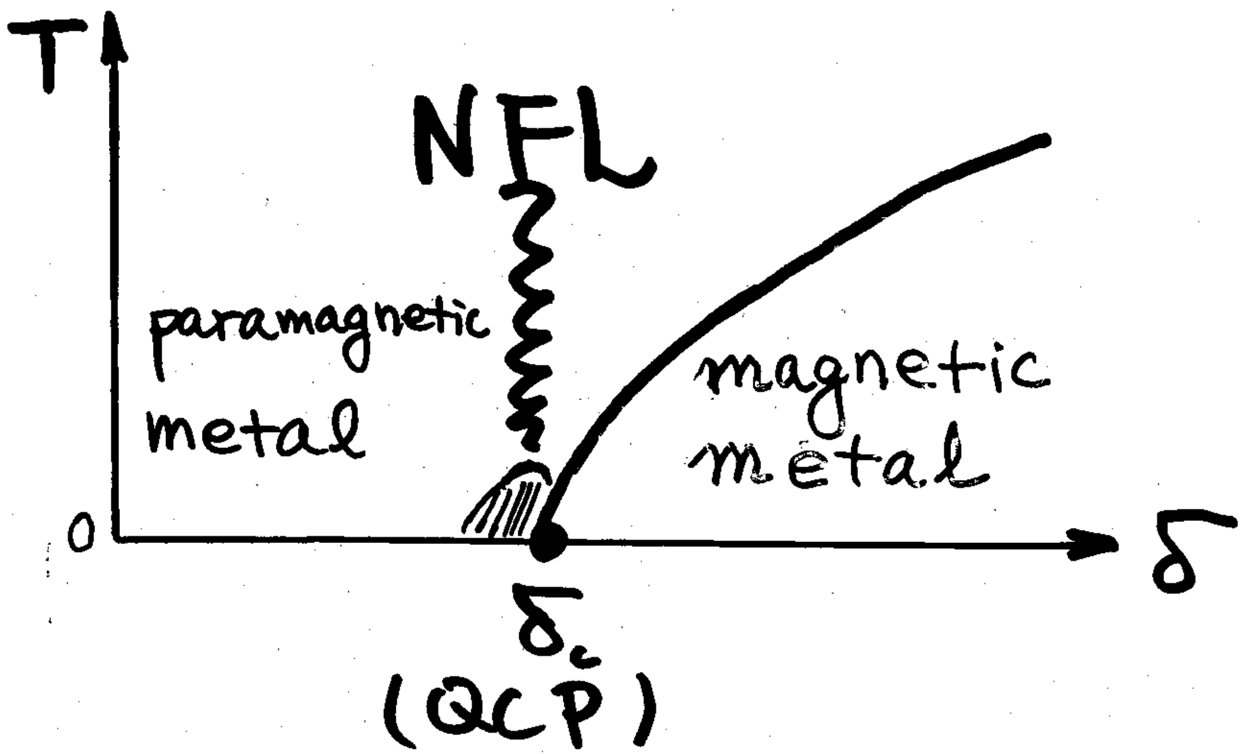
Heavy fermions close to a QCP

- Schematic phase diagram:



- eg. $CePd_2Si_2$, $CeNi_2Ge_2$, $CeCu_{6-x}Au_x$, $\cdots$

- Non-Fermi liquid behavior in the QC regime:
  - Specific heat coefficient C_v/T singular
  - Temperature dependence of resistivity anomalous
  - ...

- Cf. Other routes toward NFL behavior

Standard picture:

- Lattice of local moments
  + conduction electrons

- Doniach phase diagram

  – Kondo: energy scale $T_K^0 \sim W e^{-W/J_K}$

  $\Rightarrow$ paramagnetic metal

  – RKKY: energy scale $I \sim J_K^2/W$

  $\Rightarrow$ magnetic metal

  – The transition is of SDW type: Stoner instability associated with a "large" Fermi surface.

- $\Rightarrow$ Same QC behavior as for ordinary itinerant electron systems

  – $D + z$ dimensional GL theory (Hertz, Millis, $\cdots$)

  – Expected spin susceptibility in the QC regime:

$$\chi(\mathbf{q}, \omega) = \frac{1}{\kappa(T) + b\,(\mathbf{q} - \mathbf{Q})^2 - i\,a\,\omega}$$

Neutron scattering in $\mathrm{CeCu_{6-x}Au_x}$ **at** $\mathrm{x} =$

(Schroder et al '98; '99; Stockert et al, '98)

- Frequency & temperature dependence:

fit with

anomalous exponent

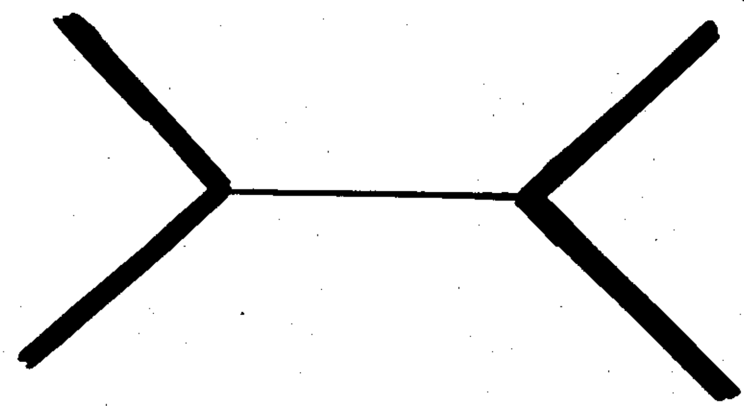
$$\chi(\mathbf{q},\omega) = \frac{1}{f(\mathbf{q}) + A\,(\omega + icT)^{0.75}}$$

for all momentum $\mathbf{q}$

- Momentum dependence:

peaks of $\chi''(q\omega)$:

$\perp \vec{q}$ in a^*c^* plane



c^* ↑ → a^*

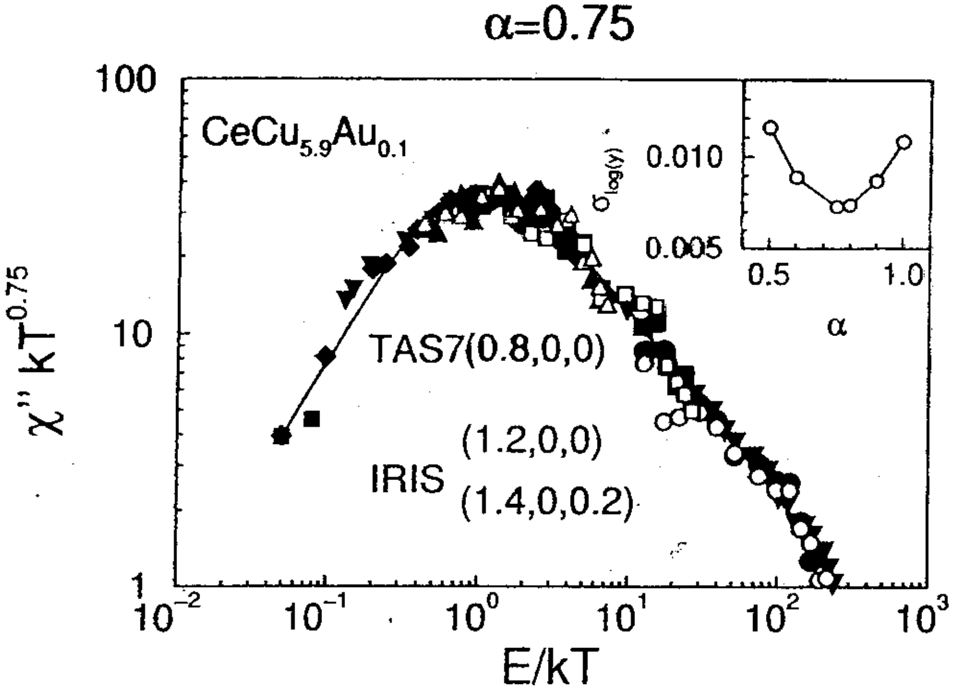
quasi-1D in $\vec{q}$ space

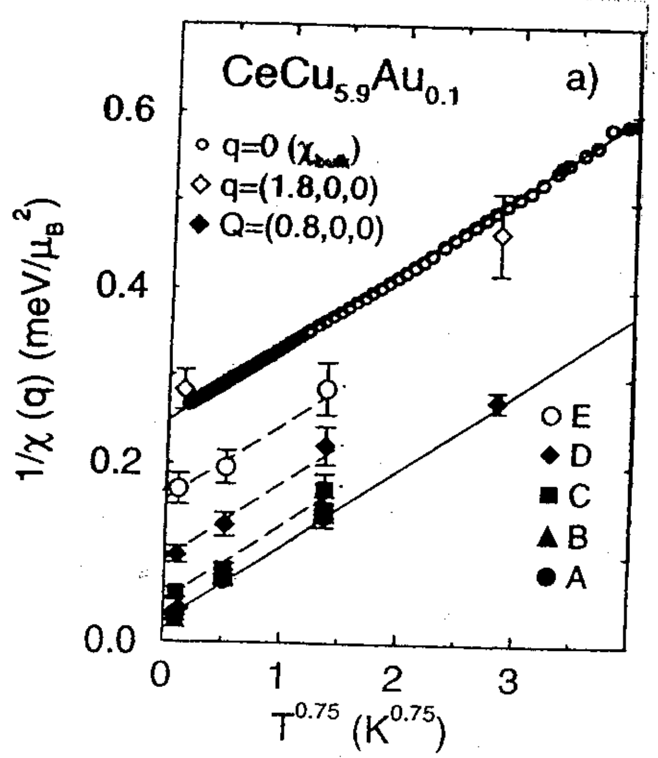
⇒ quasi-2D in $\vec{x}$ space

cf Rosch

Neutron scattering in $CeCu_{6-x}Au_x$ at $x = x_c$

(Schroder et al '98; '99; Stockert et al, '98)





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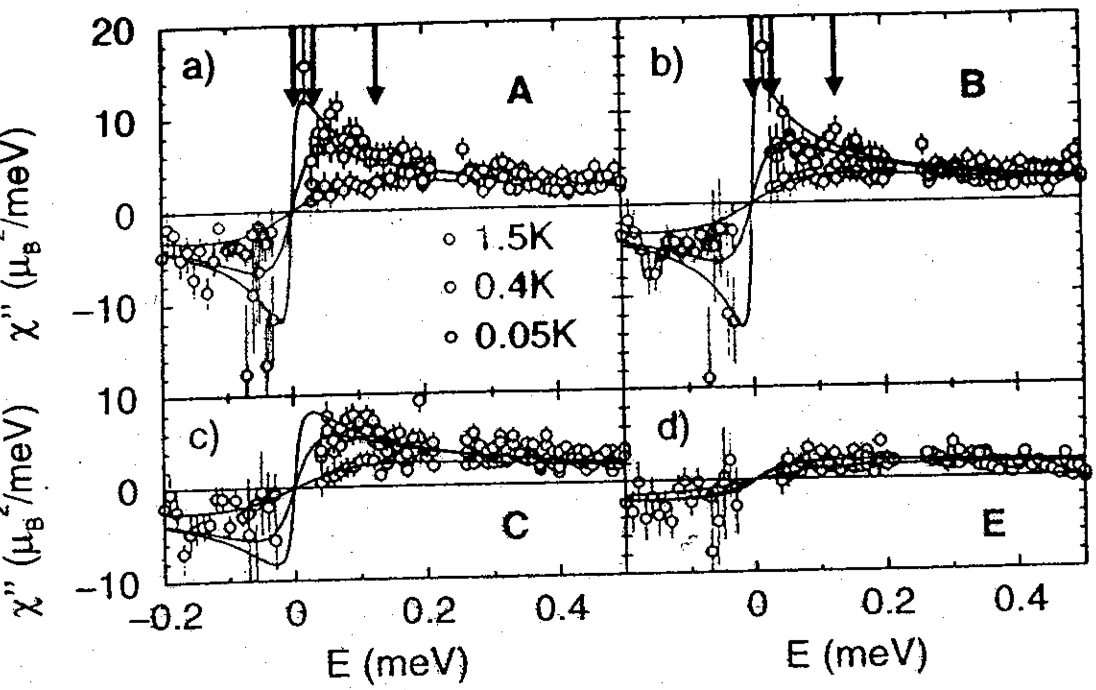

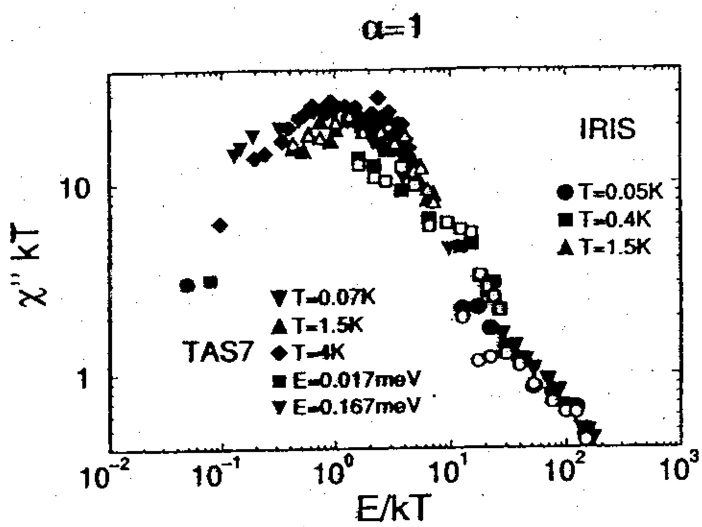

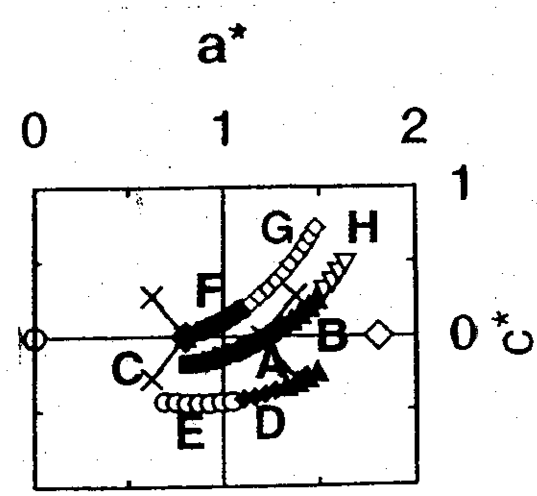

Neutron scattering in $CeCu_{6-x}Au_x$ **at** $x = x_c$

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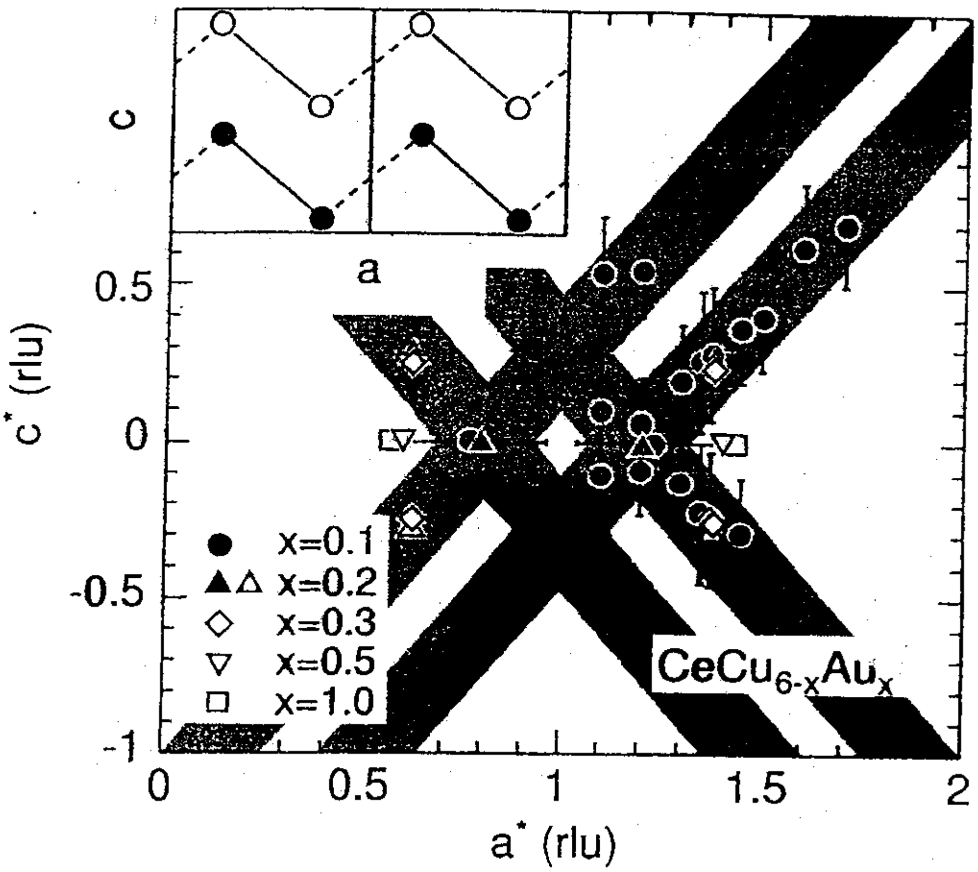


- The question we address: **Is there more than one type of QCPs in Kondo lattices?**

  (Also P. Coleman et al.)

- Main finding: two types of quantum critical behavior can occur

  – first type: SDW transition

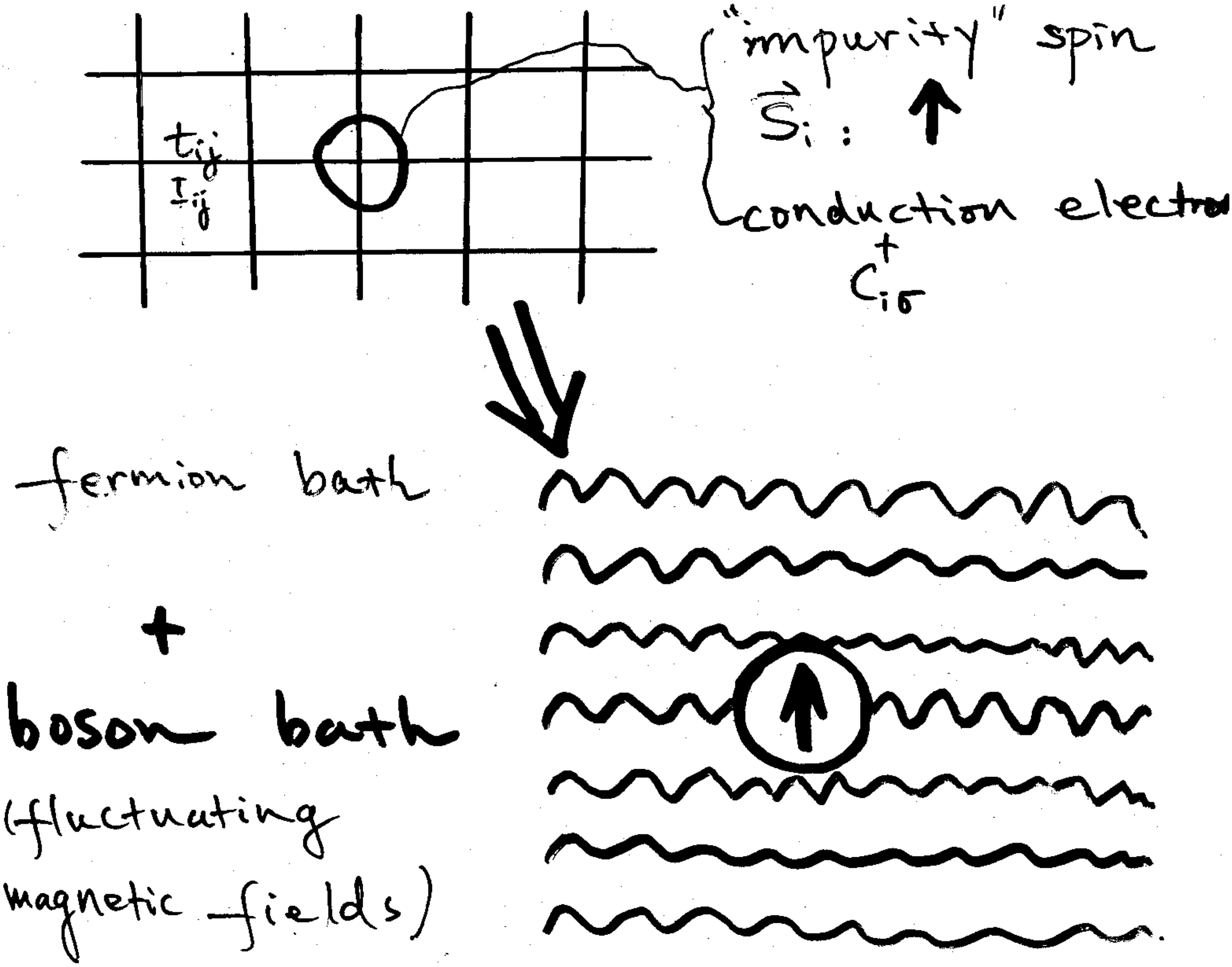
  – second type: local (Kondo) physics also critical

Extended DMFT* of the Kondo lattice: Qualitative picture

(* Smith & QS; Chitra & Kotliar)

$$\mathcal{H} = \sum_{ij,\sigma} t_{ij}\, c_{i\sigma}^{\dagger}\, c_{j\sigma} + \sum_{i} J_K\, \mathbf{S}_i \cdot \mathbf{s}_{c,i}$$

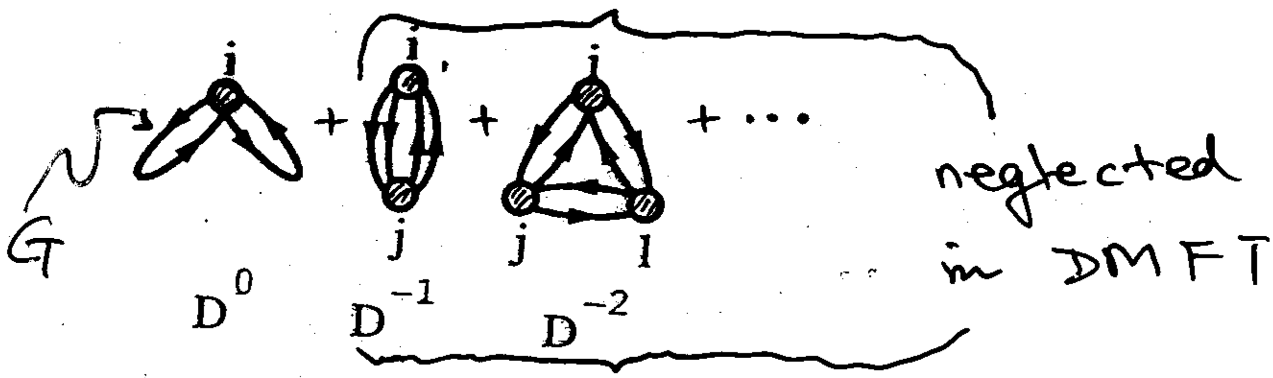
$$- \sum_{ij} I_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j$$



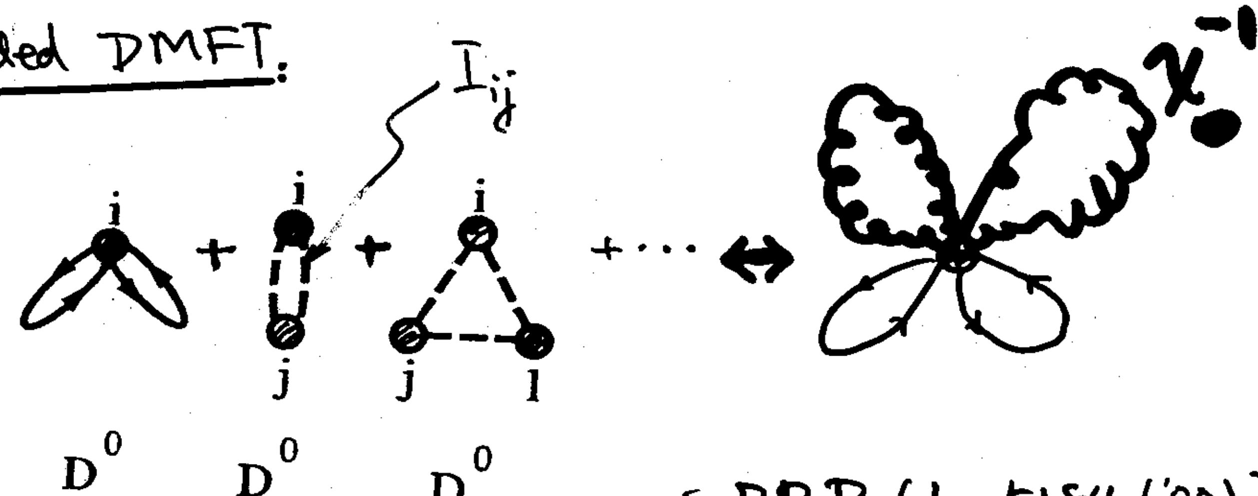
Extended DMFT of the Kondo lattice:
(Cont'd)

- Conserving resummation of $1/D$ expansion:

DMFT (Georges, Kotliar et al RMP '96)



Extended DMFT:



[PRB 61, 5184 ('00)]

- Implemented by taking the large D limit with $t_{<ij>} = t_0/\sqrt{2D}$ and $I_{<ij>} = I_0/\sqrt{2D}$.

Effective impurity problem

- The RKKY interactions lead to an additional retarded interaction:

$$\Delta\mathcal{S}_{\rm imp} = -\int d\tau \int d\tau' \, \chi_0^{-1}(\tau-\tau') \, \mathbf{S}(\tau)\cdot\mathbf{S}(\tau')$$

- Effective impurity Hamiltonian:

$$\mathcal{H}_{\rm imp} = J_K \, \mathbf{S}\cdot\mathbf{s}_c + \sum_{k,\sigma} E_k \, c^\dagger_{k\sigma} c_{k\sigma}$$
$$+ g \sum_k \mathbf{S}\cdot\left(\vec{\phi}_k + \vec{\phi}^{\,\dagger}_{-k}\right) + \sum_k w_k \, \vec{\phi}^{\,\dagger}_k \cdot \vec{\phi}_k$$

fluctuating magnetic fields

where

$$g^2 \sum_k \delta(\omega - w_k) = {\rm Im}\chi_0^{-1}(\omega)$$

- Self-consistently,

  – g and w_k determined by I_0 and χ

  – E_k determined by t_0 and G

RKKY

Self-consistency condition

- $$\frac{1}{N_{site}} \sum_{\mathbf{k}} G(\mathbf{k},\omega) = G_{loc}(\omega)$$

  $$\frac{1}{N_{site}} \sum_{\mathbf{q}} \chi(\mathbf{q},\omega) = \chi_{loc}(\omega)$$

- Lattice Green function

$$G(\mathbf{k},\omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma(\omega)}$$

- Lattice spin susceptibility

$$\boxed{\chi(\mathbf{q},\omega) = \frac{1}{M(\omega) - I_{\mathbf{q}}}}$$

$M(\omega)$ is "spin self-energy", which satisfies

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

(Cf. RPA $\quad M^{-1}_{RPA} =$ )

Step I: Characterizing two types of QCPs

The form $\chi(\mathbf{q},\omega) = \frac{1}{M(\omega)-I_{\mathbf{q}}} \Longrightarrow$ QCP can be characterized in terms of the behavior of the "spin self-energy" $M(\omega)$:

- first type:

$$\mathrm{Im} M^{-1}(\omega) = \frac{1}{(E^*_{loc})^2}\,\omega$$

E^*_{loc} is the effective Fermi energy

- second type:

$$\mathrm{Im} M^{-1}(\omega) \sim |\omega|^{\alpha}\,\mathrm{sgn}\omega \quad \text{with} \; 0 < \alpha < 1$$

$E^*_{loc} = 0$: a QCP with anomalous local dynamics

Step II: Origin of the anomalous local dynamics

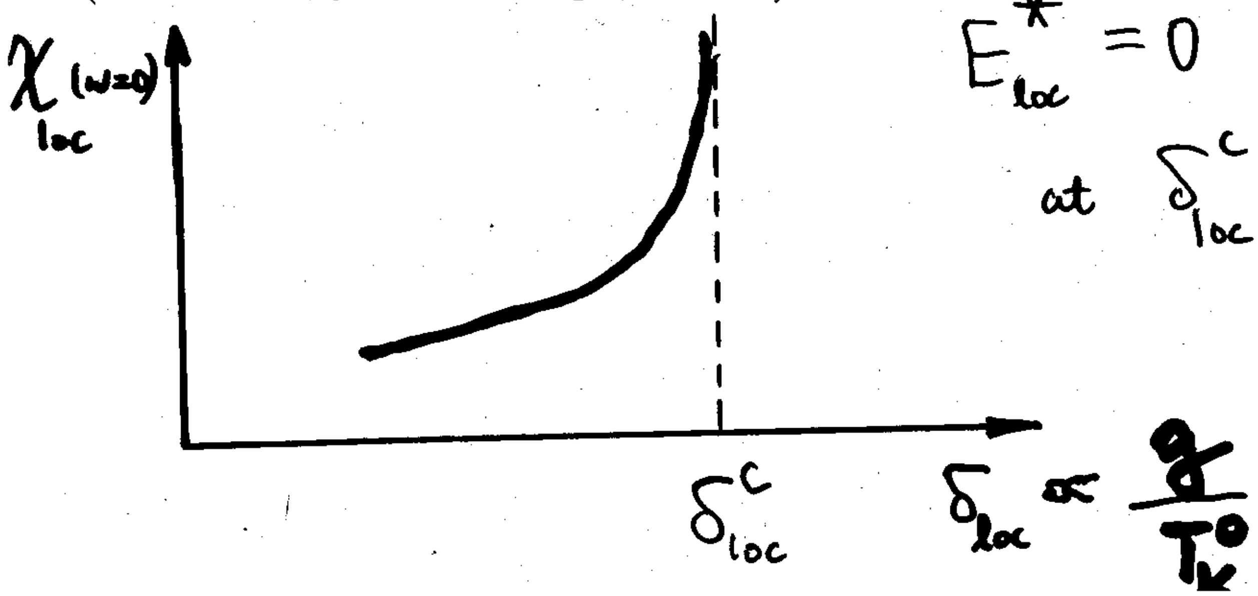
- Effective impurity problem once again:

$$\mathcal{H}_{\text{imp}} = J_K\, \mathbf{S}\cdot\mathbf{s}_c + \sum_{k,\sigma} E_k\, c_{k\sigma}^{\dagger}\, c_{k\sigma} + g \sum_{k} \mathbf{S}\cdot\left(\vec{\phi}_k + \vec{\phi}_{-k}^{\,\dagger}\right) + \sum_{k} w_k\, \vec{\phi}_k^{\,\dagger}\cdot\vec{\phi}_k$$

- If we just put in a sub-ohmic spectrum for the fluctuating magnetic field $\vec{\phi}$:

$$\sum_{k} \delta(\omega - w_k) \sim |\omega|^{\gamma}\,\text{sgn}\omega \qquad \text{with} \quad \gamma < 1$$

then $\mathcal{H}_{\text{imp}}$ does indeed have a QCP of its own (Smith & QS '97; Sengupta '97)



“RKKY- density of states”

- $$\boxed{\rho_I(\epsilon) \equiv \sum_{\mathbf{q}} \delta(\epsilon - I_{\mathbf{q}})}$$

  Cf. conduction electron d.o.s.

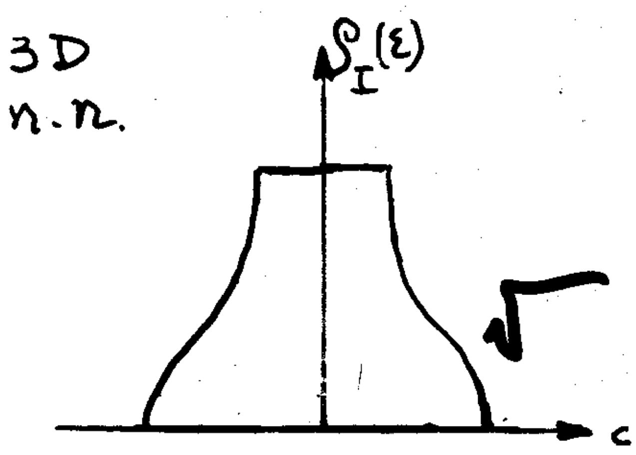
  $$\rho(\epsilon) \equiv \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}})$$

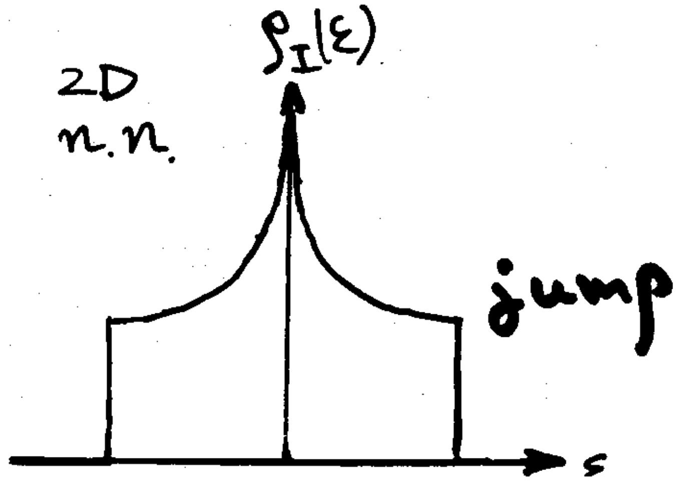
- The self-consistency condition can be rewritten as

  $$\int d\epsilon\ \rho_I(\epsilon)\ \frac{1}{M(\omega) - \epsilon} = \chi_{loc}(\omega) \quad = \sum_{q} \frac{1}{M(\omega) - I_q}$$

  $$\int d\epsilon\ \rho(\epsilon)\ \frac{1}{\omega + \mu - \Sigma(\omega) - \epsilon} = G_{loc}(\omega)$$

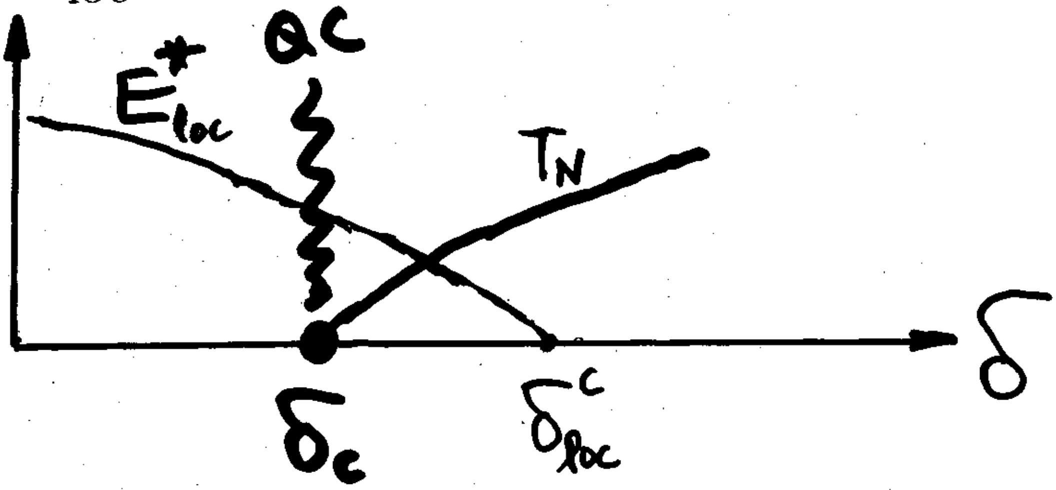
- Extended DMFT as an approximation for finite D systems:





Step III: Self-consistent solution – two types of QCPs

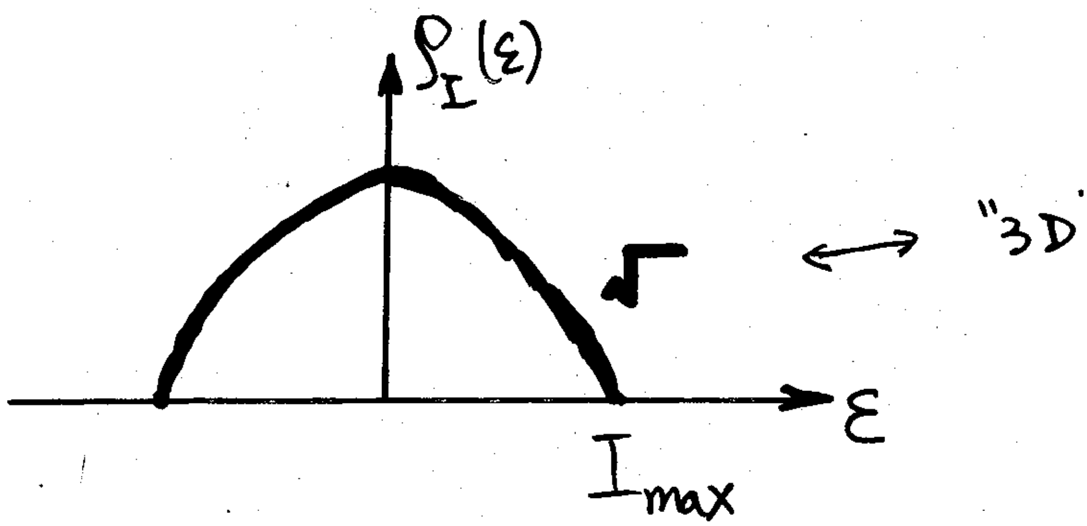
- If $\chi(\mathbf{Q}, \omega = 0) = \frac{1}{M(\omega=0) - I_{\max}} \to \infty$ at $\delta_c < \delta_{\rm loc}^c$,



then

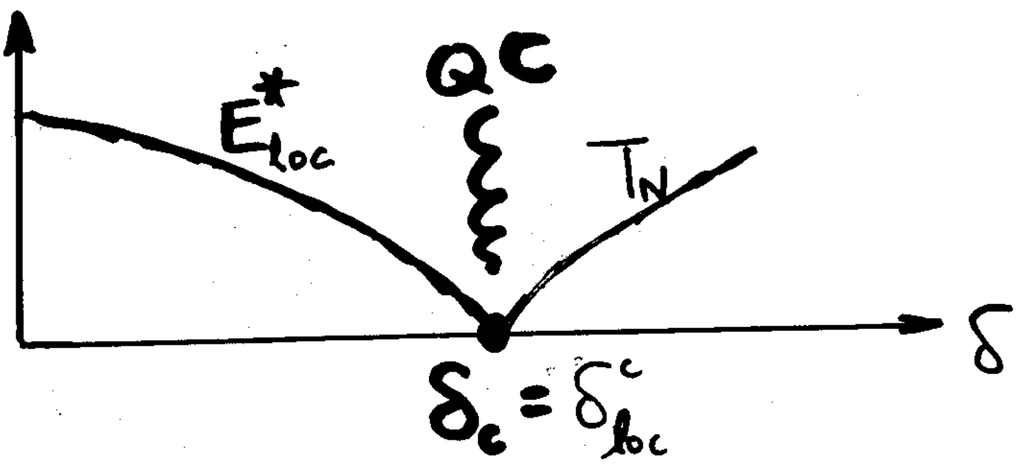
- at δ_c, the local problem is not critical; local moments completely quenched
- $\Rightarrow$ the QCP is of SDW (or Hertz) type

- This occurs for a semi-circular "RKKY-d.o.s."



Step III: Self-consistent solution – two types of QCPs (Cont'd)

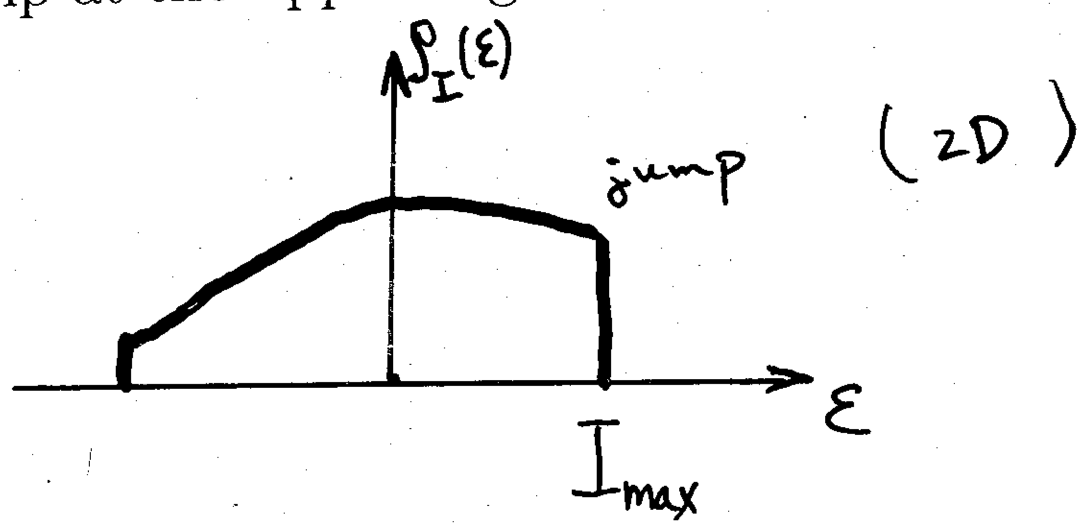
- If $\chi(\mathbf{Q}, \omega = 0) = \frac{1}{M(\omega=0) - I_{\max}} \to \infty$ exactly at $\delta_c = \delta_{\text{loc}}^c$,



then

- at δ_c, the local problem is also critical; vestiges of local moments remain.
- $\Rightarrow$ non-SDW (or non-Hertz) QCP.

- This occurs whenever the "RKKY-d.o.s." has a jump at the upper edge:



Dynamical spin susceptibility at the non-Hertz QCP

- Local susceptibility

$$\chi_{loc}(\omega) = \frac{1}{2\Lambda}(\ln \frac{\Lambda}{|\omega|} + i\frac{\pi}{2} \text{ sgn } \omega)$$

- "spin self-energy"

$$M(\omega) \approx I_{\text{max}} + A\,\omega^{\alpha}$$
$$\text{where } \alpha = [2\rho_I(I_{\text{max}})\Lambda]^{-1}$$

- $\mathbf{q}$–dependent susceptibility

$$\boxed{\chi(\mathbf{q},\omega) = \frac{1}{(I_{\text{max}} - I_{\mathbf{q}}) + A\,\omega^{\alpha}}}$$

- Cf. $CeCu_{6-x}Au_x$ at $x = x_c$:
  - $\alpha \approx 0.75$
  - quasi-2D

Summary

- Extended DMFT of the Kondo lattice:
  - conserving resummation of $1/D$ expansion
  - captures the dynamical competition between Kondo and RKKY interactions

- Two types of QCPs:
  - SDW (Hertz) type
  - non-SDW (non-Hertz) type: local Kondo physics is also critical

- 2D fluctuations facilitate the realization of non-Hertz QCPs

- Cf. neutron scattering in $CeCu_{6-x}Au_x$