Local Fluctuations and non-Fermi Liquid Properties in Quantum Critical Metals

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Heavy fermions as prototype QC metals:

- QCPs explicitly identified
  - mostly (T=0) transition from a paramagnetic metal to an AF metal

- Stoichiometric/nearly stoichiometric systems: $YbRh_2Si_2$, $CeCu_{6-x}Au_x$, $CePd_2Si_2$, $CeIn_3$, . . .

- Non-Fermi liquid behavior in the QC regime:
  - Resistivity anomalous (e.g., linear in T)
  - Specific heat anomalous – two classes:
    * C_v/T singular (e.g., $\ln\frac{T_0}{T}$)
    * C_v/T non-analytic ($\gamma_0 - \gamma_1 T^\beta$)

- Fermi liquid behavior recovered away from the QCP

Traditional picture

Consider AF case, ordering wavevector $\mathbf{Q} \neq \mathbf{0}$

- $T = 0$ SDW transition (Hertz '76, Millis, Moriya, Lonzarich, Continentino, Lavagna $\cdots$)

  – Critical d.o.f: long-wavelength fluctuations of the order parameter $\mathbf{m}(\mathbf{q} \sim \mathbf{Q}, \omega \sim 0)$ (paramagnons)

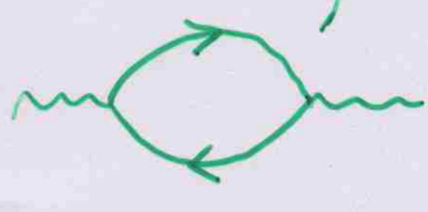
- ϕ^4 theory with $D_{eff} = D + z \geq 4$
  $\Rightarrow$ Gaussian fixed point

  dynamic exponent $z = 2$

  mixed {
  – statics: $\xi \to \infty$
  – (quantum) dynamics: $\xi_\tau \sim \xi^z \to \infty$

- Expected dynamical spin susceptibility

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



Some key puzzles from heavy fermions

- Anomalous exponent $\alpha < 1$ & ω/T scaling:
  - implying non-Gaussian fixed point
- The same α seen essentially everywhere in the Brillouin zone:
  - suggesting new local physics

A new class of QCP, beyond ϕ^4 theory

Remainder of the talk:

- Microscopic model & comparison w/ expts
- Beyond microscopics

Cf. also Coleman *et al.*; Sachdev *et al.*

Revisiting on the $T = 0$ SDW picture:

- ϕ^4 theory appears internally consistent
  - cf. however, Chubukov *et al.*; Belitz & Kirkpatrick
- fermions are by-standers

Fermions and local moments

- "Kondo-logy" (single local moment)
  - Kondo temperature T_K^0
  - Kondo singlet $\frac{1}{2}(|\uparrow>_f |\downarrow>_c - |\downarrow>_f |\uparrow>_c)$
  - Kondo resonance
- Heavy fermions: a lattice of local moments in a conduction electron sea

Q: Do "heavy fermions" remain as by-standers at QCP?

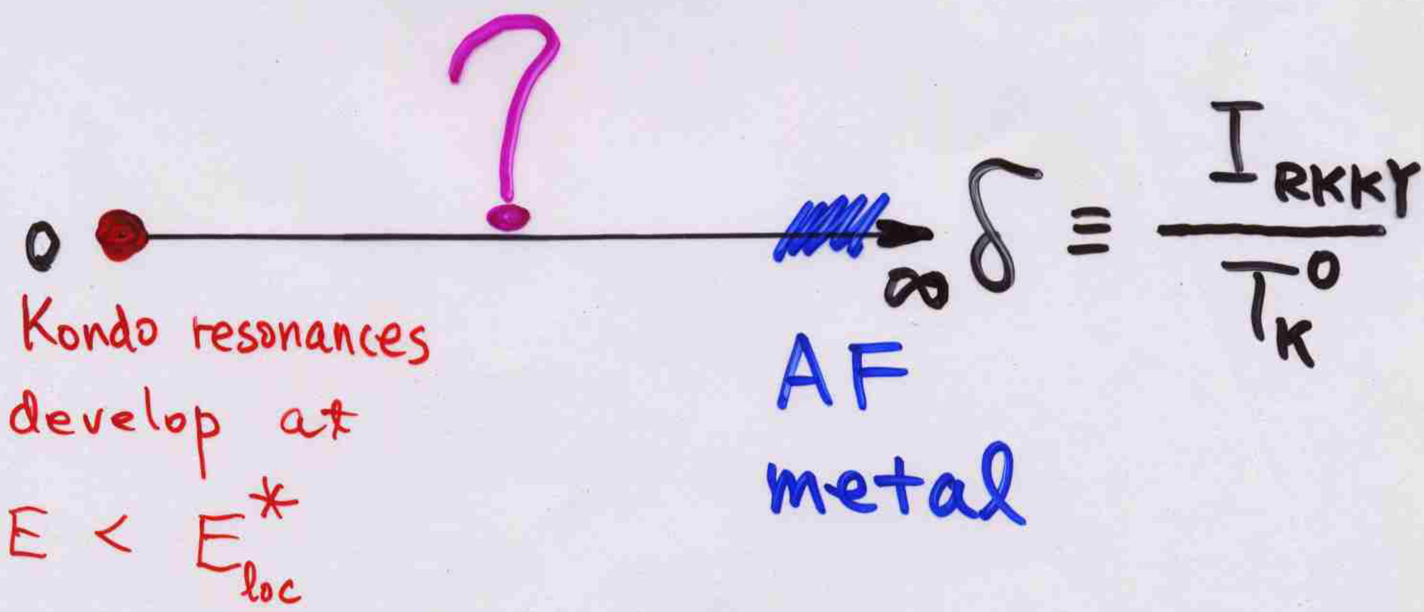
- Kondo lattice:

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

local moments

away from half-filling

- Kondo vs. RKKY
  - When $\delta \equiv \frac{\mathrm{I_{rkky}}}{\mathrm{T_K^0}}$ is small: Kondo resonance develops $\Rightarrow$ paramagnetic metal with heavy quasiparticles (Doniach, Varma, $\cdots$)
  - When δ is very large: AF metal

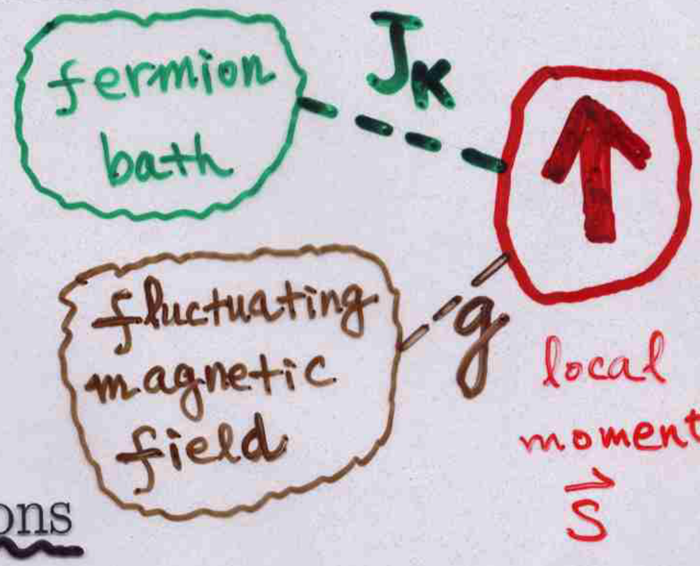


Extended-DMFT* of Kondo lattice

(* Smith & QS; Chitra & Kotliar)

- Mapping to a Bose-Fermi Kondo model

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



+ self-consistency conditions

- The effective impurity problem determines
  - electron self-energy $\Sigma(\omega)$
  - "spin self-energy" $M(\omega)$
- Dynamical spin susceptibility

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

(Cf. Contrast to RPA:

$M^{-1}_{RPA} =$ 

$\sim$ const $- i\omega$)

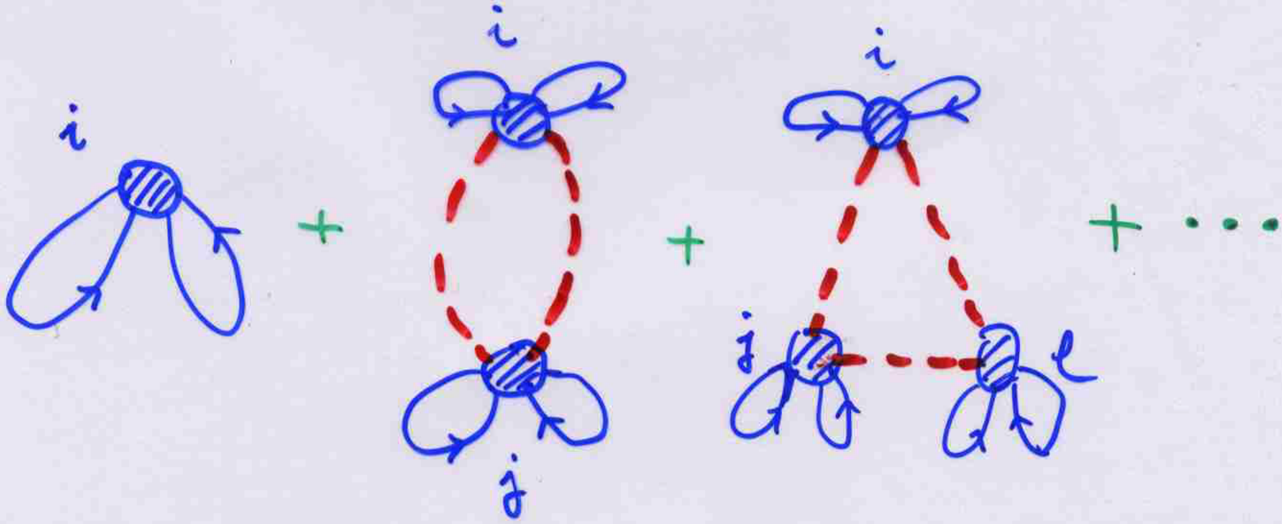
Extended DMFT

Take Kondo lattice as an example:

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

$$+\frac{1}{2}\sum_{ij} I_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j$$

- Conserving resummation of diagrams:



Dynamical susceptibility

- The effective impurity problem determines
  - electron self-energy $\Sigma(\omega)$
  - "spin self-energy" $M(\omega)$:

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

- Lattice dynamical spin susceptibility

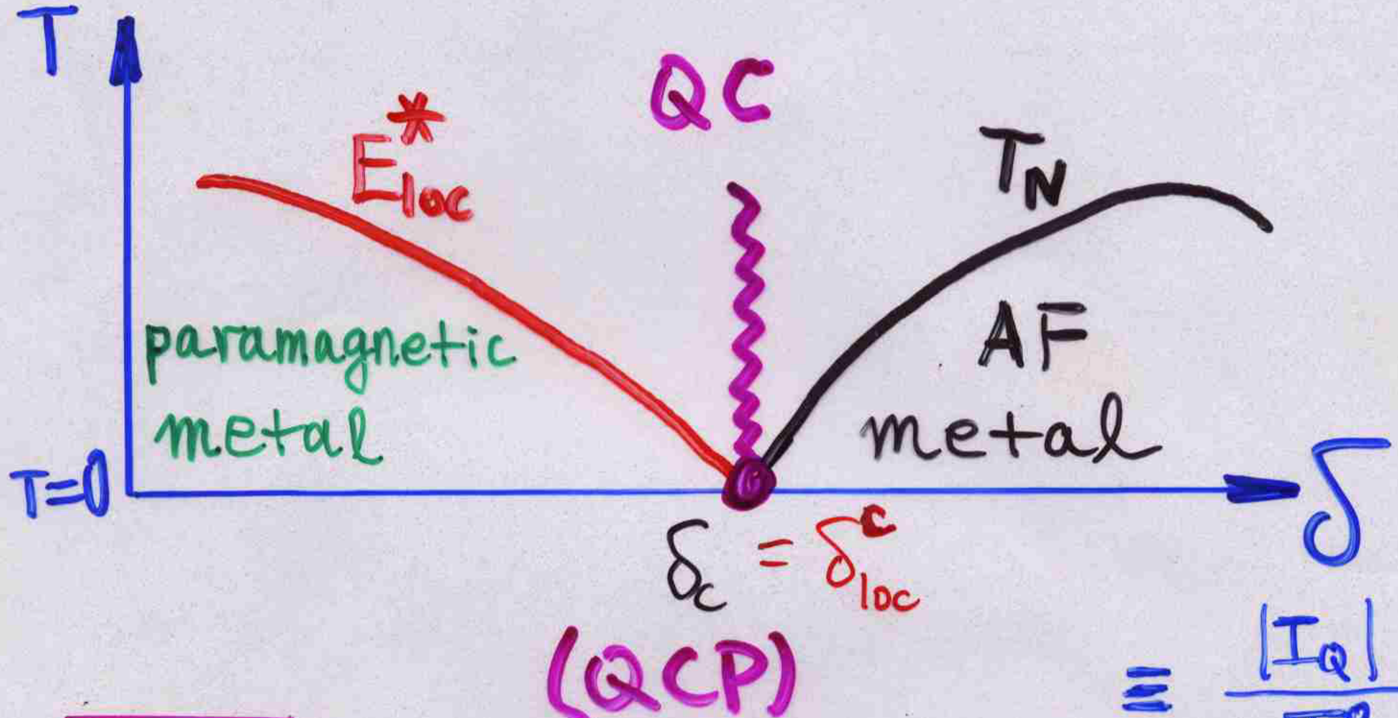
$$\chi(\mathbf{q},\omega) = \frac{1}{M(\omega) + I_{\mathbf{q}}}$$

Self-consistency equations

$$\langle\, G(\mathbf{k},\omega)\,\rangle_{\mathbf{k}} \;=\; G_{loc}(\omega)$$

$$\langle\, \chi(\mathbf{q},\omega)\,\rangle_{\mathbf{q}} \;=\; \chi_{loc}(\omega)$$

Locally quantum critical point

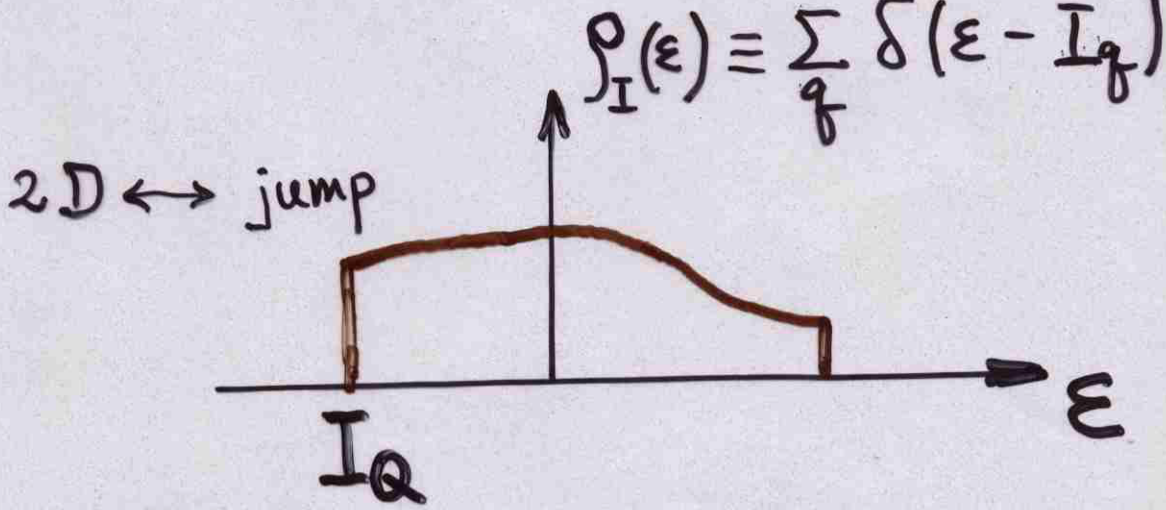


$\equiv \frac{|I_Q|}{T_K^0}$

$\delta_c = \delta^c_{loc}$: at the QCP, E^*_{loc} vanishes

(cf: 3D)

This occurs for 2D magnetic fluctuations:

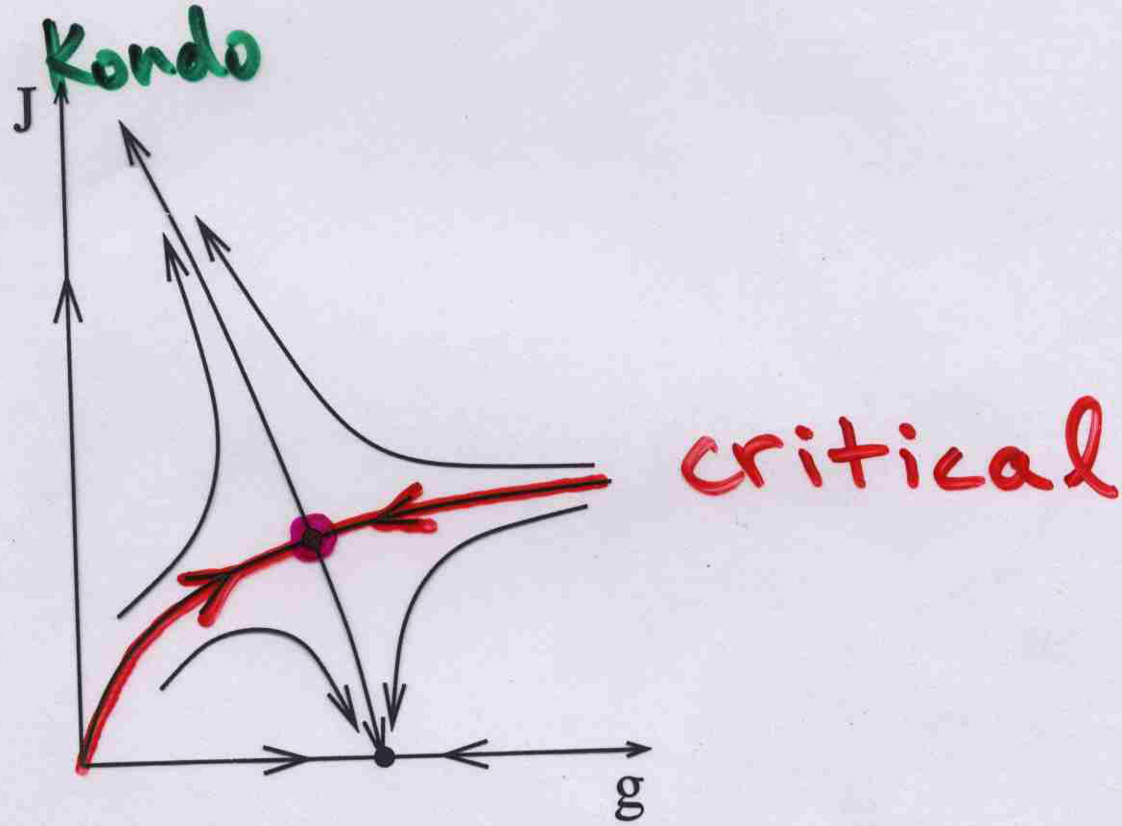


QS, S. Rabello, K. Ingersent, & J. L. Smith, Nature, '01 ;

– – –, cond-mat/0202414 (containing the details)

$\epsilon(\equiv 1-\gamma)$ expansion of the Bose-Fermi Kondo model

$$\sum_p \left[\delta(\omega - w_p) - \delta(\omega + w_p)\right] \sim |\omega|^\gamma \,\mathrm{sgn}\omega$$



order ϵ:	J. L. Smith & QS '97
	A. M. Sengupta '97
higher orders:	L. Zhu & QS '02
	G. Zarand & E. Demler '02
$J = 0$:	S. Sachdev & J. Ye '93 (large N)
	M. Vojta, C. Buragohain, & S. Sachdev '00

At the QCP:

- Local susceptibility

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

where $\Lambda \approx T_K^0$

- "spin self-energy"

$$M(\omega) \approx -I_{\mathbf{Q}} + A\,(-i\omega)^{\alpha}$$

with

$$\alpha = \frac{1}{2\rho_I(I_{\mathbf{Q}})\Lambda} \sim \frac{1}{2}$$

Numerical identification of LCP

(D. Grempel & QS, cond-mat/0207493)

- Anisotropic Kondo lattice:

$$\mathcal{H} = \sum_{ij,\sigma} t_{ij}\, c_{i\sigma}^{\dagger}\, c_{j\sigma} + \sum_i J_K\, \mathbf{S}_i \cdot \mathbf{s}_{c,i} + \sum_{ij} \frac{I_{ij}}{2} S_i^z\, S_j^z$$

- EDMFT $\Rightarrow$

$$Z_{\text{imp}} \sim \int \mathcal{D}n \int d\lambda\ \exp[-\int_0^{\beta} d\tau\, \mathcal{L}/2\,]$$

where

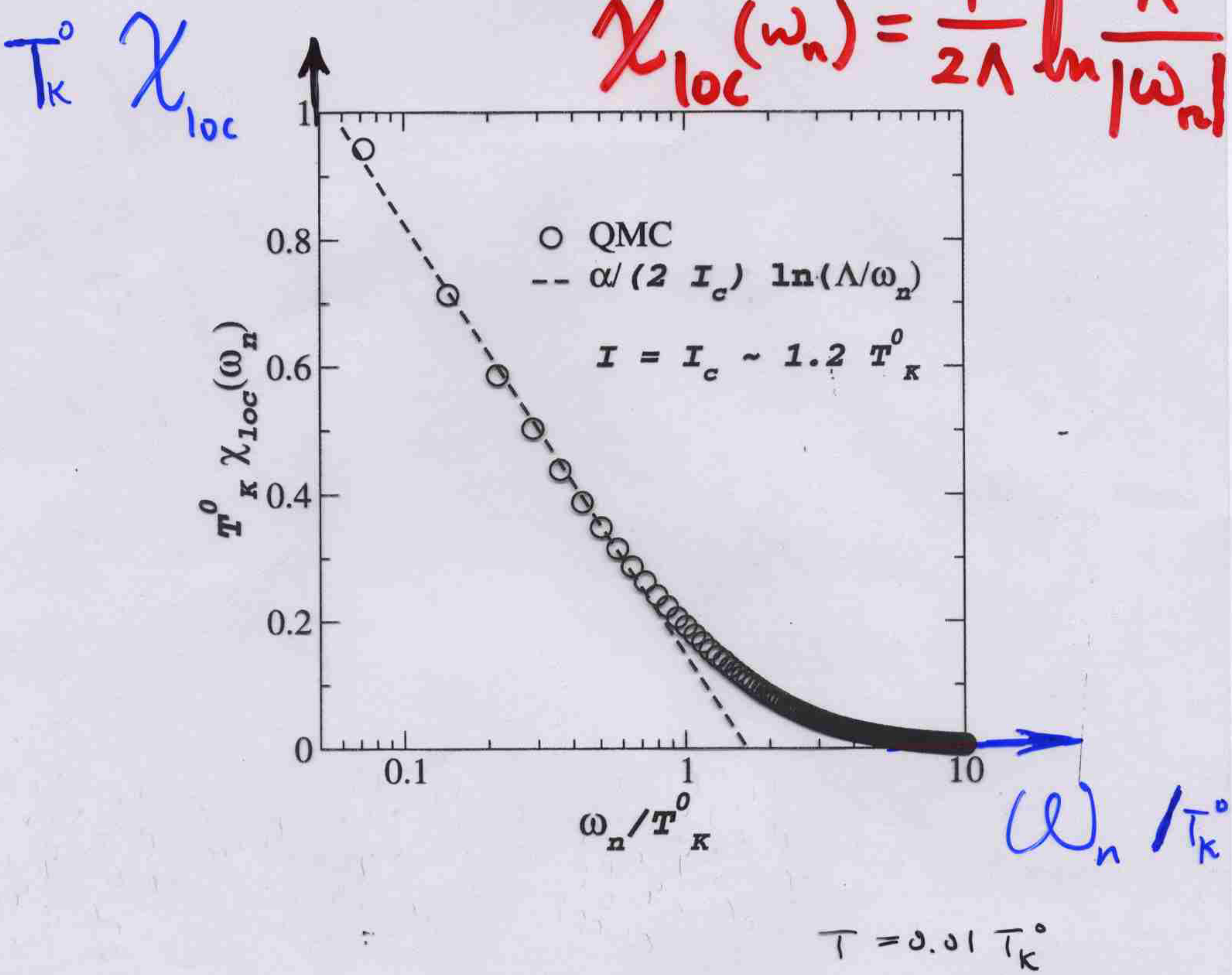
$$\mathcal{L} = i\lambda(n^2 - \frac{1}{4}) + \frac{1}{g}(\partial_\tau n)^2 - \int d\tau' n(\tau) n(\tau') \times \times [\chi_0^{-1}(\tau - \tau') - \mathcal{K}_c(\tau - \tau')]$$

and self-consistency conditions

- QMC (Grempel & Rozenberg)

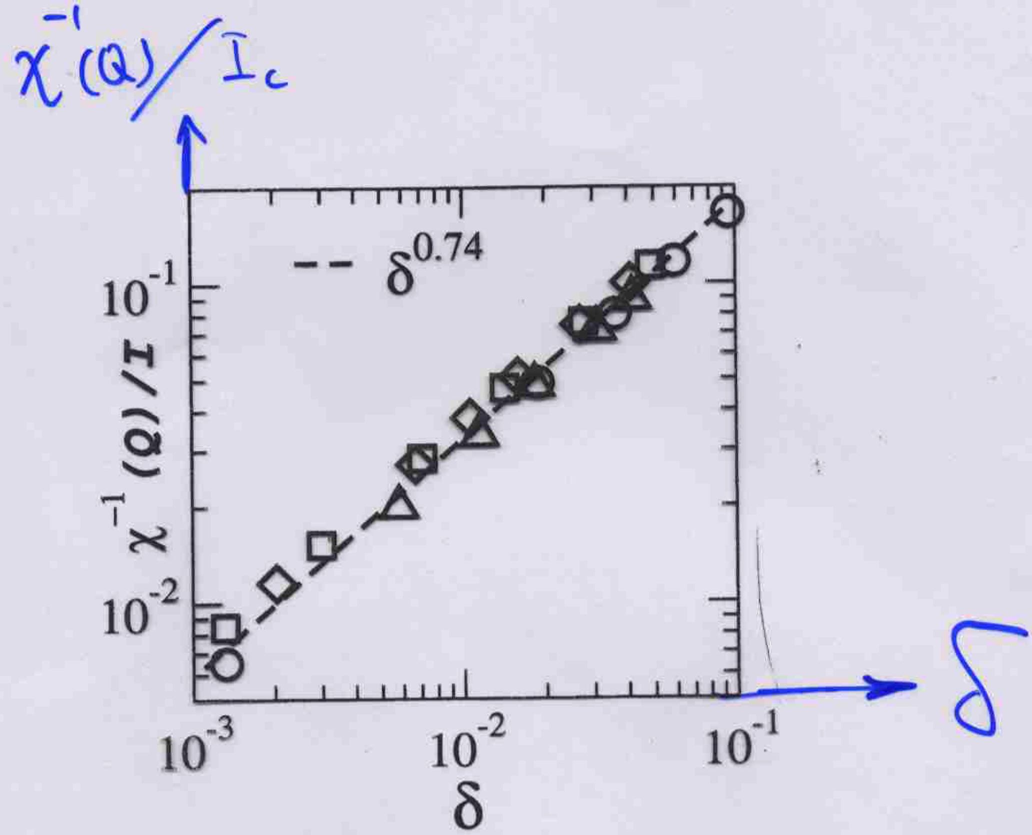
- Large N limit (Ye, Sachdev & Read; Sengupta & Georges)

• Local susceptibility at $\mathrm{I} = \mathrm{I_c}$:



• also consistent with large N saddle-point results

- Inverse peak susceptibility at $I \sim I_c$



$\chi^{-1}(Q, \omega=0) \sim \delta^{\alpha}$

w/ $\alpha \approx 0.7$

- $\delta(T=0) \propto (I_c - I)$

- $\delta(T, I_c) \propto T$

- Importance of treating both Kondo and RKKY (unstable fixed point of $H_{\rm imp}$):
  - Locally critical solution is numerically stable to T=0

- Spin-isotropic case: numerical algorithms capable of treating both Kondo and RKKY are yet to be developed
  - Cf. complementary results from S. Burdin, M. Grilli, and D. R. Grempel, cond-mat/0206174
    * EDMFT w/ RKKY alone (stable fixed point of $H_{\rm imp}$):
    * solution for the spin-liquid phase develops instability at $T < T_{\rm inst}$

Spin dynamics at the locally QCP:

- Dynamical spin susceptibility

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

- Static uniform spin susceptibility

$$\chi(T) = \frac{1}{\Theta + B\,T^{\alpha}}$$

- NMR relaxation rate:

$$\frac{1}{T_1} \sim A_{hf}^2\,\frac{\pi}{8\Lambda}$$

Scaling function

- "spin self-energy"

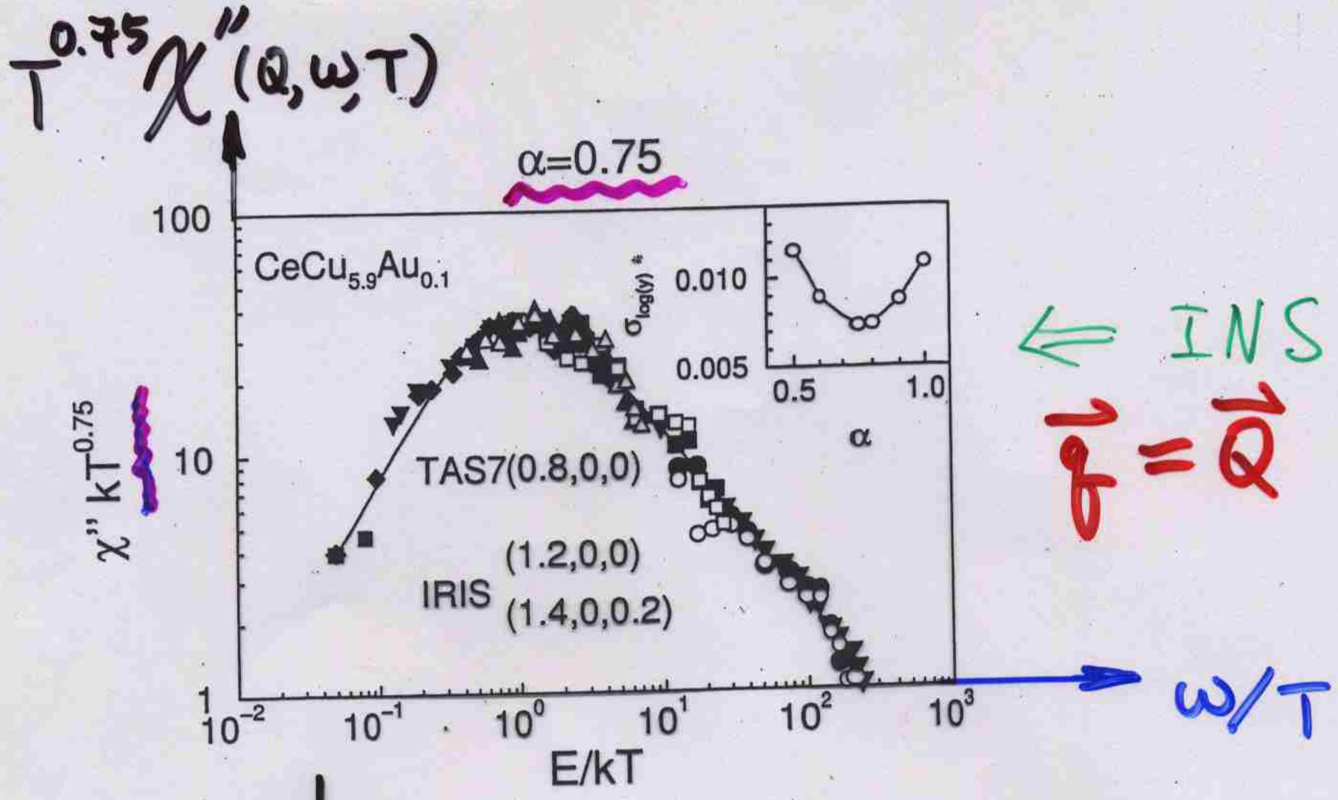
$$M(\omega) \;\approx\; -I_{\mathbf{Q}} + C\,T^{\alpha}\,\mathcal{M}(\omega/T)$$

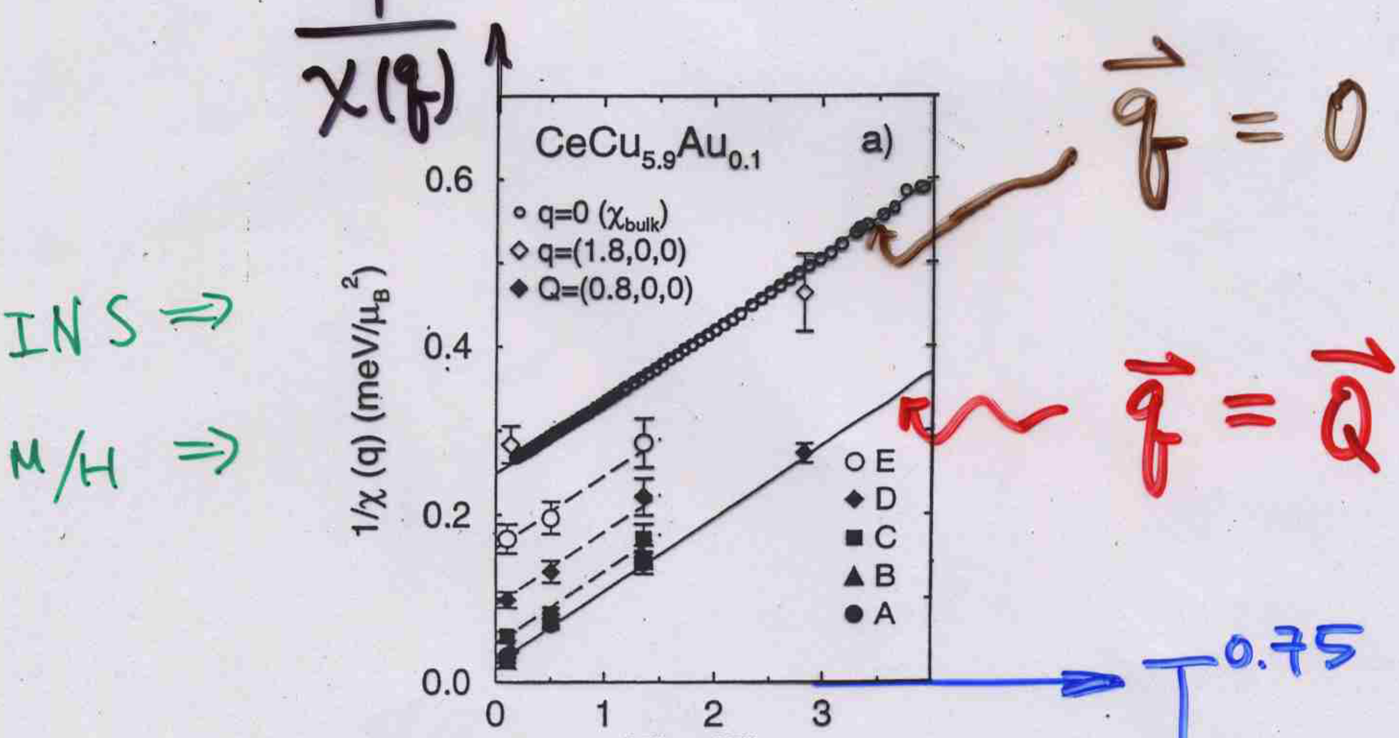
where

$$\mathcal{M}(\omega/T) = \exp[\alpha\;\psi(1/2 - i\omega/2\pi T)]$$

- at the peak wavevector:

$$\chi(\mathbf{Q},\omega,T) \propto \frac{1}{T^{\alpha}}\,\frac{1}{\mathcal{M}(\omega/T)}$$





A. Schröder *et al.*, Nature '00; A. Schröder, G. Aeppli, E. Bucher, R. Ramazashvili, & P. Coleman, PRL '98 ; O. Stockert, H. v. Löhneysen, A. Rosch, N. Pyka, & M. Loewenhaupt, PRL '98

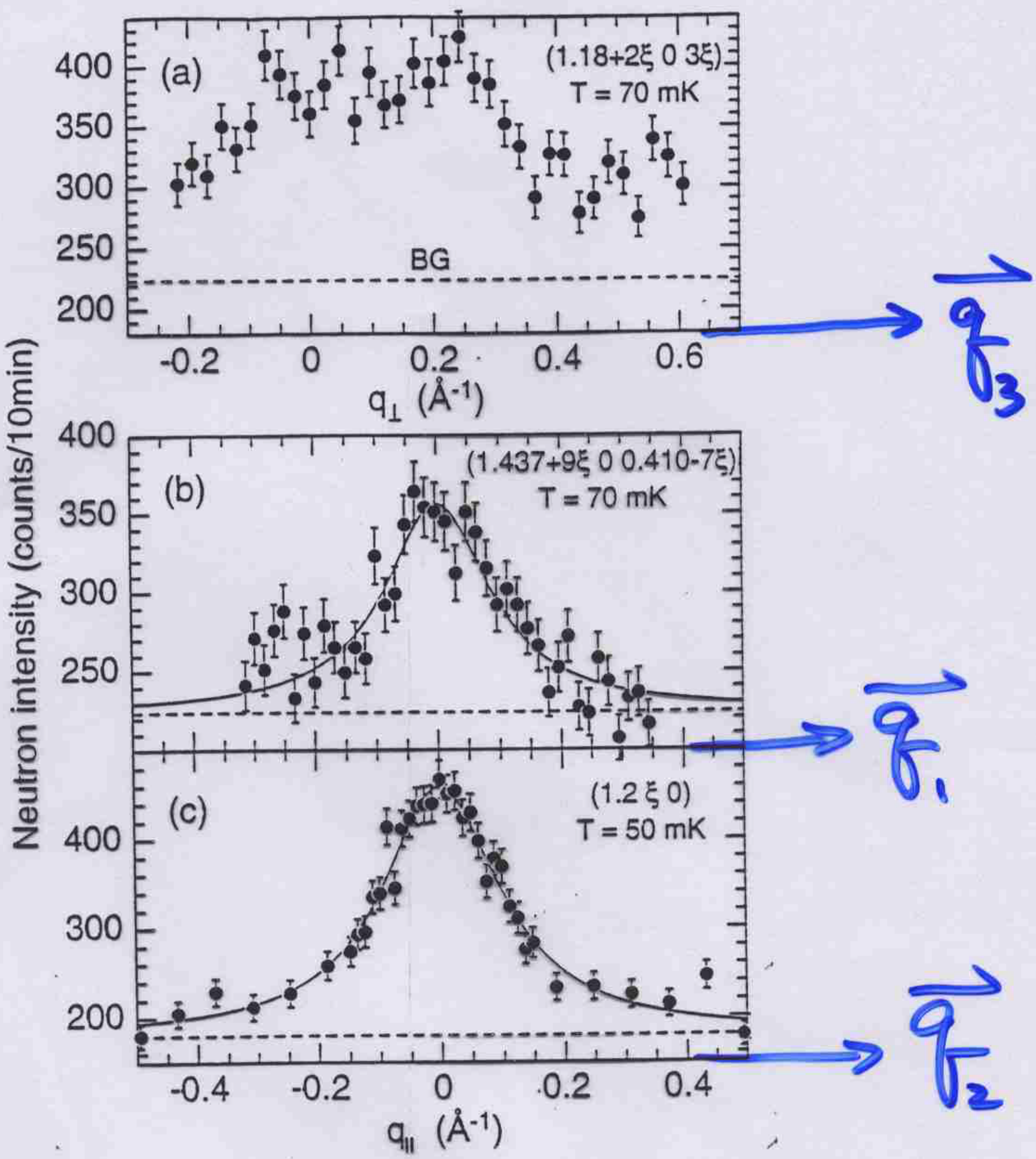
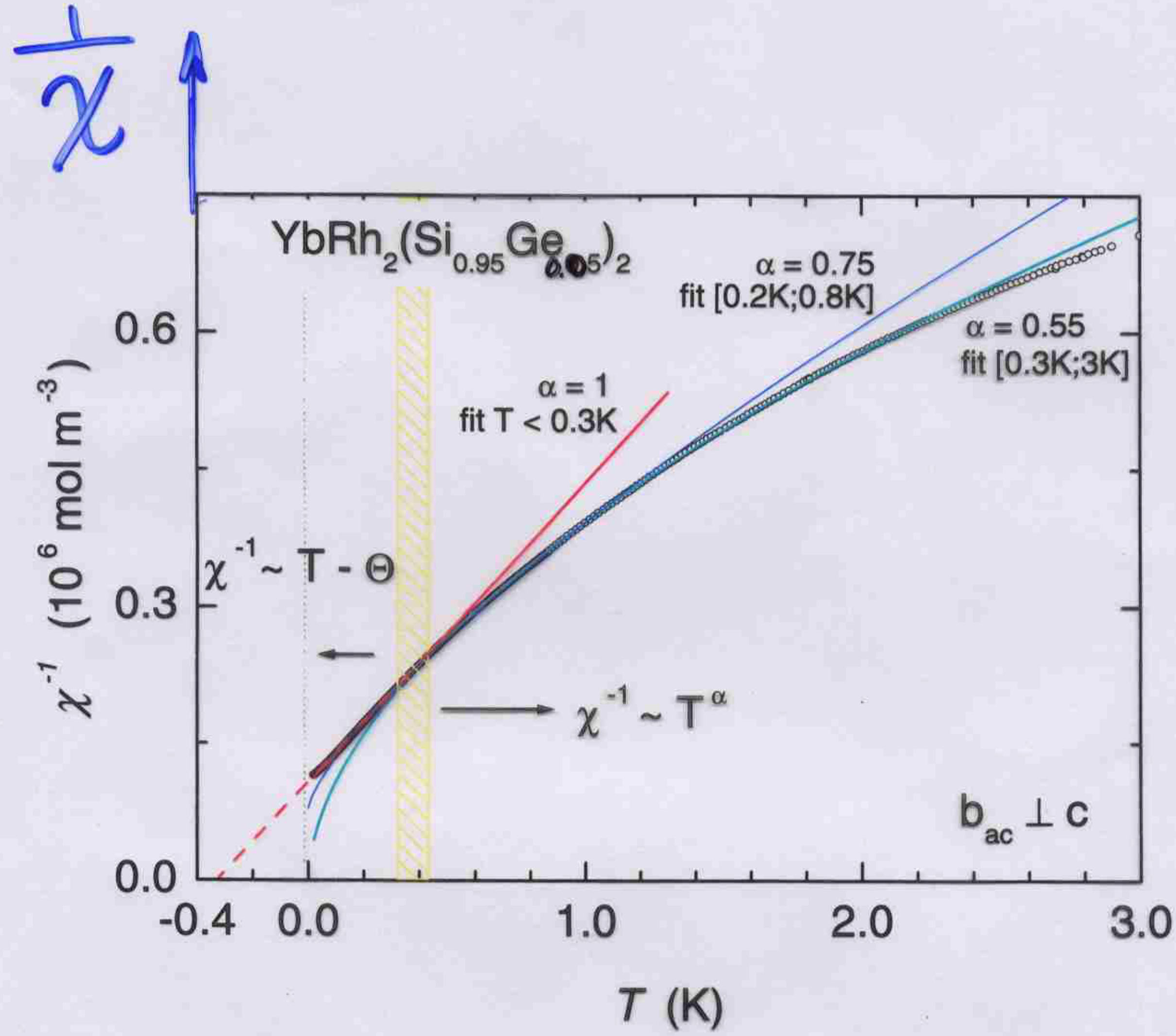


FIG. 3. q scans along (a) and across [(b) and (c)] the rodlike feature in $CeCu_{5.9}Au_{0.1}$ for $\hbar\omega = 0.1$ meV and $k_f = 1.15$ Å^{-1} ($T = 50/70$ mK). There is only a weak q dependence along the rods, while transverse scans show peaks with nearly the same linewidth.

A. Rosch, A. Schröder, O. Stockert, and H. v. Lohneysen, PRL '97;

O. Stockert *et al.*, PRL '98; A. Schröder *et. al.*, Nature '00

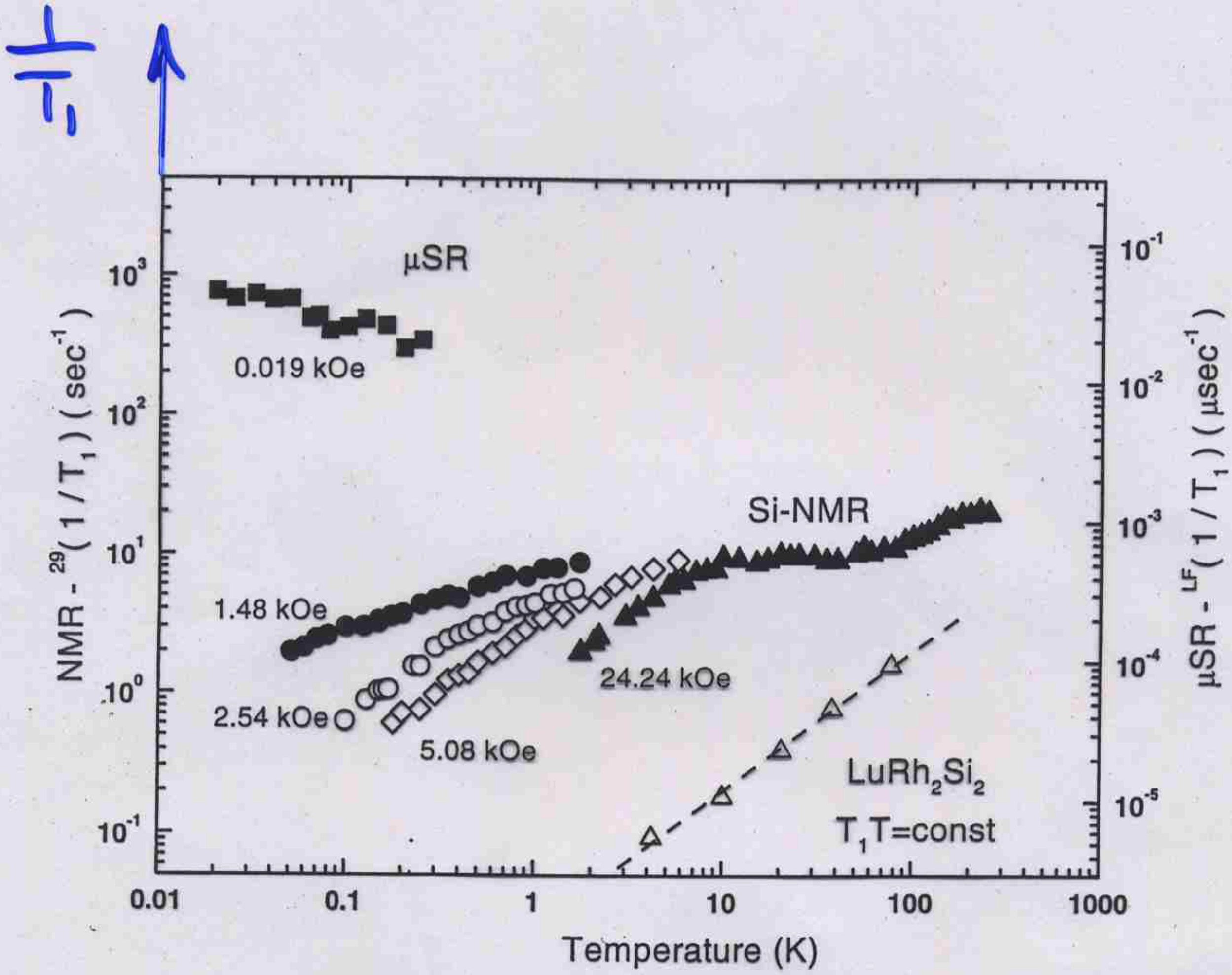
susceptibility in $YbRh_2(Si_{0.95}Ge_{0.05})_2$



P. Gegenwart, J. Custers, T. Tayama, K. Tenya, C. Geibel, O. Trovarelli, F. Steglich, & K. Neumeier, '02;

O. Trovarelli, C. Geibel, S. Mederle, C. Langhammer, F. M. Grosche, P. Gegenwart, M. Lang, G. Sparn, & F. Steglich, PRL '00

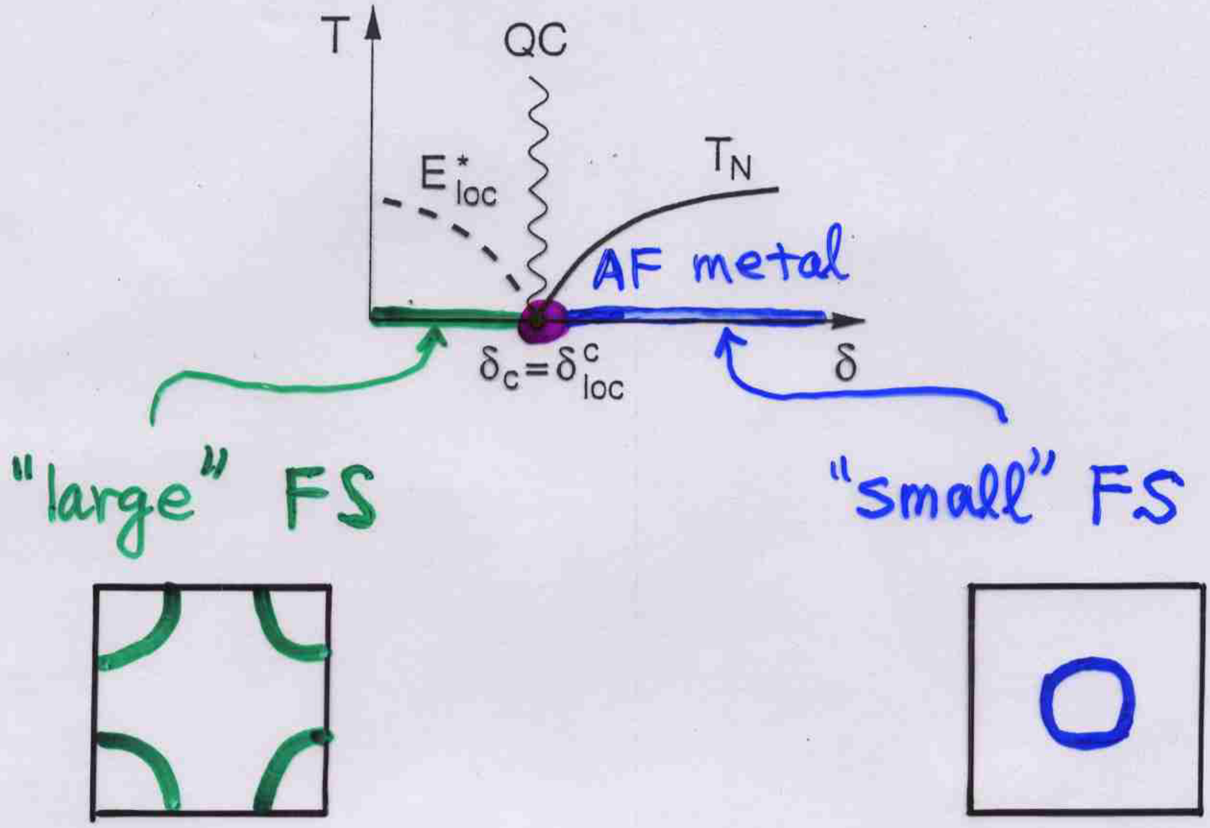
NMR & μSR in $YbRh_2Si_2$



NMR: K. Ishida, K. Okamoto, Y. Kawasaki, Y. Kitaoka, O. Trovarelli, C. Geibel, & F. Steglich, PRL '02;

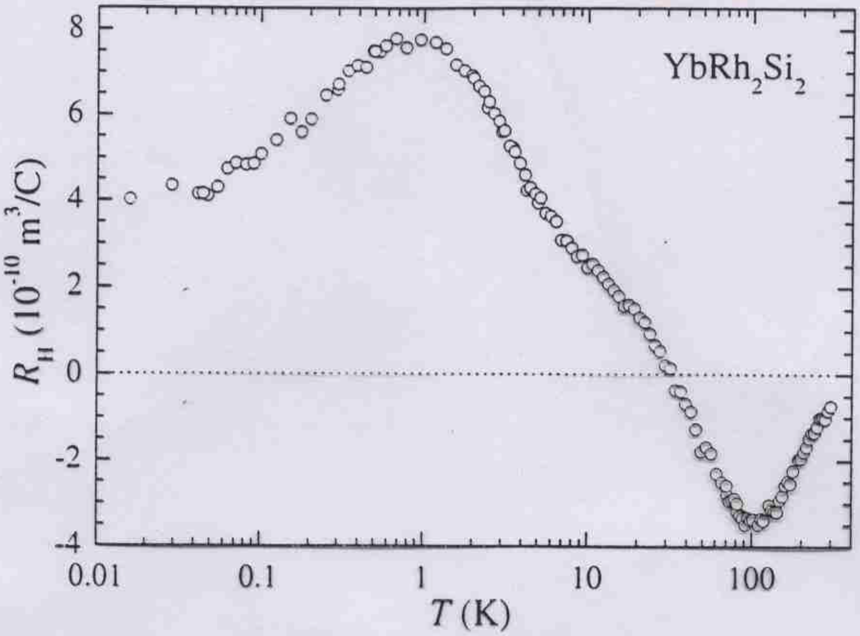
μSR: K. Ishida, D. E. MacLaughlin, O. O. Bernal, R. H. Heffner, G. J. Nieuwenhuys, O. Trovarelli, C. Geibel, & F. Steglich, '02

- **Fermi surface evolution**

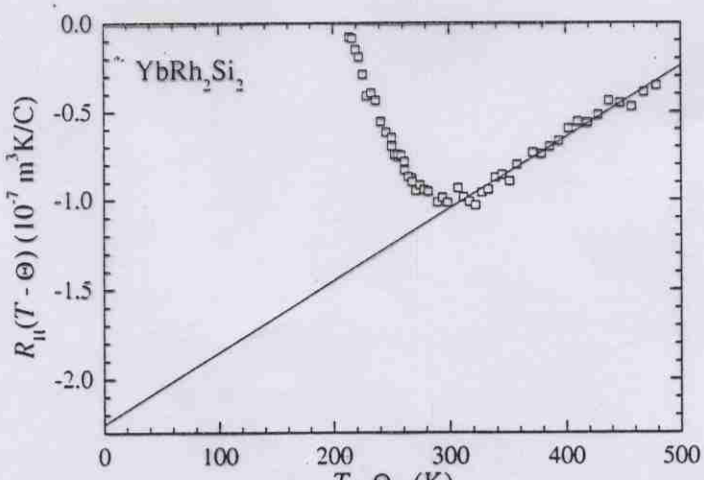


- Fermi surface probes
  - Hall coefficient expected to jump
    - ∗ P. Coleman, C. Pépin, QS, & R. Ramazashvili, JPCM '01
    - ∗ QS, S. Rabello, K. Ingersent, & J. L. Smith, cond-mat/0202414
    - ∗ for $Cr_{1-x}V_x$: A. Yeh, Y. A. Soh, J. Brooke, G. Aeppli, T. F. Rosenbaum, & S. M. Hayden '02
  - de Haas-van Alphen
  - Residual resistivity vs. δ

S. Paschen et al.
SCES '02



$$R_H(T \to 0) \approx R_{cond}$$



$R_H(T) = R_0 + R_s \chi(T)$

presumably $R_0 \approx R_{cond}$

Fig. 2. Hall coefficient R_H multiplied by the difference of temperature T and paramagnetic Weiss temperature Θ vs $T - \Theta$. The linear behaviour above 120 K allows for the separation of R_H into a normal and an anomalous contribution.

Outlook

- More Local probes and Fermi surface studies

- Dimensionality and frustration:

  cf. $Ce_{1-x}La_xRu_2Si_2$ is 3D and appears to be Gaussian: S. Raymond *et al.* '01

- The effect of disorder and frustration.

  cf. $UCu_{5-x}Pd_x$:

  – Neutron scattering: ω/T scaling (M. Aronson *et al.* '95)

  – μSR: $T-$independent relaxation rate (D. MacLaughlin *et al.* '01)

  – Cu-site NMR: $1/T_1 \sim T$ (J. L. Gavilano *et al.* '97; N. Büttgen *et al.* '00)

Beyond microscopics

Weak-coupling indications for local criticality

- Gaussian theory

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

$\Rightarrow$ in 2D, the local (i.e., $\mathbf{q}$−averaged) susceptibility at the Gaussian level is singular:

$$\chi^G_{loc} \sim \ln \frac{1}{-i\omega}$$

- This singularity can lead to important non-linear effects in the dynamics of *local degrees of freedom* — such as local moments in heavy fermion metals.

Robustness of the locally critical point

- GL action:

$$\mathcal{S}_{\mathrm{LCP}} = \mathcal{S}_{lw}\left[\phi(\mathbf{q} \sim \mathbf{Q}, \omega)\right] + \mathcal{S}_{loc} + \mathcal{S}_{mix}$$

- For $\alpha < 1$, the long-wavelength part is Gaussian: $D + z > 4$
  - yields a contribution to the spin self-energy with a non-singular $\mathbf{q}$-dependence

- The contribution to the spin self-energy from the coupling to the local modes should also have a smooth $\mathbf{q}-$dependence

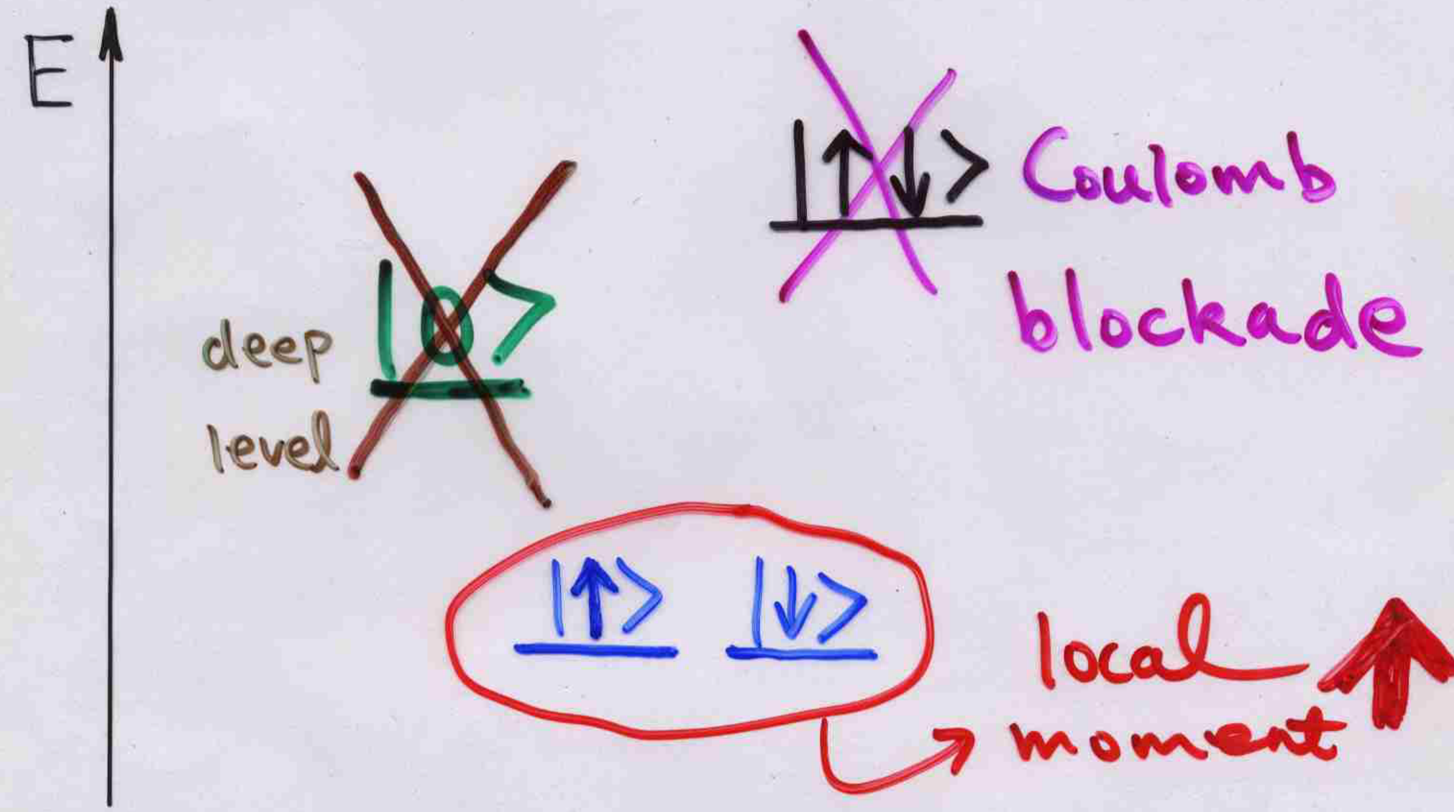
- $\Rightarrow$ The spatial anomalous dimension $\eta = 0$,

$$\chi(\mathbf{q} \sim \mathbf{Q}) \sim 1/|\mathbf{q} - \mathbf{Q}|^2$$

- $\Rightarrow$ Singular χ_{loc} is robust, so is local criticality

Broader implications

- What is a local moment anyway?



- Local physics in Mott-Hubbard systems
- QC in Ruthenates [Grigera *et al.* '01] and (?)Cuprates

Summary

- Experiments: non-Gaussian QC metals
- Two types of quantum phase transitions
  - T=0 SDW transition (Gaussian)
  - Locally critical: local critical modes co-exist with long-wavelength fluctuations of the order parameter (interacting)
- The locally critical picture provides a natural understanding of some outstanding puzzles in heavy fermion metals
- A jump in the Hall coefficient is predicted
- Broader implications of local criticality