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ICTP 40th Anniversary

SMR.1572 - 29

Workshop on
Novel States and Phase Transitions in Highly Correlated Matter

12 - 23 July 2004

Local quantum criticality and non-fermi liquid properties

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These are preliminary lecture notes, intended only for distribution to participants

Local Quantum Criticality and Non-Fermi Liquid Properties

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Rice University

Outline:

1. Quantum critical heavy fermions
2. Destruction of Kondo effect: EDMFT
3. Beyond the microscopics
4. More experiments
5. Bose-Fermi Kondo in magnetic quantum dots

ICTP, July 22, 2004

Lijun Zhu, Stefan Kirchner,
Eugene Pivovarov,
Silvio Rabello, J. L. Smith — **(Rice University)**

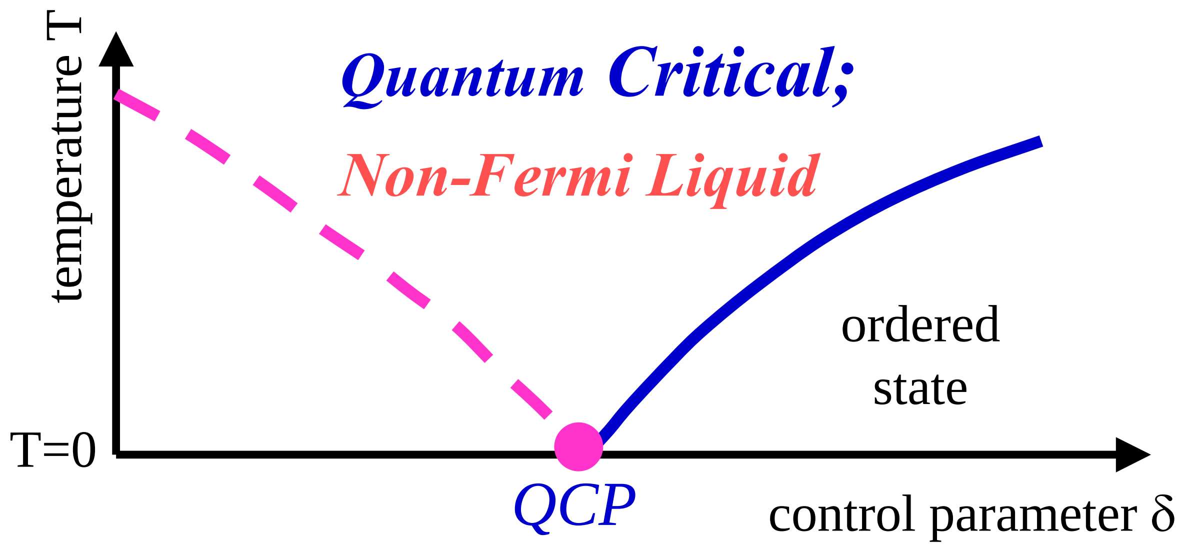
Kevin Ingersent — **(Univ. of Florida)**

Daniel Grempel — **(CEA-Saclay)**

Jianxin Zhu — **(Los Alamos)**

S. Paschen	**P. Gegenwart**	**R. Küchler**
T. Lühmann	**S. Wirth**	**N. Oeschler**
T. Cichorek	**K. Neumaier**	**O. Tegus**
O. Trovarelli	**C. Geibel**	**J. A. Mydosh**
F. Steglich	**P. Coleman**	

Quantum Critical Electron Systems



- **Quantum criticality** ⟹ **breakdown of Fermi liquid theory**
- **Non-Fermi liquid excitations** ⟹ **new types of quantum critical points**
- **High Tc superconductors (?), heavy fermions, ...**

- **Kondo lattices:**

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

- **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 fermions near a magnetic QCP:**
  - $YbRh_2Si_2$ (critical Bab=60mT, Bc=0.7T)

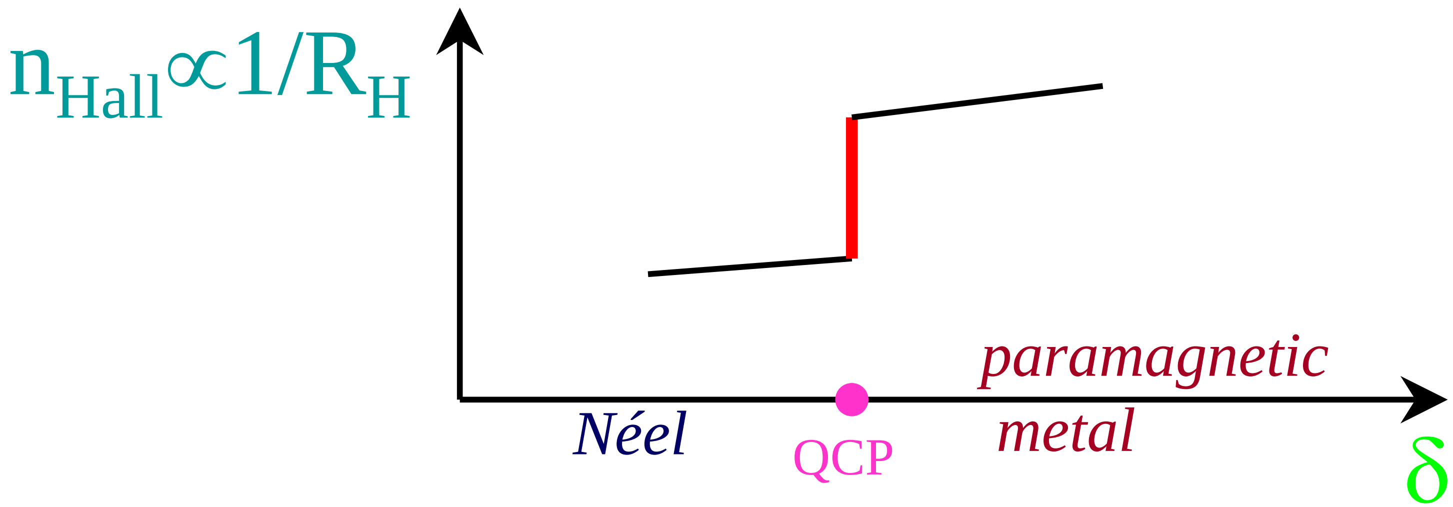
    tetragonal; easy-plane anisotropy (Mab:Mc≈100:1 at low T); $T_K^0 \approx 20$ K
  - $Ce(Cu_{1-x}Au_x)_6$ (critical x ≈0.017)

    nearly orthorhombic; Ising-anisotropy (Mc:Ma:Mb ≈10:2:1); $T_K^0 \approx 6$ K
  - Phases: AF metal; paramagnetic metal

- **Heavy fermions near a magnetic QCP (cont'd):**
  - $CePd_2Si_2$
  - $CeIn_3$
  - $CeNi_2Ge_2$
  - YbAgGe [new toy – frustrated (hexagonal) lattice]
  - CeMIn5 (?)

Hall Effect in $YbRh_2Si_2$

- **The Hall number has a sharp jump @ QCP in the T =0 limit (by extrapolation):**



- **Suggesting a sudden collapse and reconstruction of the Fermi surface at the QCP**

S. Paschen et al., preprint '04

Dynamics of the quantum critical $CeCu_{5.9}Au_{0.1}$

- **Frequency and temperature dependences of the dynamical spin susceptibility:**
  - **an anomalous exponent $\alpha < 1$**
  - **ω/T scaling**

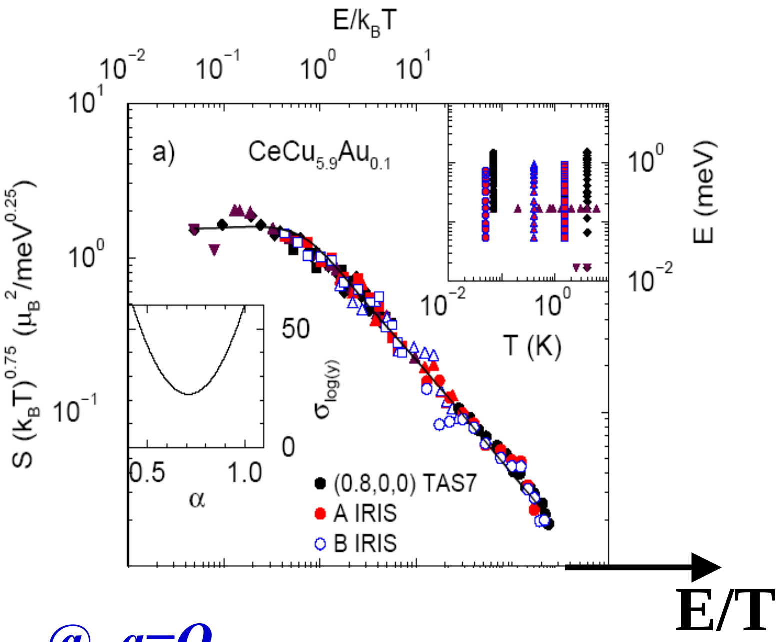
  → implying non-Gaussian fixed point

- **The anomalous exponent α is seen essentially \`everywhere' in the momentum space**

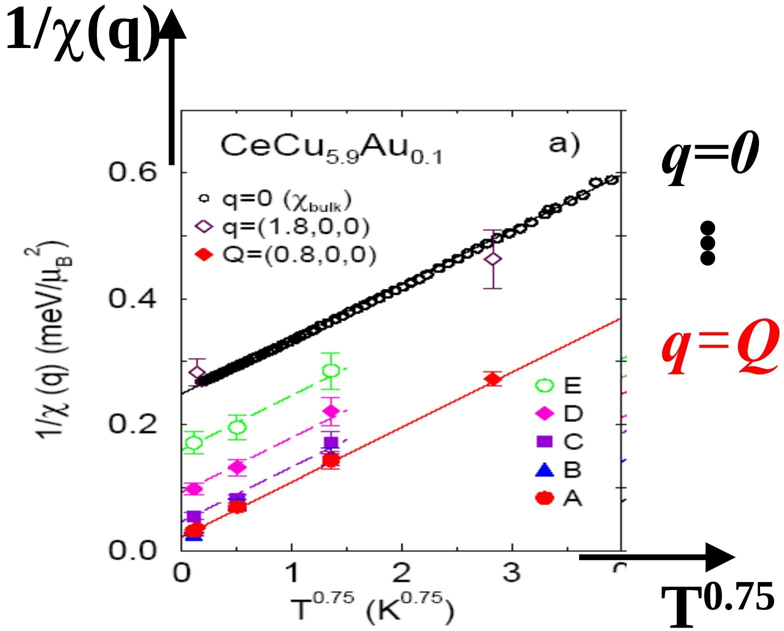
Dynamical and Static Susceptibilities in $CeCu_{5.9}Au_{0.1}$

- E/T scaling
- Fractional exponent α=0.75

- α=0.75 `everywhere' in **q**.

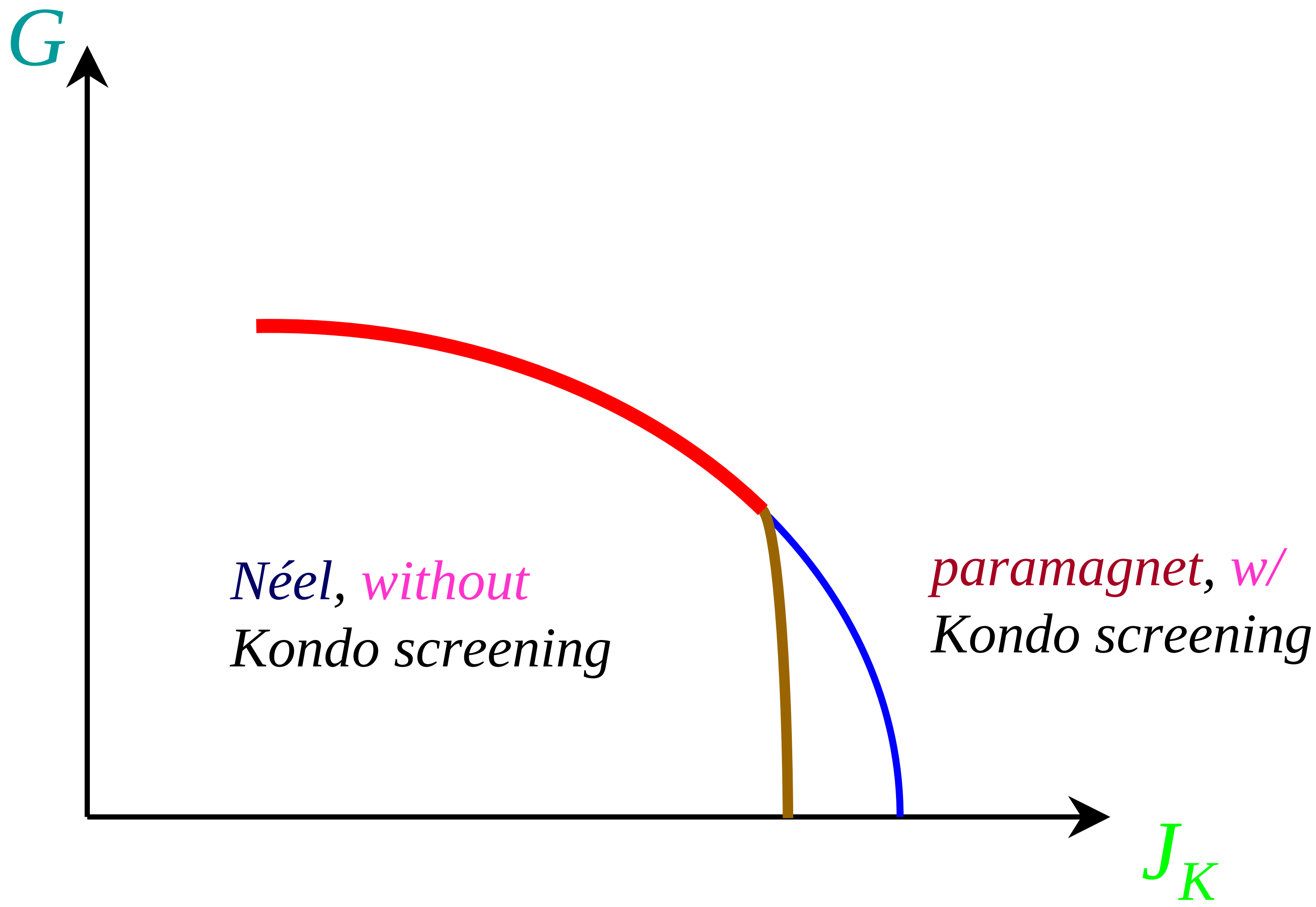


INS @ q=Q



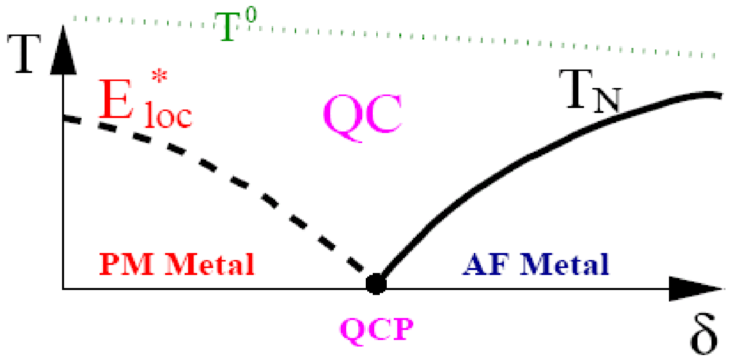
INS and M/H

A. Schröder et al., Nature '00; PRL '98; O. Stockert, H. v. Löhneysen, A. Rosch, N. Pyka, & M. Loewenhaupt, PRL '98



G
Néel, without
Kondo screening
paramagnet, w/
Kondo screening
J_K

Local Quantum Critical Point



Destruction of Kondo effect ($E_{loc}^* \rightarrow 0$) at the QCP

- **Local susceptibility also diverges:**

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

where $\Lambda \approx T_K^0$

- **"spin self-energy" has anomalous exponent**

$$M(\omega) \approx -I_Q + A(-i\omega)^{\alpha}$$

where $\alpha = \frac{1}{2\rho_I(I_Q)\Lambda}$

QS, S. Rabello, K. Ingersent, & J. L. Smith, Nature 413, 804 (2001)

DMFT* of Kondo Lattice

(* Georges and Kotliar, Metzner and Vollhardt, …)

- **Mapping to a self-consistent Kondo model**

$$\mathcal{H}_{\text{eff}} = J_K \, \mathbf{S} \cdot \mathbf{s}_c + \sum_{p,\sigma} E_p \, c^\dagger_{p\sigma} c_{p\sigma}$$

+ self-consistency conditions

- **Correctly describes Kondo screening: heavy fermion phase with large Fermi surface**

- **But: no competing mechanism against Kondo effect: Kondo screening is too robust**

- **No dynamical competition between Kondo and RKKY**

Extended-DMFT* of Kondo Lattice

(* Smith & QS;   Chitra & Kotliar; Sengupta & Georges)

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

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

+ self-consistency conditions

- **The effective impurity problem determines**
  - **Electron self-energy *Σ (ω)***
  - **"spin self-energy" *M (ω)***

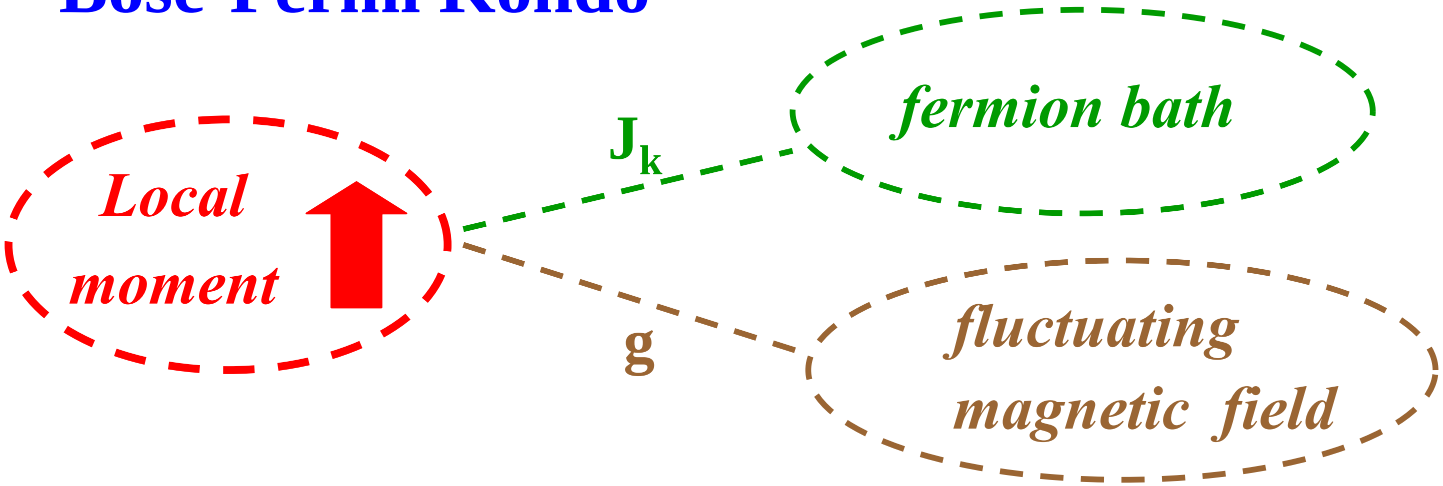
- **Dynamical spin susceptibility:**

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

Extended-DMFT of Kondo Lattice

Kondo Lattice

Bose-Fermi Kondo



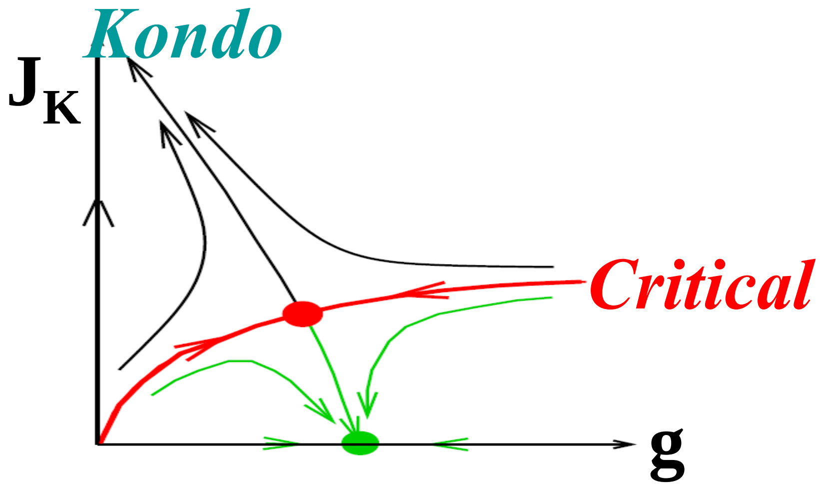
+ self-consistency

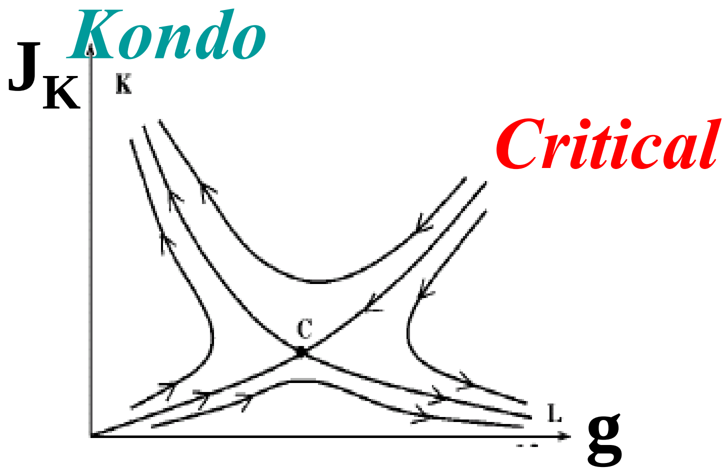
Cf. QS, S. Rabello, K. Ingersent and J.L.Smith, Phys. Rev. B '03 for details

ε-expansion of Bose-Fermi Kondo model:

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

SU(2) & XY **Ising**





Critical: $\chi_{\text{loc}}(\tau) \sim 1/\tau^{\epsilon}$ ⟷ *Crucial for LQCP solution*

Order ε: *J. L. Smith & QS '97; A. M. Sengupta '97;* **Higher orders in ε and spin anisotropies:** *L. Zhu & QS '02; G. Zarand & E. Demler '02*

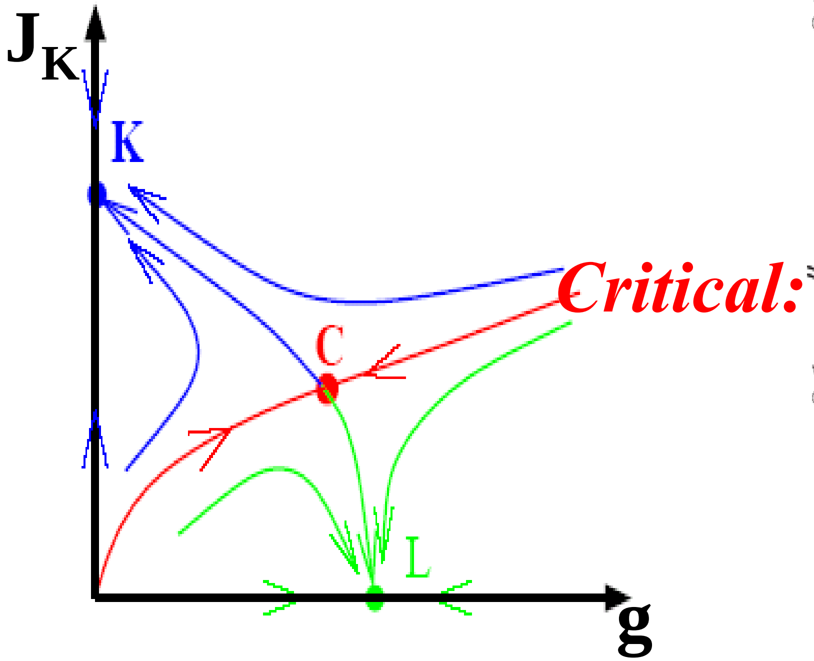
$J_K = 0$: *S. Sachdev & J. Ye '93 (large N); M. Vojta, C. Buragohain & S. Sachdev '00*

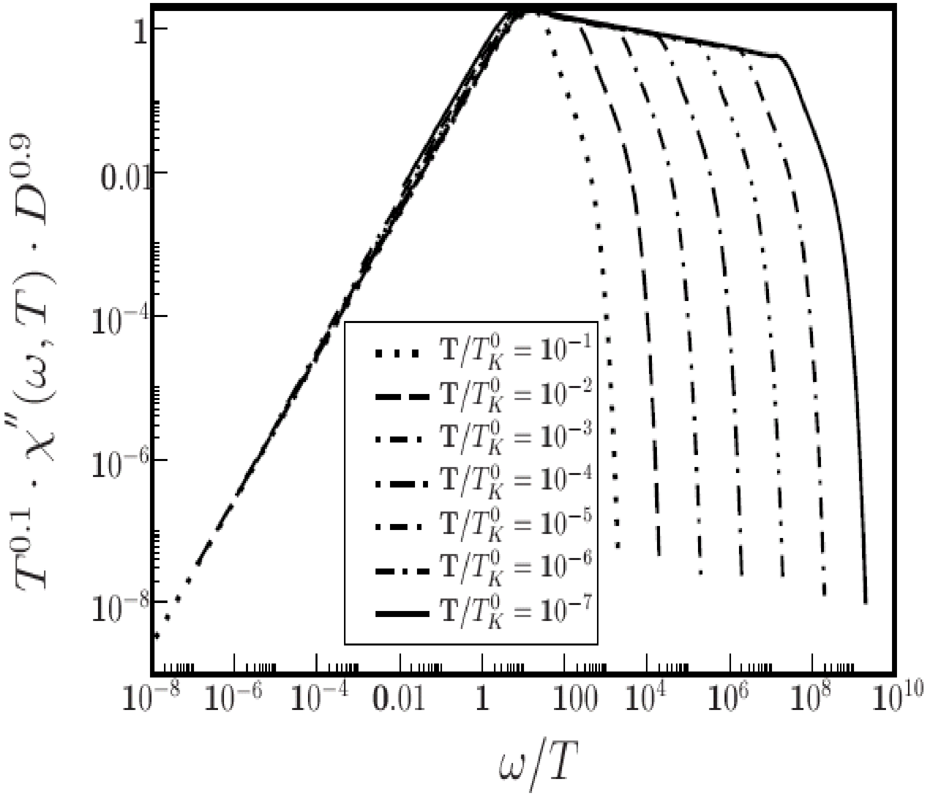
Dynamical large-N of Bose-Fermi Kondo

$SU(N)\times SU(\kappa N)$

(Parcollet & Georges, PRL '97; Cox & Ruckenstein, PRL '93)

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



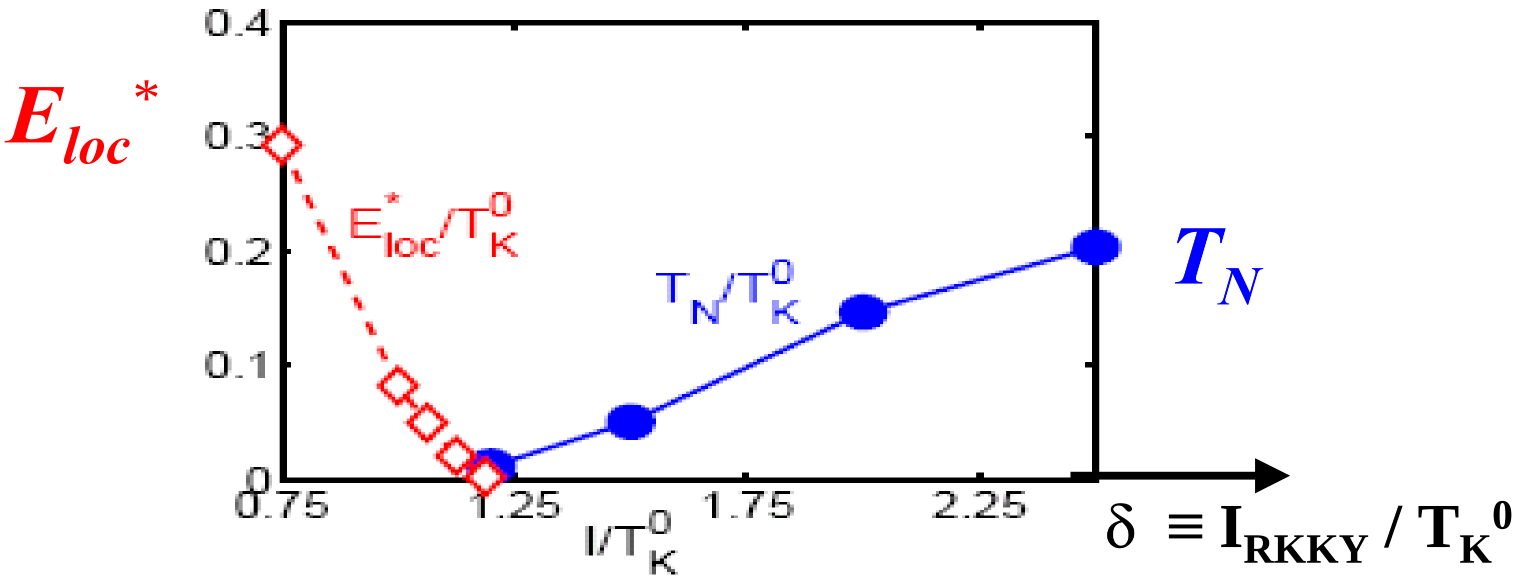


L. Zhu, S. Kirchner, QS, & A. Georges, cond-mat 0406293;
S. Kirchner, L. Zhu, & QS, cond-mat 0407307

Kondo lattice with Ising anisotropy

EDMFT of $\mathcal{H} = \mathcal{H}_0(c) + \sum_i J_K \mathbf{S}_i \cdot \mathbf{s}_{c,i} + \sum_{ij} I_{ij} S_i^z S_j^z$

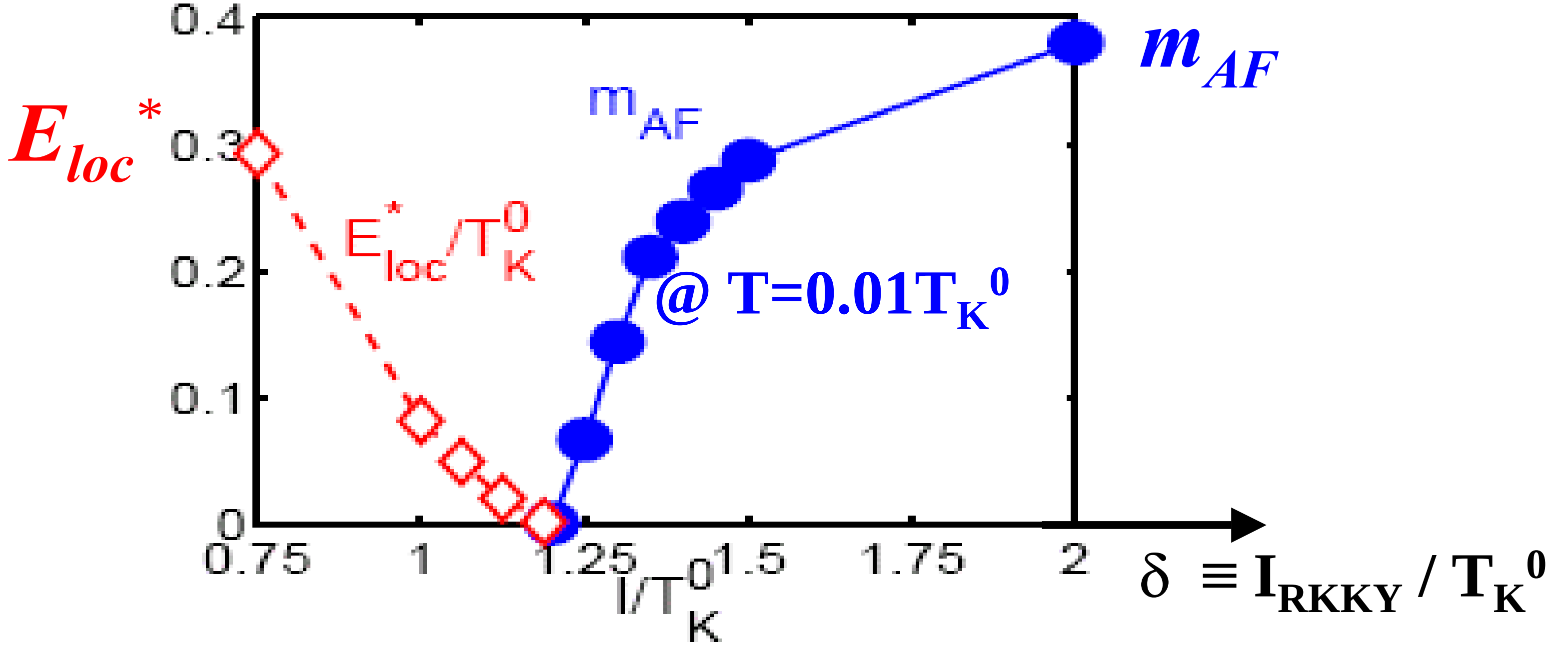
(Quantum Monte Carlo algorithm of Grempel and Rozenberg '99)



The destruction of Kondo resonances ($E_{loc}^* \rightarrow 0$)
meets with the vanishing of the Néel temperature

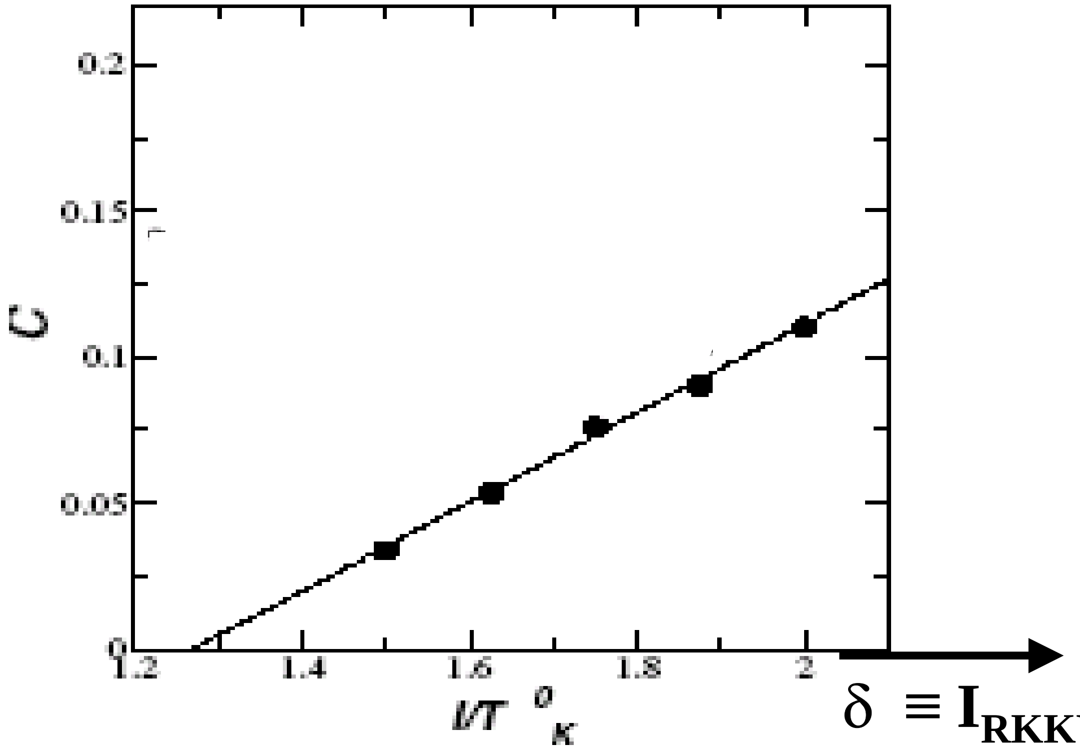
J.-X. Zhu, D. Grempel, & QS, Phys.Rev.Lett. '03

Kondo lattice with Ising anisotropy: Evidence for 2nd-order transition at T=0 (cont'd)



- m_{AF} → 0: continuous AF transition
- E_{loc}^* → 0: destruction of Kondo resonances

Kondo lattice with Ising anisotropy: Evidence for 2nd-order transition at T=0 (cont'd)



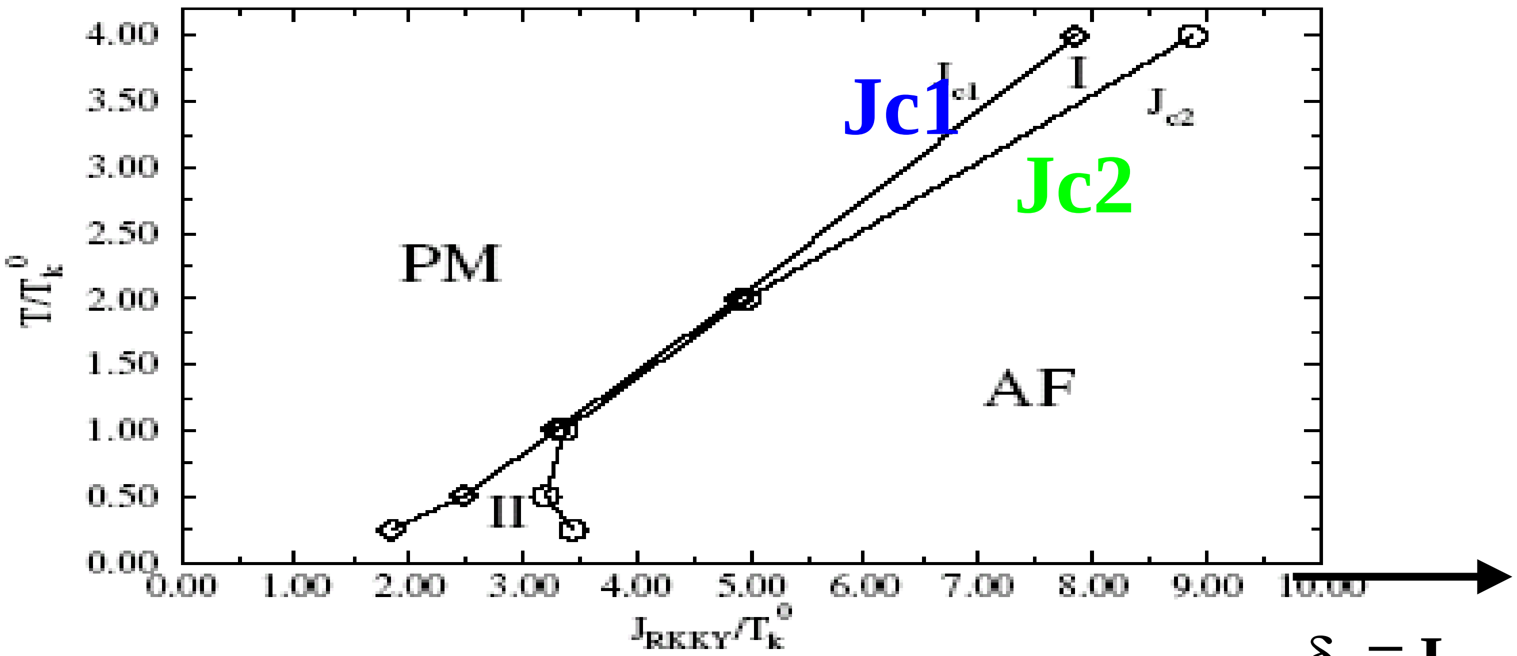
$\delta \equiv I_{RKKY} / T_K^0$

Curie constant C in the nominally "paramagnetic" solution as a function of I/T_K^0.

EDMFT of Anderson lattice with Ising anisotropy

(P. Sun and G. Kotliar, Phys.Rev.Lett. '03)

EDMFT of $\mathcal{H} = \mathcal{H}_{\text{Anderson-lattice}} + \sum_{ij} I_{ij} S_i^z S_j^z$



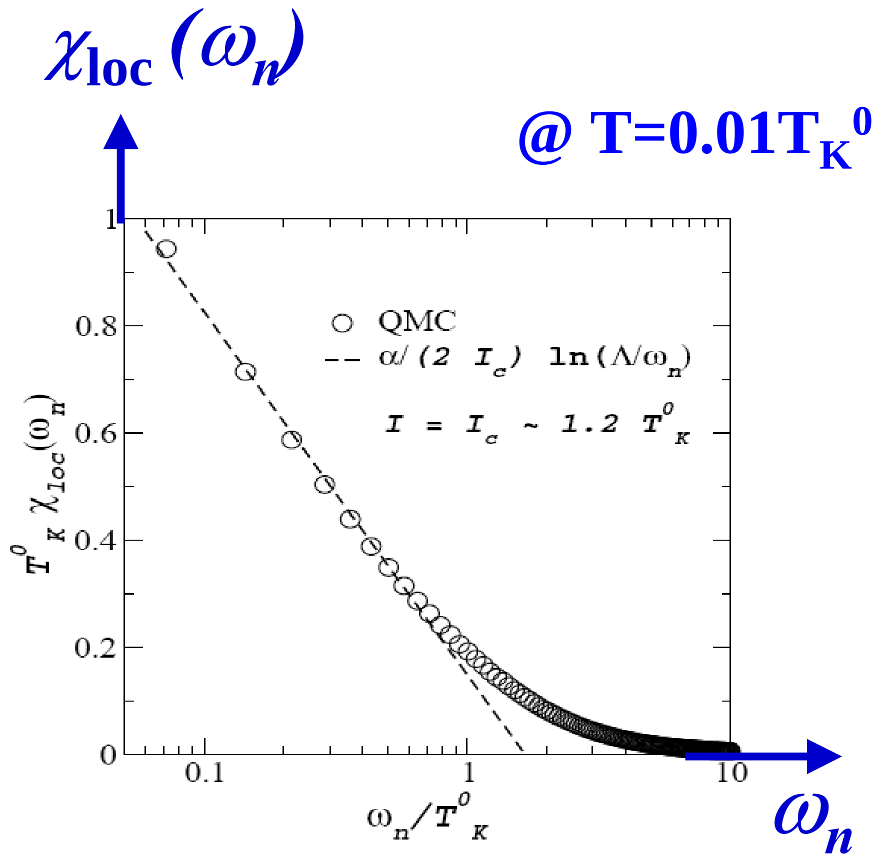
$\delta \equiv I_{RKKY} / T_K^0$

- Along Jc1 line, weaker first order at lower T
- If Jc1 line terminates at a 2nd order transition at T=0, then Jc2(T=0) must be equal to Jc1(T=0)

Quantum Critical Dynamics

- **Local spin susceptibility at $I \approx I_c \approx 1.2\ T^0_K$:**

$$\chi_{loc}(\omega_n) = \frac{1}{2\Lambda}\ln\frac{\Lambda}{|\omega_n|}$$

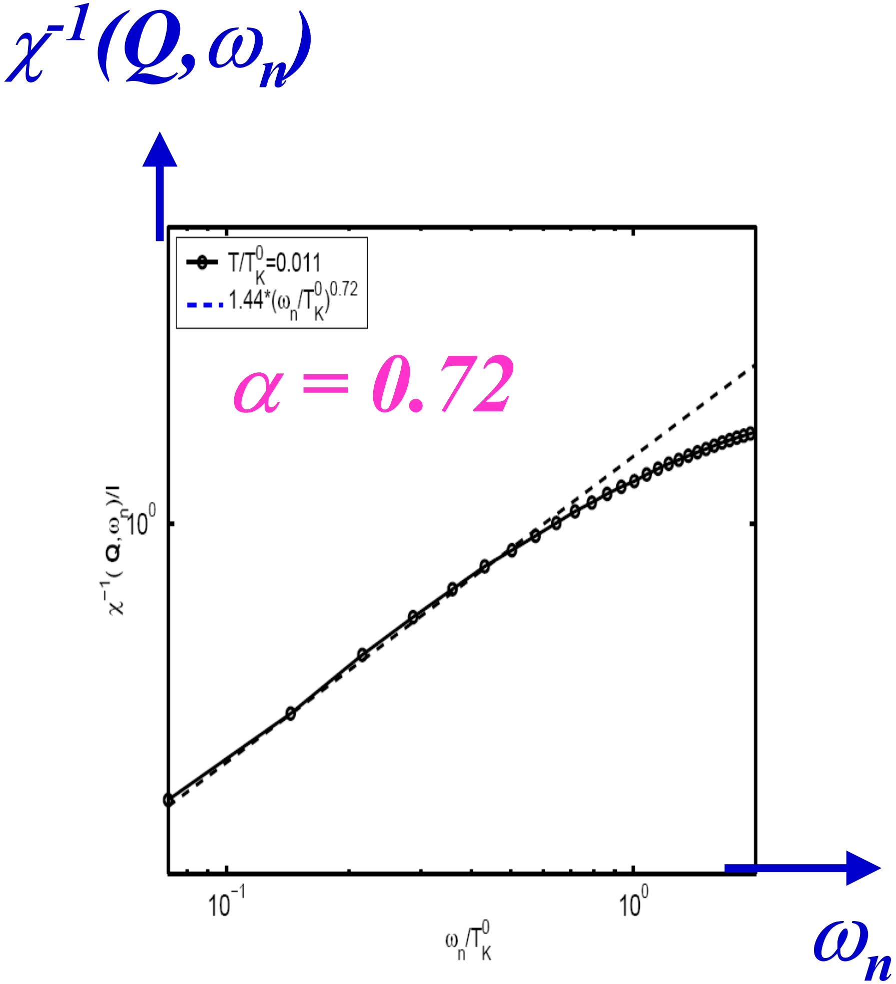


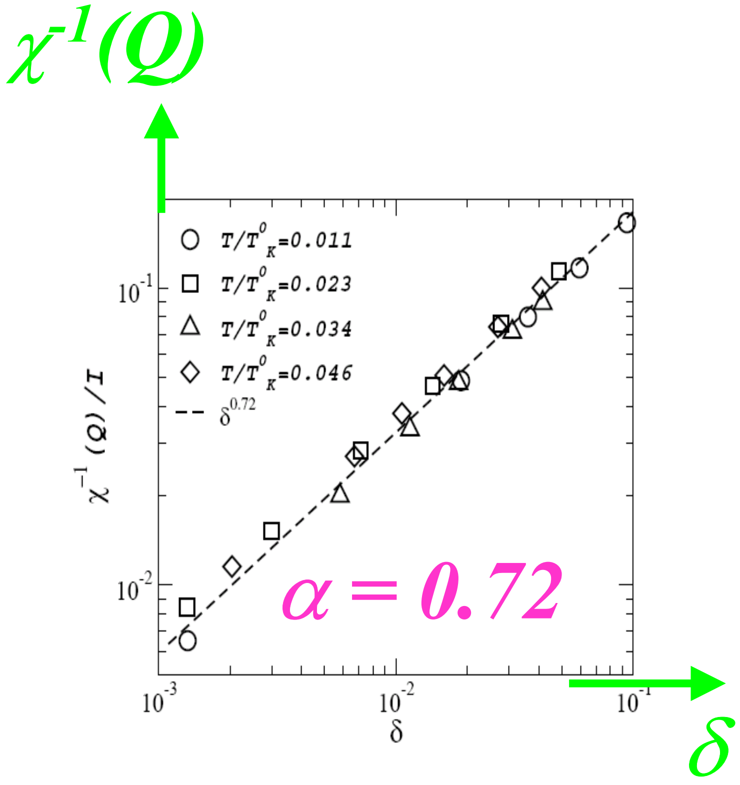
- **Calculated $\alpha \approx 0.7$**

D. Grempel and QS, Phys. Rev. Lett. '03

Fractional exponent in the dynamics

- **Inverse peak susceptibility at I ≈ Ic**

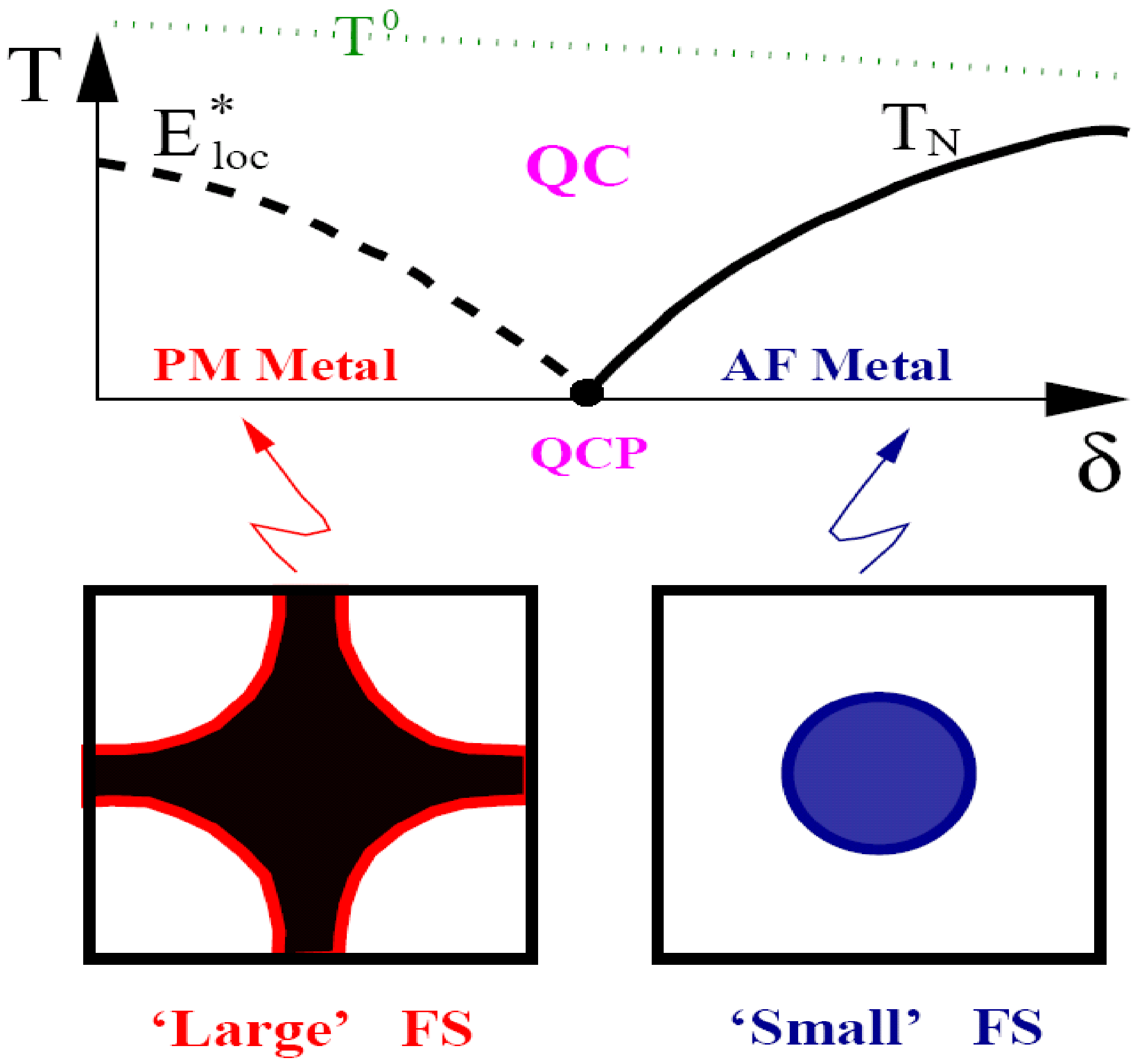




$\delta(T, I_c) \propto T;$

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

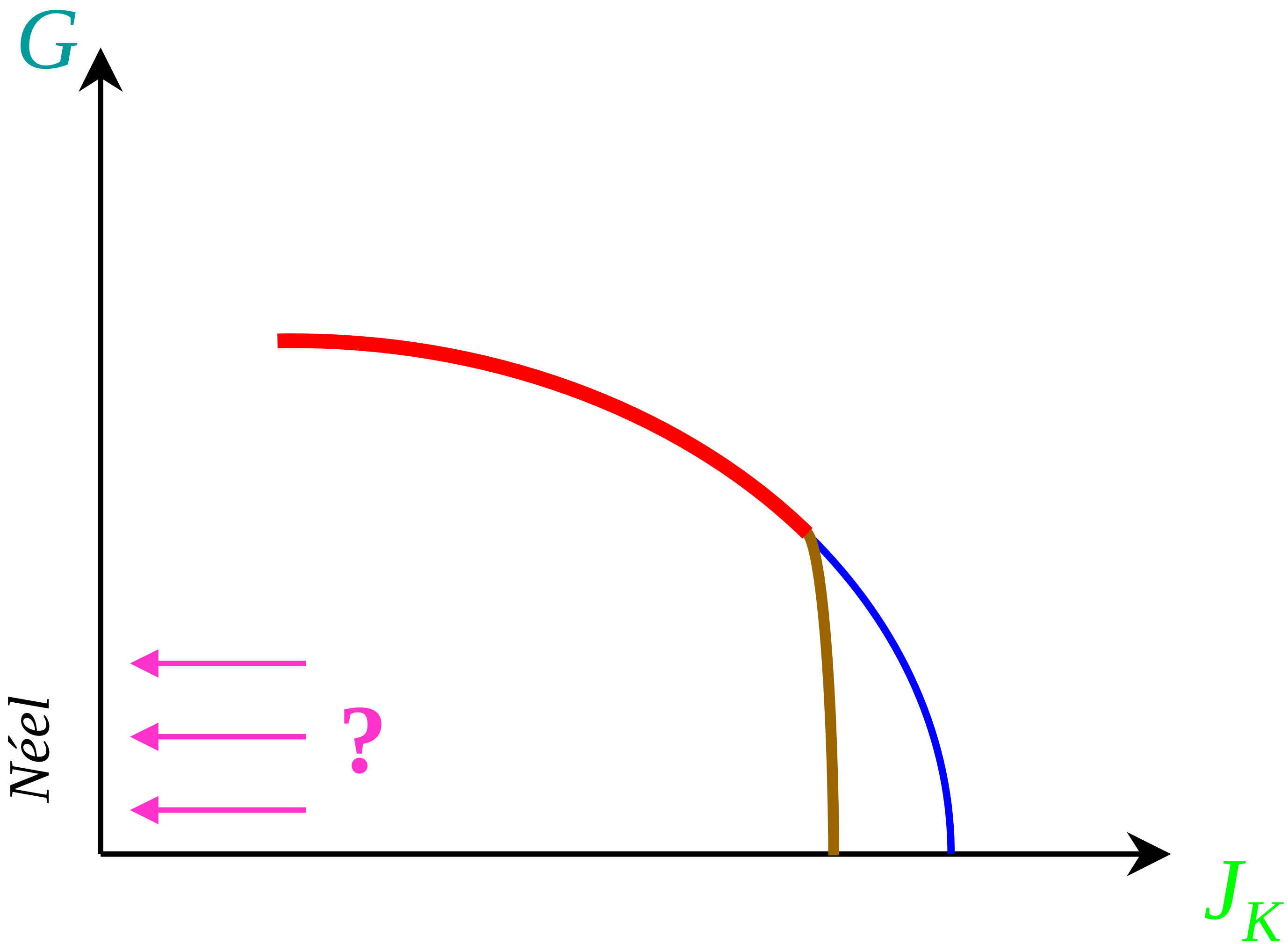
Fermi Surface Evolution



In what sense is the QCP local?

- **Localization of f-electrons**
  - $m^* \rightarrow \infty$ over the entire Fermi surface as $\delta \rightarrow \delta_{QCP}$
  - Reconstruction of the Fermi surface across δ_{QCP}
- **Anomalous spin dynamics everywhere in q.**
- **Destruction of Kondo effect** ➡
  - Non-Fermi liquid excitations part of the quantum-critical spectrum.

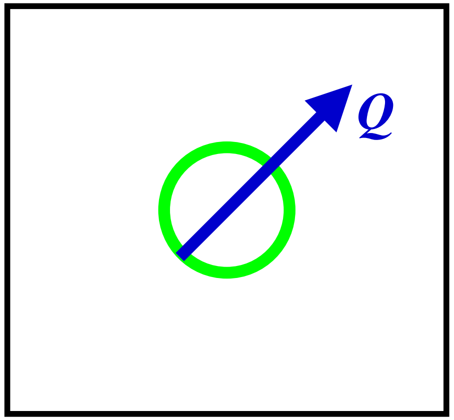
- **What happens beyond EDMFT?**



- ***Ising case:*** Kondo coupling to fermions irrelevant

- ***Heisenberg case:***

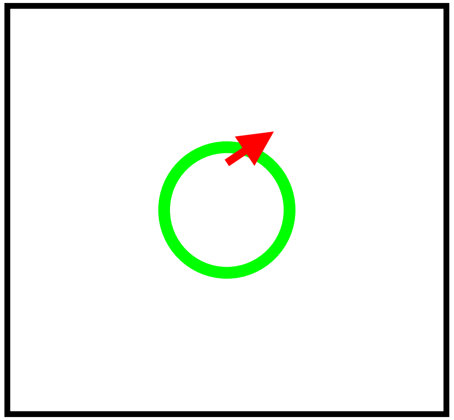
$$\boldsymbol{S}(\boldsymbol{x},\tau) \approx \boldsymbol{m} + \boldsymbol{n}\, e^{i\boldsymbol{Q}\bullet\boldsymbol{x}}$$



  – Coupling of fermions to *n* irrelevant:

  – Coupling of fermions to *m*:

$$\sum_a y^a \int d\boldsymbol{x}\, d\tau\; m^a(\boldsymbol{x},\tau)\, m_c^a(\boldsymbol{x},\tau)$$



Related problem in 1D:

$$\beta(y_\perp) = \left(1 - \frac{K_T}{2} - \frac{1}{2K_T}\right) y_\perp + u K_T y_z y_\perp$$

$$\beta(y_z) = u K_T^2 y_\perp^2$$

$$\beta(K_T) = \left(1 - K_T^2\right) y_\perp^2$$

where $u = \sqrt{2\pi} v_S / (v_S + v_T)$

E. Pivovarov, & QS, Phys.Rev. B '04;
O. Zachar, & A. M. Tsvelik, Phys. Rev. B '01;
A. E. Sikkema, I. Affleck, & S. R. White, Phys. Rev. Lett. '97;
O. Zachar, S. A. Kivelson, & V. J. Emery, Phys. Rev. Lett. '96

Spin dynamics at the LQCP

- **Dynamical spin susceptibility:**

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

  - *cf. $CeCu_{6-x}Au_x$ (A. Schröder et al ’98; O. Stockert et al. ’98)*
  - *$UCu_{5-x}Pd_x$(?) (M. Aronson et al. ’95; D. MacLaughlin et al. ’00)*

- **Static bulk spin susceptibility:**

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

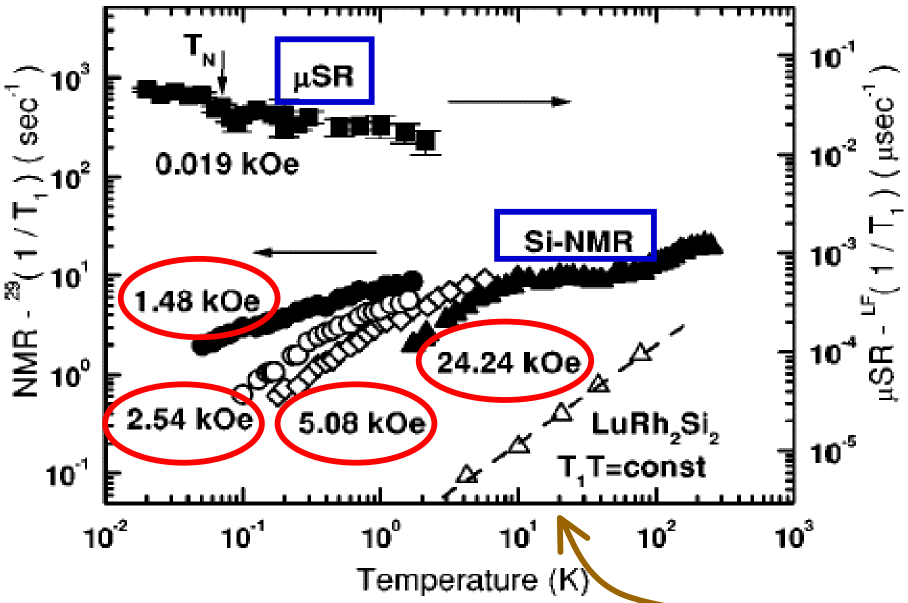
  - *cf. $CeCu_{6-x}Au_x$ (A. Schröder et al. ’00)*
  - *$YbRh_2Si_2$ (P. Gegenwart et al. ’02)*
  - *$CeCoIn_5$(?) (J. Thompson et al. ’02, S. Nakatsuji et al. ’02)*

- **NMR relaxation rate:**

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

  - *cf. $YbRh_2Si_2$ (K. Ishida et al. ’03)*
  - *$CeCu_{6-x}Au_x$ (R. Walstedt et al.’03): $(1/T_1)_{Cu} \sim T^{\alpha}$*
    [sum over generic q – transfer hyperfine coupling?]

NMR and μSR relaxation rates in $YbRh_2Si_2$



- B/T scaling
- $1/T_1$ extrapolates to const. as field B→Bc

T_K^0

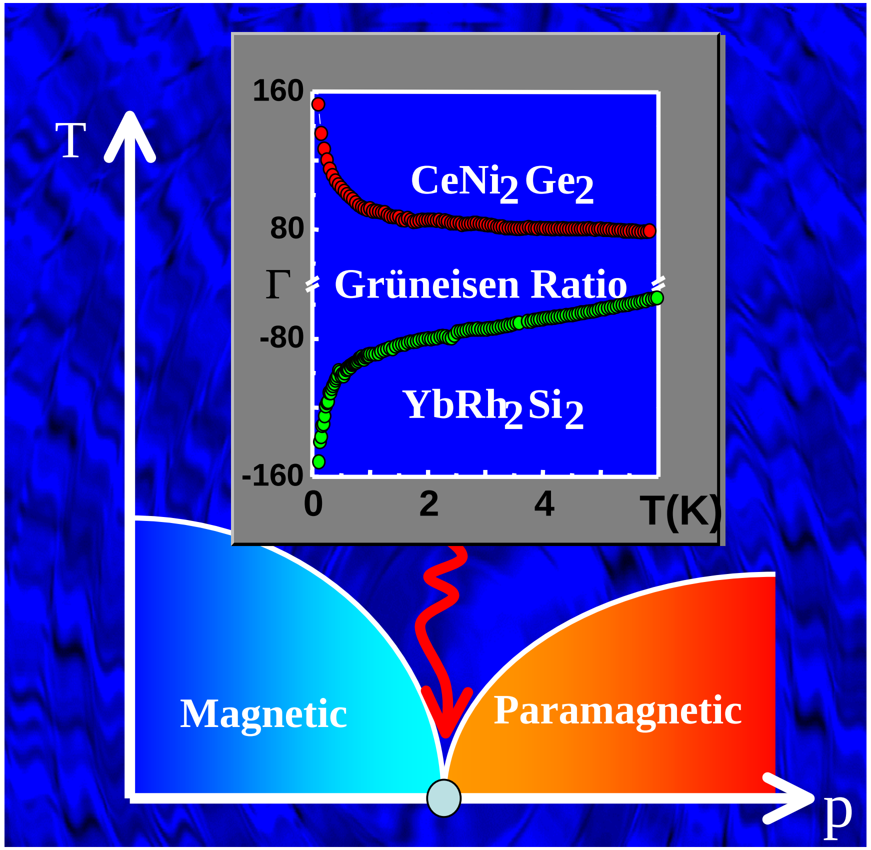
NMR: K. Ishida, K. Okamoto, Y. Kawasaki, Y. Kitaoka, O. Trovarelli, C. Geibel, & F. Steglich, PRL '02; PRB '03

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

Divergence of the Grüneisen Ratio

$$\Gamma \sim \frac{\text{thermal expansion } \alpha \equiv \frac{1}{V}\frac{\partial V}{\partial T}}{\text{specific heat } c}$$

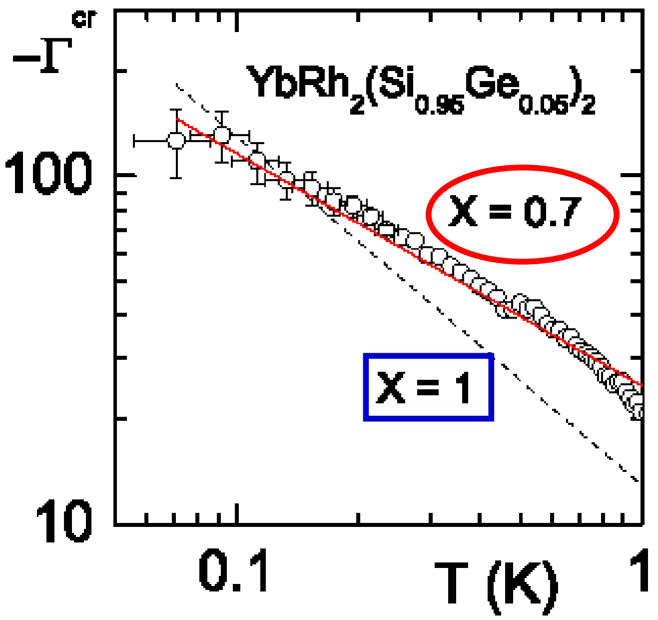
$$\sim \frac{\partial S/\partial p}{T\partial S/\partial T} \quad \rightarrow \frac{1}{T^{x}}$$



L. Zhu, M. Garst, A. Rosch, and QS, Phys. Rev. Lett. '03

R. Küchler et al., Phys. Rev. Lett. '03

Grüneisen exponent in Ge-doped $YbRh_2Si_2$



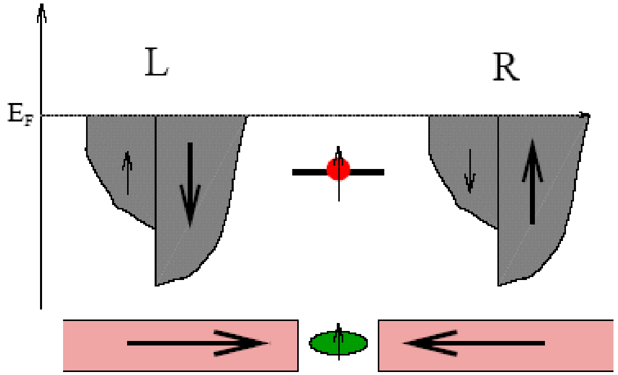
- **LQCP: $x_{loc} \approx 0.66$ to 2nd order in ε-expansion for the XY case**

- **Cf. AF-SDW: $x = 1 / \nu z = 1$**

R. Küchler et al., Phys. Rev. Lett. '03

Quantum criticality in magnetic quantum dot

(S. Kirchner, L. Zhu, QS, and D. Natelson, unpublished '04)



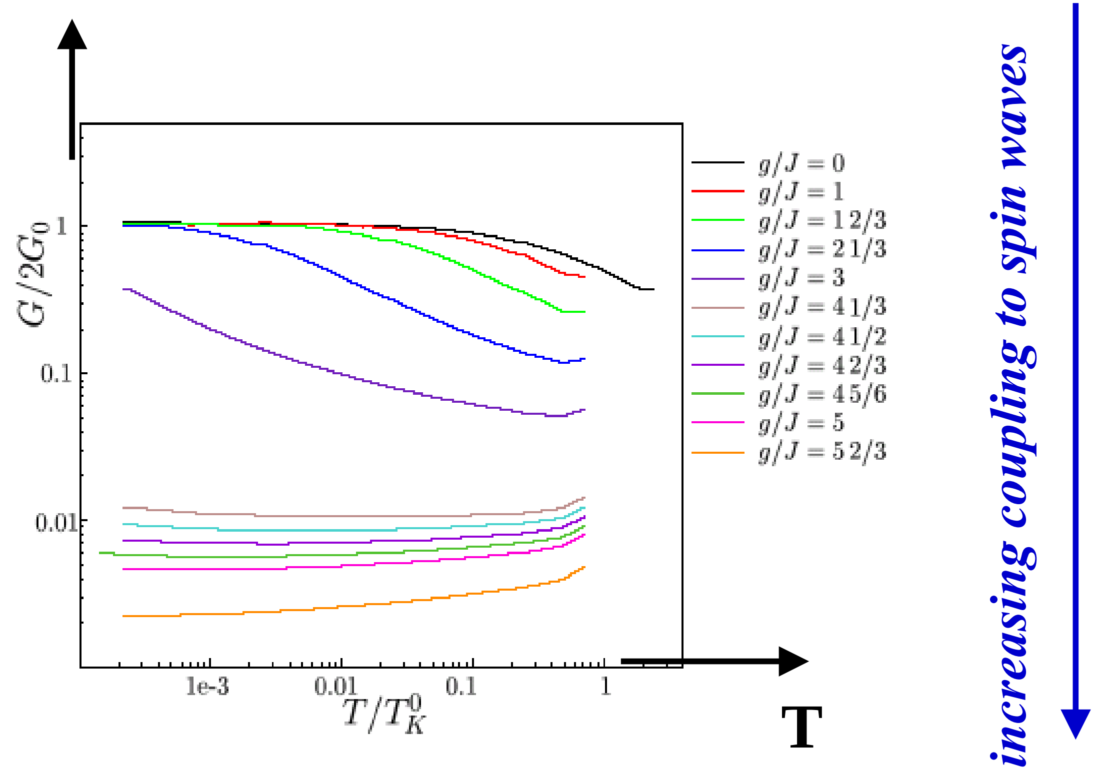
Cf. for parallel configuration: Splitting of Kondo resonance (J. Martinek et al, PRL '03; P. McEwen, D. Ralph, et al., APS March Meeting '04)

- **Spin waves: Sub-ohmic dissipation bath (γ=0.5)**
- **Bose-Fermi Kondo model w/ xy-symmetry**
- **Tuning the relative couplings of the dot spin to spin waves and fermions leads to a QCP**

For mixed-valence quantum dot with Ohmic bath: K. Le Hur '04

Quantum criticality in magnetic quantum dot (cont'd)

Linear-response conductance



SUMMARY

- **Two types of quantum critical metals**
  - T=0 SDW transition (Gaussian)
  - Locally quantum-critical: destruction of Kondo effect exactly at the magnetic QCP (interacting)
- **Microscopic (EDMFT) results of Kondo lattice models**
- **Evidence from Hall effect, inelastic neutron scattering, NMR, and Grüneisen ratio**
- **Beyond microscopics**
- **Relevance to other strongly correlated metals?**

How can the Hertz picture* break down?

[* paramagnons fluctuating in (d+z) dimensions]

- ***Non-Fermi liquid electronic excitations may be part of the quantum-critical spectrum:***
  - **Such electronic excitations arise exactly at the QCP**

- ***Quantum temporal fluctuations may not simply be extra z-dimensions of classical fluctuations:***

$$Z \sim \sum_{\text{config in } (x,\tau)} Z(\text{config})$$

The partition function for an individual configuration in space and time may not be positive semidefinite (cf, the “minus sign problem” of quantum Monte Carlo).

- Robustness of the LQCP (for α < 1): GL

- Kondo versus Mott-Hubbard systems: