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Workshop on
Novel States and Phase Transitions in Highly Correlated Matter

12 - 23 July 2004

Grüneisen ratio divergence at heavy fermion quantum critical points

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

Grüneisen ratio divergence at heavy fermion quantum critical points

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Outline

- Introduction
- $CeNi_2Ge_2$
- $YbRh_2Si_2$
- $CeCu_{6-x}Ag_x$
- Outlook

Collaborators

R. Küchler, N. Oeschler	Thermal expansion
J. Custers, F. Weickert	Electrical resistivity, χ_{ac}, $\Delta L(B)$
T. Cichorek, K. Neumaier[1], E.-W. Scheidt[2]	Specific heat
J. Ferstl, C. Geibel	$YbRh_2Si_2$ single crystals
J.A. Mydosh	$CeNi_2Ge_2$ single crystals
K. Heuser[2], G.R. Stewart[3]	$CeCu_{6-x}Ag_x$ polycrystals
F. Steglich	

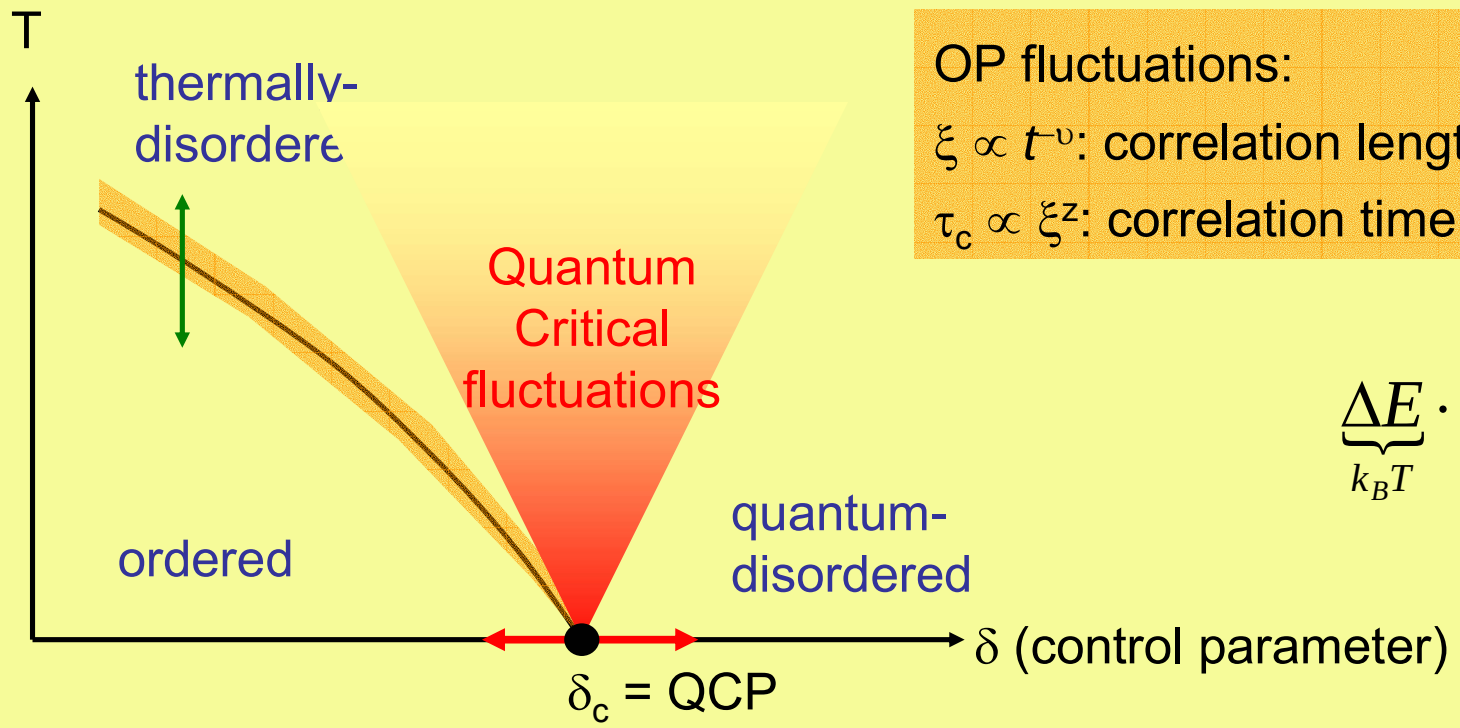
[1]*Walther Meissner Institute, Garching, Germany*

[2]*Augsburg University, Germany*

[3]*University of Florida, Gainesville FL, USA*

C. Pépin, P. Coleman, M. Garst, I. Paul, Q. Si, …	Theory

Quantum phase transitions



OP fluctuations:

$\xi \propto t^{-\upsilon}$: correlation length

$\tau_c \propto \xi^z$: correlation time

$$\underbrace{\Delta E}_{k_B T} \cdot \tau_{\text{therm}} \geq \hbar$$

classical phase transition: driven by thermal fluctuations

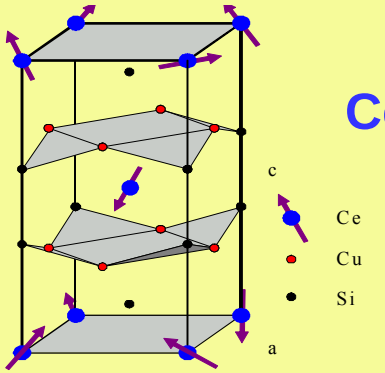
$\tau_c > \tau_{\text{therm}} \rightarrow$ static description

quantum phase transition: driven by quantum fluctuations , $\tau_c < \tau_{\text{therm}}$ ($\rightarrow \infty$)

QC fluctuations: wide-reaching influence on finite-T properties, dynamic

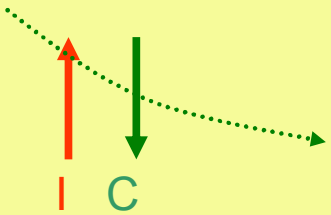
Kondo effect and Heavy Fermion systems

- lattice of *f*-moments (most Ce, Yb or U)
- high *T*: Curie-Weiss-behavior
- Upon cooling: Kondo-interaction between *f*-moments and conduction electrons

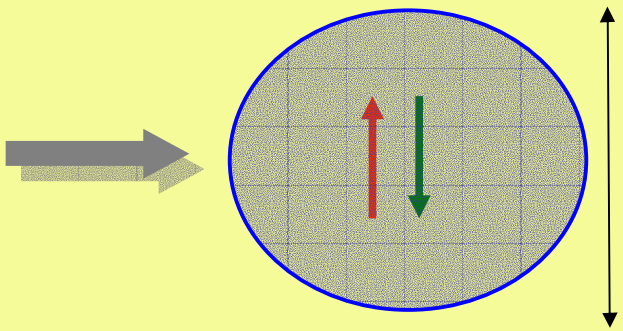


$CeCu_2Si_2$

$T \gtrsim T_K$



$T \ll T_K$



$$\xi_K = \frac{\hbar v_F}{k_B T_K} \sim 100\,\text{nm}$$

for $T_K \sim 50$ K

I: „impurity“ spin
C: conduction electron

(Jun Kondo ´63)

→ Spin-singlet ground-state
→ strong correlations (large ξ)

Landau Fermi liquid

Lev Landau ´57

Excitations of system with strongly interacting electrons

1:1 correspondence ⟷

Free electron gas

→ Definition of quasiparticles near E_F with renormalized mass m^*

→ specific heat: $C / T = \gamma = \frac{k_B^2}{3\hbar^2} k_F \cdot m^* \sim \frac{1}{T^*}$

→ electrical resistivity: $\Delta\rho = aT^2$ mit $a \sim \frac{1}{T^{*2}}$

Heavy Fermion systems

HFS: lattice of *f*-electrons

two competing interactions:

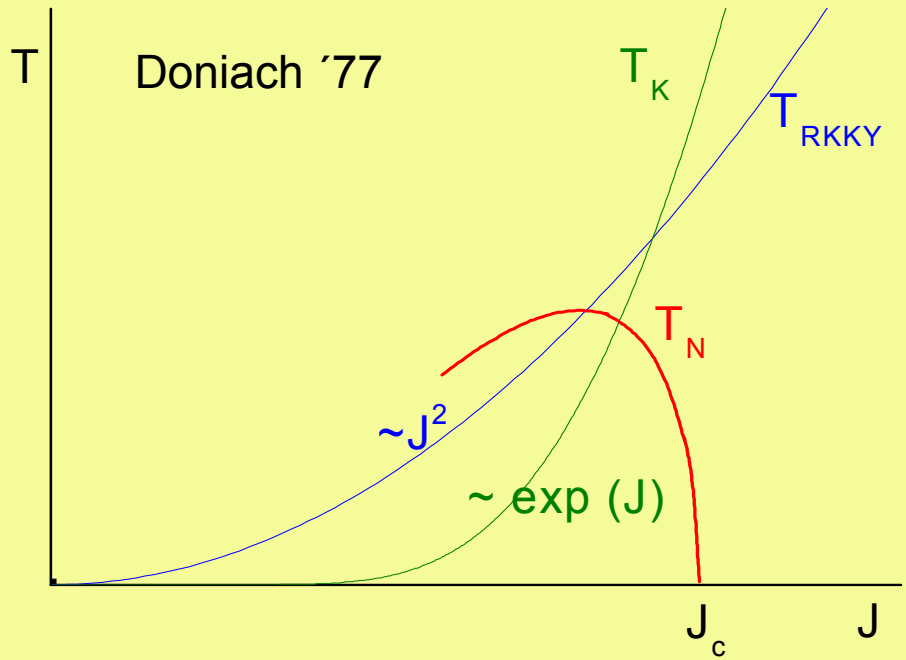
Kondo → local singlet state

$T_K \sim \exp(-1/(N(E_F)J)$

RKKY → magnetic order

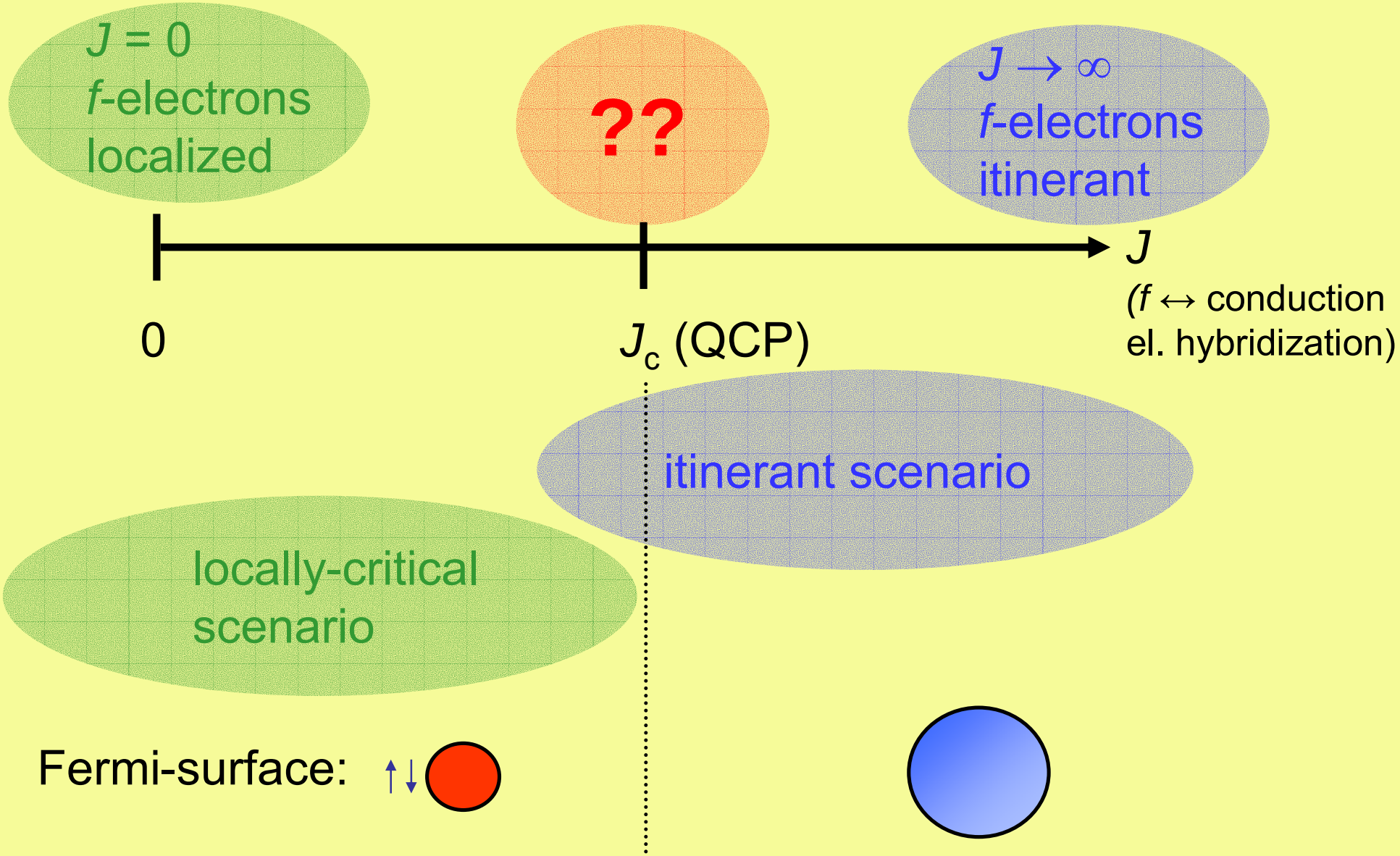
$T_{RKKY} \sim J^2 N(E_F)$

J: *f*-cond. el. hybridization



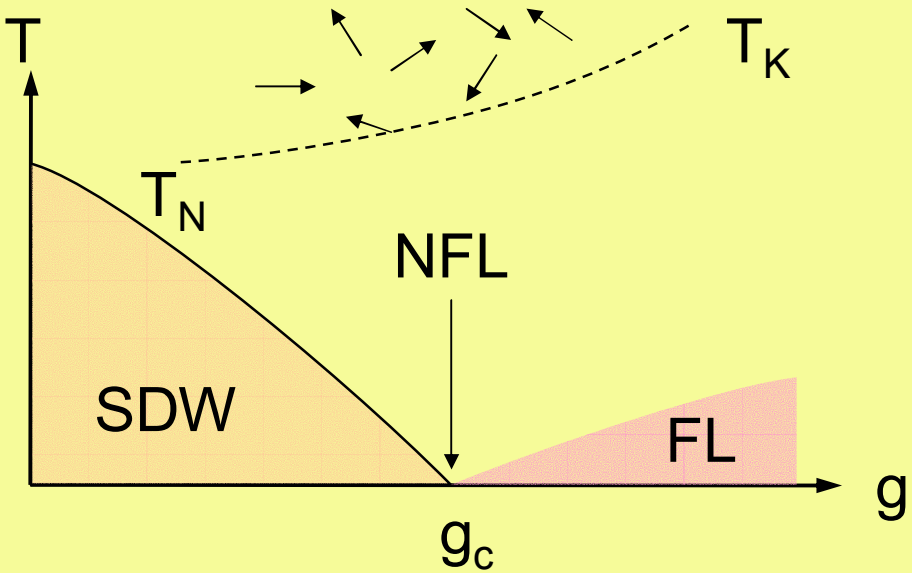
HF systems ideally suited to study quantum criticality

QCP in HF systems



Itinerant *vs* locally critical scenario

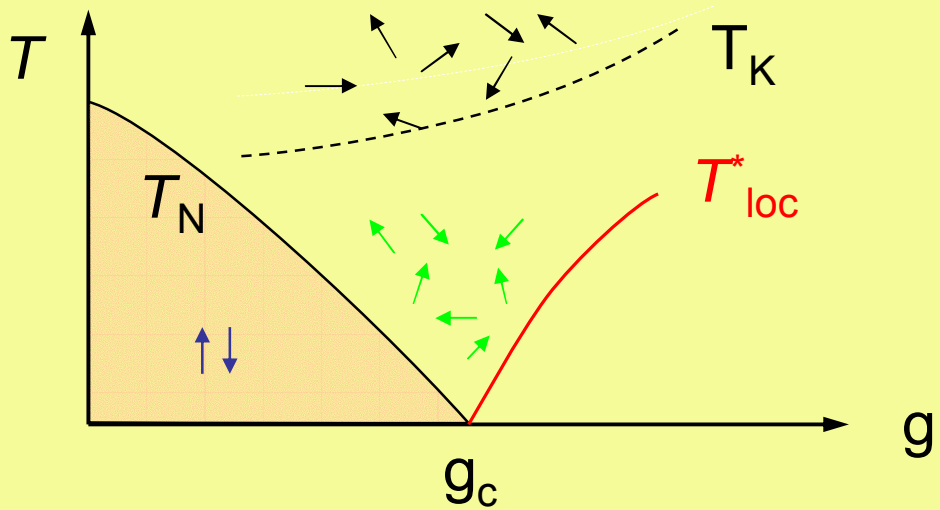
Hertz, Millis, Moriya, Lonzarich, …

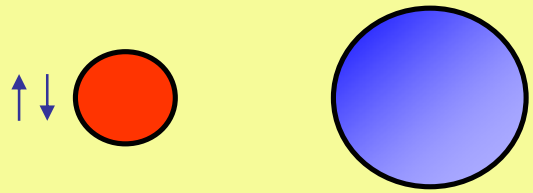


AF: z=2 (d_{eff} = d+z)

	$d=2$	$d=3$
C/T	$\ln(T_0/T)$	$\gamma_0 - \alpha\sqrt{T}$
ρ	T	$T^{3/2}$

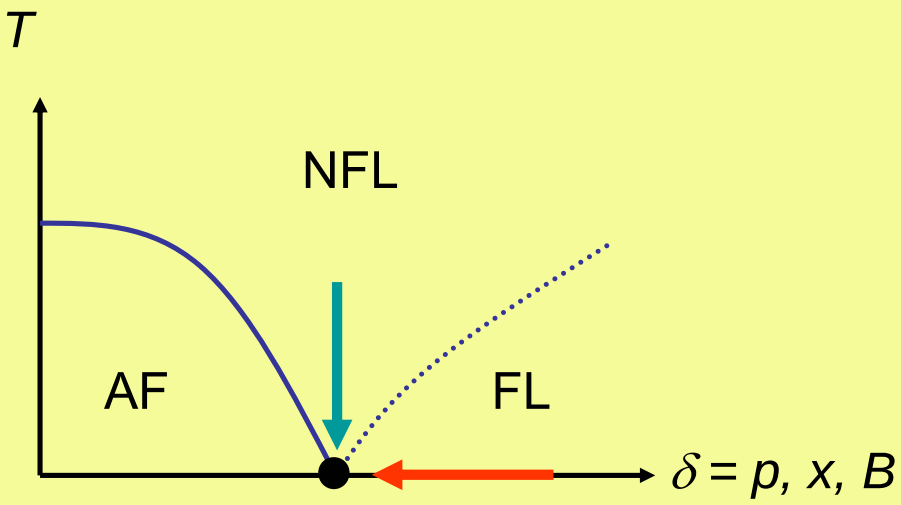
P. Coleman, C. Pépin, J. Phys. Cond. Matt. (2001)
Q. Si et al., Nature 413 (2001)





- Heavy quasiparticles decompose at QCP
- spatially locally critical excitations

Grüneisen ratio analysis



Thermal expansion

$\beta = -1/V\ \partial S/\partial p$ $\beta = V^{-1}\, dV/dT$

Specific heat: $C/T = \partial S/\partial T$

$$\Gamma \sim \frac{\beta}{C} = -\frac{1}{V_{mol}} \frac{(\partial S/\partial p)_T}{T(\partial S/\partial T)_p} = \frac{1}{V_{mol} E^*} \frac{\partial E^*}{\partial p}$$

$\rightarrow \infty$ at QCP!

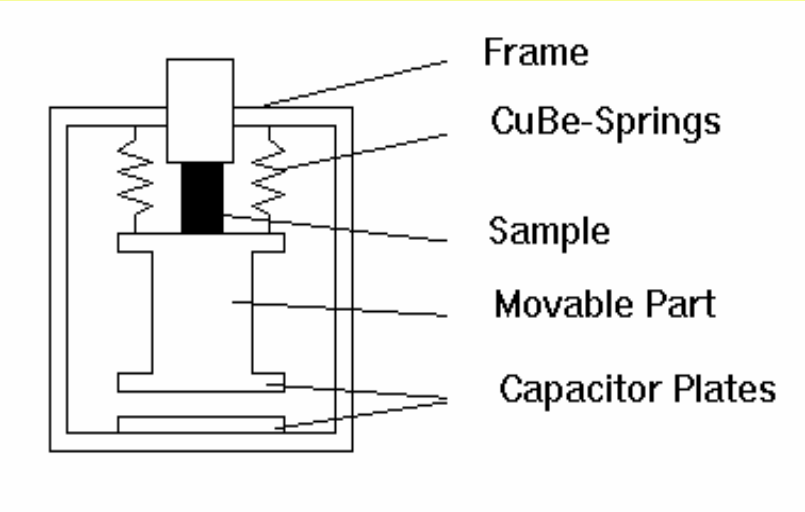
Itinerant theory: $\Gamma \sim T^{-\upsilon z} \sim T^{-1}$ (L. Zhu *et al.*, PRL 2003)

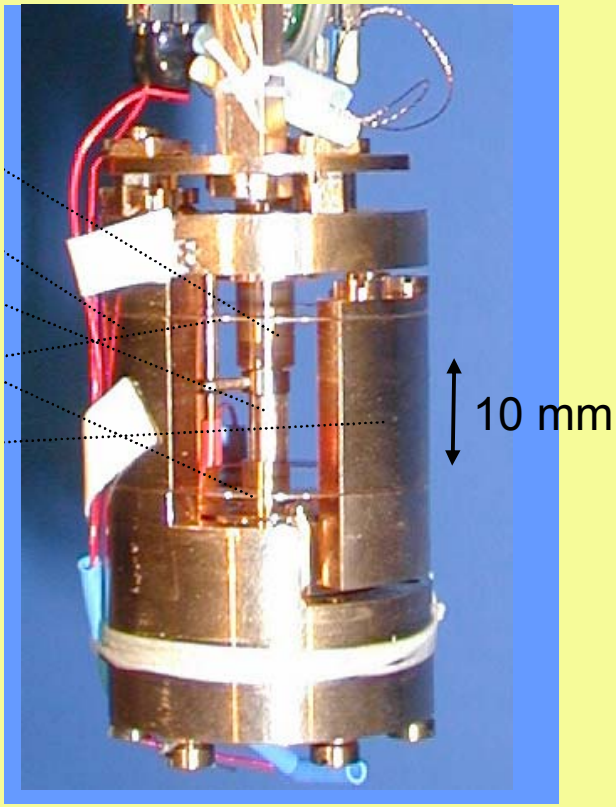
$$\Gamma_H = -\frac{(\partial S/\partial H)_T}{T(\partial S/\partial T)_H} = -\frac{(\partial M/\partial T)_H}{C|_H} = \frac{1}{T}\frac{\partial T}{\partial H}\Big|_S$$

$\rightarrow \infty$ at QCP!

Thermal expansion

Principle of operation:





$$\Delta l = -\Delta d = \varepsilon \cdot A \cdot \frac{\Delta C}{C^2}$$

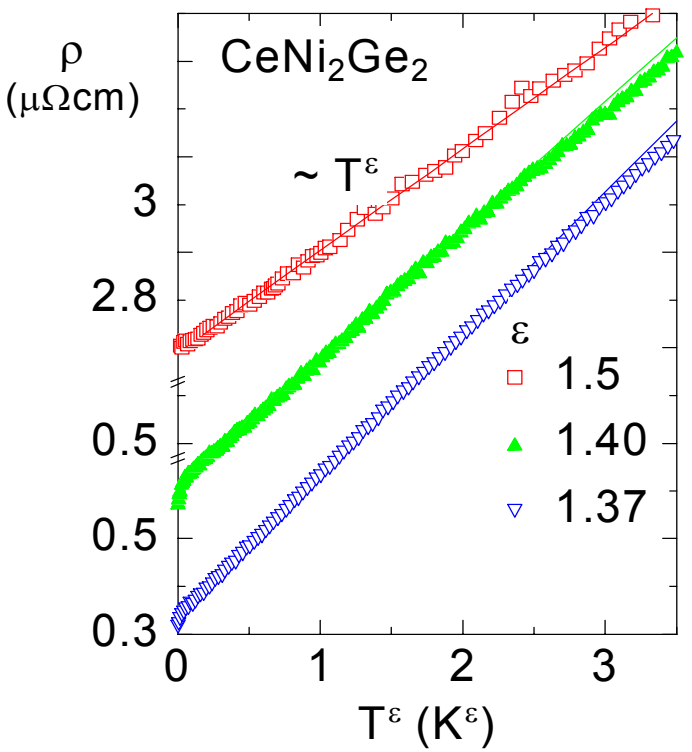
$$\alpha(T) = \frac{1}{l} \cdot \left(\frac{\partial \Delta l(T)}{\partial T} \right)_p$$

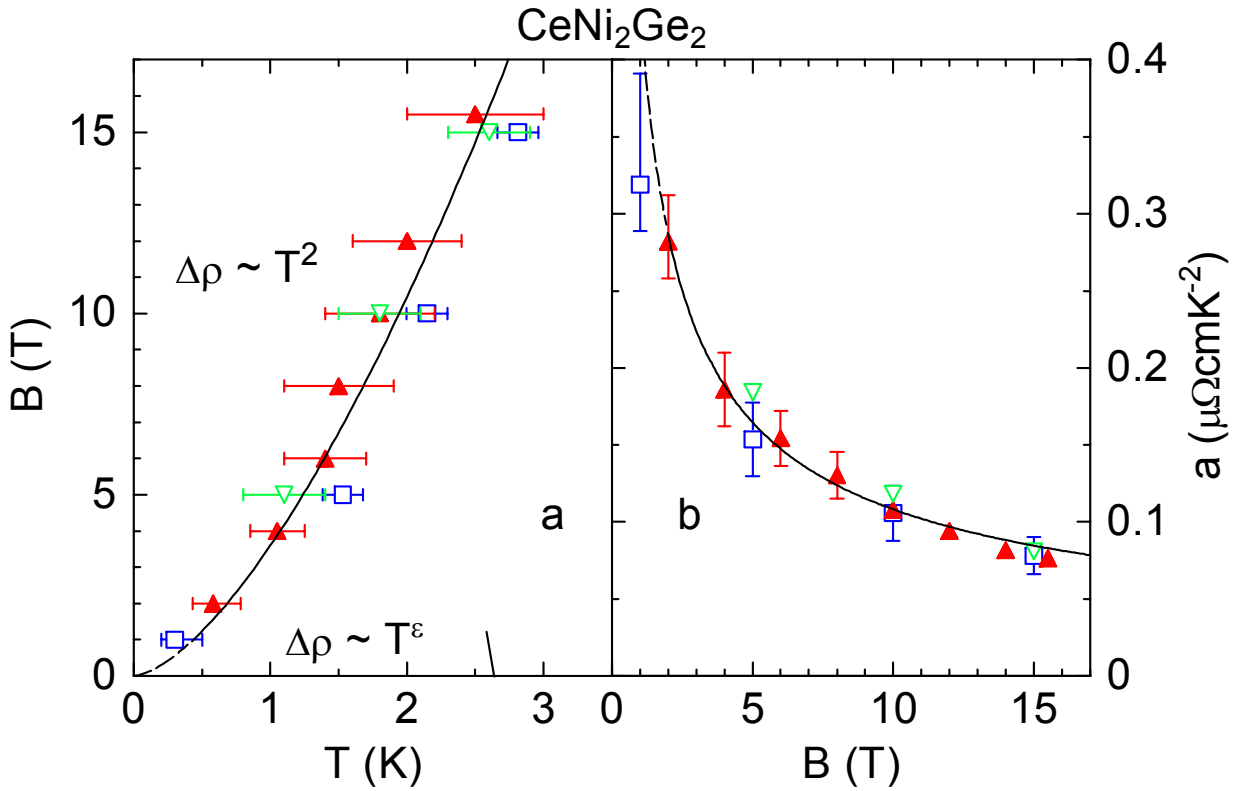
→ Resolution: < 0.01Å

$\Delta l/l$ = 10^{-10} (l = 5 mm) at $B \leq$ 20 T

$CeNi_2Ge_2$: close to zero-field QCP

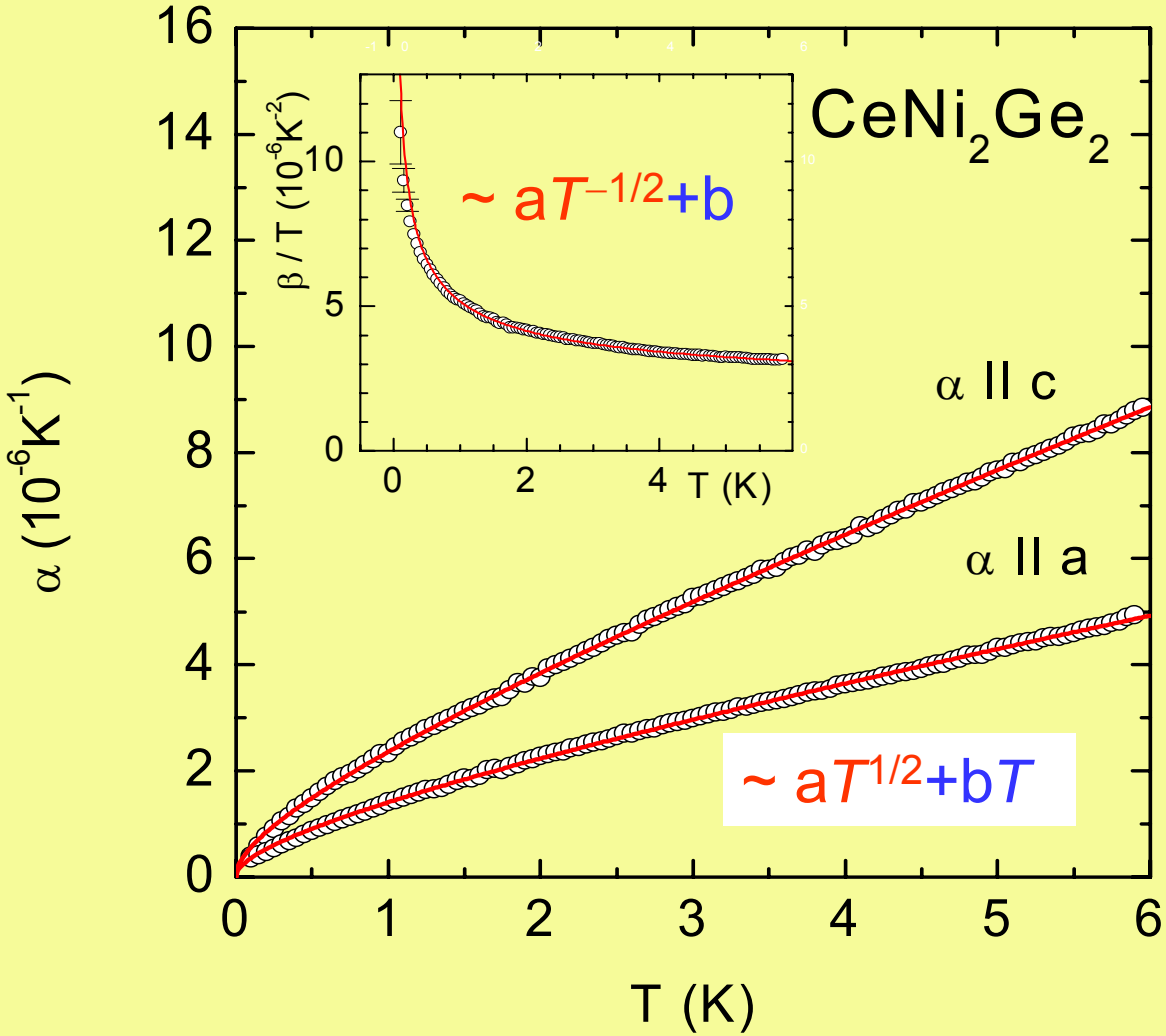
T_K = 30 K, paramagnetic ground state





P. Gegenwart, F. Kromer, M. Lang, G. Sparn, C. Geibel, F. Steglich, Phys. Rev. Lett. **82**, 1293 (1999)

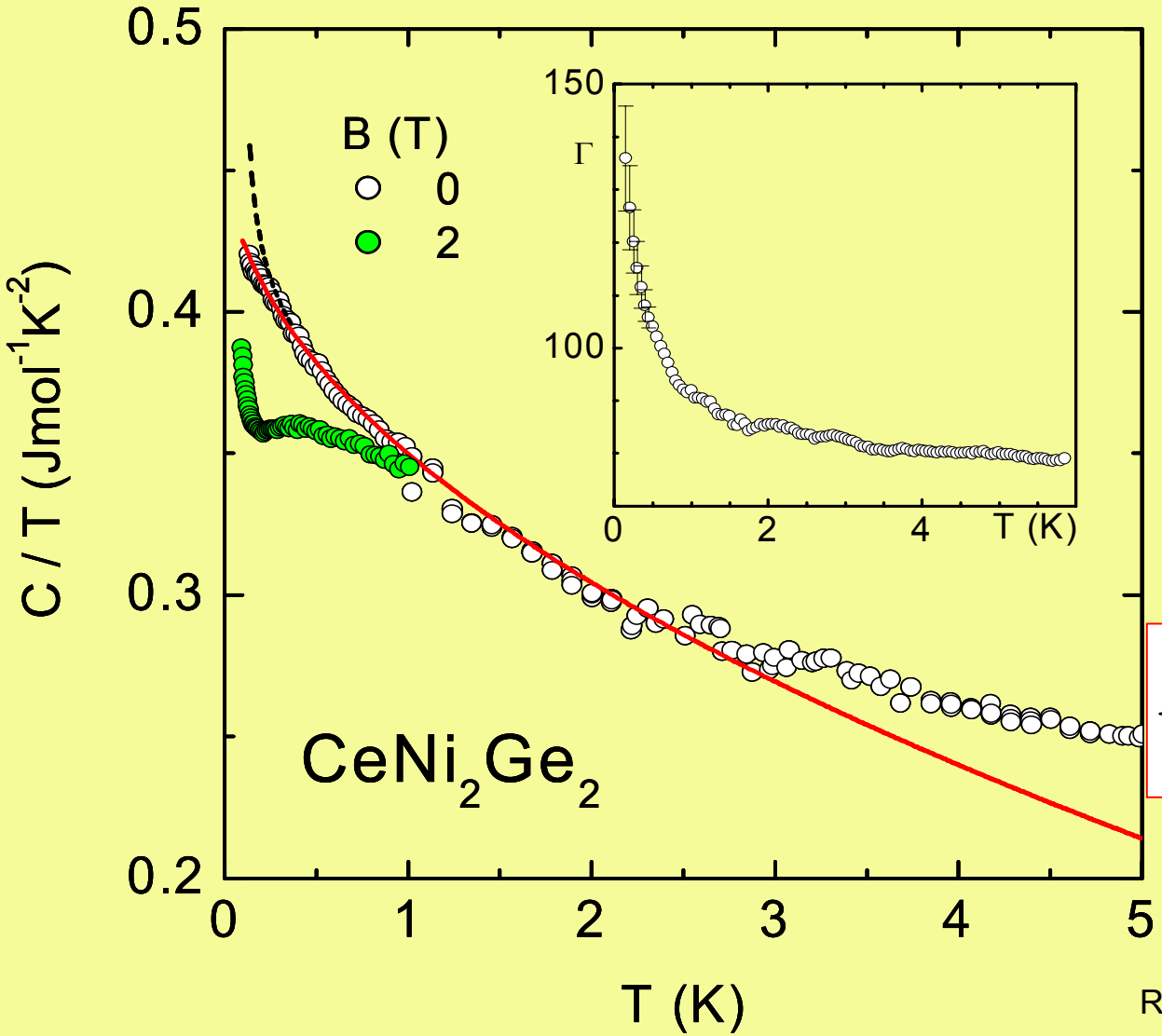
$CeNi_2Ge_2$: thermal expansion



In accordance with prediction of itinerant theory

R. Küchler, N. Oeschler, P. Gegenwart, T. Cichorek, K. Neumaier, O. Tegus, C. Geibel, J.A. Mydosh, F. Steglich, L. Zhu, Q. Si, Phys. Rev. Lett. **91**, 066405 (2003)

$CeNi_2Ge_2$: specific heat



$\Gamma \rightarrow \infty$ for $T \rightarrow 0$

$$\frac{C}{T} = \gamma_0 - \alpha\sqrt{T} + \frac{d}{T^3}$$

R. Küchler *et al.*, PRL **91**, 066405 (2003).

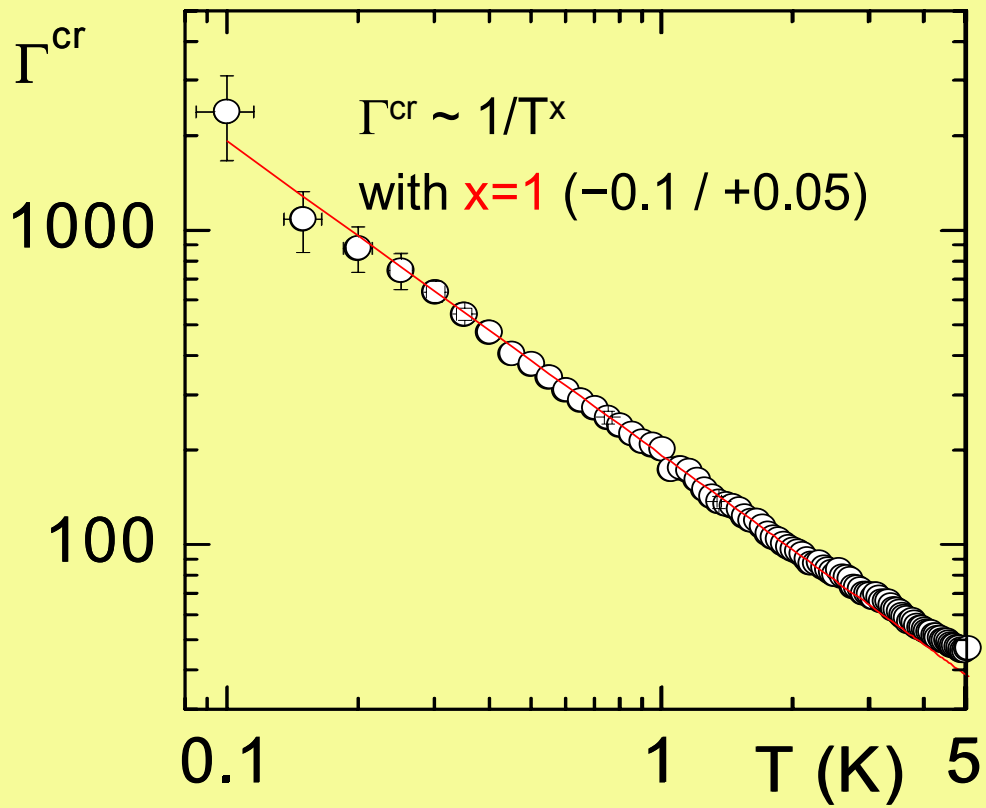
T. Cichorek *et al.*, Acta. Phys. Pol. **B34**, 371 (2003).

$CeNi_2Ge_2$: Grüneisen ratio

critical components: $\beta^{cr}=\beta(T)-bT$

$C^{cr}=C(T)-\gamma T$

$\Gamma^{cr} = V_{mol}/\kappa_T \cdot \beta^{cr}/C^{cr}$



- correlation length $\xi \sim |r|^{-\nu}$

  e.g. $r = (p-p_c)/p_c$
- correlation time $\tau_c \sim \xi^z$ (z: dynamical critical exponent)

$\rightarrow$ $\Gamma^{cr}(T) \sim T^{-1/(\nu z)}$

- prediction:

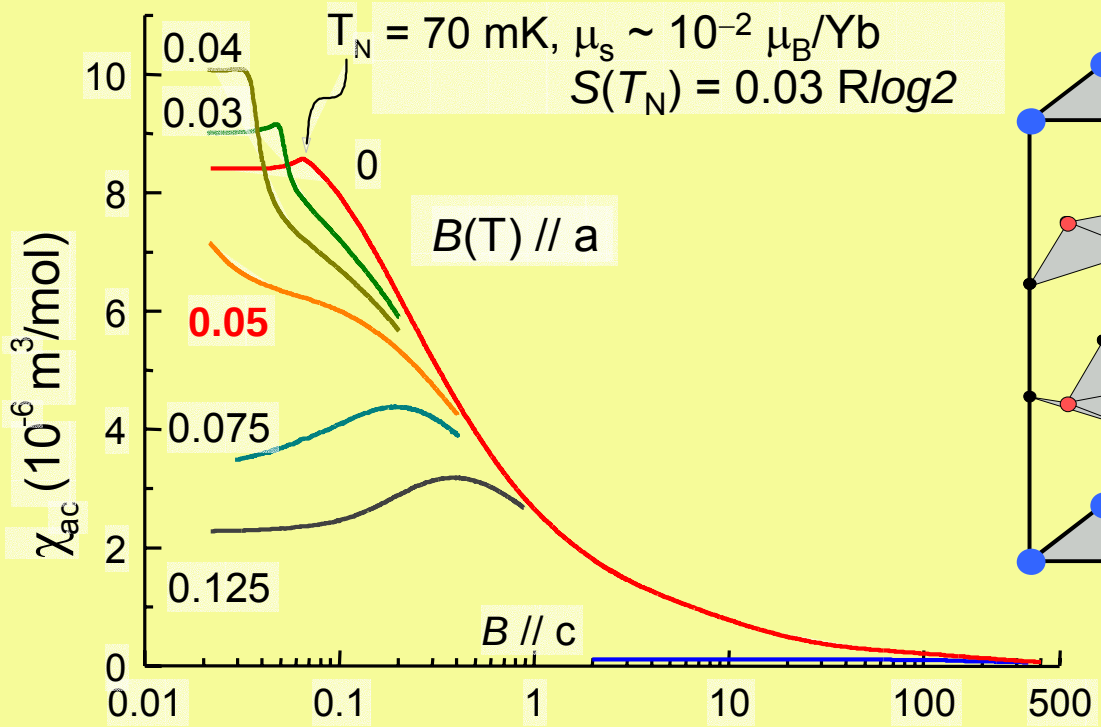
  $\nu = ½$, $z = 2 \rightarrow x = 1$

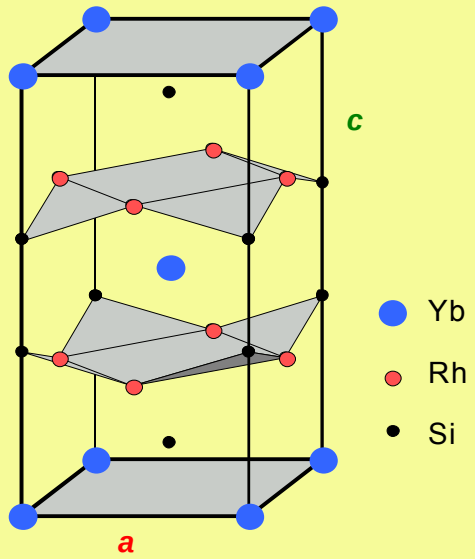
$\rightarrow$ all observations in accordance with the itinerant scenario

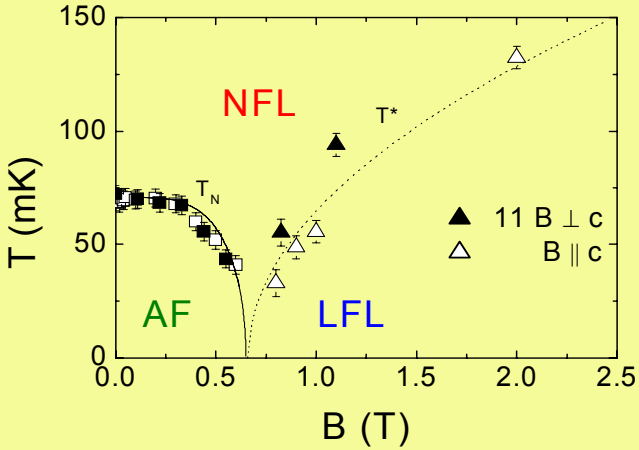
$YbRh_2Si_2$

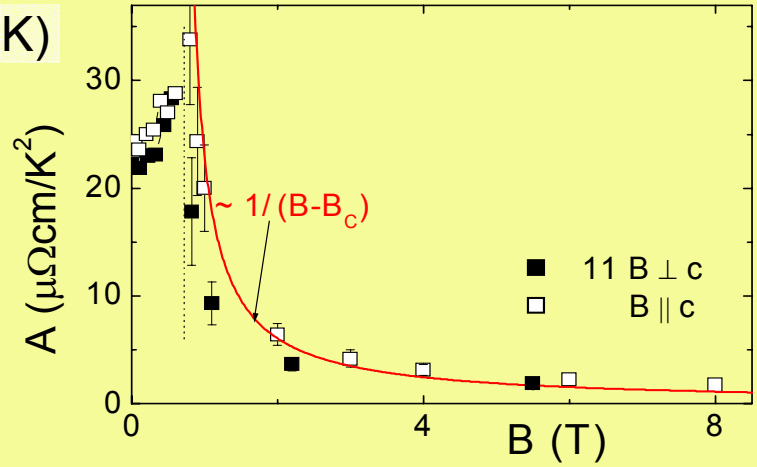
O. Trovarelli *et al.*, PRL **85**, 626 (2000).

P. Gegenwart *et al.*, PRL **89**, 056402 (2002).

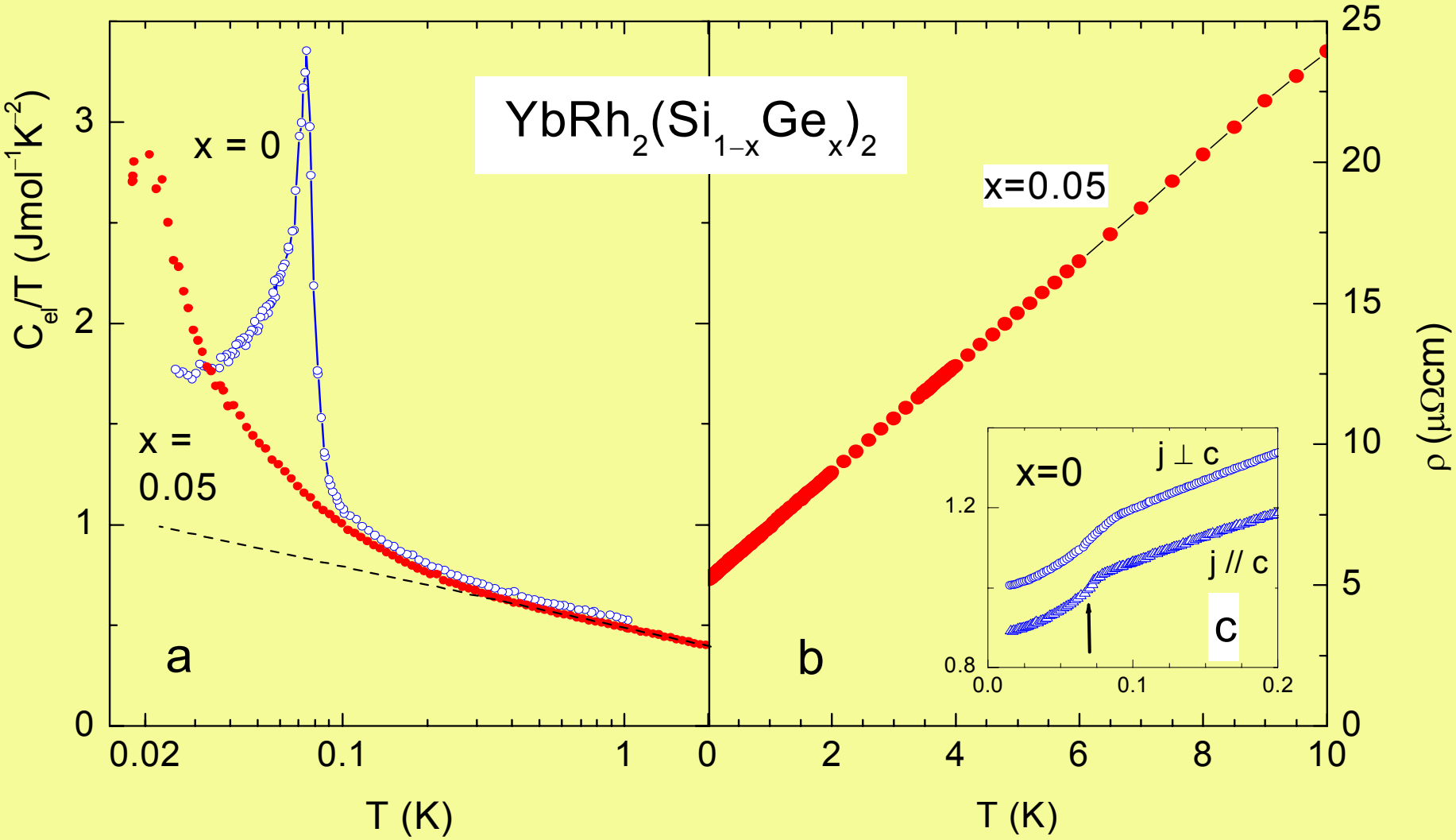






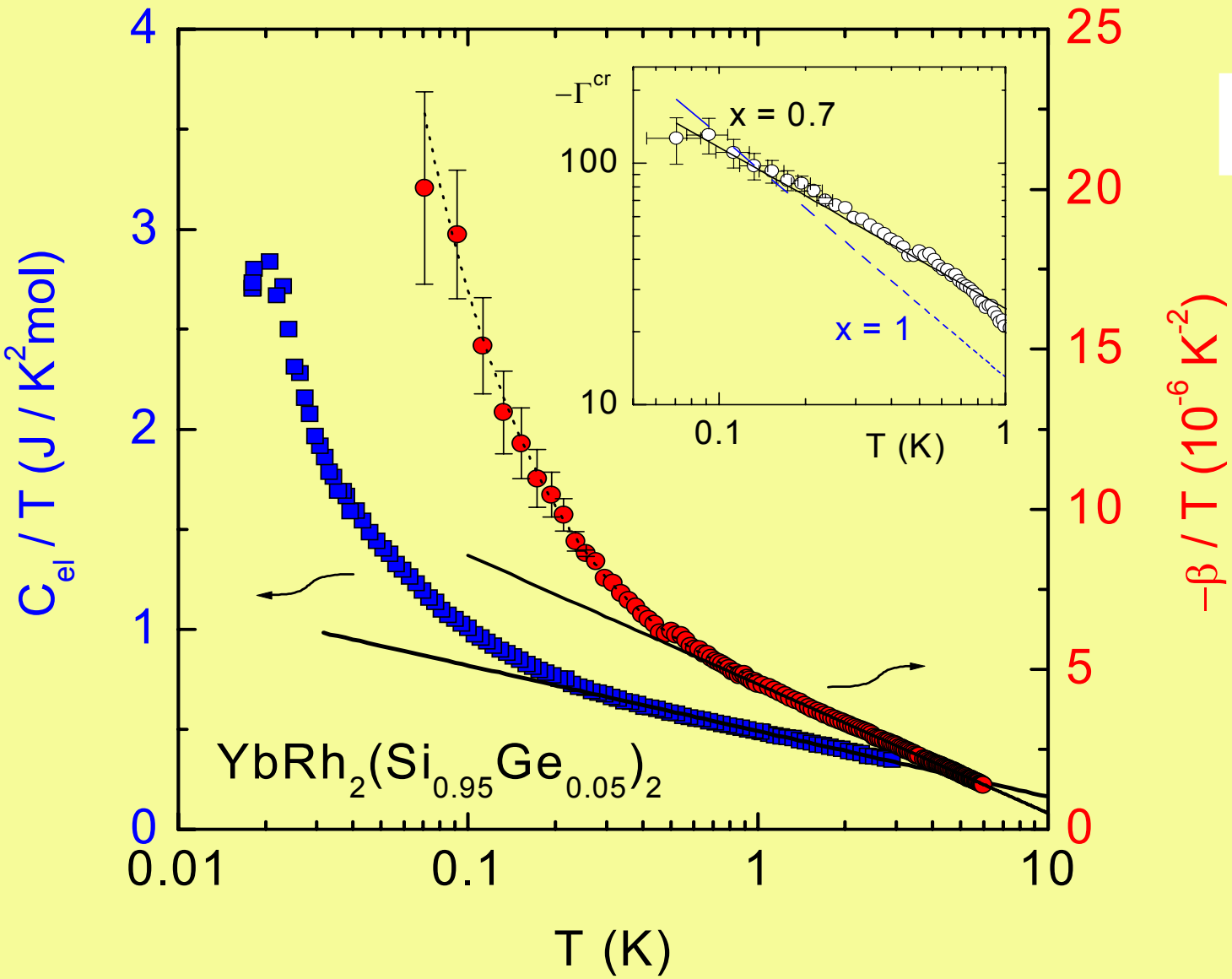


$YbRh_2(Si_{0.95}Ge_{0.05})_2$



Disparate behavior (spin part → *C*, charge part → ρ) at QCP !

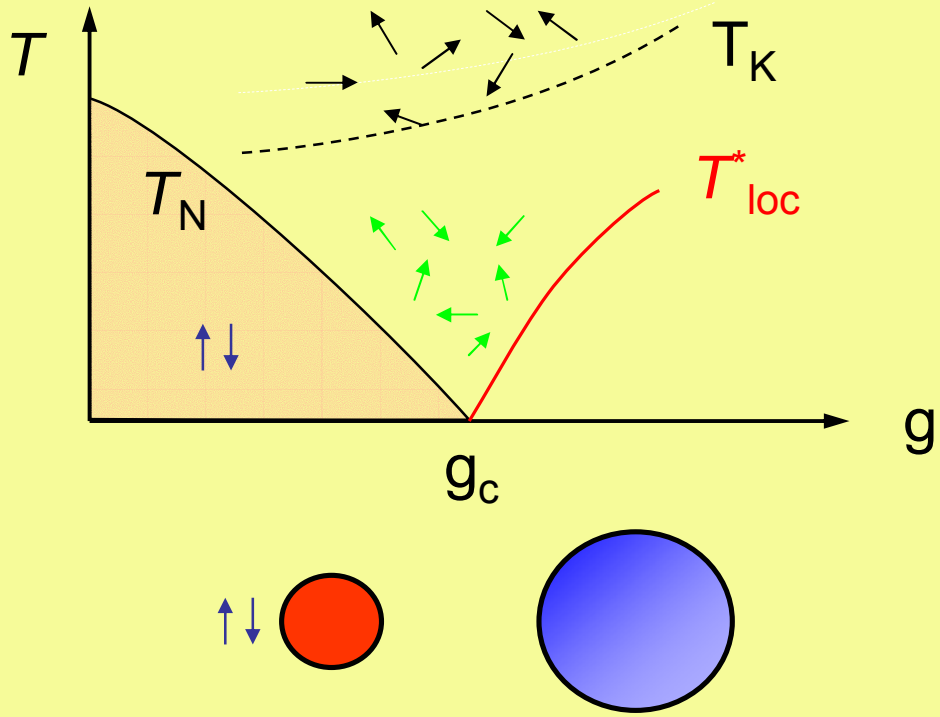
$YbRh_2(Si_{0.95}Ge_{0.05})_2$: Thermal expansion and Grüneisen ratio



R. Küchler et al.,
PRL **91**, 066405 (2003)

Locally-critical QCP in $YbRh_2Si_2$?

P. Coleman, C. Pépin, J. Phys. Cond. Matt. (2001)
Q. Si et al., Nature 413 (2001)



$YbRh_2Si_2$:

J. Custers *et al.*, Nature **424**, 524 (2003)

- $C \leftrightarrow \rho$ disparity: quasiparticle decomposition
- T/b scaling suggests $T^*_{loc} \rightarrow 0$ at QCP

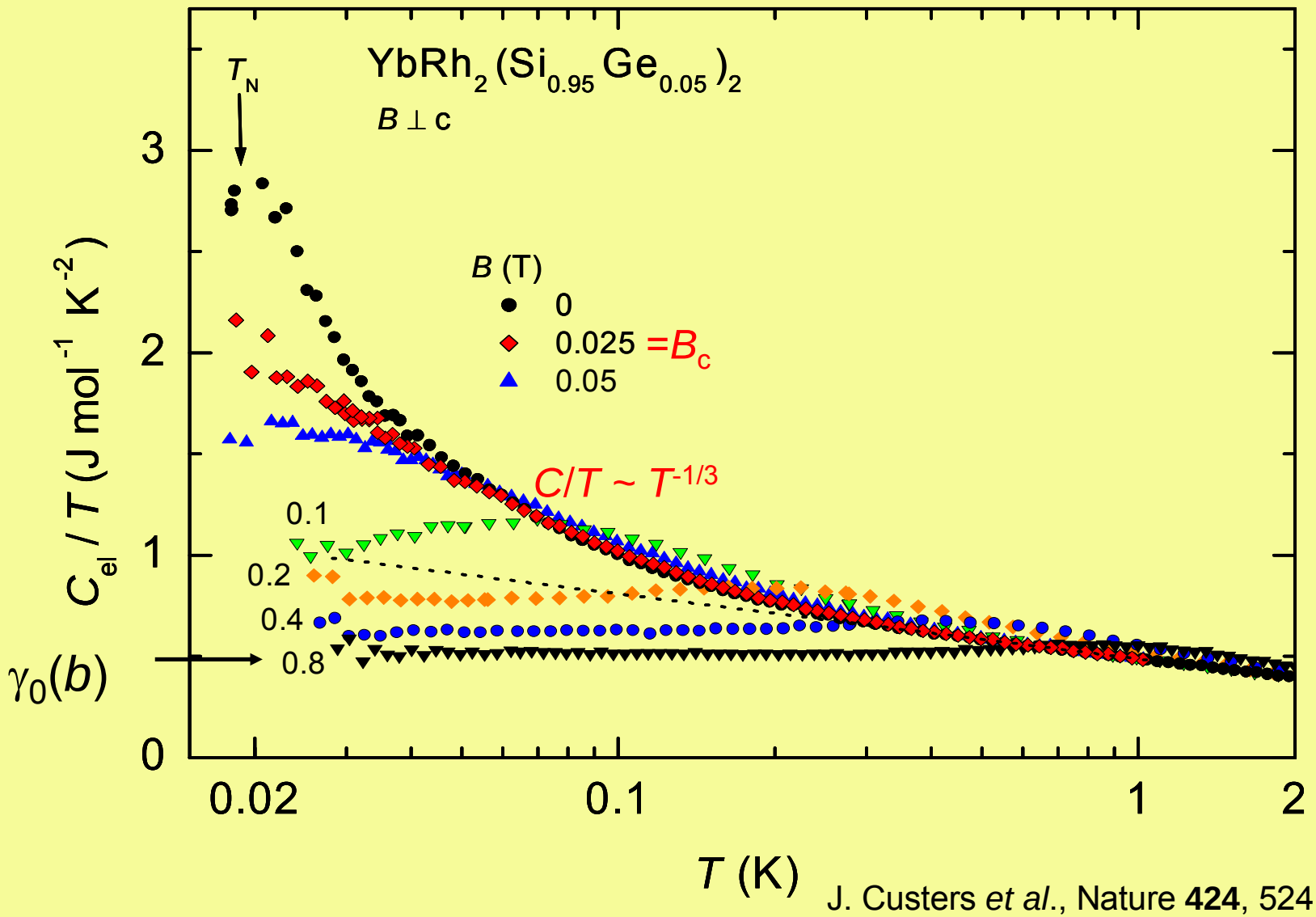
J. Sichelschmidt et al. PRL **91**, 156401 (2003)

- local moments in Yb^{3+} ESR

S. Paschen et al., to be published

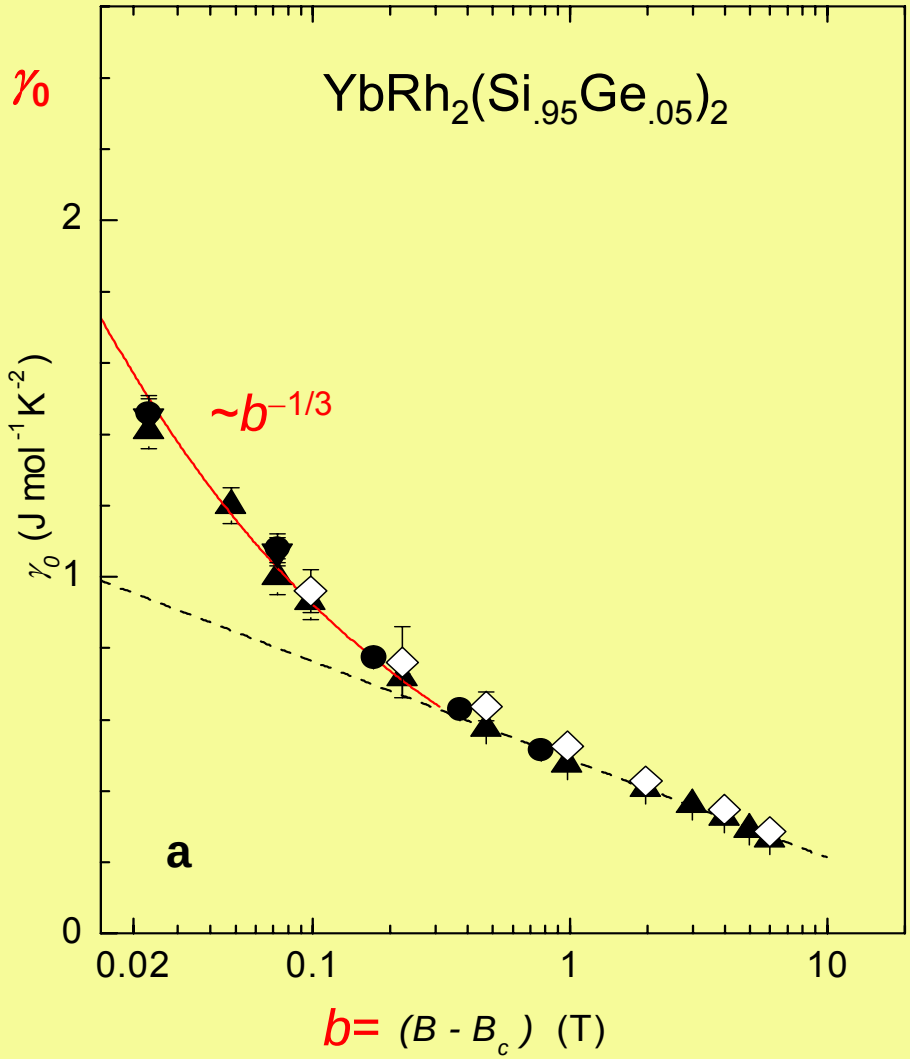
- ρ_H: abrupt destruction of renormalized Fermi surface

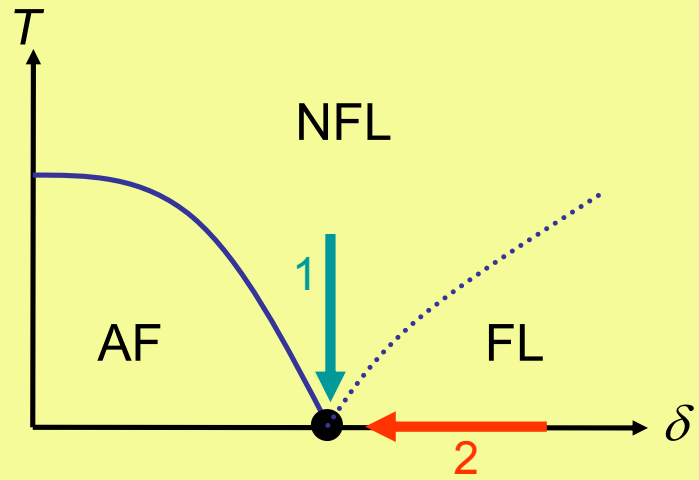
$YbRh_2(Si_{0.95}Ge_{0.05})_2$



J. Custers *et al.*, Nature **424**, 524 (2003)

Stronger than logarithmic mass divergence

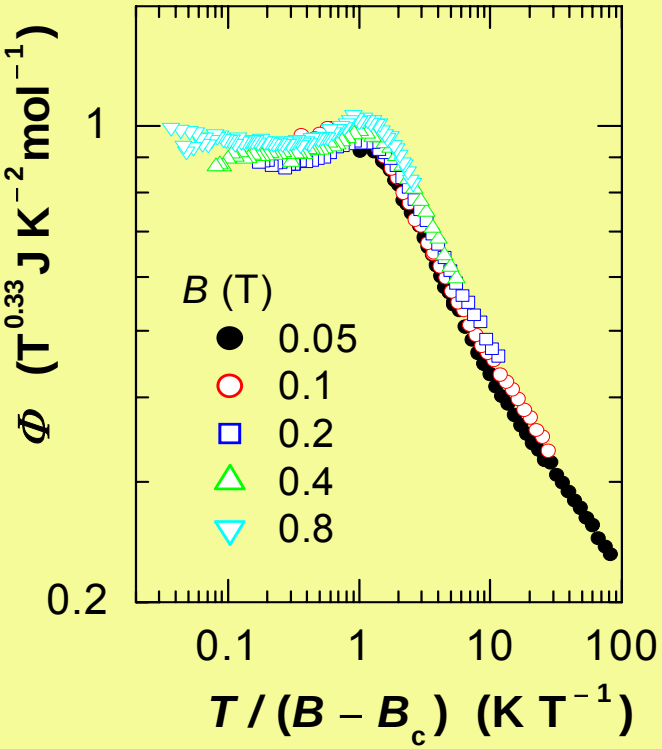




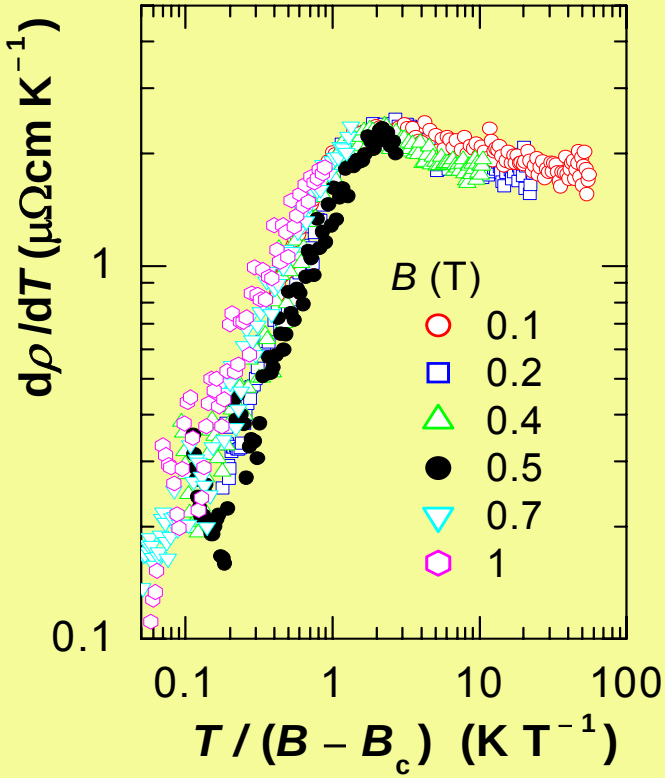
- similar divergence in C/T
- T or B, respectively, define energy scale

Temperature over magnetic field scaling

Specific heat



Electrical resistivity

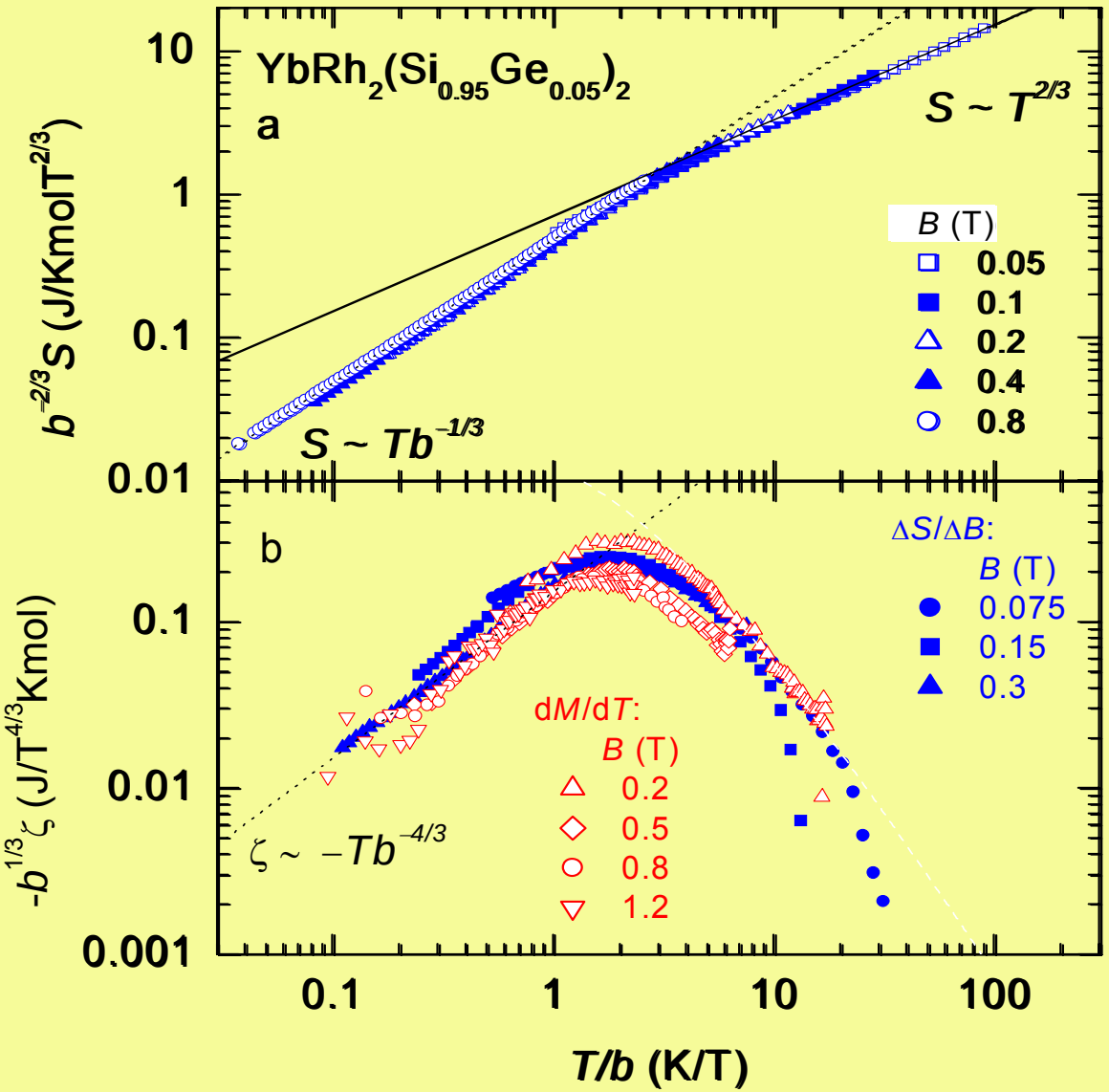


Characteristic energy scale for heavy QP, $T_0(b) \sim b$, vanishes at QCP

$\Rightarrow T/T_0$ Scaling for $\Phi(T,b)$ with $\Phi(T,b) = b^{1/3} \cdot C(T,b)/T$

J. Custers *et al.*, Nature **424**, 524 (2003)

Temperature over magnetic field scaling



P. Gegenwart, cond-mat/0406260

Magnetic entropy

Comparison with M_{DC}

$$\zeta \overset{!}{=} \frac{\partial^2 F}{\partial T \partial B} = \frac{\partial S}{\partial B} = \frac{\partial M}{\partial T}$$

Thermal and magnetic properties consistent

$$\chi = \chi_0(b) + T^2 b^{-7/3}$$

$CeCu_{6-x}M_x$

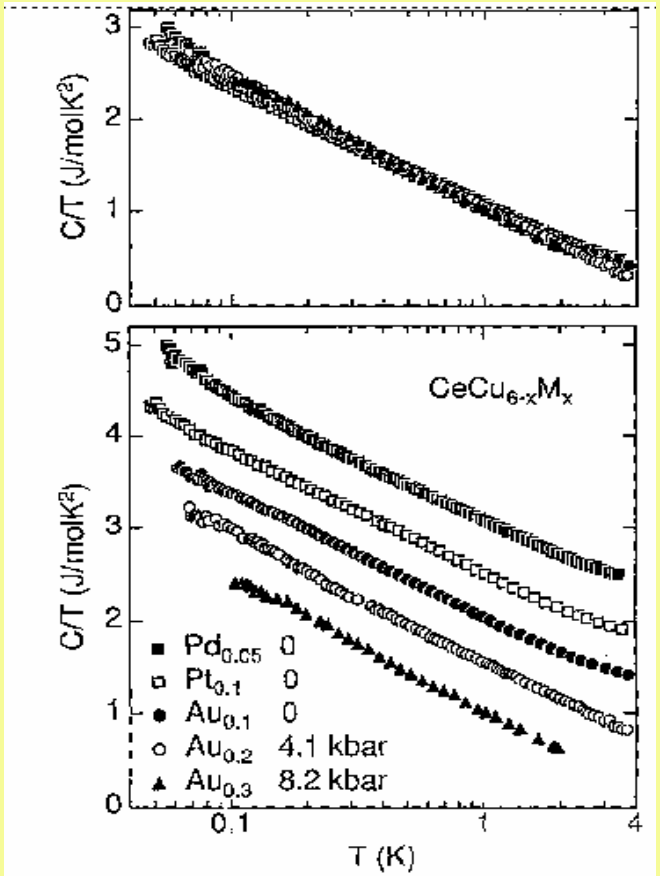


Figure 13. C/T versus $\log T$ for various $CeCu_{6-x}M_x$ samples and pressures as indicated. The upper frame shows the universality of the logarithmic divergence of C/T for $T \to 0$. The lower frame shows the same data shifted by 0.5 J mol^{-1} K^{-2} each for clarity (after [43]).

C/T ~ log *T*
(universal!)

H.v. Löhneysen et al., PRL 1994, 1996
A. Rosch et al., PRL 1997
O. Stockert et al., PRL 1998

2D-SDW scenario ?

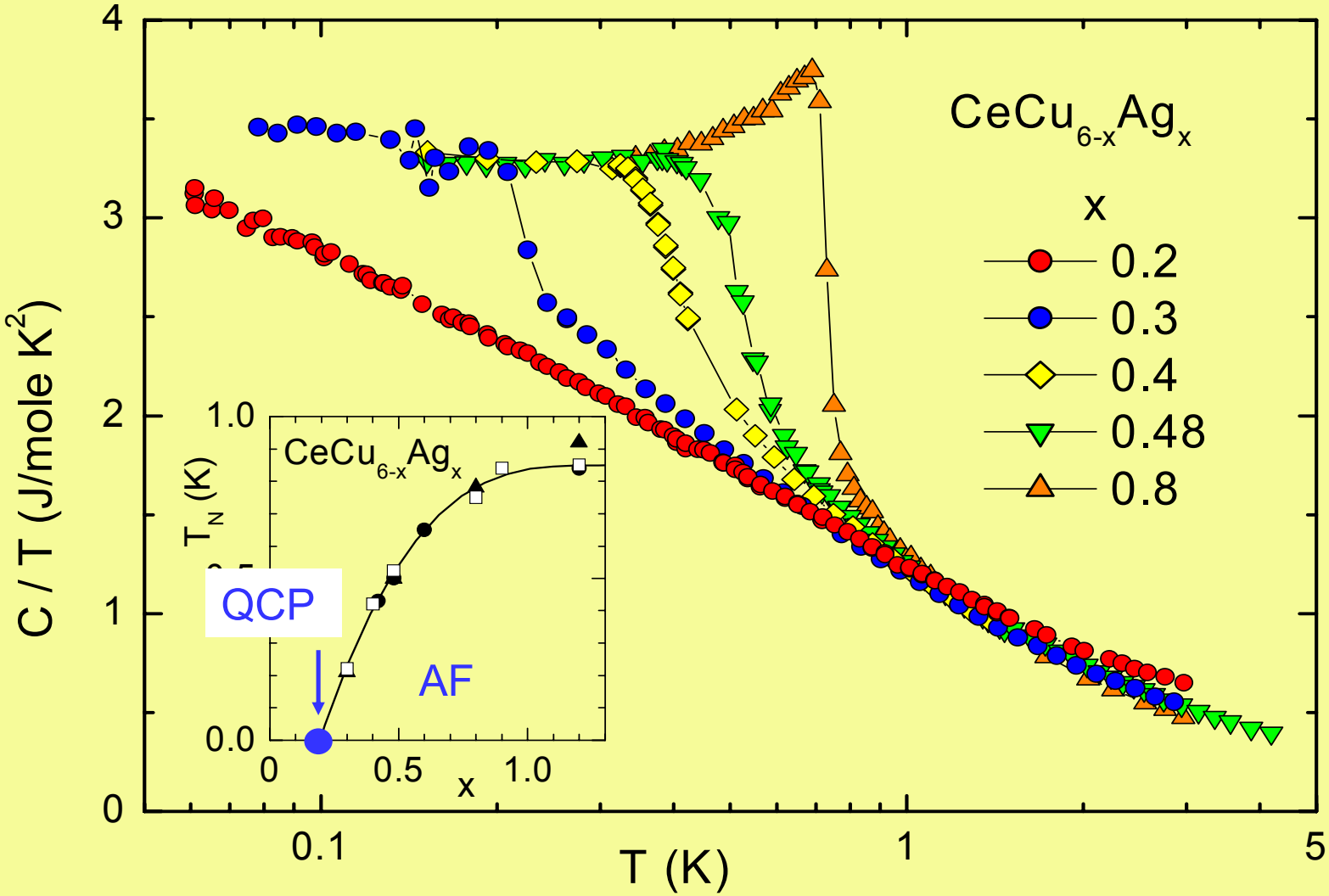
A. Schröder et al., Nature 2000

- E/T scaling in $\chi''(q,\omega)$
- $\chi(q) \sim \{T-\theta(q)\}^{-0.75}$ for all q

→ locally critical scenario

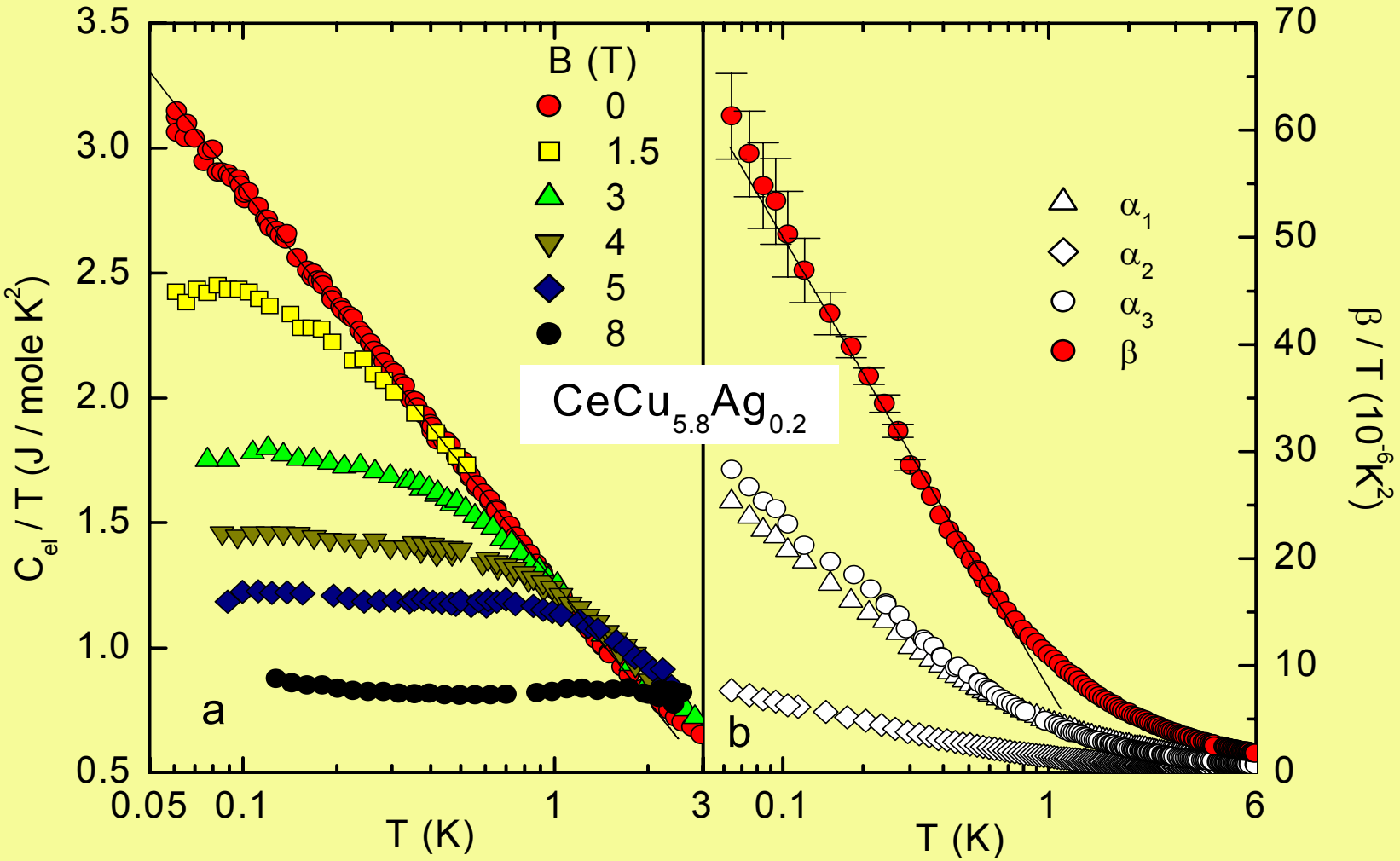
could we disprove 2D-SDW scenario thermodynamically?

$CeCu_{6-x}Ag_x$



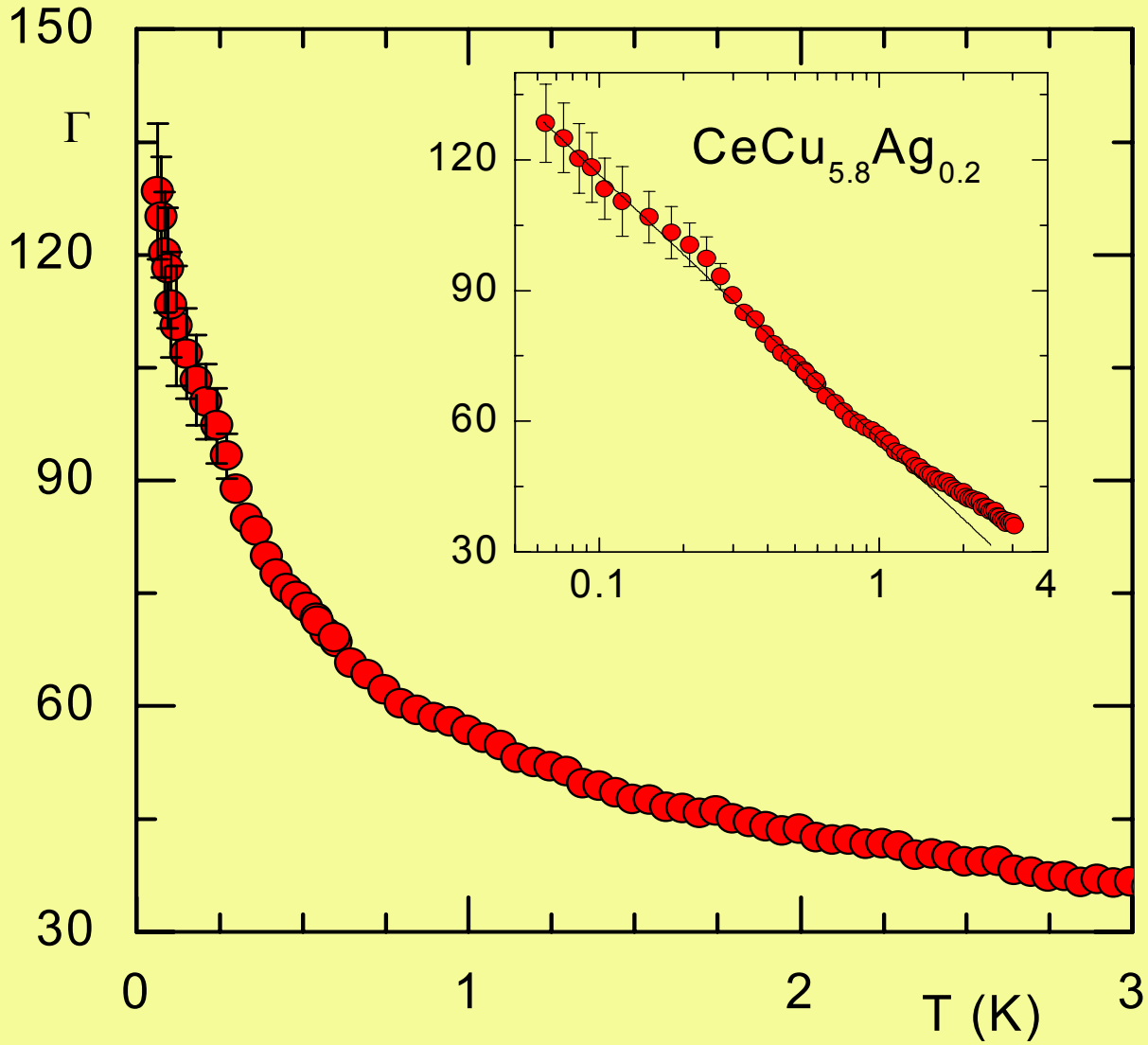
E.-W. Scheidt et al., Physica B 321, 133 (2002).

$CeCu_{5.8}Ag_{0.2}$



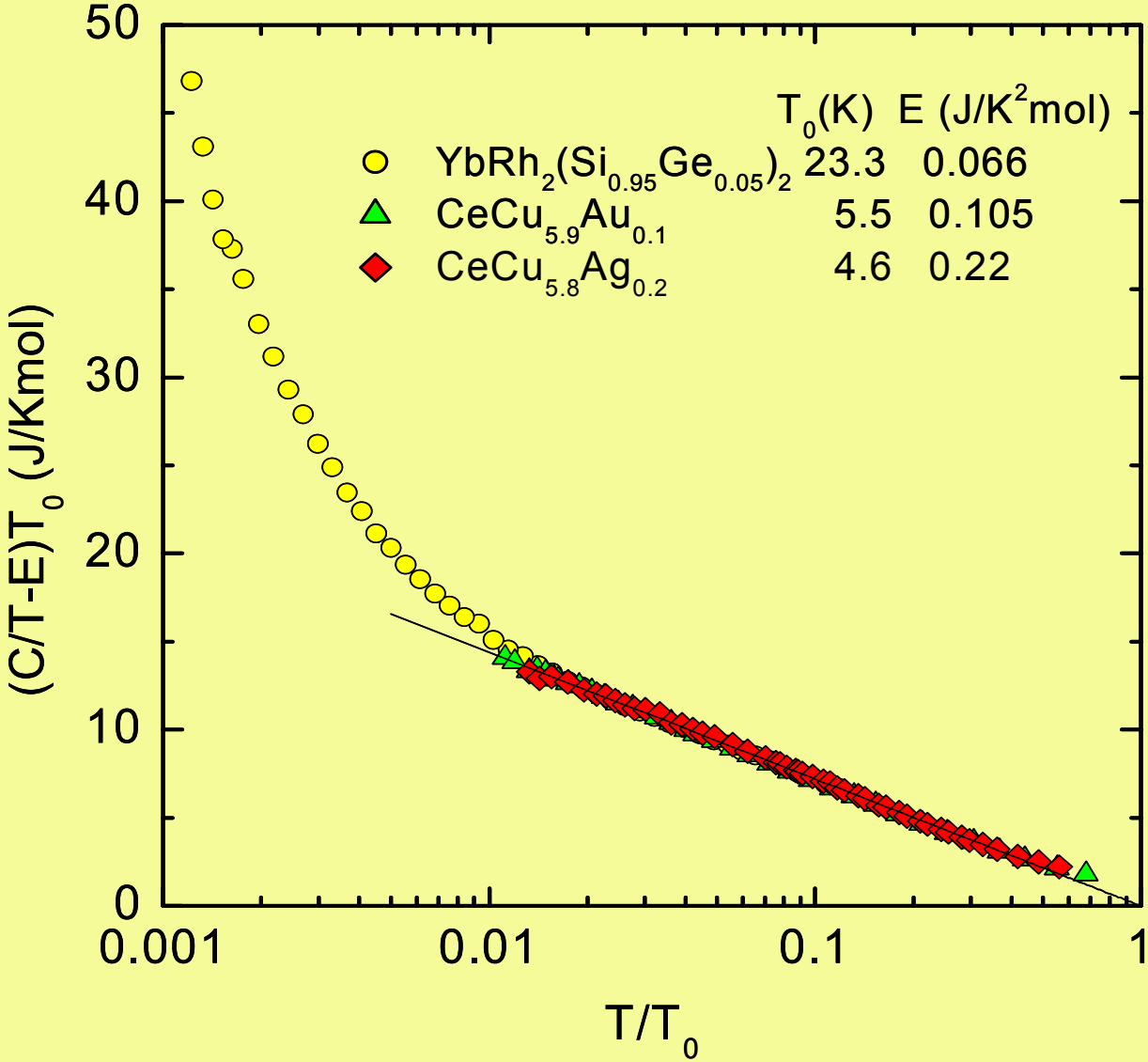
R. Küchler, P. Gegenwart, K. Heuser, E.-W. Scheidt, G.R. Stewart and F. Steglich, to be published, PRL.

$CeCu_{5.8}Ag_{0.2}$



R. Küchler, P. Gegenwart, K. Heuser, E.-W. Scheidt, G.R. Stewart and F. Steglich, to be published,PRL.

$CeCu_{5.8}Ag_{0.2}$

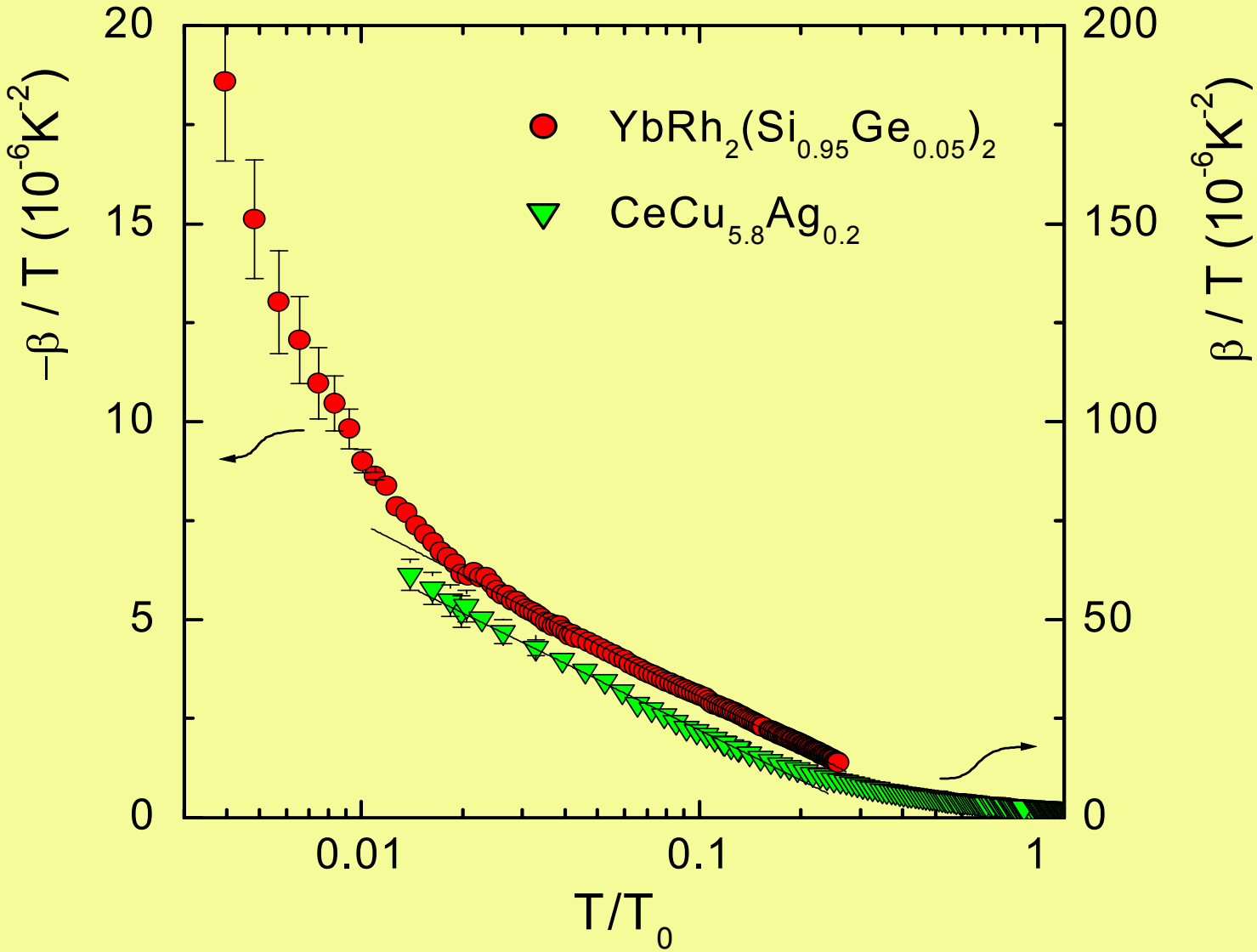


J. Sereni, Physica B 230-232, 580 (1997)

log*T* involves 55% of *R*log2

R. Küchler, P. Gegenwart, K. Heuser, E.-W. Scheidt, G.R. Stewart and F. Steglich, to be published, PRL.

$CeCu_{5.8}Ag_{0.2}$



R. Küchler, P. Gegenwart, K. Heuser, E.-W. Scheidt, G.R. Stewart and F. Steglich, to be published.

Conclusion

At any QCP: Grüneisen-ratio $\Gamma \rightarrow \infty$

- $CeNi_2Ge_2$ ($CeIn_{3-x}Sn_x$) compatible with itinerant theory (in 3D)
- $YbRh_2Si_2$, $CeCu_{6-x}Ag_x$: incompatible (both in 3D and 2D)

$\rightarrow$ two different classes of QCPs?! – why ??

$YbRh_2Si_2$:

- Disparity between *C* und ρ → Break-up of heavy quasiparticles ?
- Local magnetic moments well below T_K

→ locally-critical scenario ?