Thermodynamical signature of quantum criticality

Universally diverging Grüneisen ratio

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Phys. Rev. Lett. 91, 066404 (2003).

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R. Küchler et al Phys. Rev. Lett. 91, 066405 (2003).
Phys. Rev. Lett. 93, 096402 (2004).

Outline

- Brief introduction to Quantum Criticality
- Scaling Analysis of Thermodynamics

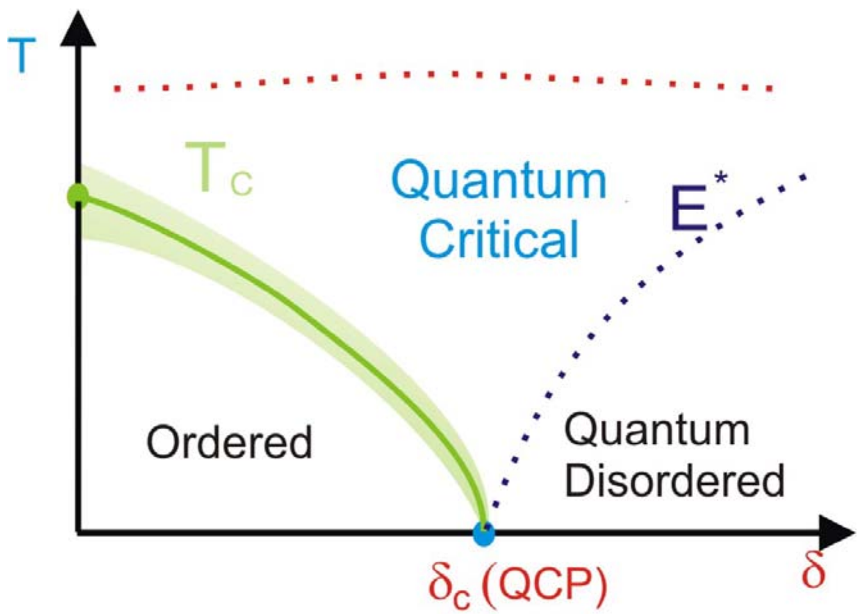
  Grüneisen ratio = thermal expansion / specific heat $\to \infty$

- Thermodynamic probe of quantum critical metals

  Experiments

  Theory
  - Spin Density Wave (SDW)
  - Local Quantum Criticality (LQCP)

Quantum phase transitions



$$\xi \sim (\delta - \delta_c)^{-\nu}$$
$$E^* \sim (\delta - \delta_c)^{\nu z} \to 0$$

Quantum fluctuations

$\tau_Q \sim \hbar / E^*$

Thermal fluctuations

$\tau_T \sim \hbar / (k_B T)$

Quantum Critical

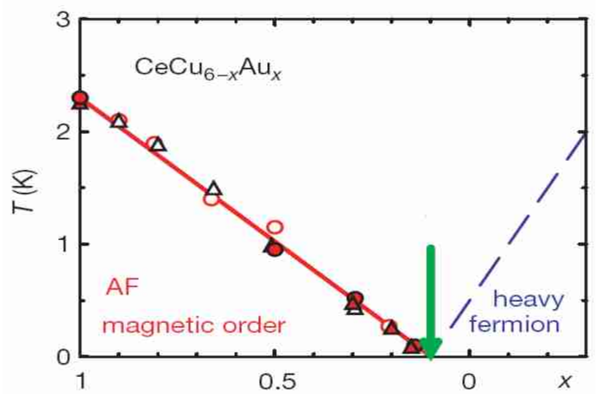
★ $\tau_Q \gg \tau_T$

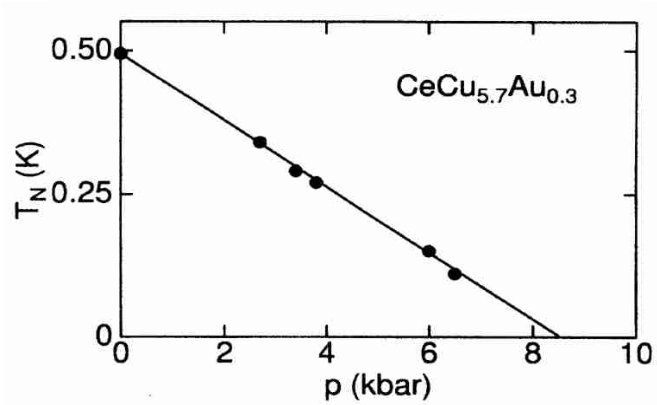
★ Non-Fermi Liquid, ...

S. Sachdev, *Quantum Phase Transitions* (Cambridge), 1998.
S. L. Sondhi, S. M. Girvin, J. P. Carini, and D. Shahar, Rev. Mod. Phys. 69, 315 (1997).

QPT in heavy fermion metals

$CeCu_{6-x}Au_x$

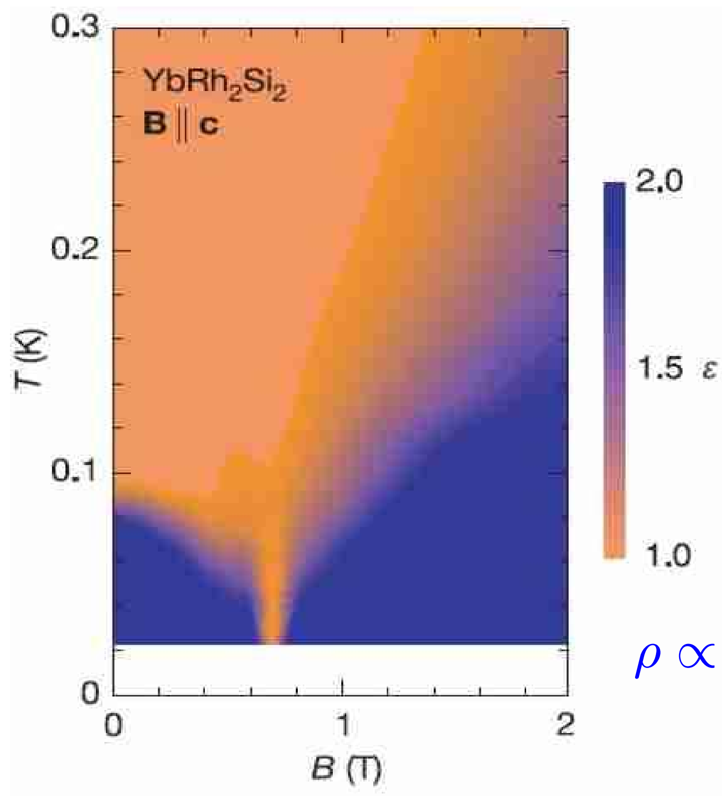




H. v. Löhneysen et al, Phys. Rev. Lett. **72**, 3262 (1994). B. Bogenberger and H. v. Löhneysen, ibid, **74**, 1016 (1995).

A. Schröder et al, Nature **407**, 351 (2000).

$YbRh_2Si_2$



$\rho \propto T^{\varepsilon}$

O. Trovarelli *et al.*, Phys. Rev. Lett. **85**, 626 (2000).

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

How to understand QCPs?

Quantum Criticality

New Physics: Non-Fermi liquid,
Unconventional superconductivity? …

Nature of QCP

$d+z$ Ginzburg-Landau Theory ?

Experimental probes

thermodynamics

Grüneisen ratio

$$\Gamma = \frac{\alpha}{c_p}$$

Thermal expansion

Specific heat

Why Grüneisen ratio particularly revealing to QCPs?

Capture two relevant directions

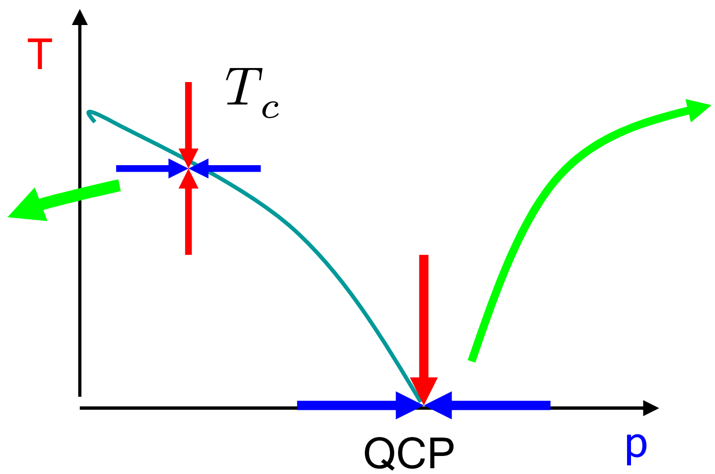
$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{p,N} = -\frac{1}{V}\left(\frac{\partial S}{\partial p}\right)_{T,N}$$

$$c_p = \frac{T}{N}\left(\frac{\partial S}{\partial T}\right)_p$$

Classical phase transition

$$t = \frac{T - T_c}{T_c}$$

$$\begin{array}{ccl} \xi & \sim & |t|^{-\nu_c} \\ c_p & \sim & |t|^{-(2-d\nu_c)} \\ & \sim & \alpha \\ \rightarrow & & \Gamma \sim const \end{array}$$



Quantum phase transition

- T, p not equivalent !
- Capture both relevant directions
- $c_p \rightarrow 0$
- α is more singular than c_p
- divergent Γ

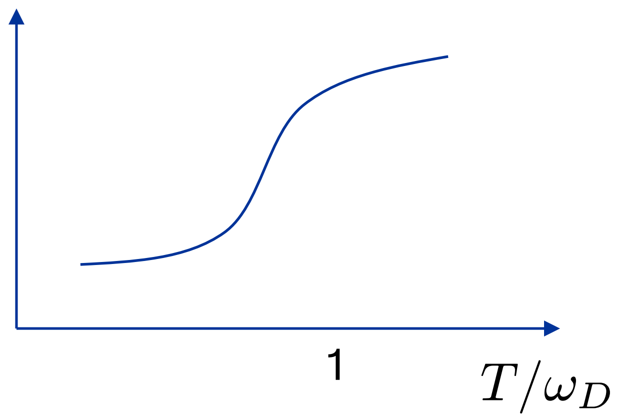
Why Grüneisen ratio particularly revealing to QCPs?

Grüneisen parameter in solids

- Phonons: Debye Frequency ω_D
- Electrons: Fermi Energy E_F

Characteristic Energy E^*

$$
\begin{aligned}
S/N &= f(T/E^*) \\
\Gamma &= \frac{1}{V_m E^*}\left(\frac{\partial E^*}{\partial p}\right).
\end{aligned}
$$



Finite!

Classical phase transition Tc

Quantum critical point

$$E^* \to 0 \Rightarrow \Gamma \to \infty$$

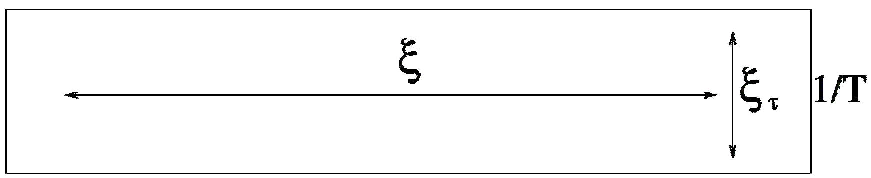
Divergent!

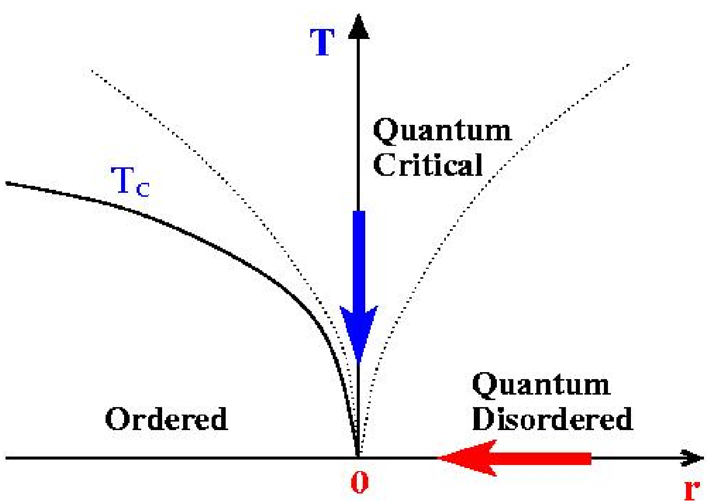
Quantum scaling (Hyperscaling)

Finite size scaling

$$\xi \sim |r|^{-\nu}, \quad \xi_\tau \sim \xi^z \sim 1/T$$

d-dim Quantum System $\Leftrightarrow$ $d+z$ Classical System





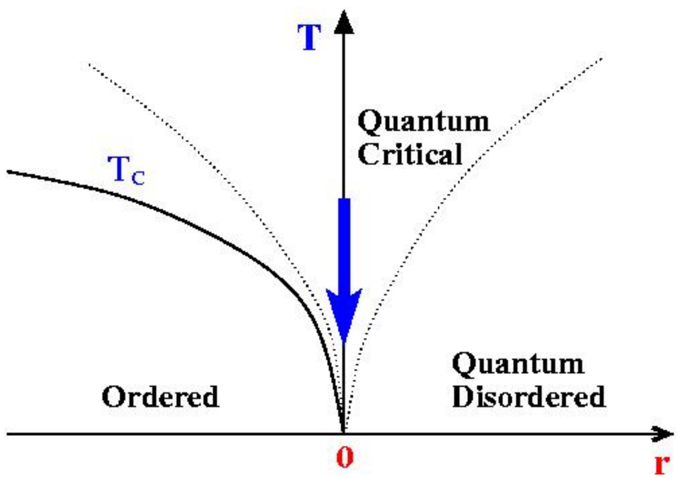
$$\frac{F_{cr}}{V} = -\frac{k_B T}{V} \ln Z$$

$$\sim \boxed{\xi^{-(d+z)}} f_1\left(\frac{1/T}{\xi^z}\right)$$

$$= -\rho_0\, r^{\nu(d+z)}\, \tilde{f}\left(\frac{T}{r^{\nu z}}\right)$$

$$= -\rho_0 T^{\frac{d+z}{z}}\, f\left(\frac{r}{T^{1/\nu z}}\right)$$

Quantum critical regime



$$F_{cr} = -\rho_0 T^{\frac{d+z}{z}} f\left(\frac{r}{T^{\boxed{\frac{1}{\nu z}}}}\right)$$

$$f(x \to 0) \approx f(0) + x f'(0) + \ldots$$

$$c_{cr}(T, r=0) \sim T^{d/z}$$

$$\alpha_{cr}(T, r=0) \sim T^{(d-\frac{1}{\nu})/z}$$

$$r = (p - p_c)$$

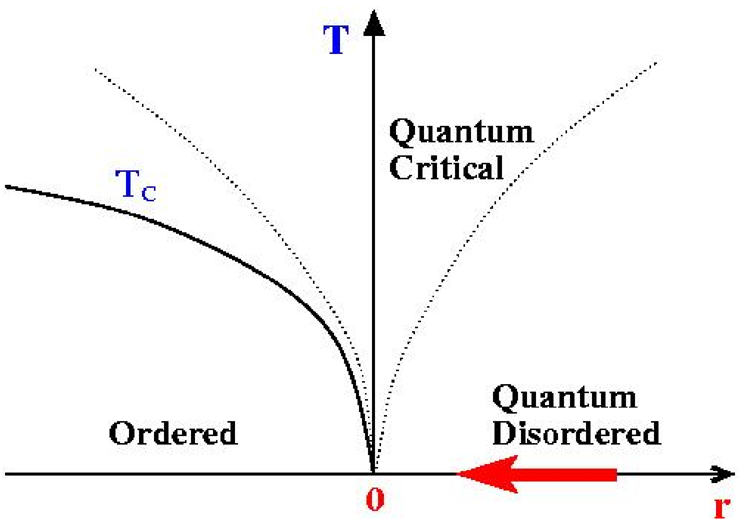
$$\alpha \sim \frac{\partial^2 F}{\partial r \partial T}$$

$$\Gamma_{cr}(T, r=0) = \frac{\alpha_{cr}}{c_{cr}} = -G_T \frac{1}{T^{\boxed{1/(\nu z)}}}$$

$\Gamma \sim 1/T^x, \quad x = 1/(\nu z)$

Measures the scaling dimension of the tuning parameter

Quantum disordered regime



$$F_{cr} = -\rho_0\, r^{\nu(d+z)}\, \tilde{f}\left(\frac{T}{r^{\nu z}}\right)$$

$$\tilde{f}(x \to 0) = \tilde{f}(0) + c\, x^{y_0+1}$$

$$c_{cr}(T \to 0, r) \sim T^{y_0} r^{\nu(d-y_0 z)}$$

$$\alpha_{cr}(T \to 0, r) \sim T^{y_0} \frac{r^{\nu(d-y_0 z)}}{p_c r}$$

$$\Gamma_{cr}(T \to 0, r) = -G_r \frac{1}{V_m(p-p_c)}.$$

$$G_r = \boxed{\frac{\nu(d-y_0 z)}{y_0}}.$$

Results for hyperscaling

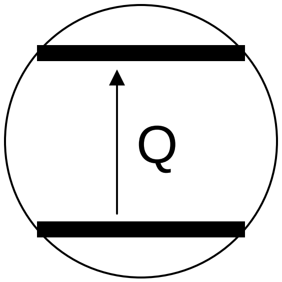
- Any generic QCP, $\Gamma \to \infty$ $\Rightarrow$ identify a QCP
- Characterize a QCP
  - QC, $\Gamma \sim 1/T^x$, x relates the most relevant parameter
  - QD, $\Gamma = G_r/[V_m(p - p_c)]$, G_r universal

Questions:

Whether hyperscaling holds

Spin-density-wave Picture

Hertz, Millis, Moriya, ……
An effective d+z Ginzburg-Landau Theory



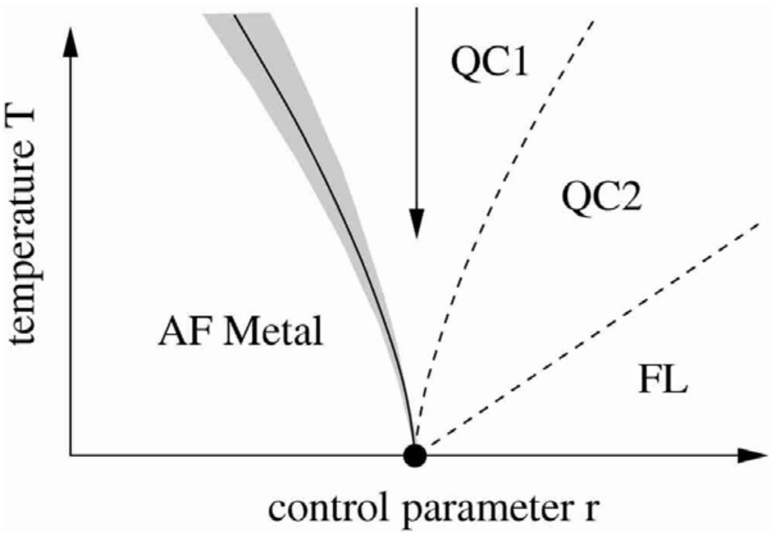
Long-wavelength fluctuations of the order parameter $\vec{\phi}$
$d_{\text{eff}} = d + z \geq 4$

$$S[\vec{\phi}] = \frac{1}{2} \sum_{\mathbf{q}, i\omega_l} \chi_0^{-1}(\mathbf{q}, i\omega_l) |\vec{\phi}(\mathbf{q}, i\omega_l)|^2 + u \int_0^\beta d\tau \int d^d\mathbf{r}\ |\vec{\phi}(\mathbf{r}, \tau)|^4,$$

$$\chi_0^{-1}(\mathbf{q}, i\omega_l) = \delta + (q\xi_0)^2 + \frac{|\omega_l|}{\Gamma_q}$$

$\omega \sim q^z$
AFM fluctuation $Q = (\pi, \ldots, \pi)$ $\Gamma_q = \Gamma_0 Q$ $\quad z = 2$
$\delta \sim q^{1/\nu} \quad \nu = 1/2$

SDW – 3D Antiferromagnetic fluctuation



$$F_{cr} \sim T^{(d+z)/z} f\left(\frac{r}{T^{1/(\nu z)}}, uT^{(d+z+\frac{1}{\nu}-4)/z}\right)$$

FL regime

$$F_{cr} \sim r^{(d+z)\nu}\left(\frac{T}{r^{\nu z}}\right)^2$$

QC regime

$$F_{cr} \sim T^{(d+z)/z}\left(1+\frac{r}{T^{1/\nu z}}+uT^{(d+z-4)/z}\right)$$

SDW - Results

FL Regime

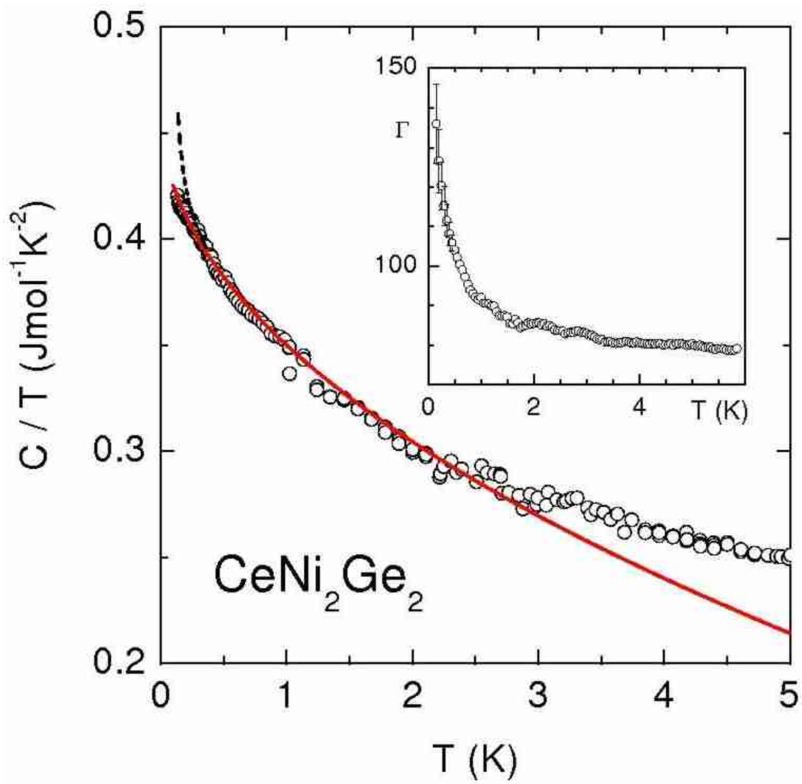
	$d=3, z=2$	$d=2, z=2$
α_{cr}	$Tr^{-1/2}$	Tr^{-1}
$c_{cr} \sim$	$-Tr^{1/2}$	$T \log \frac{1}{r}$
$\Gamma_{r,cr} =$	$-(2r)^{-1}$	$\left(r \log \frac{1}{r}\right)^{-1}$

QC Regime

	$d=3, z=2$	$d=2, z=2$	Hyperscaling
$\alpha_{cr} \sim$	$T^{1/2}$	$\log\log\frac{1}{T}$	$T^{\left(d-\frac{1}{\nu}\right)/z}$
$c_{cr} \sim$	$-T^{3/2}$	$T\log\frac{1}{T}$	$T^{d/z}$
$\Gamma_{r,cr} \sim$	$-T^{-1}$	$\frac{\log\log\frac{1}{T}}{T\log\frac{1}{T}}$	$T^{-1/(\nu z)}$

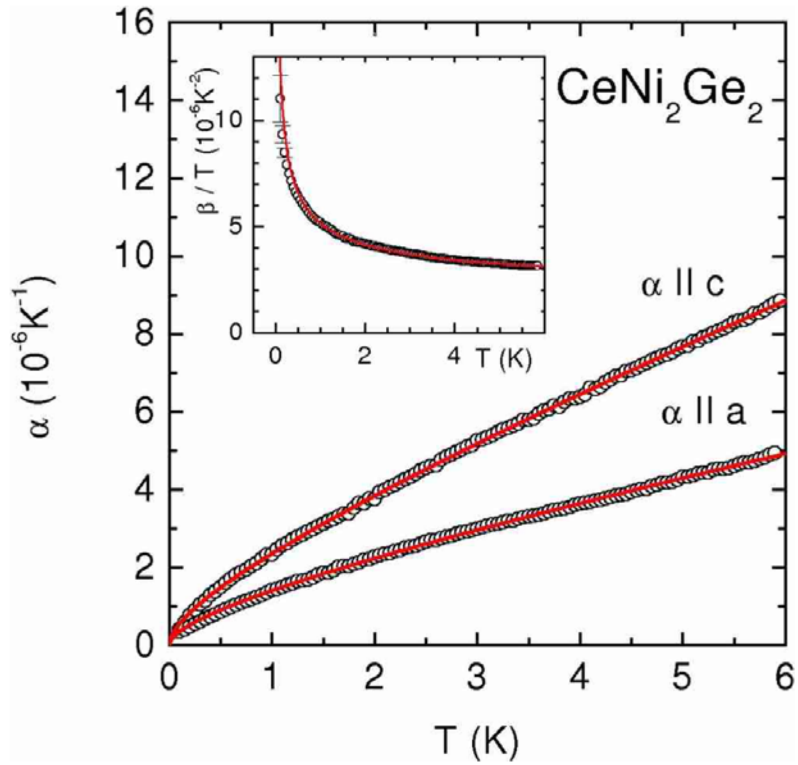
$CeNi_2Ge_2$

Specific heat



$$C/T = \text{const} \ - T^{1/2}$$

Thermal expansion

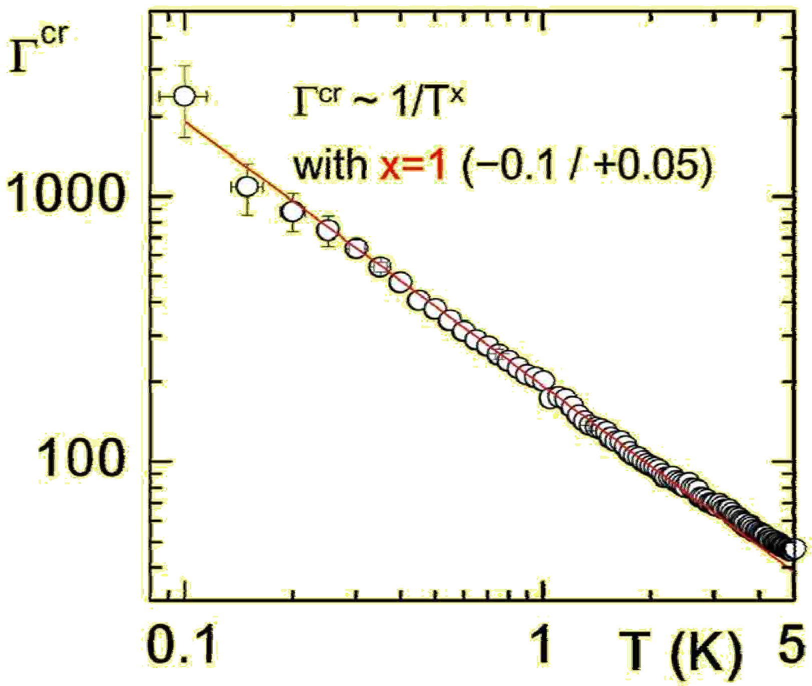


$$\alpha = aT^{1/2} + bT$$

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

$CeNi_2Ge_2$ - *cont'd*

Grüneisen ratio



Consistent with

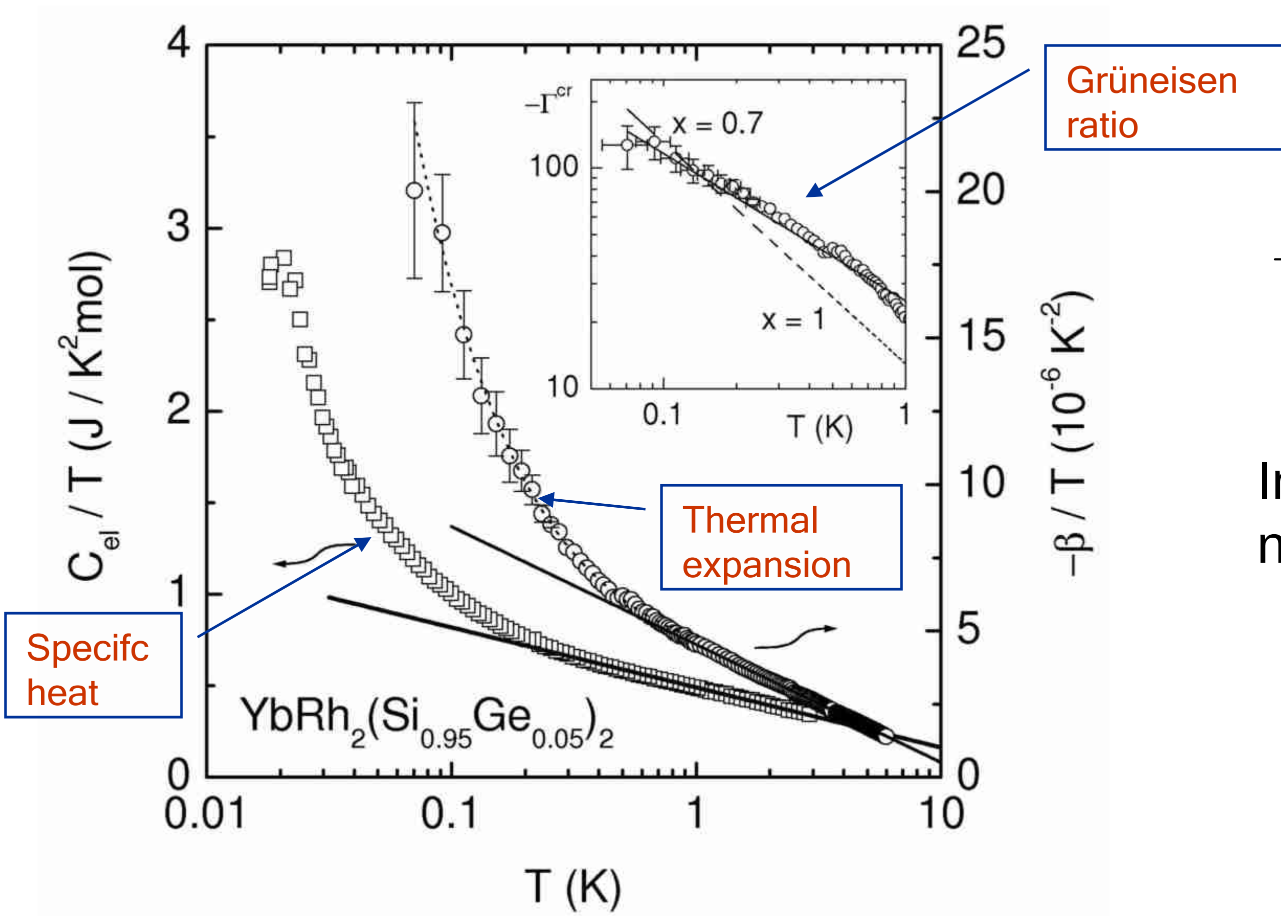
3d SDW picture

$z = 2$, $\nu = 1/2$

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

R. Küchler et al., Phys. Rev. Lett. 91, 066405 (2003).

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



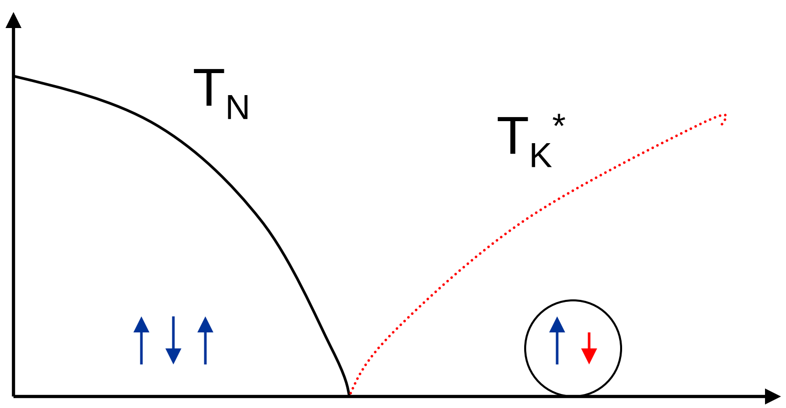
$$-\Gamma \sim 1/T^{0.7}$$

Inconsistent with neither 3D or 2D SDW

R. Küchler et al., Phys. Rev. Lett. 91, 066405 (2003).

Theories

- Locally quantum criticality



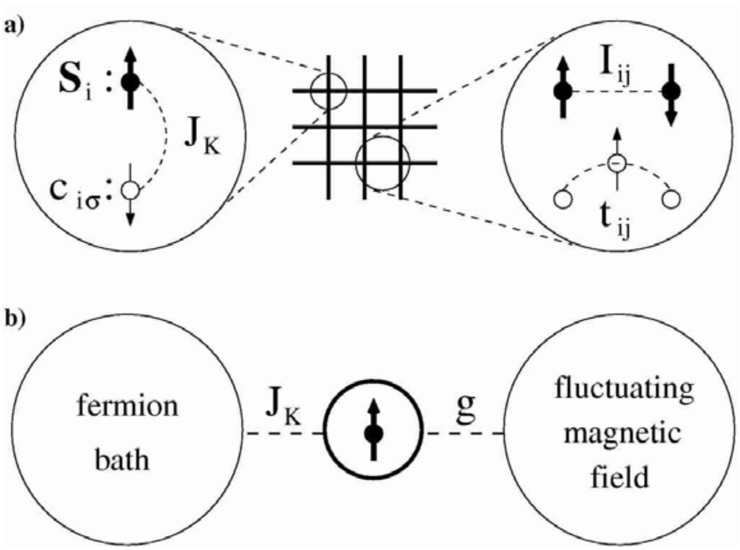
- critical local dynamics
- ω/T scaling, fractional exponent
- T_K^* finite for SDW transition

Q. Si, S. Rabello, K. Ingersent, and J.L. Smith, Nature (London) 413, 804 (2001).
P. Coleman, C. Pépin, Q. Si, and R. Ramazashvili, J. Phys.: Condens. Matter 13, R723 (2001).

Other theories
T.Senthil, M. Vojta, and S. Sachdev, Phys. Rev. B 69, 035111 (2004)
C. Pépin, Phys. Rev. Lett. 94, 066402 (2005)
V.R. Shaginyan JETP LETTERS 79, 286 (2004)

Locally critical scenario

Self-consistent Bose-Fermi Kondo Model



$$J_K\ \mathbf{S}\cdot\mathbf{s}_c + \sum_{p,\sigma} E_p\ c^{\dagger}_{p\sigma}\ c_{p\sigma}$$

$$+\,g\sum_p \mathbf{S}\cdot\left(\vec{\phi}_p + \vec{\phi}^{\,\dagger}_{-p}\right) + \sum_p w_p\,\vec{\phi}^{\,\dagger}_p\cdot\vec{\phi}_p.$$

$$\sum_p \delta(\omega - w_p) = (K_0^2/\pi)|\omega|^{1-\epsilon}$$

Free energy $f_{imp} \sim T\Phi(r/T^{\lambda_r})$

Grüneisen ratio $\Gamma \sim 1/T^{\lambda_r} \leftarrow 1/(\nu z)$

anisotropic case, with g_z, $g_\perp$, J_z, $J_\perp$

XY $\quad g_z = 0$

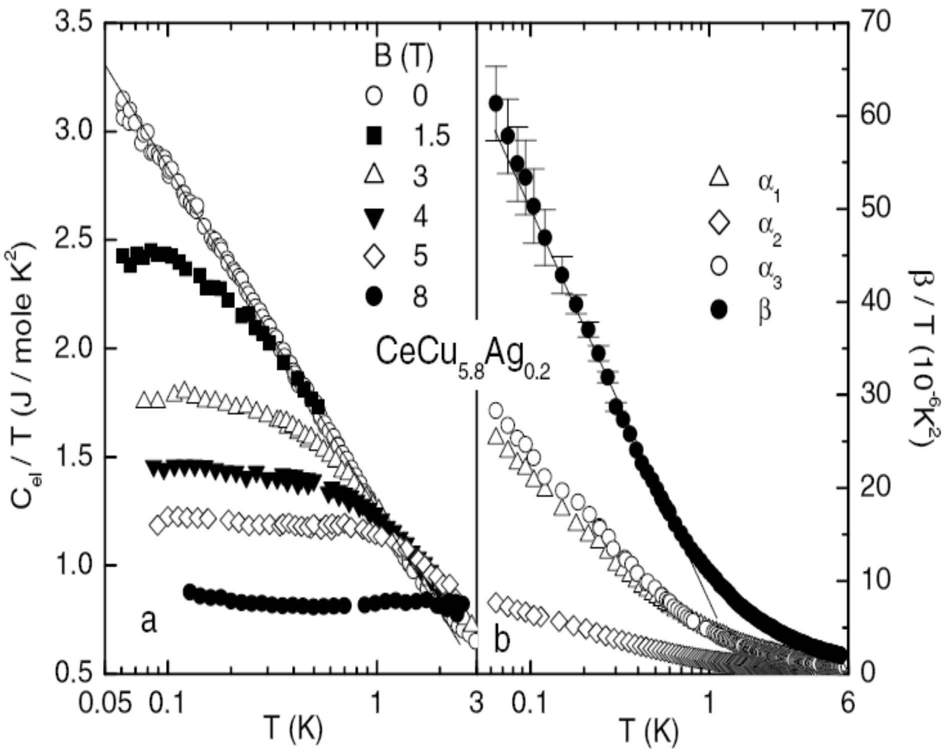
$\lambda_r \approx 0.618034\epsilon + 0.0376644\epsilon^2 \approx 0.66$

Self-consistency
when $\epsilon = 1^-$

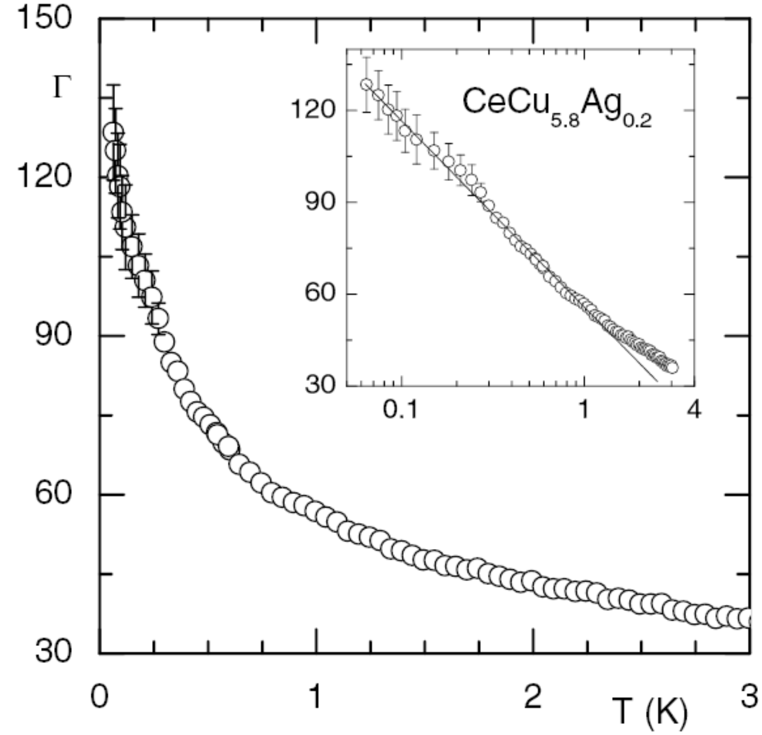
Consistent with the observation in $YbRh_2(Si_{0.95}Ge_{0.05})_2$

$CeCu_{5.8}Ag_{0.2}$

Specific heat Thermal expansion



Grüneisen ratio

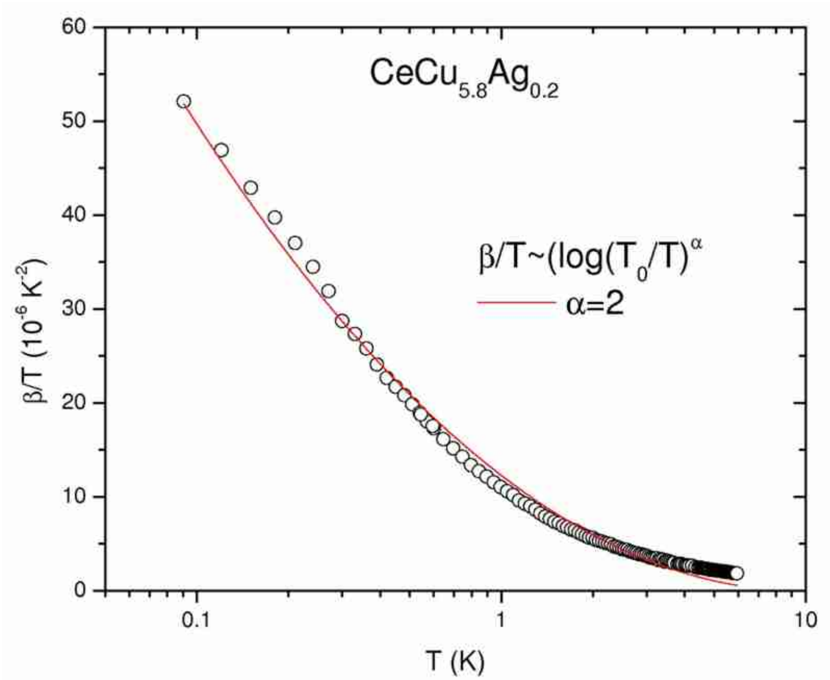


R. Küchler, P. Gegenwart, K. Heuser, E.-W. Scheidt, G. R. Stewart, and F. Steglich, Phys. Rev. Lett. 93, 096402 (2004).

Inconsistent with SDW

Different from $YbRh_2Si_2$

$CeCu_{5.8}Ag_{0.2}$ - *cont'd*



P. Gegenwart, private communication

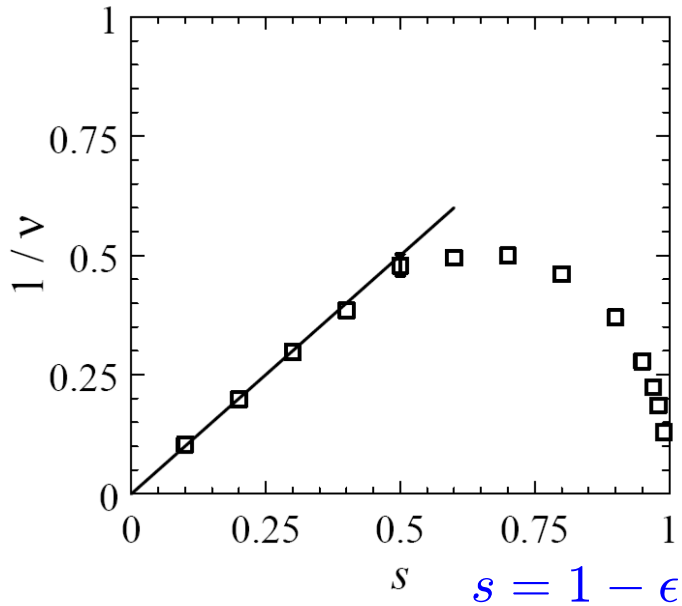
$$\mathrm{c/T} \sim \log(T_0/T)$$

$$\beta/T \sim \log^2(T_0/T)$$

$$\Gamma \sim \log(T_0/T)$$

$CeCu_{5.8}Ag_{0.2}$ - *cont'd*

Local criticality in Ising anisotropic case



R. Bulla, N.-H. Tong, and M. Vojta, Phys. Rev. Lett. 91, 170601 (2003); Phys. Rev. Lett. 94, 070604 (2005).

$$1/\nu = 1 - \epsilon$$

When $\epsilon \to 1^-$

$$\Gamma \sim 1/T^{1/(\nu z)} = 1/T^{0^+} \to \log T$$

Consistent with the observation in $CeCu_{5.8}Ag_{0.2}$

Conclusion

- Quantum critical point ⇔ universally diverging Grüneisen ratio
- Identify, characterize QCPs
- Theory
  - Hypercaling
  - Spin Density Wave
  - Local Quantum Criticality
- Experiments in quantum critical heavy fermion metals
  - Observe divergence as predicted
  - $CeNi_2Ge_2$ compatible with SDW
  - $YbRh_2(Si_{0.95}Ge_{0.05})_2$ $CeCu_{5.8}Ag_{0.2}$ Inconsistent with SDW
    Consistent with LQCP
  - LQCP XY Ising anisotropic cases
- Other strongly correlated systems