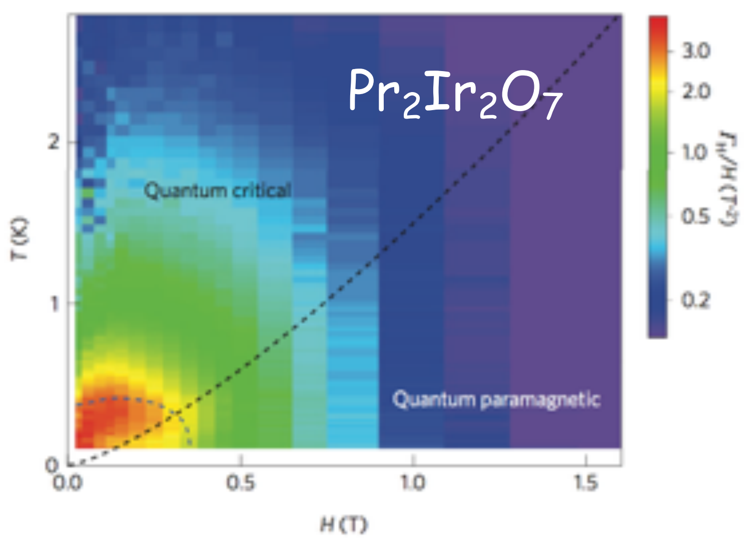
Introduction to Quantum Phase Transitions

Part I

Why are quantum phase transitions interesting?



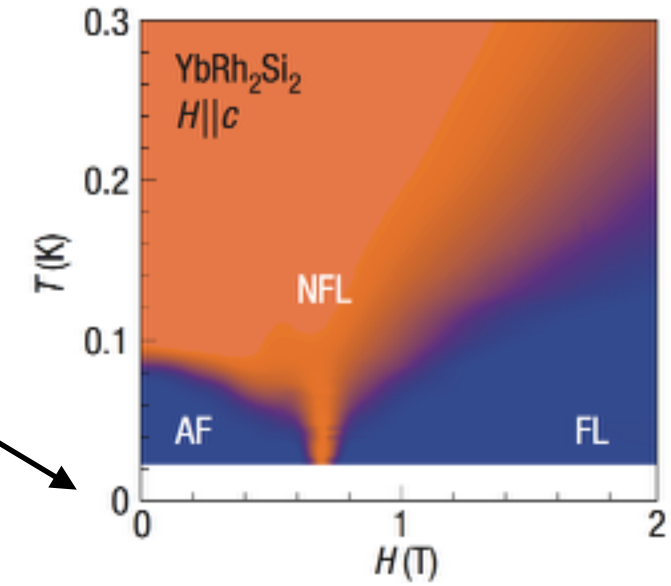
Y. Tokiwa, et al. Nat Mater (2014).

Quantum phase transition
only at strictly
zero temperature T=0

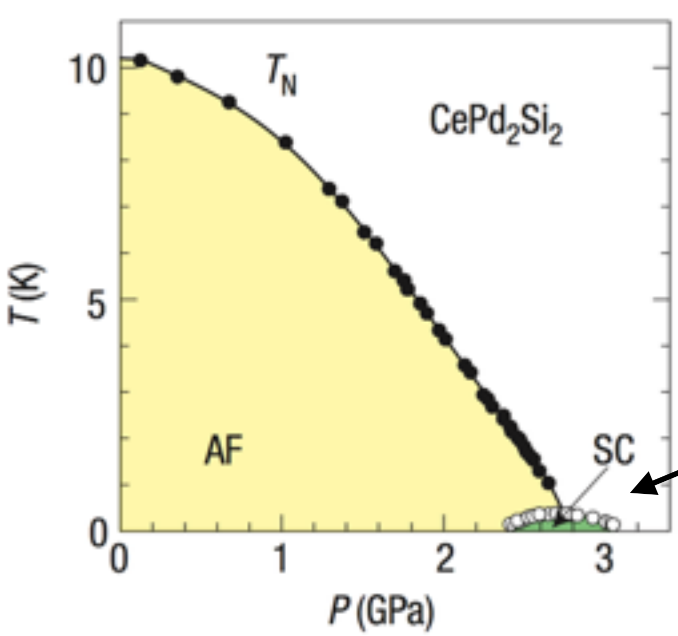
Anomalous, exotic
behaviour at finite T

at odds with
conventional properties
of materials

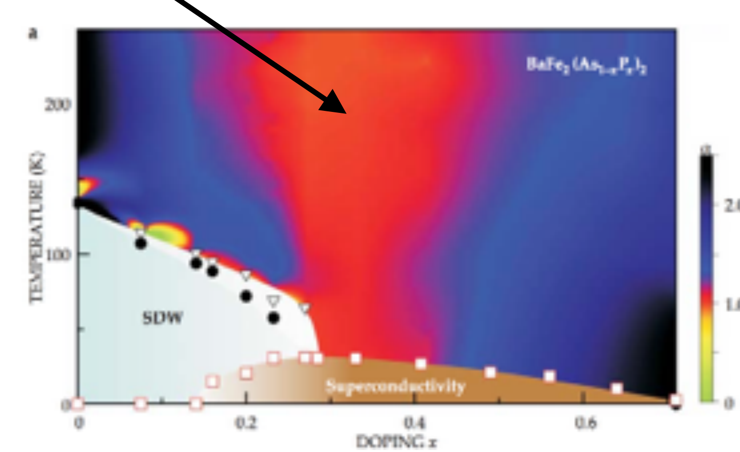
even emergent phases
like superconductivity



Custers, J. et al. Nature (2003).



Mathur, et al. Nature (1998)



S. Kasahara et al., Phys. Rev. B (2010).

Literature:

- S. Sachdev and B. Keimer, Phys. Today 64, 29 (2011).
- Quantum phase transitions, S. Sachdev (Cambridge University Press)
- Thermal and Quantum Phase transitions, M. Vojta,

  Les Houches Lecture Notes, http://statphys15.inln.cnrs.fr
- Fermi-liquid instabilities at magnetic quantum phase transitions

  H. V. Löhneysen, A. Rosch, M. Vojta, and P. Wölfle, Rev. Mod. Phys. 79, 1015 (2007).
- Focus Issue on Quantum Phase Transitions, Nat Phys, **4**, 167-204 (2008)
- …

Outline:

- Introduction:
  definition, scaling exponents, scaling hypothesis,
  phase diagram, thermodynamics

- Dilute weakly interacting Bose gas

- Insulating spin-dimer antiferromagnets

- ....

Introduction

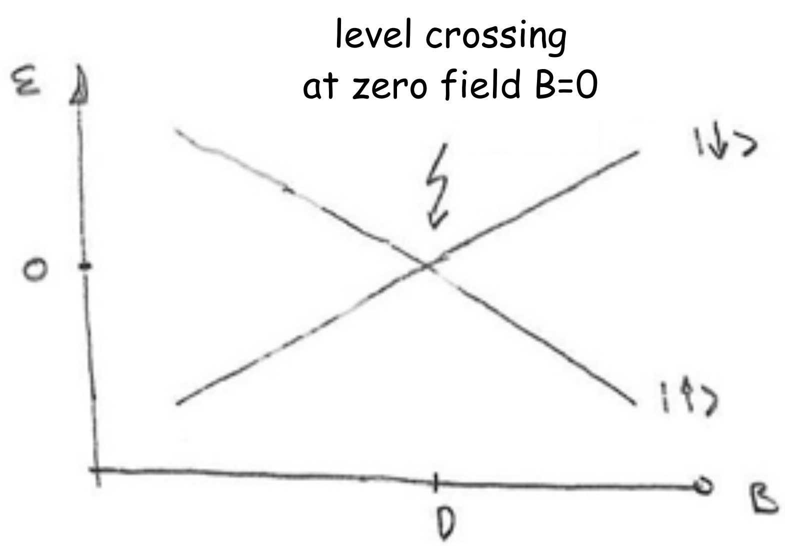
Definition of a quantum phase transition (QPT):

At a QPT the ground state energy exhibits a non-analyticity as a function of an external control parameter.

First-order QPT: level crossing

simple example: free spin 1/2 in a magnetic field ⇨ Hamiltonian $H = -g\mu_B \vec{S}\vec{B}$

energy spectrum



free energy

$$F = -k_B T \log(e^{g\mu_B B/(2k_B T)} + e^{-g\mu_B B/(2k_B T)})$$

$$= k_B T\, \Psi\left(\frac{g\mu_B B}{2k_B T}\right)$$

with scaling function $\Psi(x) = -\log(e^x + e^{-x})$

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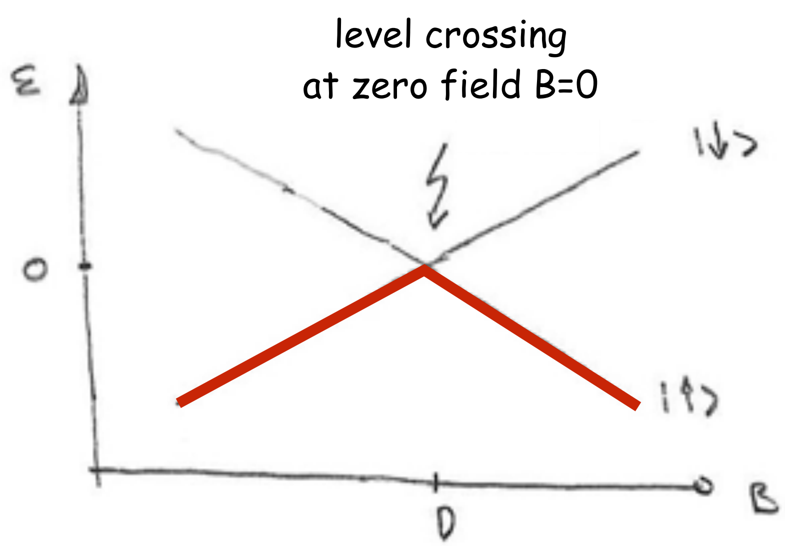

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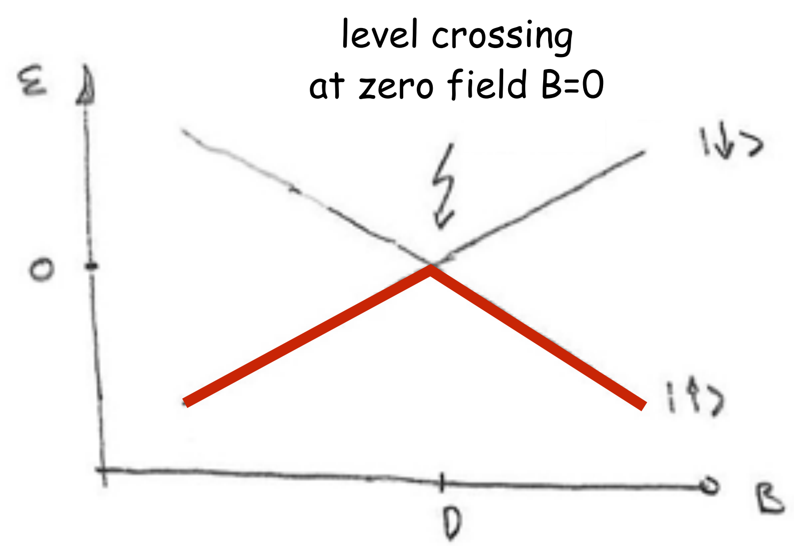

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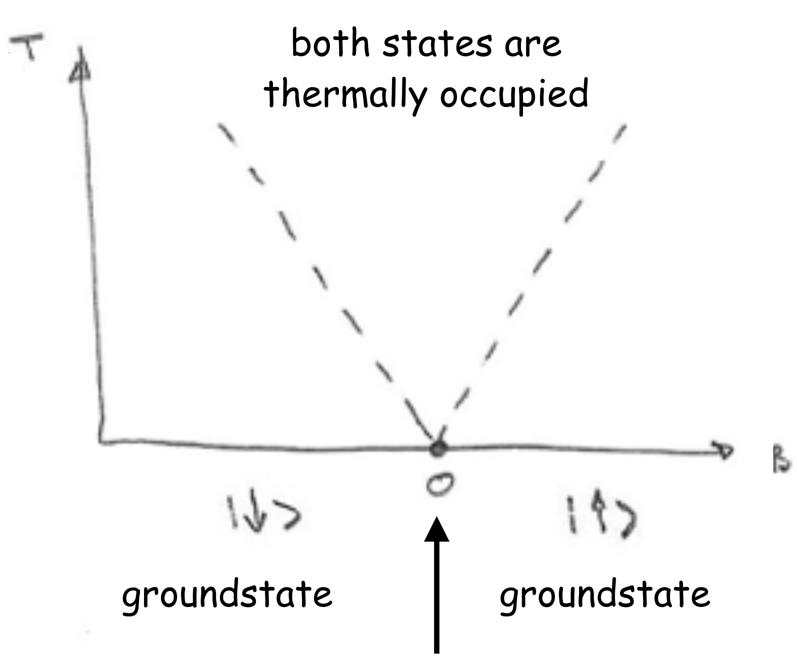
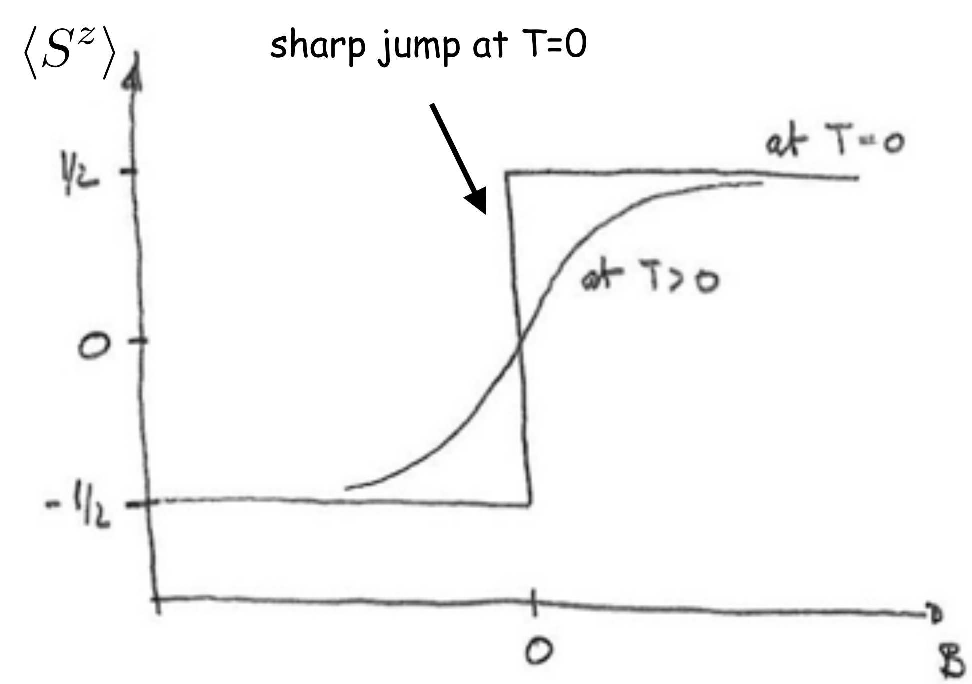
phase diagram



at B=0:
residual entropy at T=0 $S = k_B \log 2$

spin expectation value

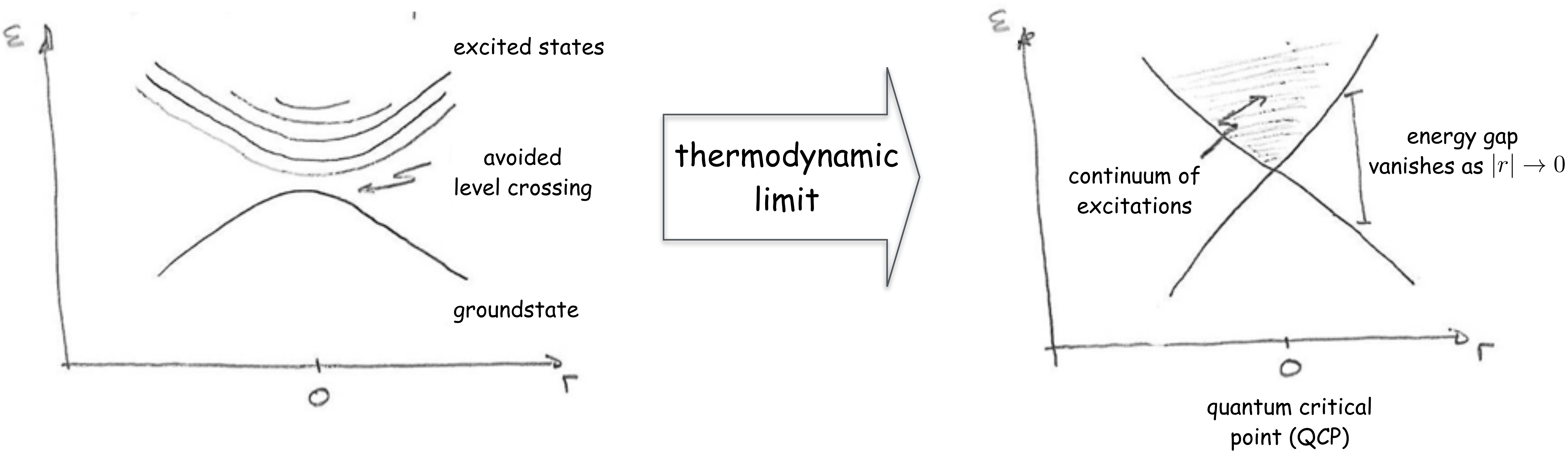


Continuous QPT

transition point at T=0, i.e., the quantum critical point (QCP) is characterised by critical continuum of excitations

Example: (with energy gap away from the QCP)

spectrum for a finite size system — spectrum for a infinite system



tuning parameter r vanishes at the QCP: r=0

e.g. for tuning by pressure $r \propto p - p_c$, for tuning by magnetic field $r \propto H - H_c$, etc.

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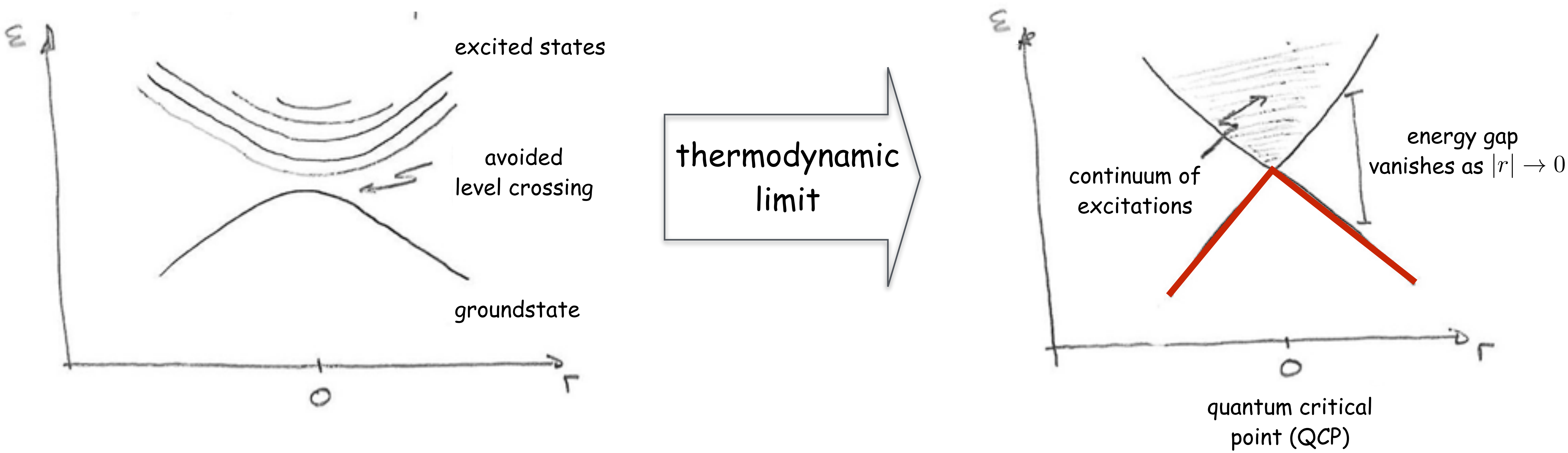

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e.g. for tuning by pressure $r \propto p - p_c$, for tuning by magnetic field $r \propto H - H_c$, etc.

Continuous QPT: diverging length and time scales

critical continuum of excitation characterised by scales that diverge at the QCP

at T=0 diverging length scale

$$\xi_r \propto |r|^{-\nu}$$

correlation length exponent ν

at T=0 diverging time scale

$$\tau \propto \xi_r^z \propto |r|^{-\nu z}$$

dynamical exponent z

Heisenberg uncertainty principle: vanishing energy scale $\varepsilon_r \propto \xi_r^{-z} \propto |r|^{\nu z}$

e.g. excitation gap in the above example

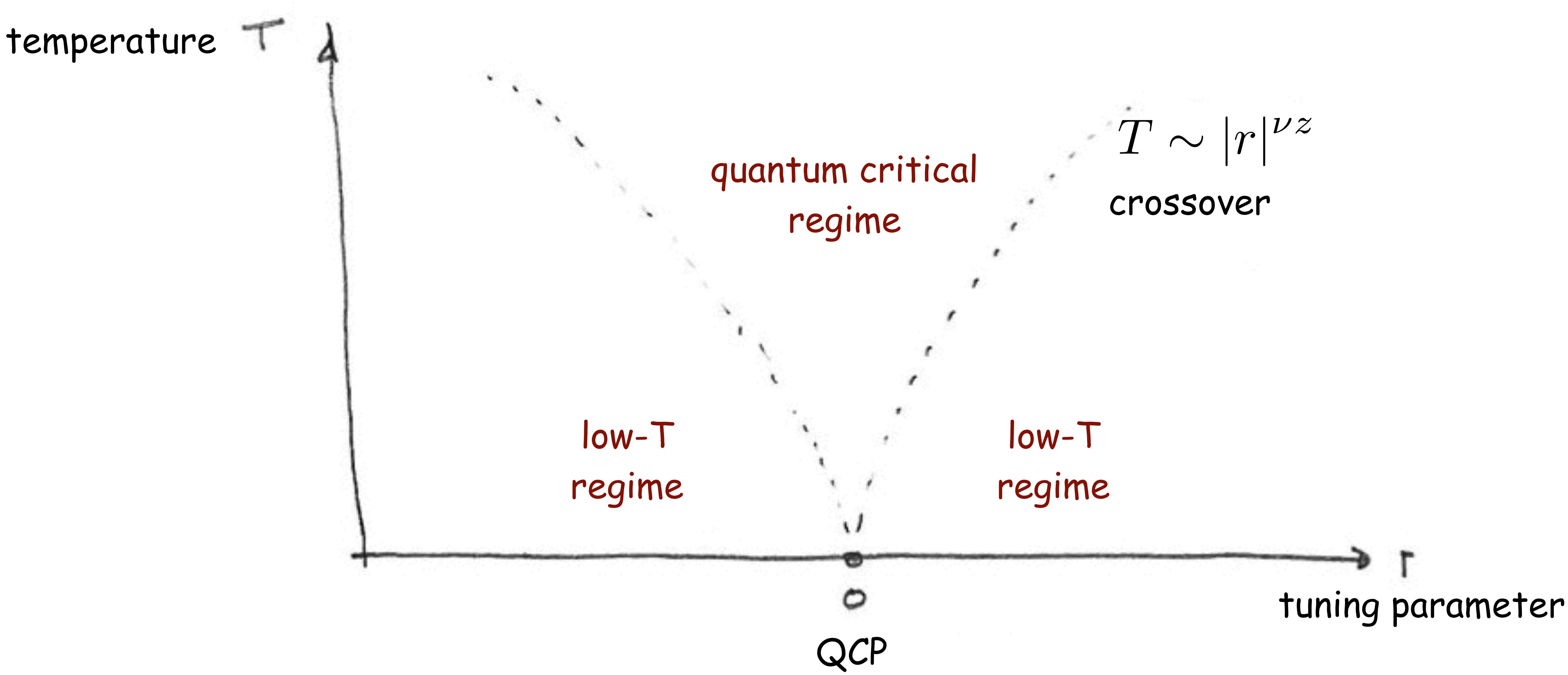
Consequences at finite T: phase diagram

comparing vanishing energy scale with temperature T: $T \sim \varepsilon_r \propto |r|^{\nu z}$

equivalent to comparing length scales: $\xi_T \sim \xi_r$

with thermal length $\xi_T \propto T^{-\frac{1}{z}}$

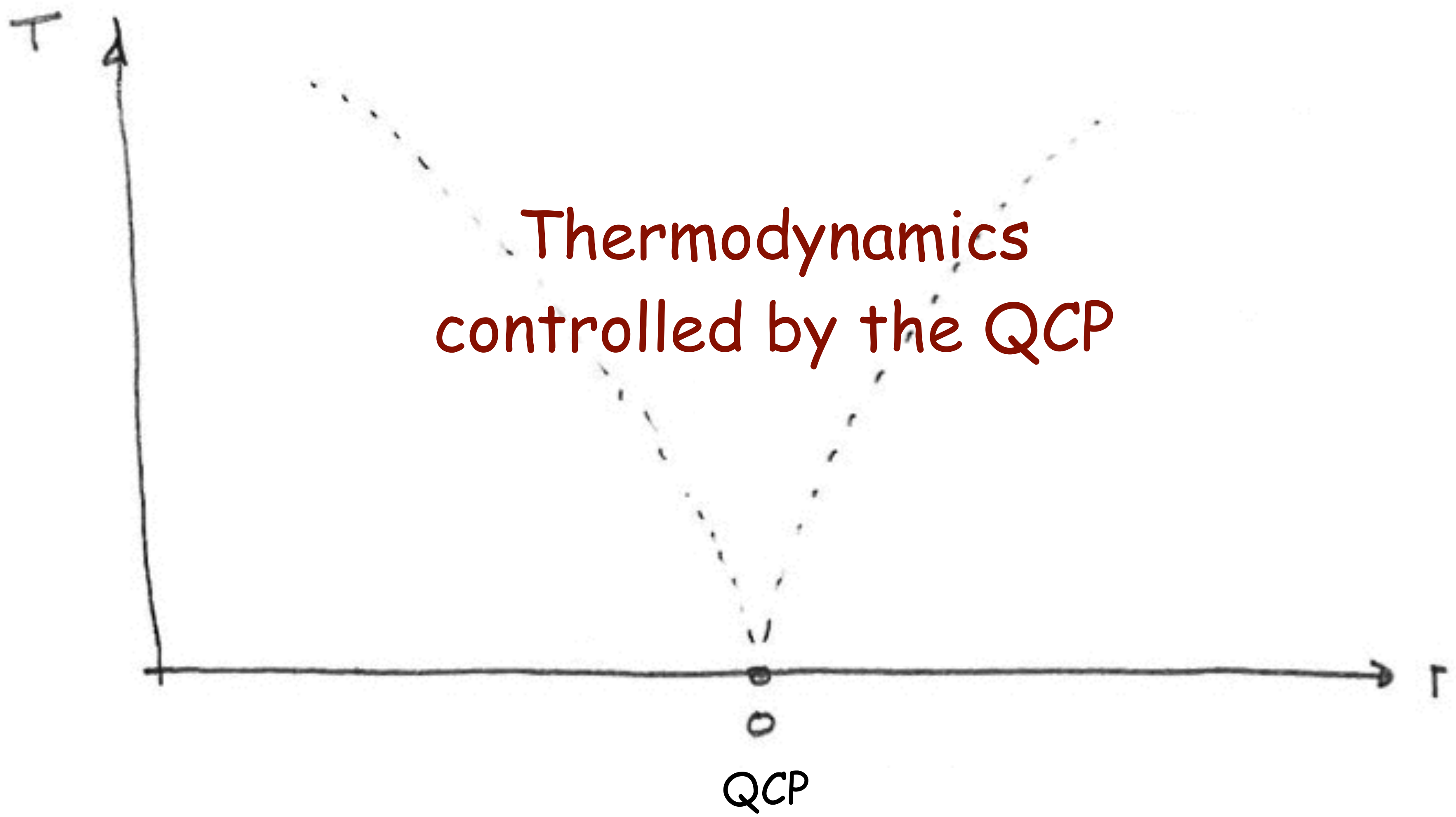
phase diagram:



Consequences at finite T: phase diagram

Although quantum phase transition only occurs at T=0
thermal excitation of the critical continuum determine the finite T properties!

⇨ anomalous behaviour of observable quantities at finite T!

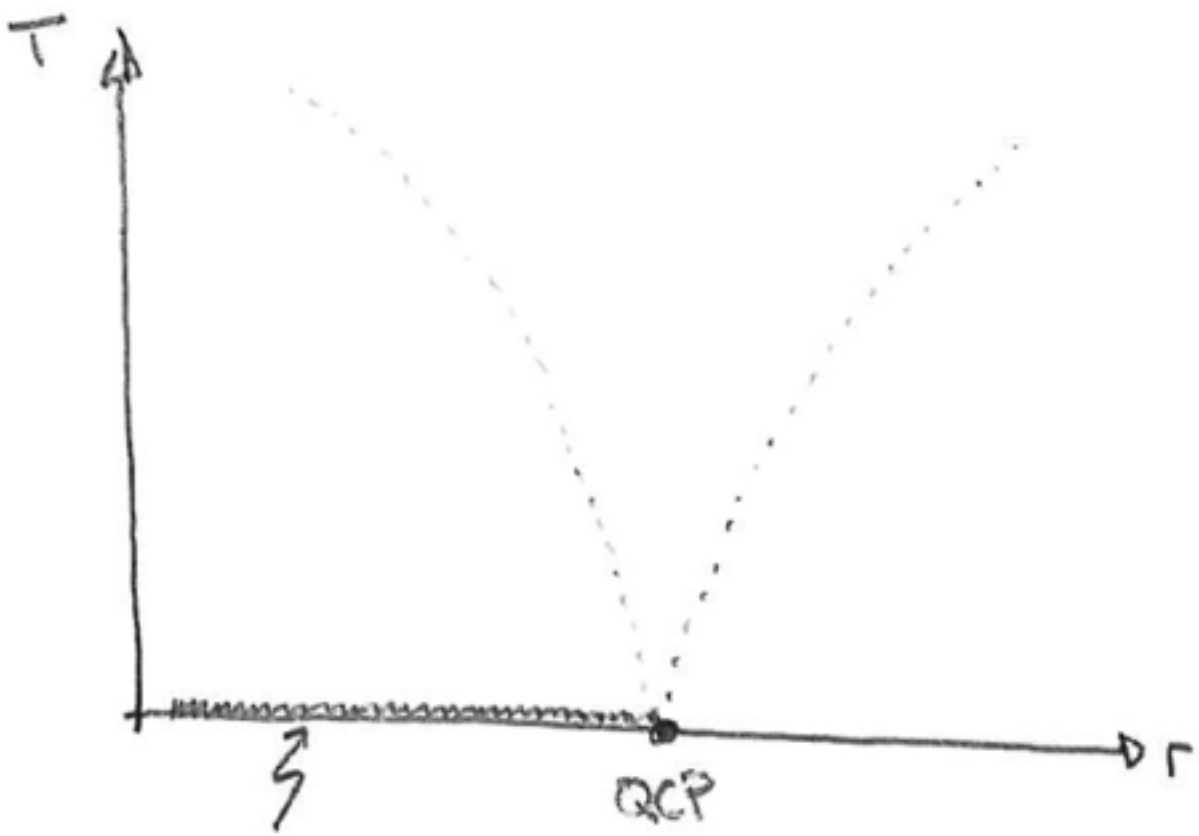


Phase diagram: type I

often the quantum phase transition is accompanied with the development of long-range order like ferromagnetism, antiferromagnetism, superconductivity etc. (exceptions: topological transitions!)

⇨ expectation value of a local order parameter is finite $\langle \Phi \rangle \neq 0$

type I



$\langle \Phi \rangle \neq 0$
only at T=0

singular thermodynamics only
at the QCP: T=r=0

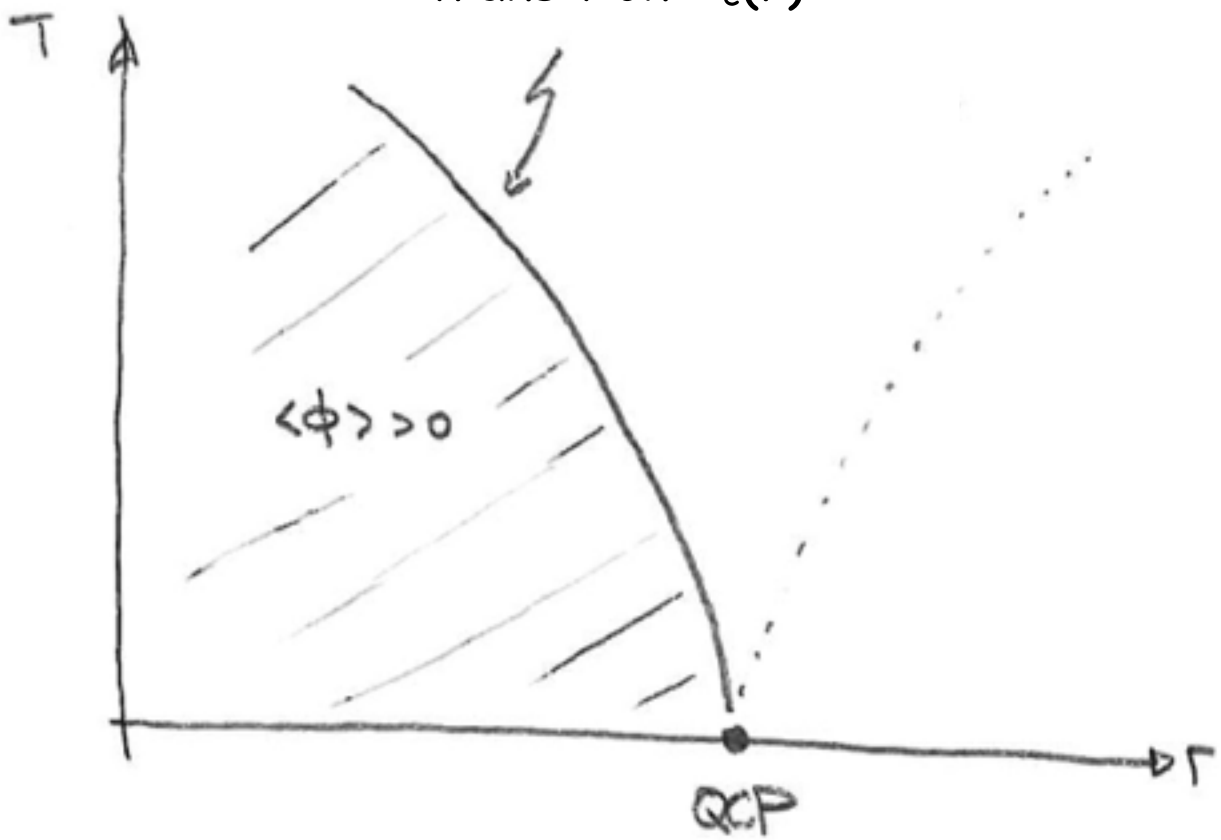
Phase diagram: type II

often the quantum phase transition is accompanied with the development of long-range order like ferromagnetism, antiferromagnetism, superconductivity etc. (exceptions: topological transitions!)

⇨ expectation value of a local order parameter is finite $\langle \Phi \rangle \neq 0$

type II

classical phase transition $T_c(r)$



finite $\langle \Phi \rangle \neq 0$ also at finite T

QCP is the endpoint of a line of classical phase transitions $T_c(r) \to 0$ for $r \to 0^-$

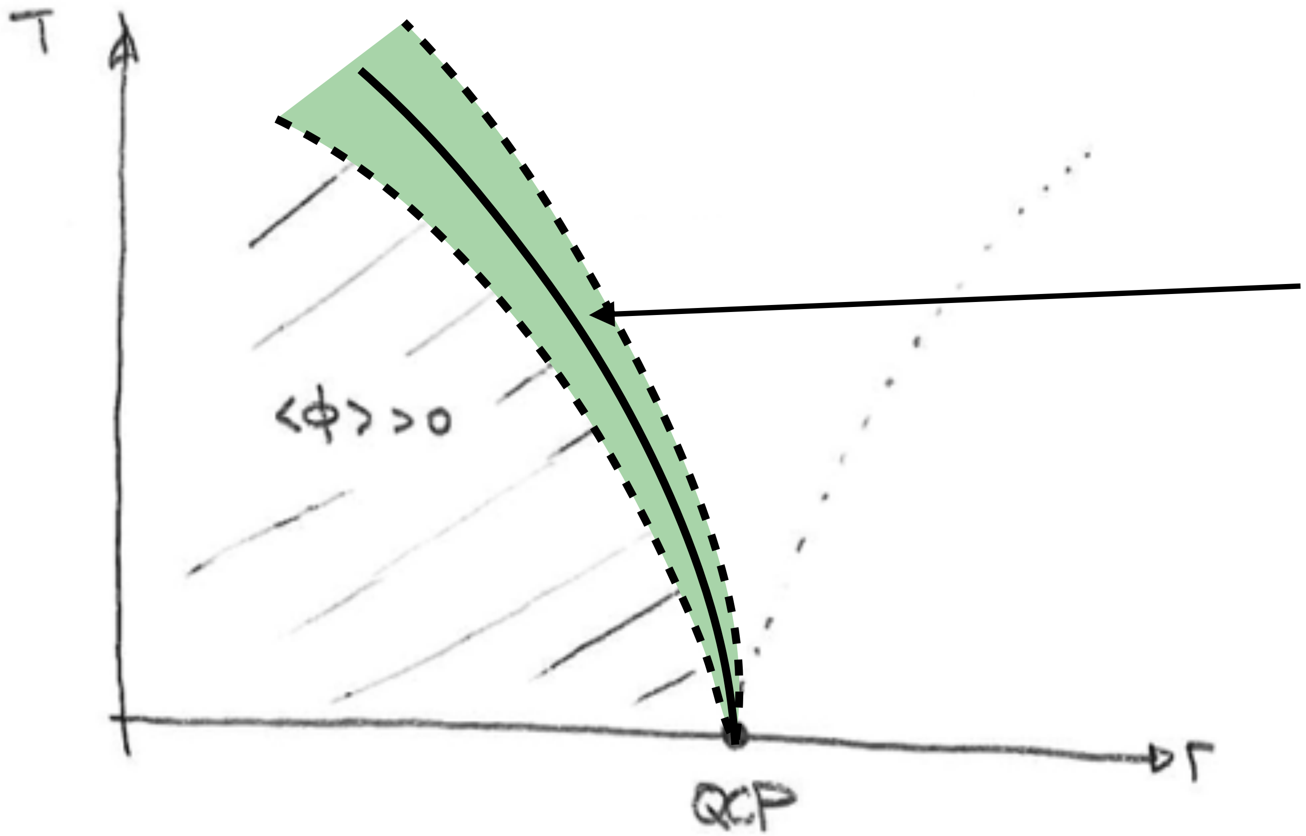
⇨ singular thermodynamics also at finite T_c!

Phase diagram: type II

often the quantum phase transition is accompanied with the development of long-range order like ferromagnetism, antiferromagnetism, superconductivity etc. (exceptions: topological transitions!)

⇨ expectation value of a local order parameter is finite $\langle \Phi \rangle \neq 0$

type II



classical criticality develops on top of a quantum critical background

thermal critical fluctuations dominate only within a tiny Ginzburg regime

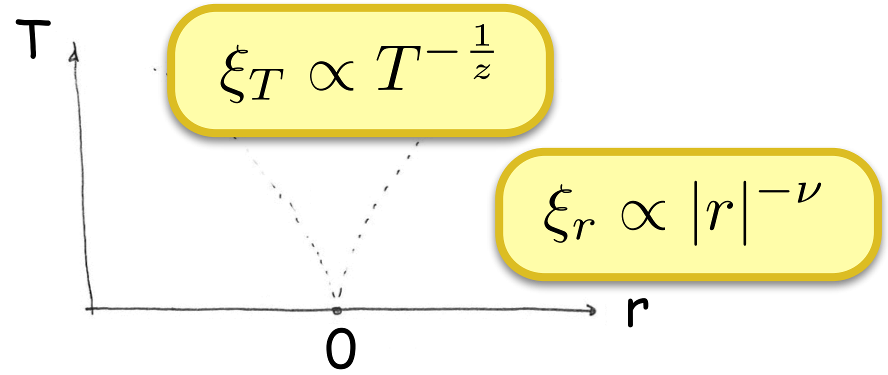
The remainder is

controlled by the QCP!

finite $\langle \Phi \rangle \neq 0$ also at finite T

Scaling hypothesis for quantum critical thermodynamics

phase diagram is two-dimensional:



critical free energy is a function of control parameter r and temperature T

from dimensional analysis follows for the critical free energy density

d: spatial dimension

for an arbitrary length ξ

scaling function

energy scale

$$f_{\rm cr} = \frac{\xi^{-z}}{\xi^{d}} \tilde{\Psi}\left(\xi_r/\xi, \xi_T/\xi\right) = \xi^{-(d+z)} \Psi\left(r\xi^{1/\nu}, T\xi^{z}\right)$$

volume

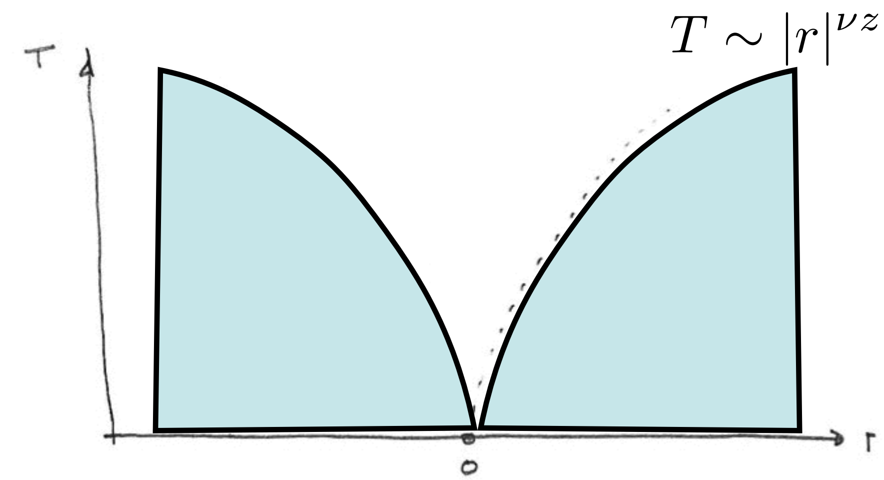
dimensionless ratios

effective dimensionality d+z

depending on relative size of r and T choose length ξ

Scaling hypothesis for quantum critical thermodynamics

low-T regime: choose $\xi = \xi_r = |r|^{-\nu}$



$$f_{\rm cr} = |r|^{\nu(d+z)} \Psi\Big(\mathrm{sgn}(r), T|r|^{-\nu z}\Big)$$

ground states on either side of the QCP might have different properties

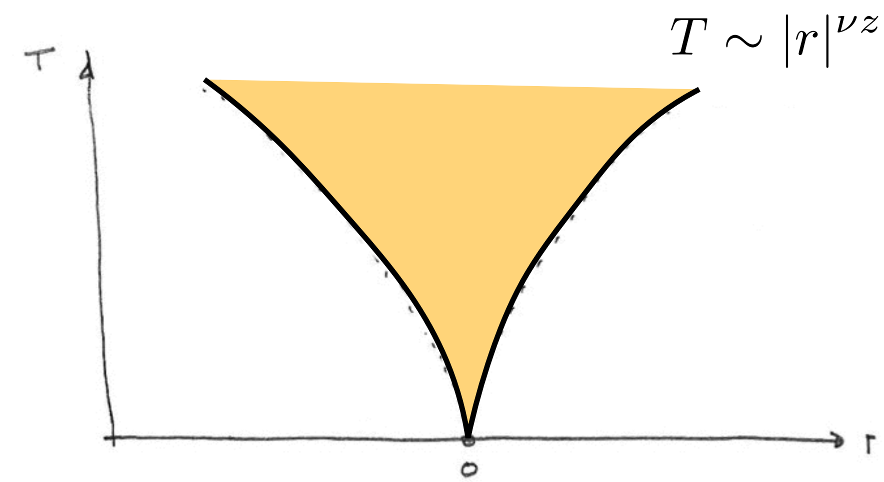
function $\Psi(\pm 1, x)$ for small x constrained by the third law of thermodynamics,

i.e., vanishing entropy at T=0: $S(T=0) = 0$

- for a gapless ground state away from the QCP (e.g. a Fermi liquid): $\Psi(\pm 1, x) \sim x^{y_0+1}$ with $y_0 > 0$
- for a gapped ground state (e.g. a Bose gas with chemical potential μ<0): $\Psi(\pm 1, x) \sim x^{z_0} e^{-1/x}$

Scaling hypothesis for quantum critical thermodynamics

quantum critical regime: choose $\xi = \xi_T = T^{-1/z}$



$$\Rightarrow \quad f_{\rm cr} = T^{\frac{d+z}{z}} \Psi\left(r T^{-1/(\nu z)}, 1\right)$$

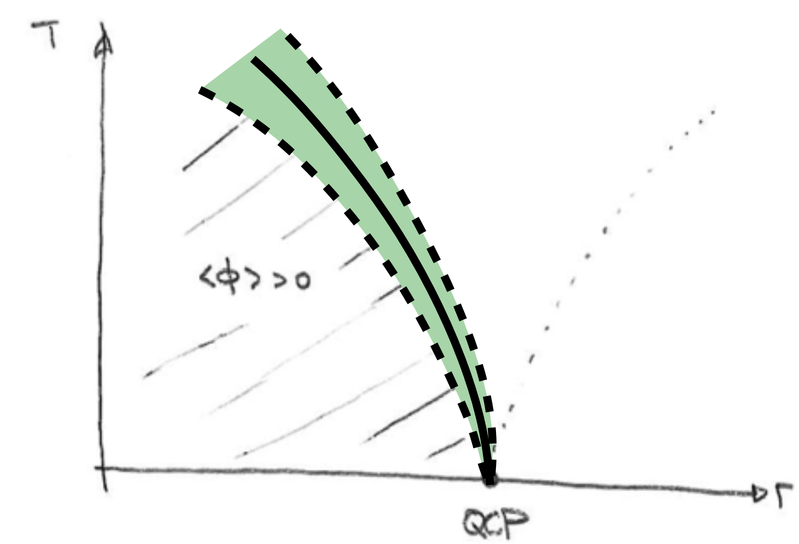
function $\Psi(x,1)$ analytic for small x: $\Psi(x,1) = \Psi(0,1) + \Psi'(0,1) x + \ldots$

However, for a phase diagram with a finite $T_c(r)$:

scaling function develops a singularity at $T_c > 0$

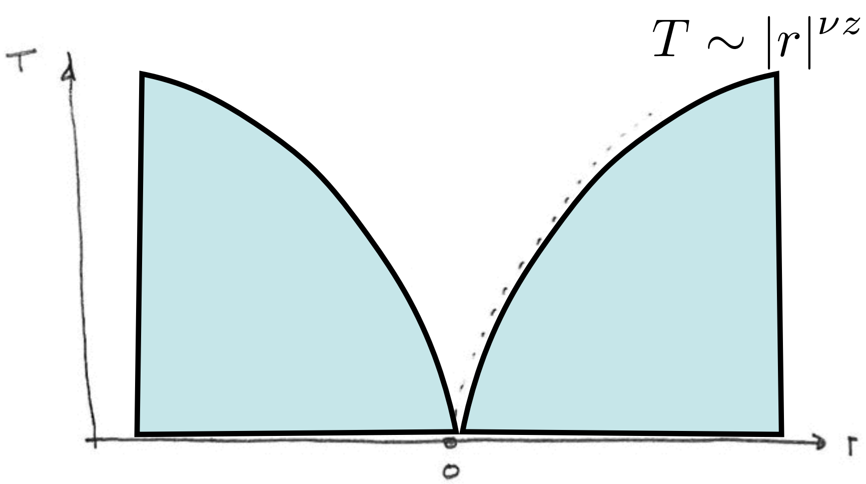
$$\Psi(x,1) \sim |x-1|^{2-\alpha}$$

α: specific heat exponent of the classical transition



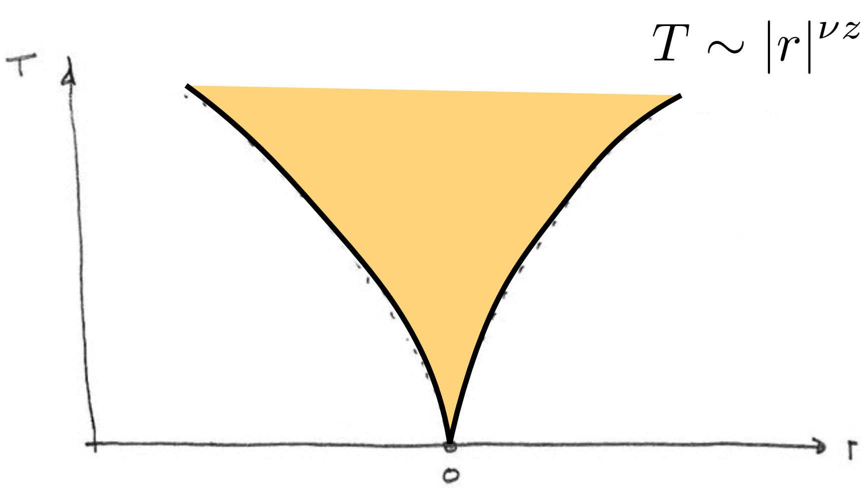
Summary:

low-T regime: choose $\xi = \xi_r = |r|^{-\nu}$



$$\Rightarrow \quad f_{\rm cr} = |r|^{\nu(d+z)} \Psi\Big(\mathrm{sgn}(r), T|r|^{-\nu z}\Big)$$

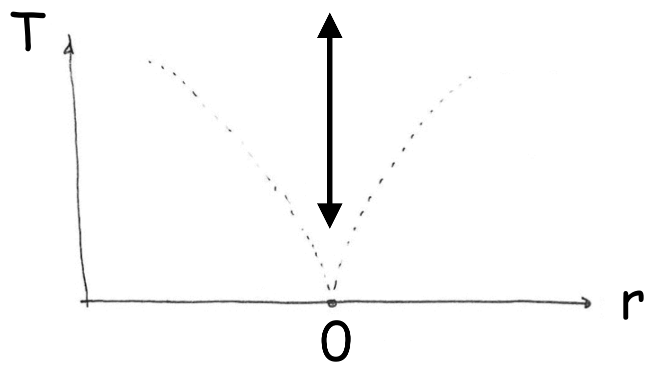
quantum critical regime: choose $\xi = \xi_T = T^{-1/z}$



$$\Rightarrow \quad f_{\rm cr} = T^{\frac{d+z}{z}} \Psi\Big(rT^{-1/(\nu z)}, 1\Big)$$

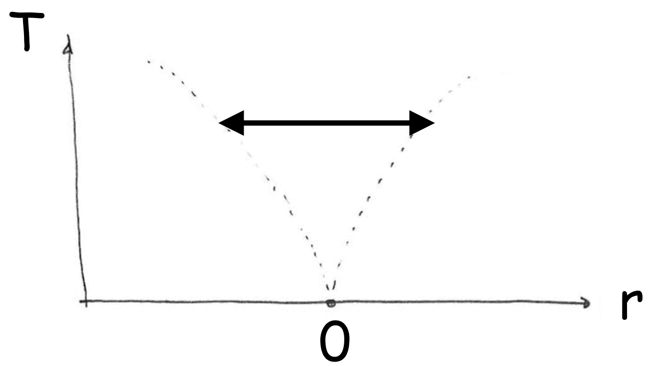
quantum critical thermodynamics

two independent first order derivatives of the free energy



variation of the free energy along the T-axis:

$$S = -\frac{\partial f}{\partial T}$$ entropy



variation of the free energy along the tuning parameter r-axis:

e.g. for pressure tuning: $r \propto p - p_c$

$$\frac{\partial f}{\partial r} \propto \frac{\partial f}{\partial p} = \frac{\Delta V}{V}$$ volume change

e.g. for tuning by magnetic field: $r \propto H - H_c$

$$\frac{\partial f}{\partial r} \propto \frac{\partial f}{\partial H} = -\mu_0 M$$ magnetization

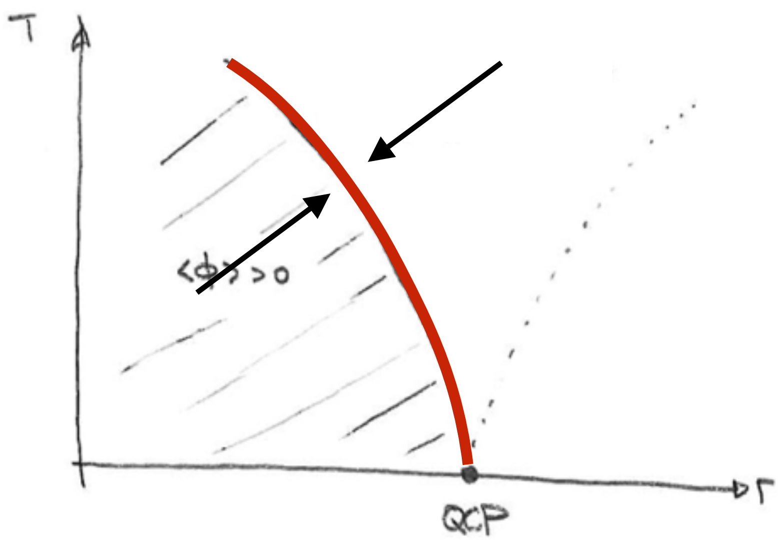
quantum critical thermodynamics

three independent second order derivatives of the free energy

transition driven by e.g.	pressure $r \sim p - p_c$	magnetic field $r \sim H - H_c$
$\frac{\partial^2 f_{\rm cr}}{\partial T^2}$	specific heat coefficient $C/T = -\frac{\partial^2 f}{\partial T^2}$	specific heat coefficient $C/T = -\frac{\partial^2 f}{\partial T^2}$
$\frac{\partial^2 f_{\rm cr}}{\partial r \partial T}$	thermal expansion $\alpha = \frac{1}{V}\frac{\partial V}{\partial T}\Big\vert_p = \frac{\partial^2 f}{\partial p \partial T}$	T derivative of magnetization $\frac{\partial M}{\partial T} = -\frac{1}{\mu_0}\frac{\partial^2 f}{\partial H \partial T}$
$\frac{\partial^2 f_{\rm cr}}{\partial r^2}$	compressibility $\kappa = -\frac{1}{V}\frac{\partial V}{\partial p}\Big\vert_T = -\frac{\partial^2 f}{\partial p^2}$	differential susceptibility $\chi = \frac{\partial M}{\partial H} = -\frac{1}{\mu_0}\frac{\partial^2 f}{\partial H^2}$

specific heat, thermal expansion, compressibility

close to classical transition

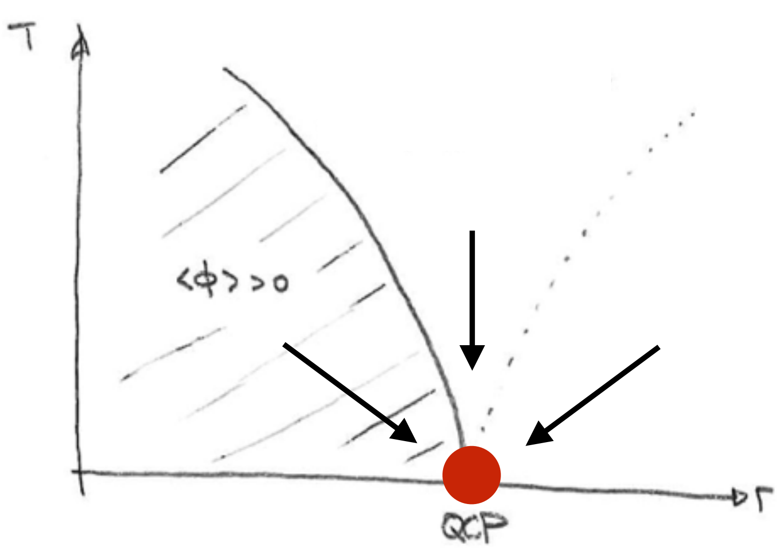


single distinguished direction

$$C_{\rm cr} \sim \alpha_{\rm cr} \sim \kappa_{\rm cr} \sim |T - T_c|^{-\alpha}$$

divergence with the same exponent

close to the quantum critical point



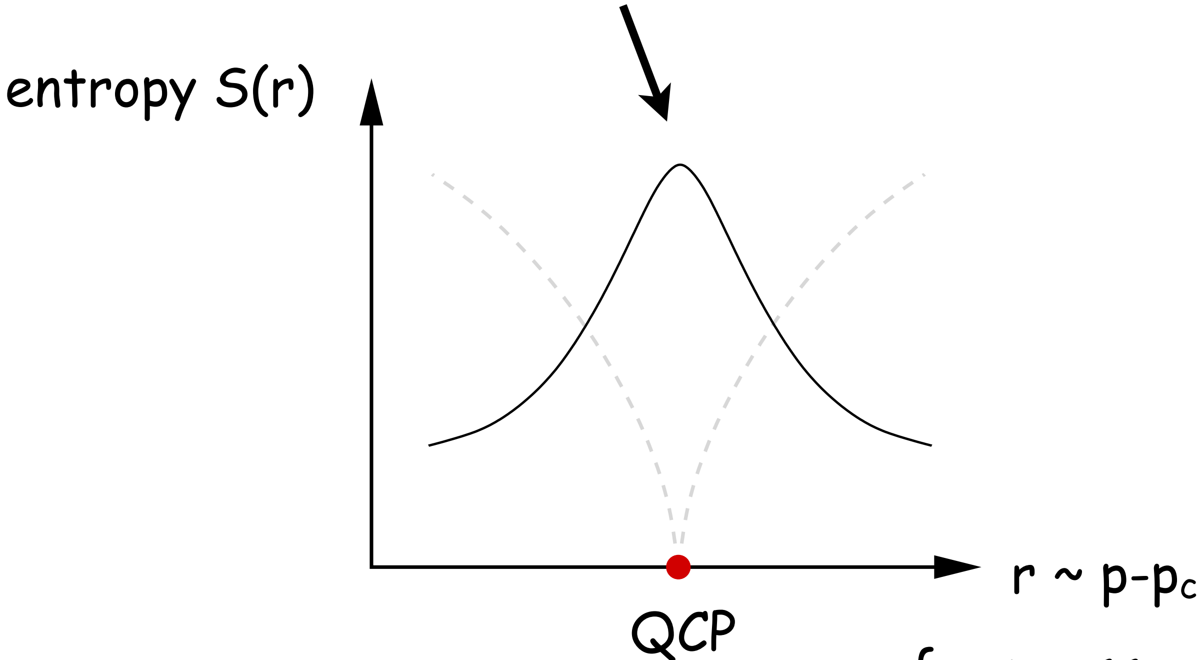
two independent directions: r = pressure and T

↓

C, α and κ yield complementary information

entropy distribution in the phase diagram

enhancement of entropy close to quantum critical point



for pressure tuning

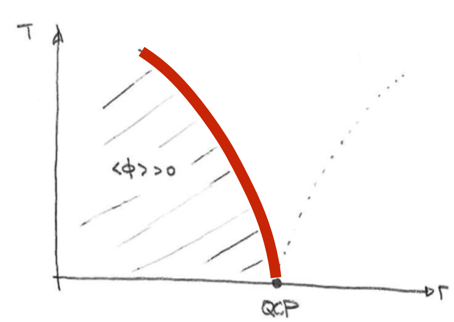
thermal expansion measures slope

$$\alpha \sim \frac{\partial S}{\partial r}$$

→ thermal expansion α changes sign

vanishing thermal expansion ⟷ positions of accumulated entropy

in the presence of a finite T_c



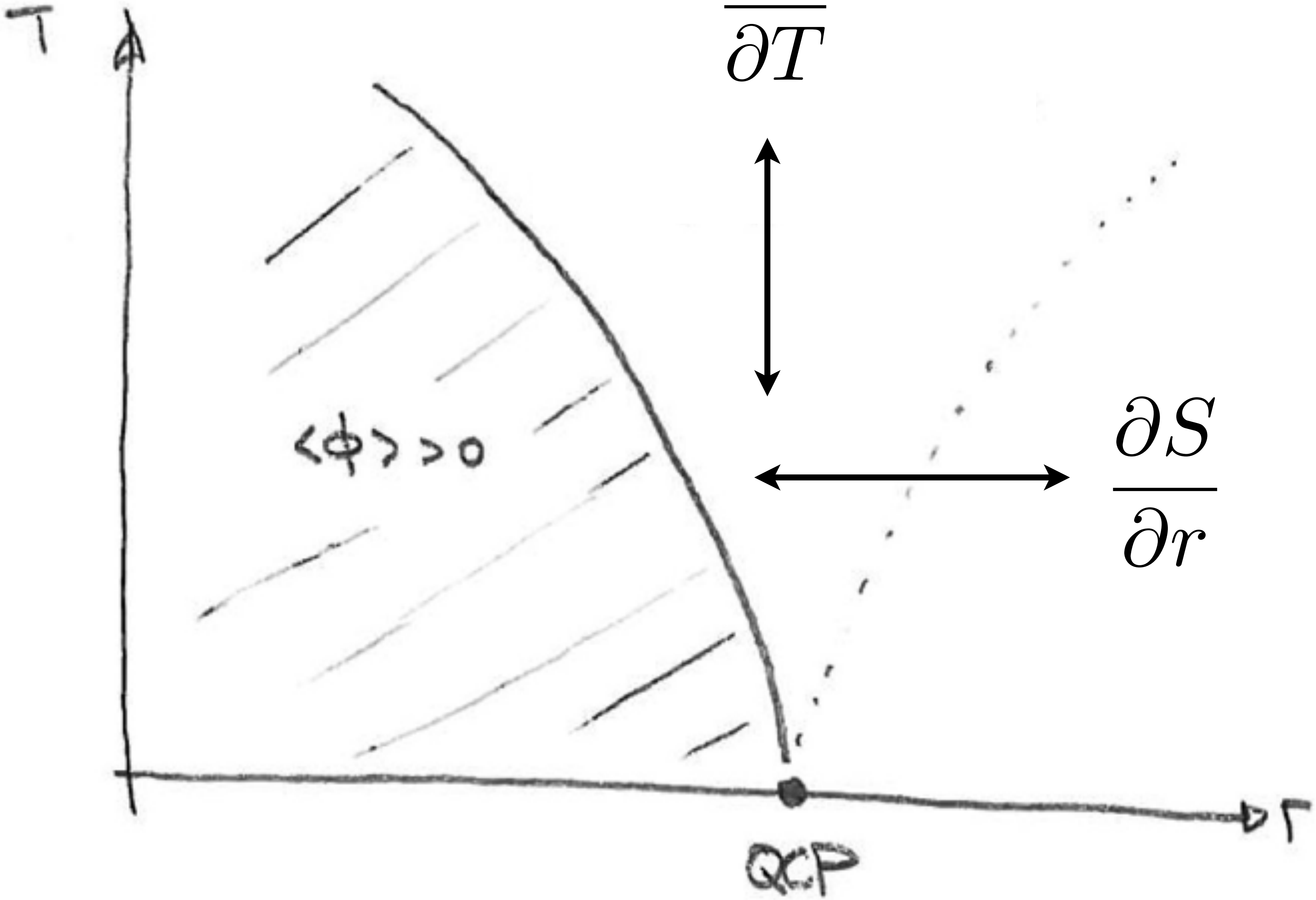
accumulation of entropy along the phase boundary

⇨ sign change close to T_c

entropy distribution in the phase diagram

consider: change of entropy S

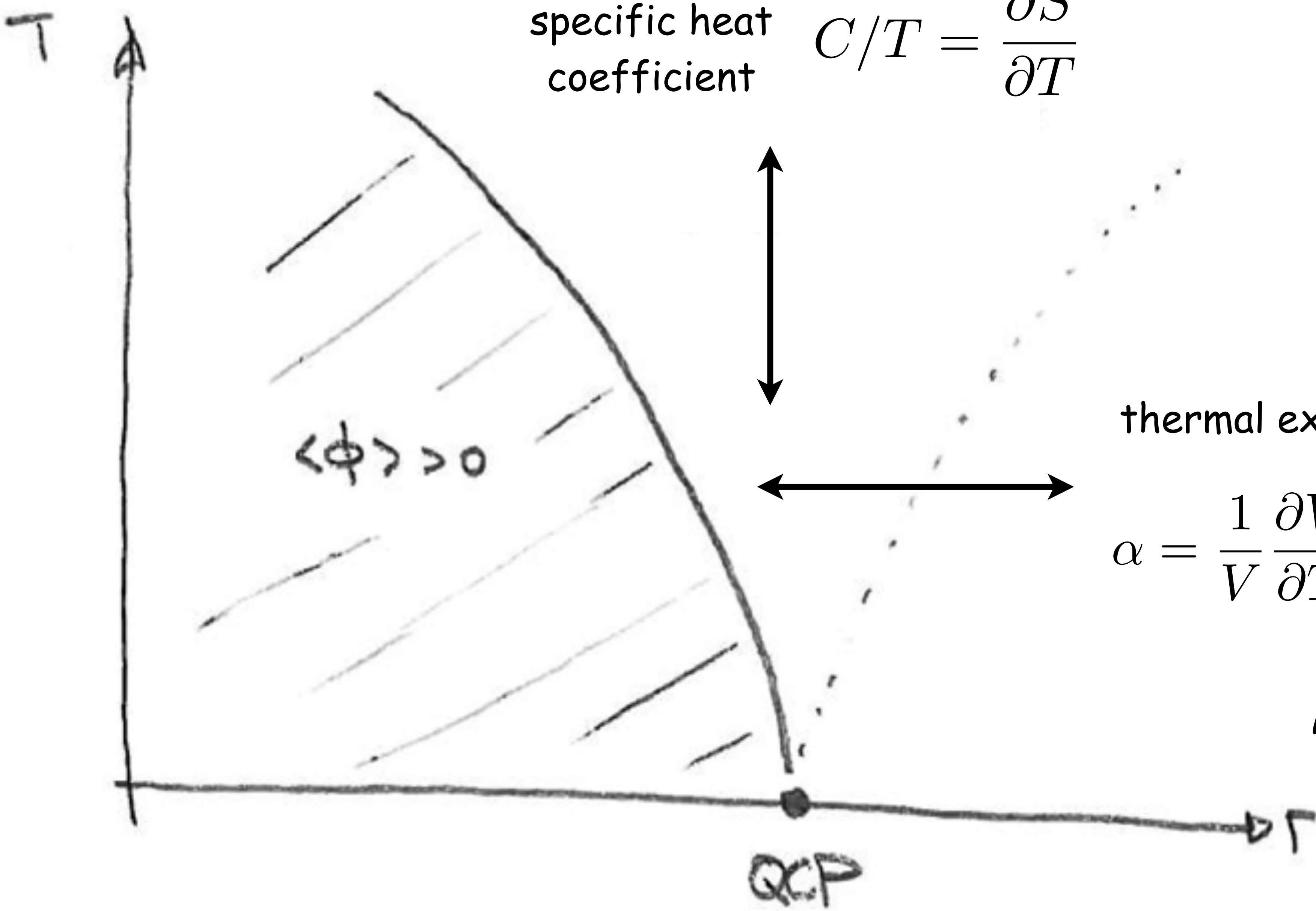
$$\frac{\partial S}{\partial T}$$



$$\frac{\partial S}{\partial r}$$

entropy distribution in the phase diagram

consider: change of entropy S



specific heat coefficient

$$C/T = \frac{\partial S}{\partial T}$$

thermal expansion

$$\alpha = \frac{1}{V}\frac{\partial V}{\partial T} = -\frac{1}{V}\frac{\partial S}{\partial p}$$

Maxwell relation

Grüneisen parameter & magnetocaloric effect

Grüneisen parameter $$\Gamma = \frac{\alpha}{C}$$ ratio of thermal expansion & specific heat

away from any quantum phase transition: Γ is constant and is a measure for the pressure dependence of the characteristic energy scale (Debye energy, Fermi energy etc.)

at a QCP tuned by pressure:

Γ changes sign and necessarily diverges with characteristic exponents

for a QCP tuned e.g. by magnetic field:

magnetic analogue: $$\Gamma_H = -\frac{\partial M/\partial T}{C} = \frac{1}{T}\frac{dT}{dH}\Big|_S$$

magnetocaloric effect

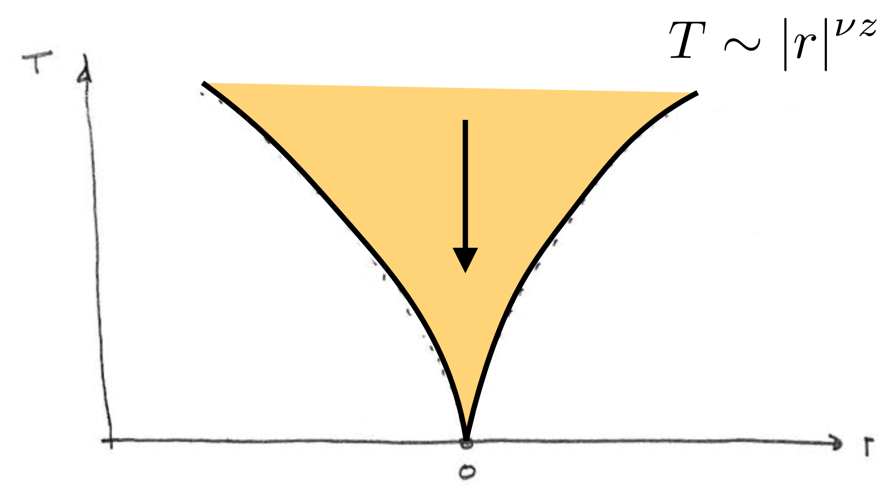
adiabatic change of temperature upon changing H

obtained using

$$dS = \frac{\partial S}{\partial H}\Big|_H dH + \frac{\partial S}{\partial T}\Big|_T dT = 0$$

Grüneisen parameter & magnetocaloric effect

quantum critical regime:



$$f_{\rm cr} = T^{\frac{d+z}{z}} \Psi\left(r T^{-1/(\nu z)}, 1\right)$$

with $\Psi(x,1) = \Psi(0,1) + \Psi'(0,1)x + \ldots$ for small x

at the QCP (r=0):

specific heat: $$C_{\rm cr} = -T \frac{\partial^2 f_{\rm cr}}{\partial T^2} \sim T^{\frac{d}{z}}$$

thermal expansion or dM/dT: $$\frac{\partial^2 f_{\rm cr}}{\partial T \partial r} \sim T^{\frac{d}{z} - \frac{1}{\nu z}}$$

Grüneisen parameter or magnetocaloric effect at r=0:

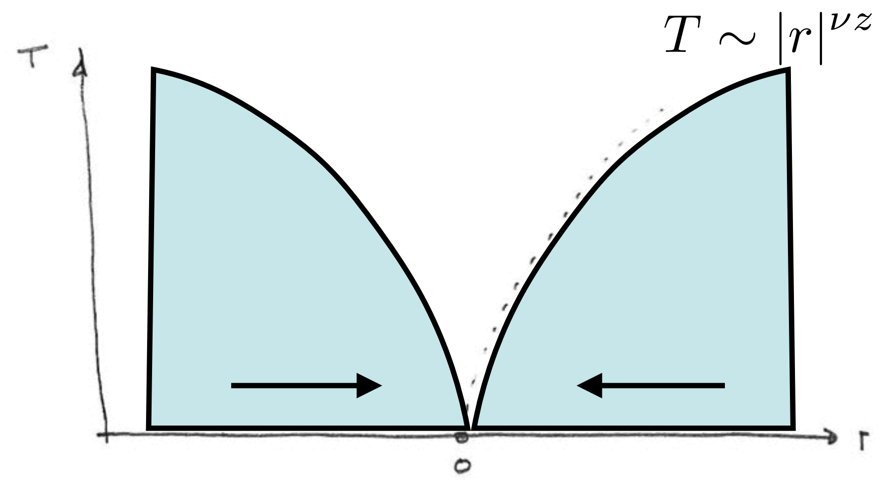
$$\Gamma \sim \frac{1}{T^{\frac{1}{\nu z}}}$$

diverges with exponent 1/(νz)

Grüneisen parameter & magnetocaloric effect

low-T regime:

$$f_{\rm cr} = |r|^{\nu(d+z)} \Psi\Big(\mathrm{sgn}(r), T|r|^{-\nu z}\Big)$$



e.g. for a system with a gapless ground state for T->0:

$$f_{\rm cr} = -\mathcal{A}|r|^{\nu(d+z)} (T|r|^{-\nu z})^{y_0+1}$$

with constant A and y_0>0.

specific heat:

$$C_{\rm cr} = -T\frac{\partial^2 f_{\rm cr}}{\partial T^2} = \mathcal{A}(y_0+1)y_0|r|^{\nu(d+z)-\nu z(y_0+1)}T^{y_0}$$

thermal expansion:

$$\alpha_{\rm cr} = \frac{\partial^2 f_{\rm cr}}{\partial p \partial T} = \mathcal{A}(y_0+1)T^{y_0}(\nu d - \nu z y_0)|r|^{\nu(d+z)-\nu z(y_0+1)-1}\frac{\partial |r|}{\partial p}$$

Grüneisen parameter for T->0:

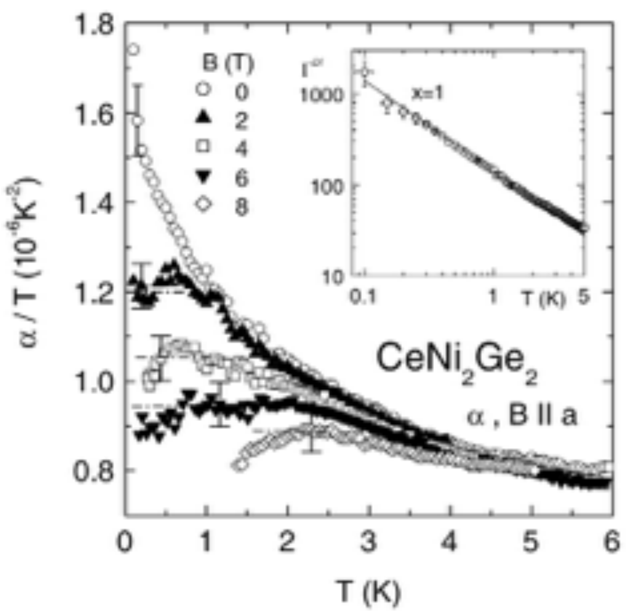
$$\Gamma = \frac{\alpha_{\rm cr}}{C_{\rm cr}} = \frac{\nu d - \nu z y_0}{y_0}\frac{1}{|r|}\frac{\partial |r|}{\partial p} = \frac{\nu d - \nu z y_0}{y_0}\frac{1}{p-p_c}$$

diverges with $1/(p-p_c)$ with universal prefactor that is given by exponents

with $r = (p-p_c)/p_0$

Examples: Sign change and divergence of the Grüneisen parameter

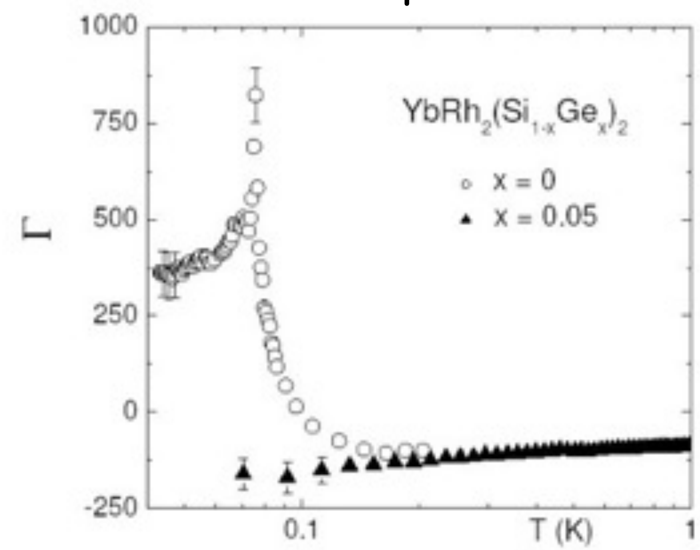
heavy-fermion compound $CeNi_2Ge_2$



Küchler et al. PRL (2003)

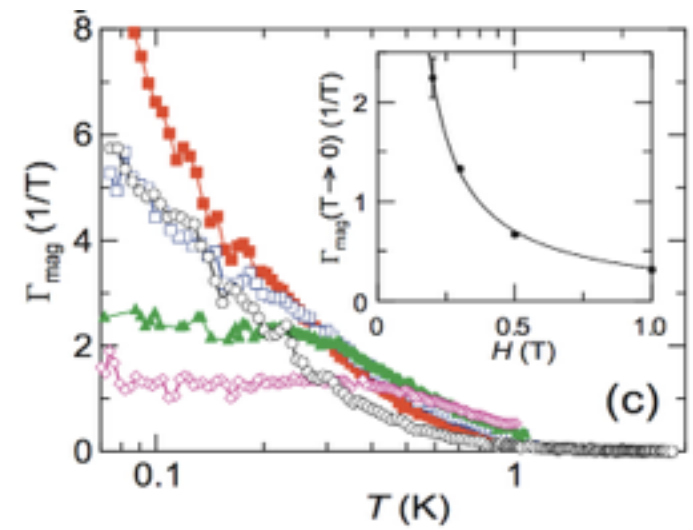
heavy-fermion $YbRh_2(Si_{1-x}Ge_x)_2$

Grüneisen parameter



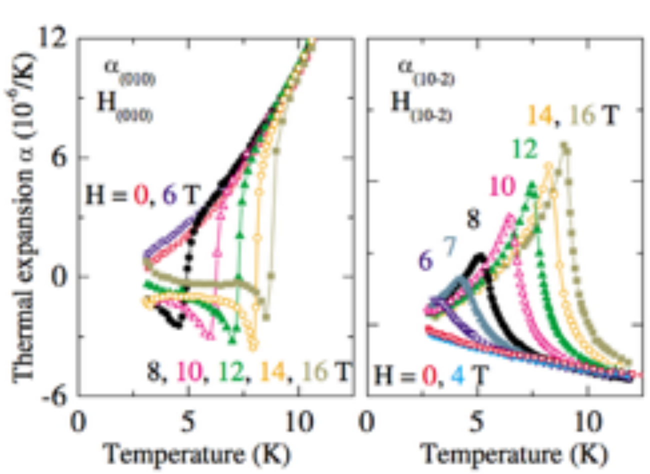
Küchler, Gegenwart

magnetocaloric effect

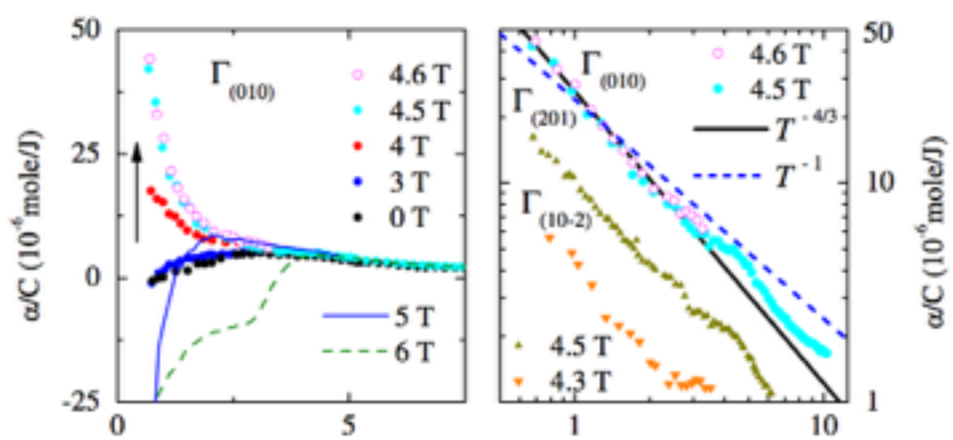


Tokiwa et al. PRL 2009

spin dimer system $TlCuCl_3$



Johannsen et al. PRL (2005)



Lorenz et al. JMMM (2007)

helimagnetic metal MnSi

absence of sign change in thermal expansion -> NO QCP

Non–Fermi Liquid Metal Without Quantum Criticality

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Dilute weakly-interacting Bose gas

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complex bosonic field ϕ governed by the Lagrangian

recovers free Schrödinger equation

$$\mathcal{L} = \phi^*(i\hbar\partial_t + \frac{\hbar^2\nabla^2}{2m} + \mu)\phi - \frac{u}{2}|\phi|^4$$

non-linearity,
interaction of bosons

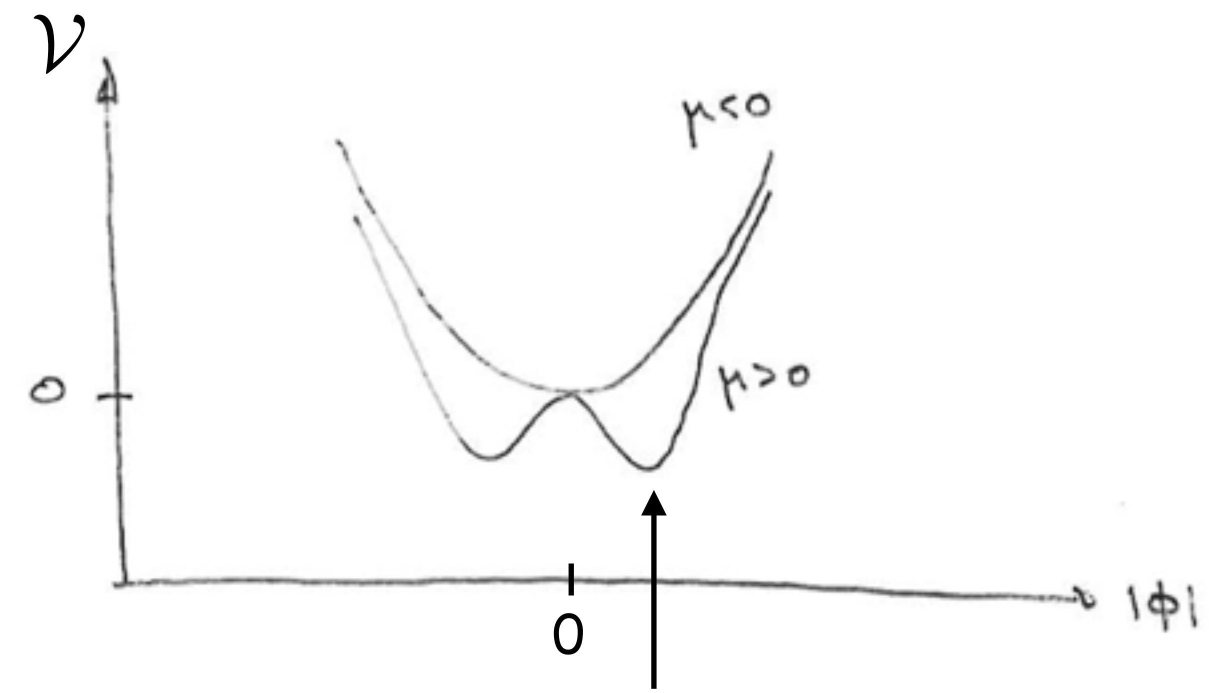
bosons with mass m and chemical potential μ that interact with amplitude u > 0

Mean-field theory

consider constant field configuration $\phi(\vec{r}, t) \equiv \phi$

effective potential

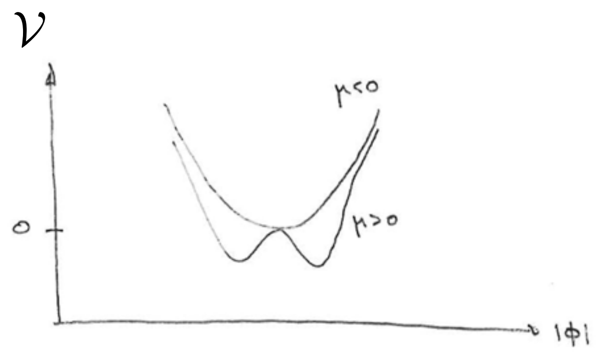
$$\mathcal{V} = -\mu|\phi|^2 + \frac{u}{2}|\phi|^4$$



quantum phase transition at μ = 0

Bose-Einstein condensation of bosons tuned by the chemical potential

Mean-field theory



for negative chemical potential μ < 0:

potential minimised for $\phi = \phi^* = 0$ ⇨ uncondensed phase

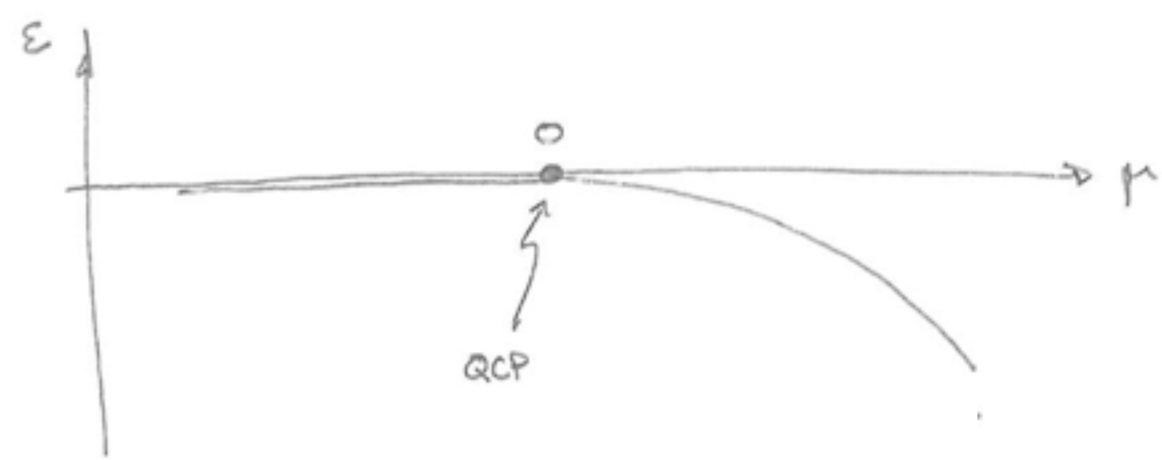
for positive chemical potential μ > 0:

mean-field attains finite value $|\phi|^2 = \frac{\mu}{u}$ ⇨ Bose condensed phase

solutions are degenerate: $\phi = \sqrt{\frac{\mu}{u}} e^{i\varphi}$ defined up to a phase factor

mean-field ground-state energy: $$\varepsilon_0 = \mathcal{V}\Big|_{\min} = \begin{cases} 0 & \text{if} \quad \mu < 0 \\ -\frac{\mu^2}{2u} & \text{if} \quad \mu > 0 \end{cases}$$

at the QCP:
non-analyticity of the ground-state energy
as a function of μ = tuning parameter



Scaling exponents

comparing chemical potential with kinetic energy with momentum $p \sim \hbar/\xi_\mu$

$$\frac{\hbar^2}{2m\xi_\mu^2} \sim \mu \quad \Rightarrow \quad \xi_\mu \sim \frac{\hbar}{\sqrt{2m|\mu|}} \sim |\mu|^{-\nu}$$

correlation length exponent $\nu = \frac{1}{2}$

comparing temperature with kinetic energy with momentum $p \sim \hbar/\xi_T$

$$\frac{\hbar^2}{2m\xi_T^2} \sim k_B T \quad \Rightarrow \quad \xi_T \sim \frac{\hbar}{\sqrt{2mk_B T}} \sim T^{-1/z}$$

thermal length

dynamical exponent $z = 2$

Attention:

For the BEC quantum phase transition in spatial dimension $d > 2$ the knowledge of the exponents v and z is not sufficient to determine the phase diagram!

The scaling hypothesis does not apply due to the presence of the "dangerously irrelevant interaction u".

Self-consistent Hartree-Fock approximation

explicit calculation: renormalization of the chemical potential at finite T>0

mean-field decoupling of the interaction:

$$H_{int} = \int dr \, \frac{u}{2} |\phi|^4 = \int dr \, \frac{u}{2} \phi^* \phi^* \phi \phi \cong 4 \frac{u}{2} \int dr \, \langle |\phi|^2 \rangle |\phi|^2$$

four possibilities to decouple the interaction

⇨ renormalization of μ

$$-\mu^R = -\mu + 2u \langle |\phi|^2 \rangle$$

Bose function

evaluation of the expectation value at finite T>0:

$$-\mu^R = -\mu + 2u \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta\left(\frac{\hbar^2 k^2}{2m} - \mu^R\right)} - 1}$$

self-consistency

phase transition occurs for μ^R=0 ⇨ critical temperature $T_c(\mu)$

$$0 = -\mu + 2u \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\frac{\hbar^2 k^2}{2mk_B T_c}} - 1}$$

substitution $\frac{\hbar^2 k^2}{2mk_B T} = x^2$

$$\Leftrightarrow \quad \mu = 2u \frac{4\pi}{(2\pi)^3} \left(\frac{2mk_B T_c}{\hbar^2}\right)^{3/2} \int_0^\infty dx \frac{x^2}{e^{x^2} - 1}$$

$$\langle |\phi|^2 \rangle = n \propto \xi_T^{-3} \sim T^{3/2}$$

density of bosons = inverse thermal volume

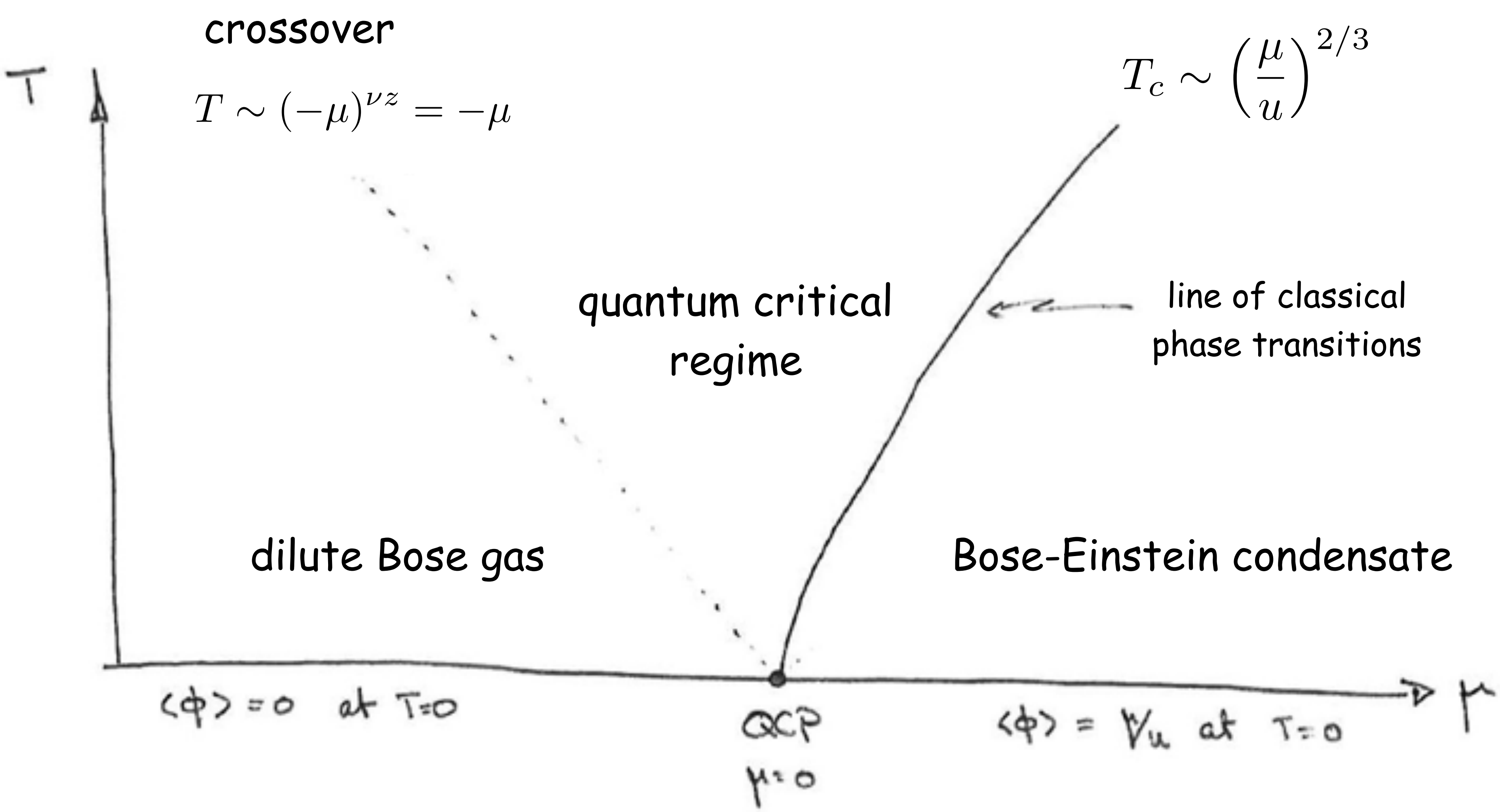
$$\rightarrow \quad \mu \sim u \, T_c^{3/2} \quad \text{or}$$

$$T_c \sim \left(\frac{\mu}{u}\right)^{2/3}$$

explicitly dependent on the interaction u!

Phase diagram

phase diagram of the dilute Bose gas in spatial dimension d=3



Generalized scaling & upper critical dimension

the presence of the scaling $T_c \sim \left(\frac{\mu}{u}\right)^{2/3}$ can also be rationalised in terms of a generalised scaling Ansatz

$$f_{\rm cr} = \xi^{-(d+z)} \Psi(\mu\, \xi^{1/\nu}, T\, \xi^z, u\, \xi^{4-(d+z)})$$

with 4 - (d+z) being the scaling dimension of the interaction u

It is irrelevant, i.e., it can be treated quasi-perturbatively as long as the effective dimension d+z exceeds the upper critical dimension 4:

$$d + z > 4 \quad \overset{z=2}{\Rightarrow} \quad d > 2$$

With the choice of the thermal wavelength: $\xi = T^{-1/z}$ and z=2 and ν=1/2

$$\Rightarrow \quad f_{\rm cr} = T^{\frac{d+2}{2}} \Psi(\frac{\mu}{T}, 1, u\, T^{(d-2)/2})$$

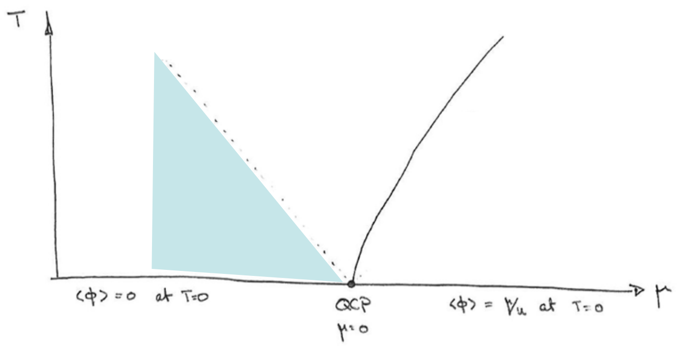
Close to the classical transition
the scaling function possesses the singularity $\Psi(x, 1, z) \sim |x + z|^{2-\alpha}$

$$\Rightarrow \quad T_c \sim \left(\frac{\mu}{u}\right)^{2/d}$$

for d=2 logarithmic corrections (BKT transition)

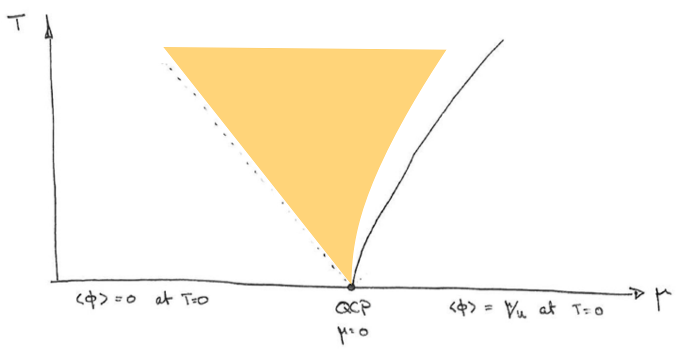
critical free energy (in d=3)

The asymptotic T dependence of the critical free energy is mostly not affected by the interaction u:



dilute Boltzmann gas

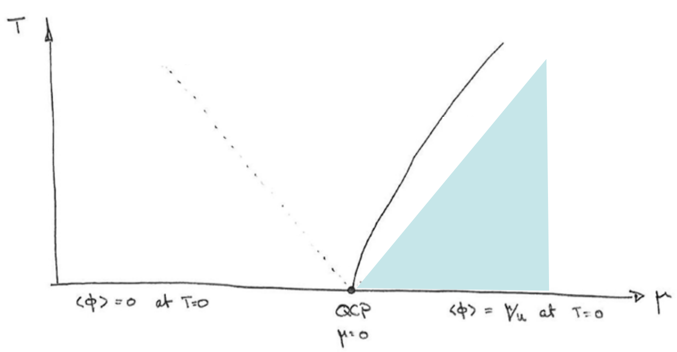
$$f_{\rm cr} \sim \frac{k_B T}{\xi_T^3} e^{\frac{\mu}{k_B T}} \sim T^{5/2} e^{\frac{\mu}{k_B T}}$$



quantum critical

$$f_{\rm cr} \sim \frac{k_B T}{\xi_T^3} \sim T^{5/2}$$

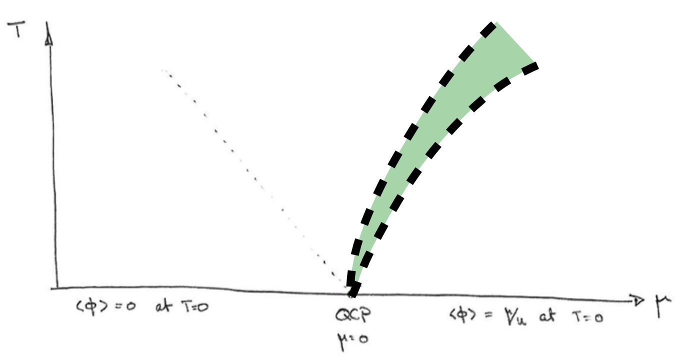
perturbative correction due to interaction $un^2 \sim uT^3$



Bogoliubov gas (not covered here)

$$f_{\rm cr} \sim \frac{k_B T}{\xi_T^3} \left(\frac{T}{\mu}\right)^{3/2} \sim \frac{T^4}{\mu^{3/2}}$$

in addition to T-independent ground state energy $-\frac{\mu^2}{2u}$



classical criticality with O(2) universality

$$f_{\rm cr} \sim |T - T_c(\mu)|^{2-\alpha}$$

specific heat exponent α