Introduction to Quantum Phase Transitions

Part II

Outline:

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

- Dilute weakly interacting Bose gas

- Insulating spin-dimer antiferromagnets

- 1d Heisenberg vs 1d Ising model in a transverse field

- Quantum critical paraelectrics

- Quantum critical metals

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Dilute weakly-interacting Bose gas

Reminder: dilute weakly-interacting Bose gas

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

mean-field exponents for d>2:

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

dynamical exponent $z = 2$

upper critical dimension d+z = 4, i.e., d=2

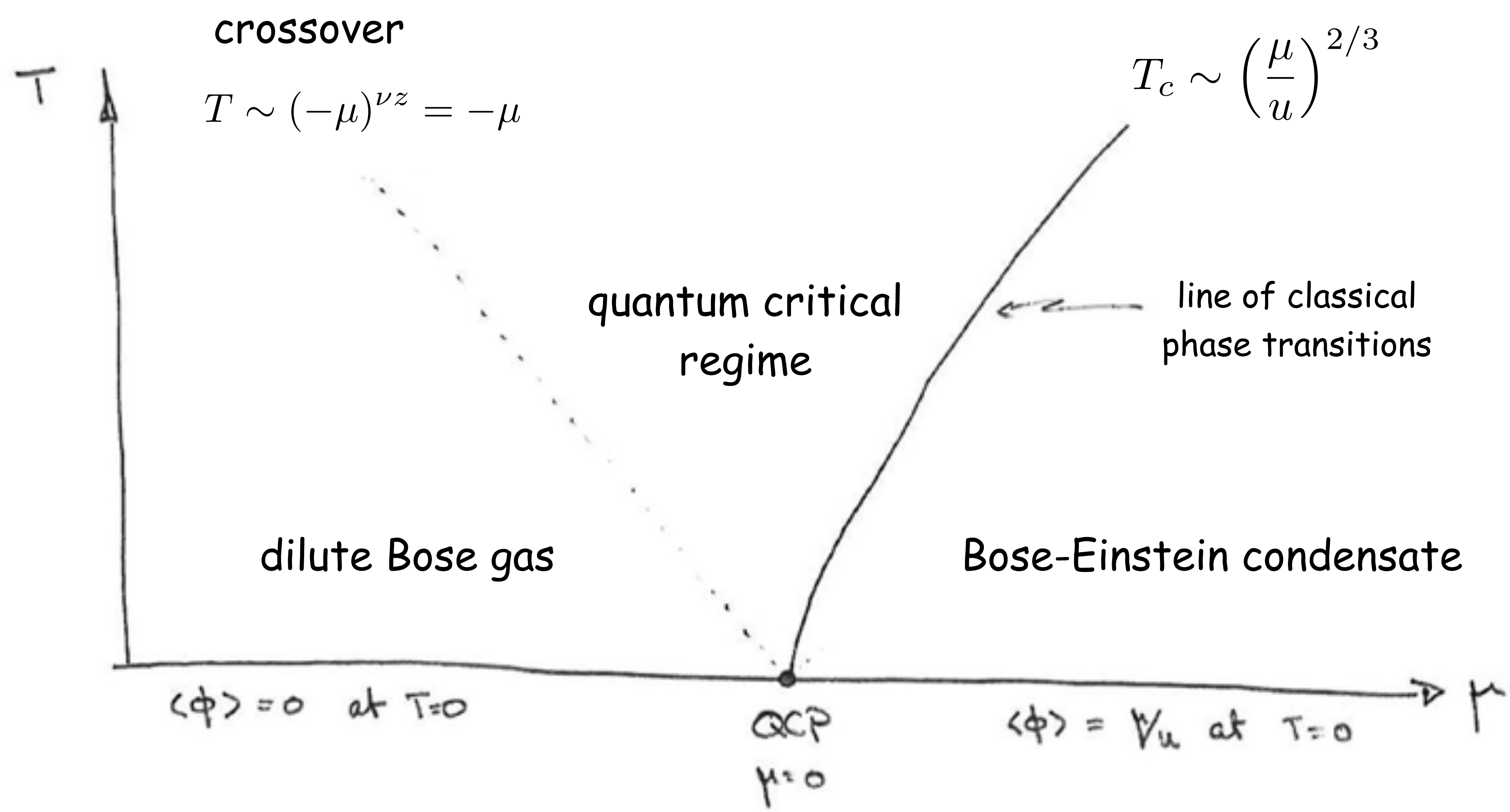
renormalization of the tuning parameter in the quantum critical regime (Hartree-Fock approximation)

$$-\mu^R = -\mu + 2u\langle|\phi|^2\rangle = -\mu + c\,uT^{\frac{d+z-2}{z}} = \mu + c\,uT^{3/2}$$

for d=3, z=2

Reminder: Phase diagram

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



Bosons in one spatial dimension

bosons in one spatial dimension at T=0:

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

consider dilute limit $\mu < 0$ with empty ground state.

First excited state contains single free boson
Next excited state contains two interacting bosons:

Two-particle wavefunction with zero total momentum only dependent on the relative coordinate $\Phi(x_1, x_2) = \Phi(x_1 - x_2)$

⇨ effective Schrödinger equation for relative coordinate $x = x_1 - x_2$

$$i\hbar\partial_t \Phi(x) = \Big(- \frac{\hbar^2 \partial_x^2}{2\mu_{\text{red}}} - \mu + u\delta(x) \Big) \Phi(x)$$

↑ reduced mass $\frac{1}{\mu_{\text{red}}} = \frac{1}{m} + \frac{1}{m}$

Quantum mechanics:

transmission coefficient $T = \frac{(ka)^2}{1 + (ka)^2}$ with scattering length $a = \frac{\mu_{\text{red}} \hbar^2}{u}$

Lifshitz transition

At low energies/momenta: $T = \frac{(ka)^2}{1+(ka)^2}$ -> 0

bosons perfectly reflect from each other!
Node develops in the two-particle wave function!

⇨ Interacting bosons in 1d behave like spinless fermions at low energies!
Emergent Pauli principle!
Example of statistical transmutation

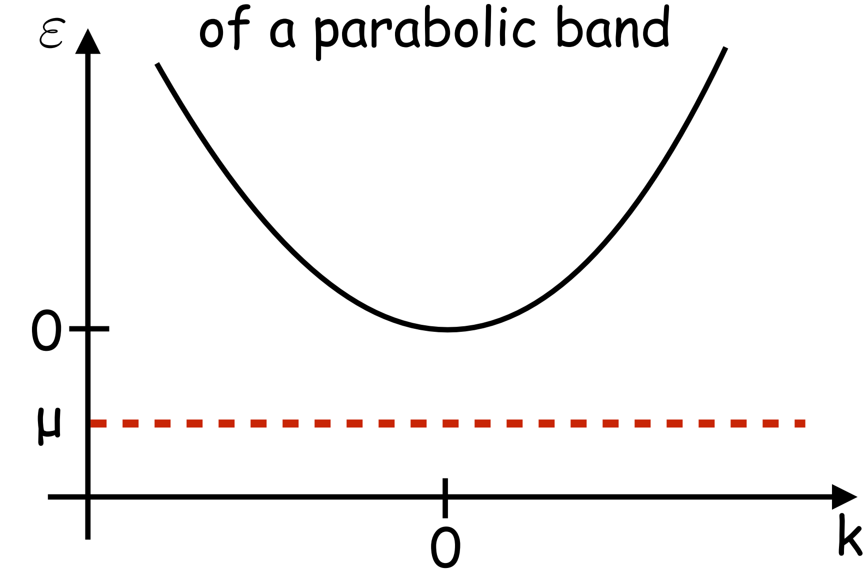
Effective theory for the quantum phase transition at μ=0:

$$H = \sum_k \Big(\frac{\hbar^2 k^2}{2m} - \mu\Big) c_k^\dagger c_k$$

← Fermionic operators

Independent of the interaction amplitude u!
Emergent universality! Scaling hypothesis applies!

Lifshitz transition:
fermions at the bottom of a parabolic band



explicit calculation:

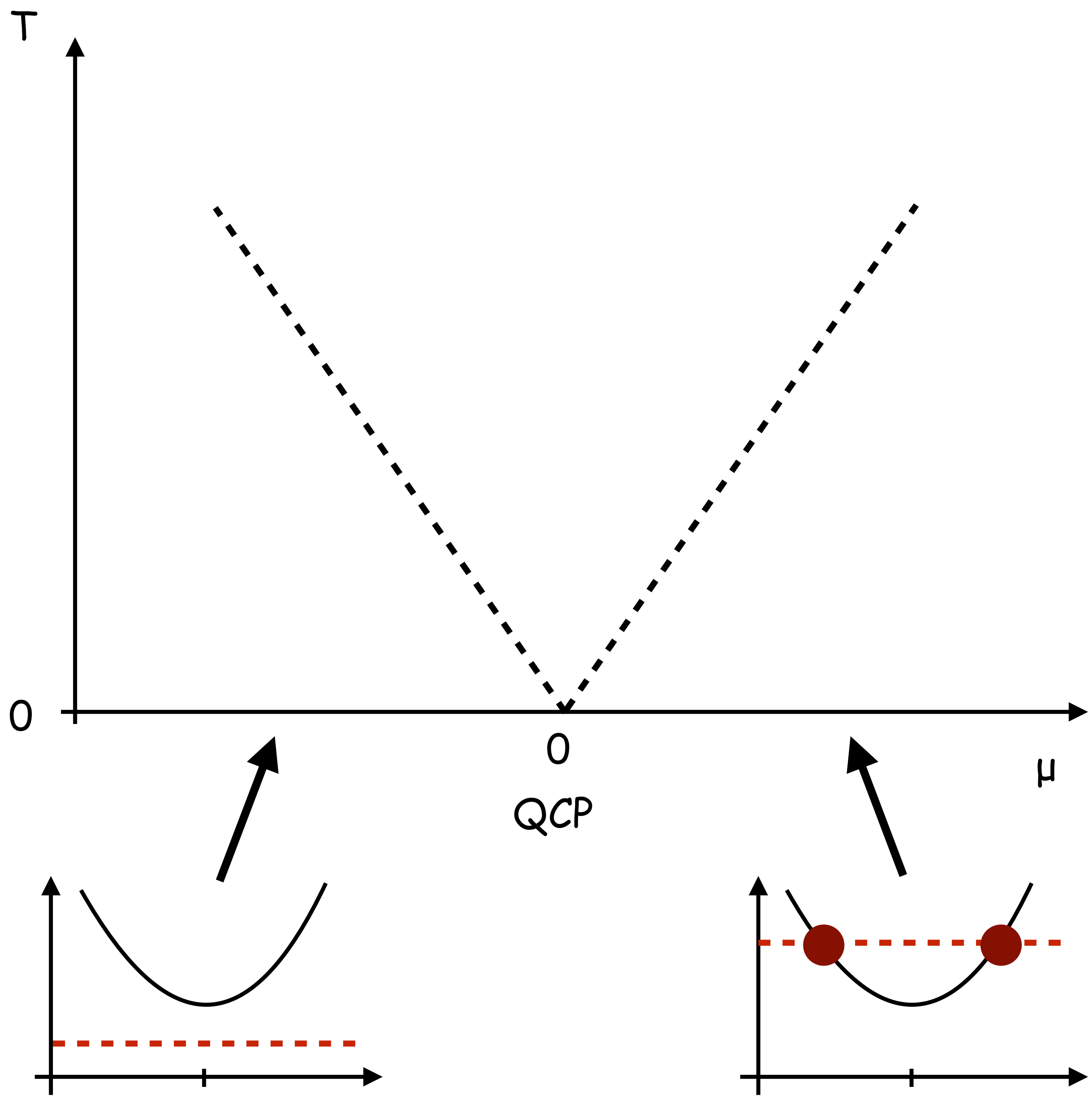
$$F = -k_B T \int_{-\infty}^{\infty} \frac{dk}{2\pi} \log(1 + \exp(-\frac{\hbar^2 k^2/(2m) - \mu}{k_B T}))$$

Free energy density
$$F = \frac{k_B T}{\xi_T} \Psi\Big(\frac{\mu}{T}\Big) \sim T^{3/2} \Psi\Big(\frac{\mu}{T}\Big)$$

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

dynamical exponent $z = 2$

Phase diagram for d=1



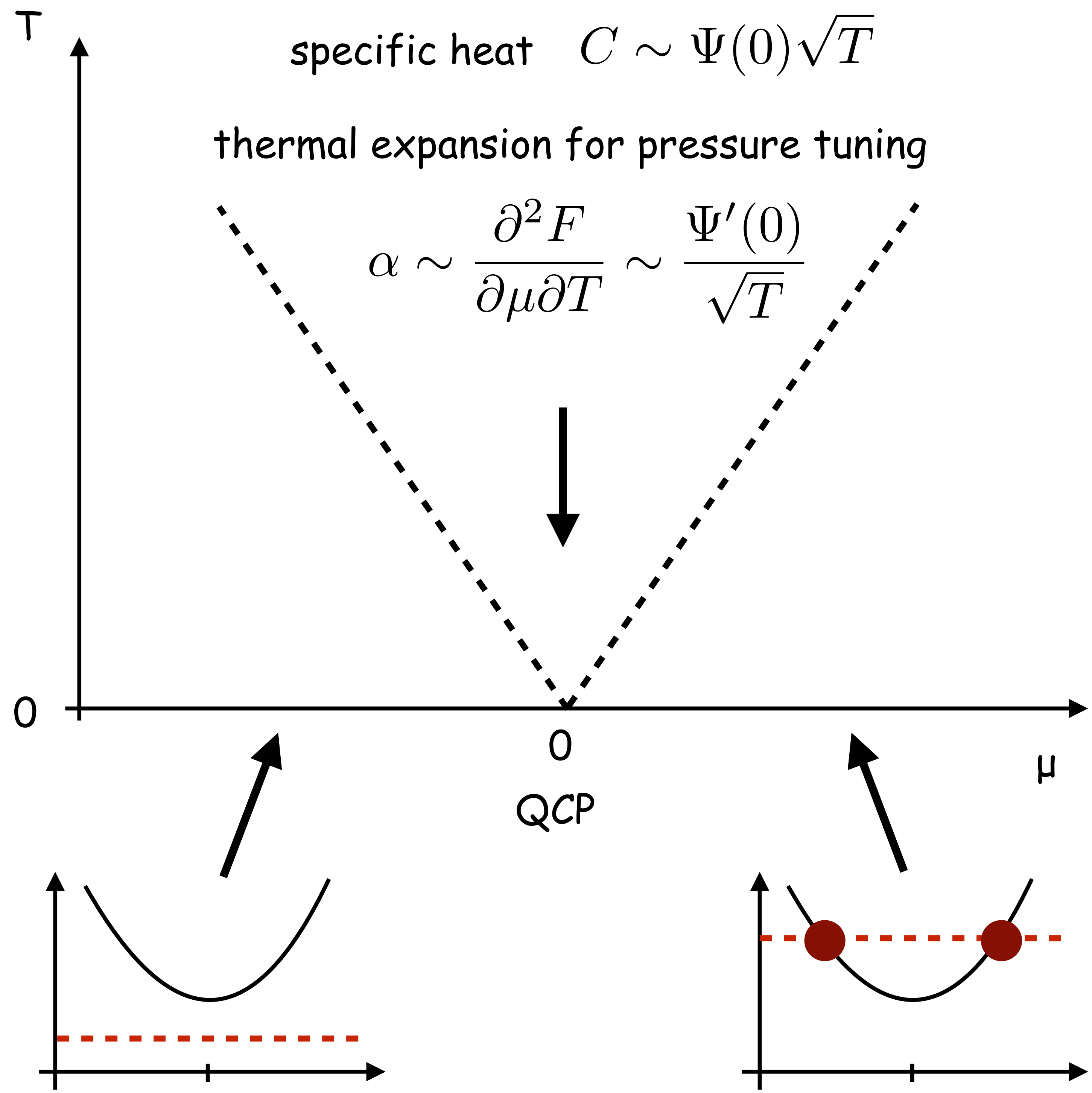
Change of the ground state at μ=0
Development of two Fermi points!

Phase diagram for d=1

specific heat $C \sim \Psi(0)\sqrt{T}$

thermal expansion for pressure tuning

$$\alpha \sim \frac{\partial^2 F}{\partial \mu \partial T} \sim \frac{\Psi'(0)}{\sqrt{T}}$$



Scaling form of the free energy:

$$F \sim T^{3/2}\Psi\left(\frac{\mu}{T}\right)$$

Change of the ground state at μ=0

Development of two Fermi points!

Residual interaction

Fermions still interact $$H_{\text{int}} = \frac{1}{4} \sum_{k,k',p,p'} \Gamma_{kk';pp'} c^\dagger_k c^\dagger_{k'} c_p c_{p'}$$

interaction amplitude at low energies has the form

$$\Gamma_{kk';pp'} = \gamma\, \delta_{k+k',p+p'} (k - k')(p - p')$$

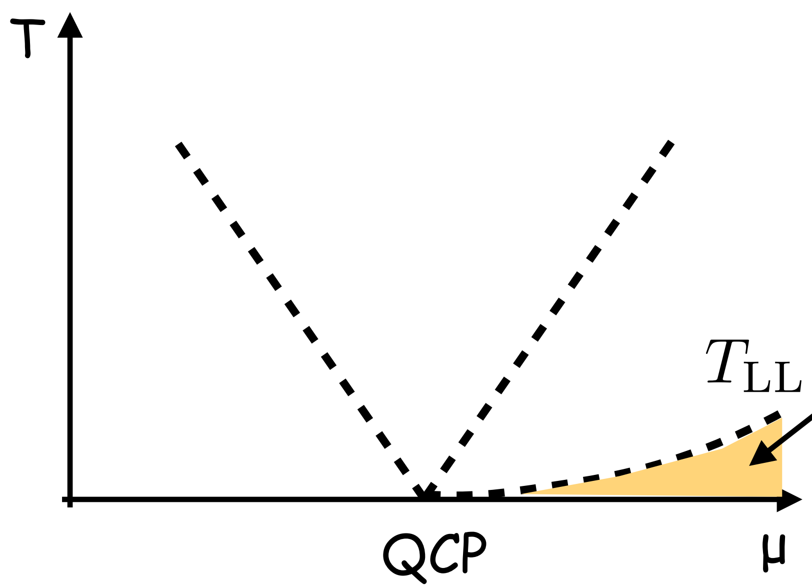
amplitude dependent on the boson interaction u

momentum conservation

factors of momentum required by Pauli principle, not possible to create/annihilate two fermions with the same momentum

⇨ Interaction irrelevant at the QCP! Does not modify the asymptotic critical behaviour!

However:



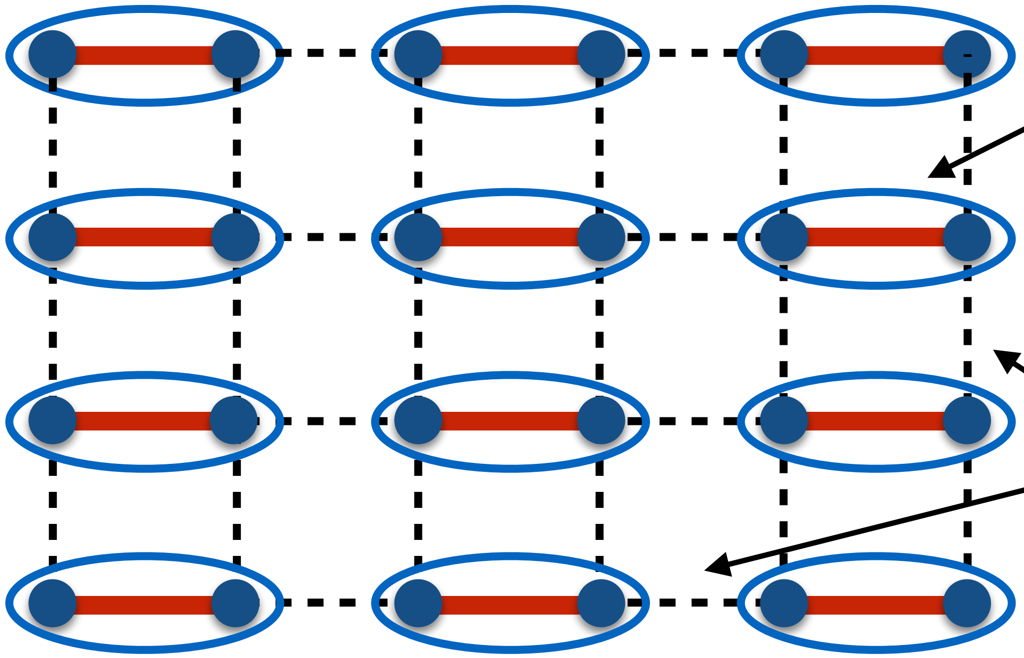
it induces Luttinger liquid correlations for μ > 0 at lowest temperatures

with crossover temperature $\log(T_{\text{LL}}/\mu) \sim 1/\mu$

Spin-dimer antiferromagnets

Weakly-coupled dimers

consider spins 1/2 on a lattice



strong antiferromagnet coupling J

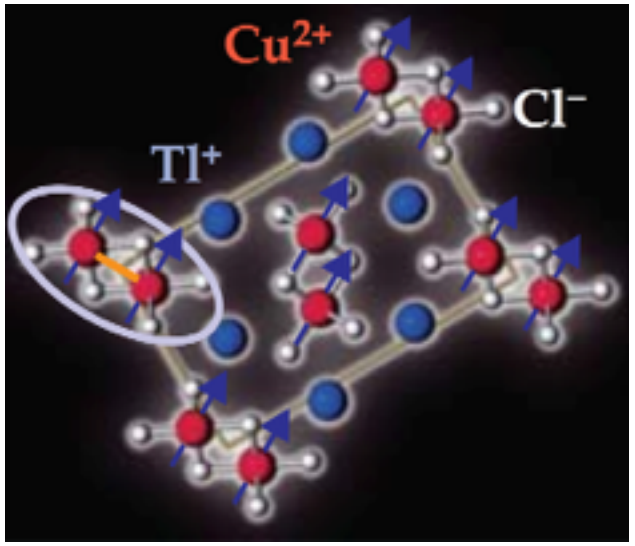
$$\Rightarrow \quad = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$

formation of a singlet state = dimer

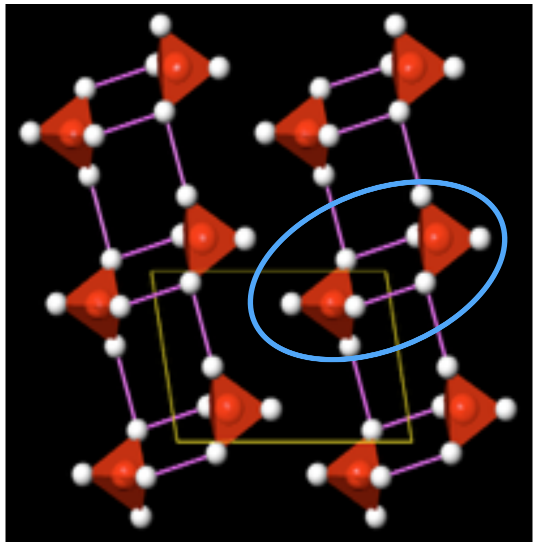
weak coupling J′ between the dimers

Examples:

dimer →



$TlCuCl_3$



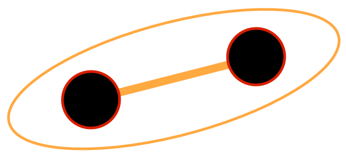
← dimer

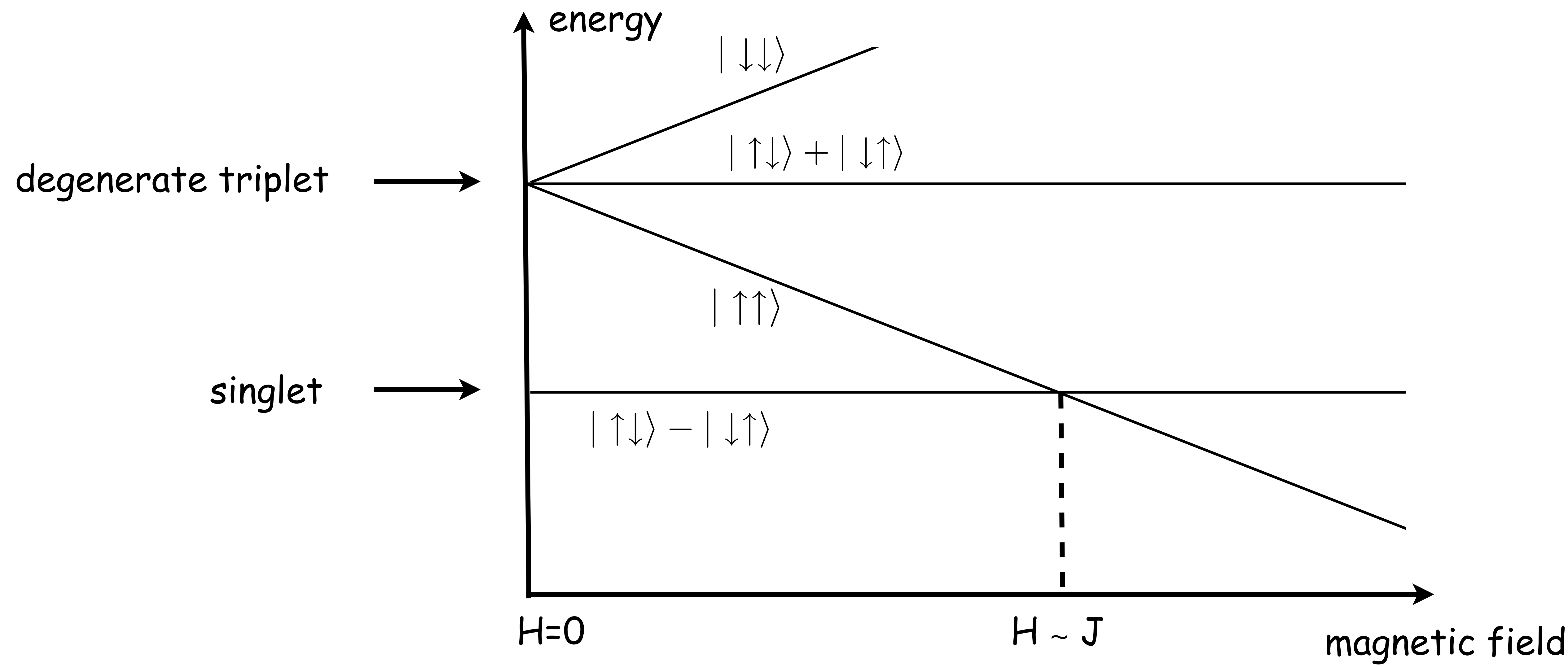
spin-ladder compound $(C_5H_{12}N)_2CuBr_4$

A single dimer in a magnetic field

neglect the inter-dimer interaction:

consider a single dimer in a magnetic field





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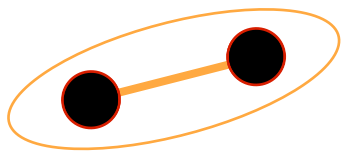
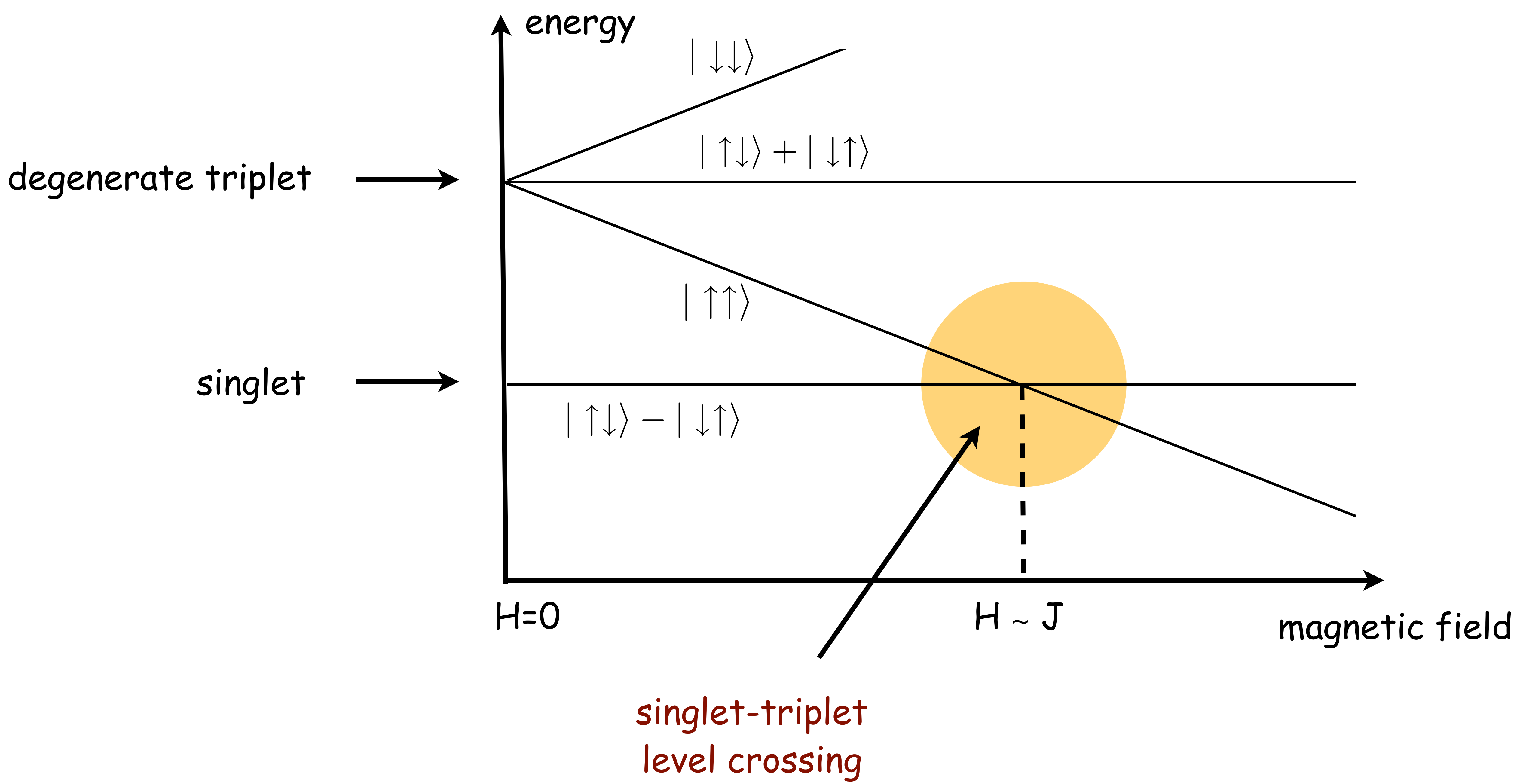
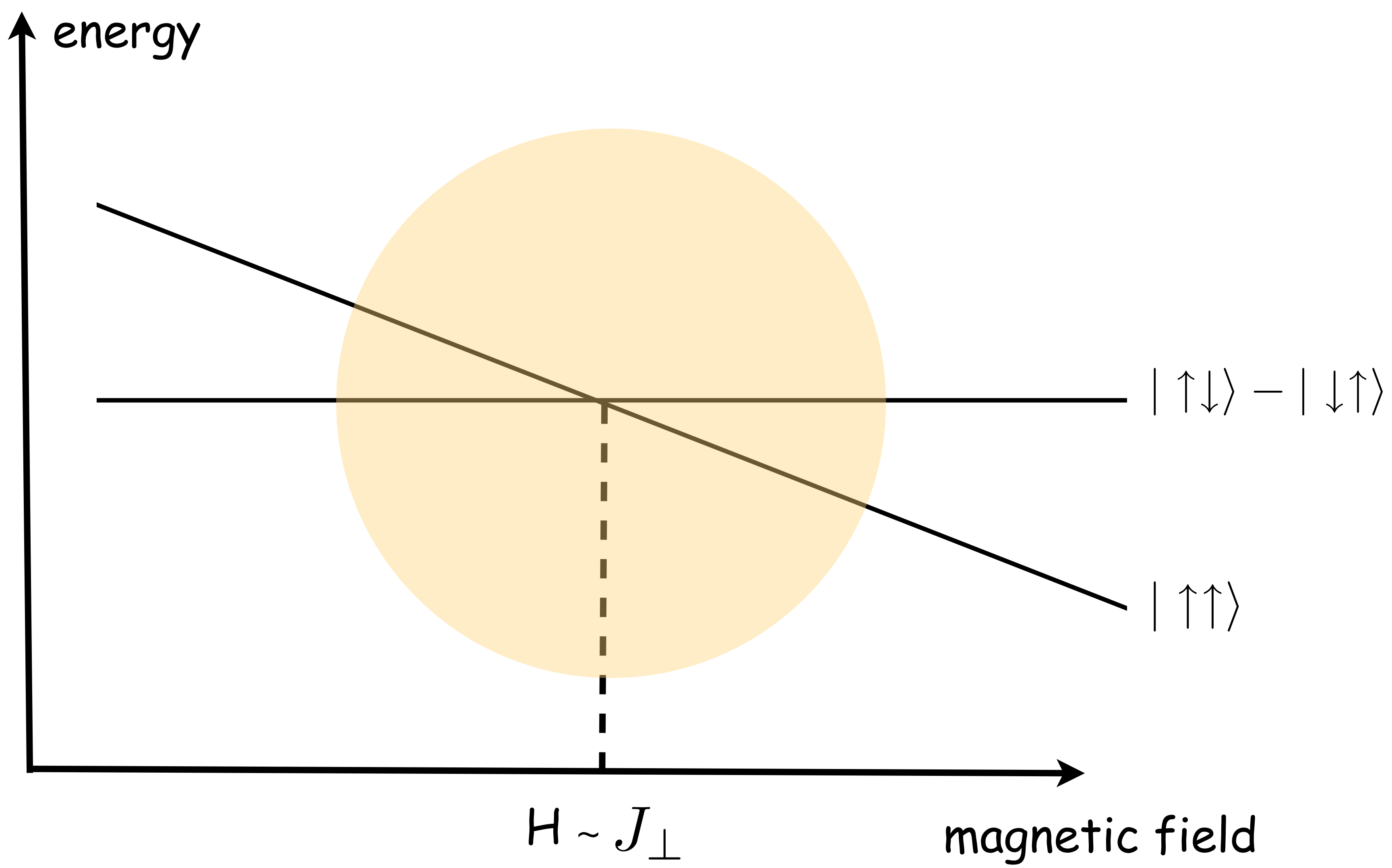




Beyond the single dimer approximation

dimers are weakly coupled by J' ⇨ triplet excitation can hop from dimer to dimer and acquire kinetic energy



Beyond the single dimer approximation

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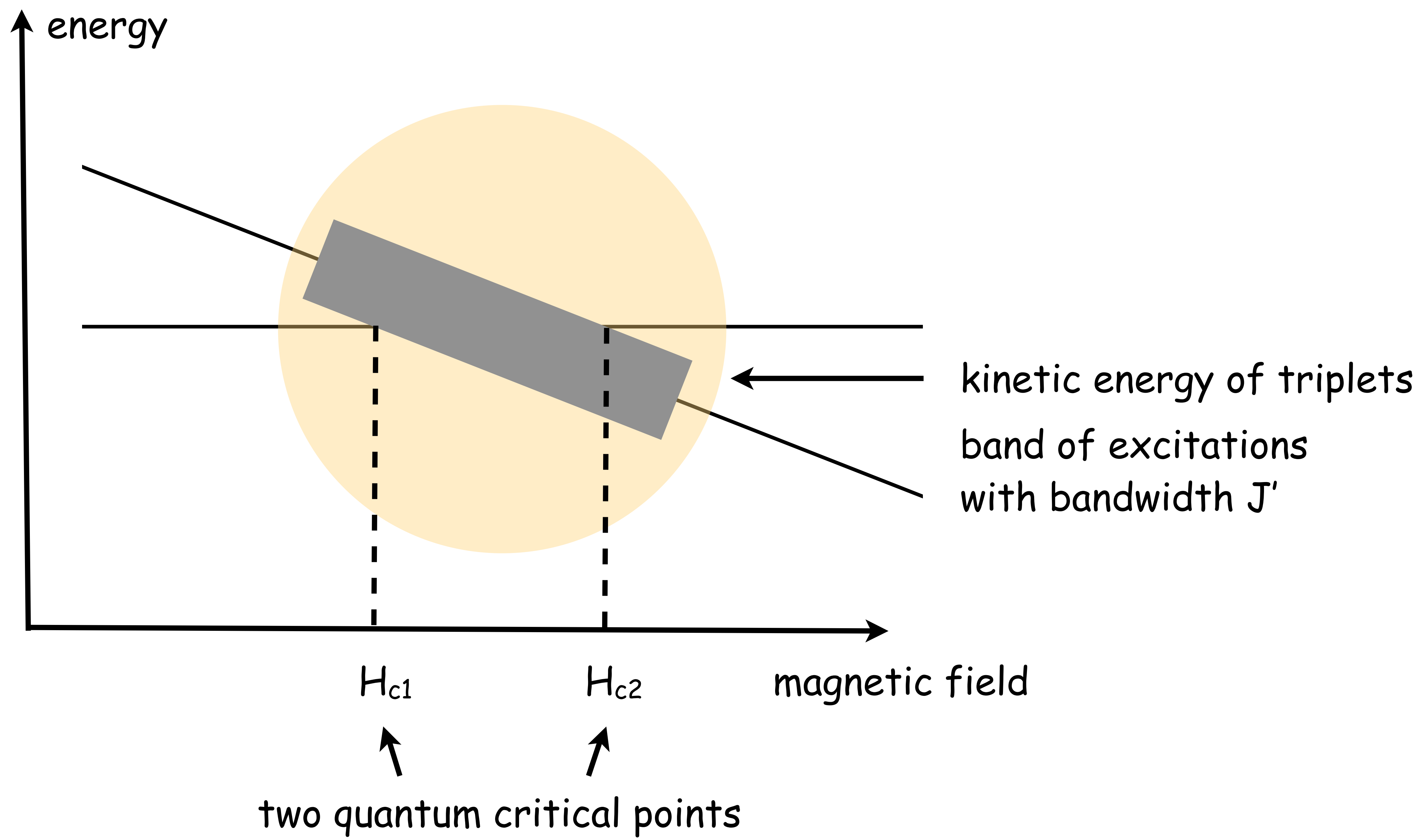
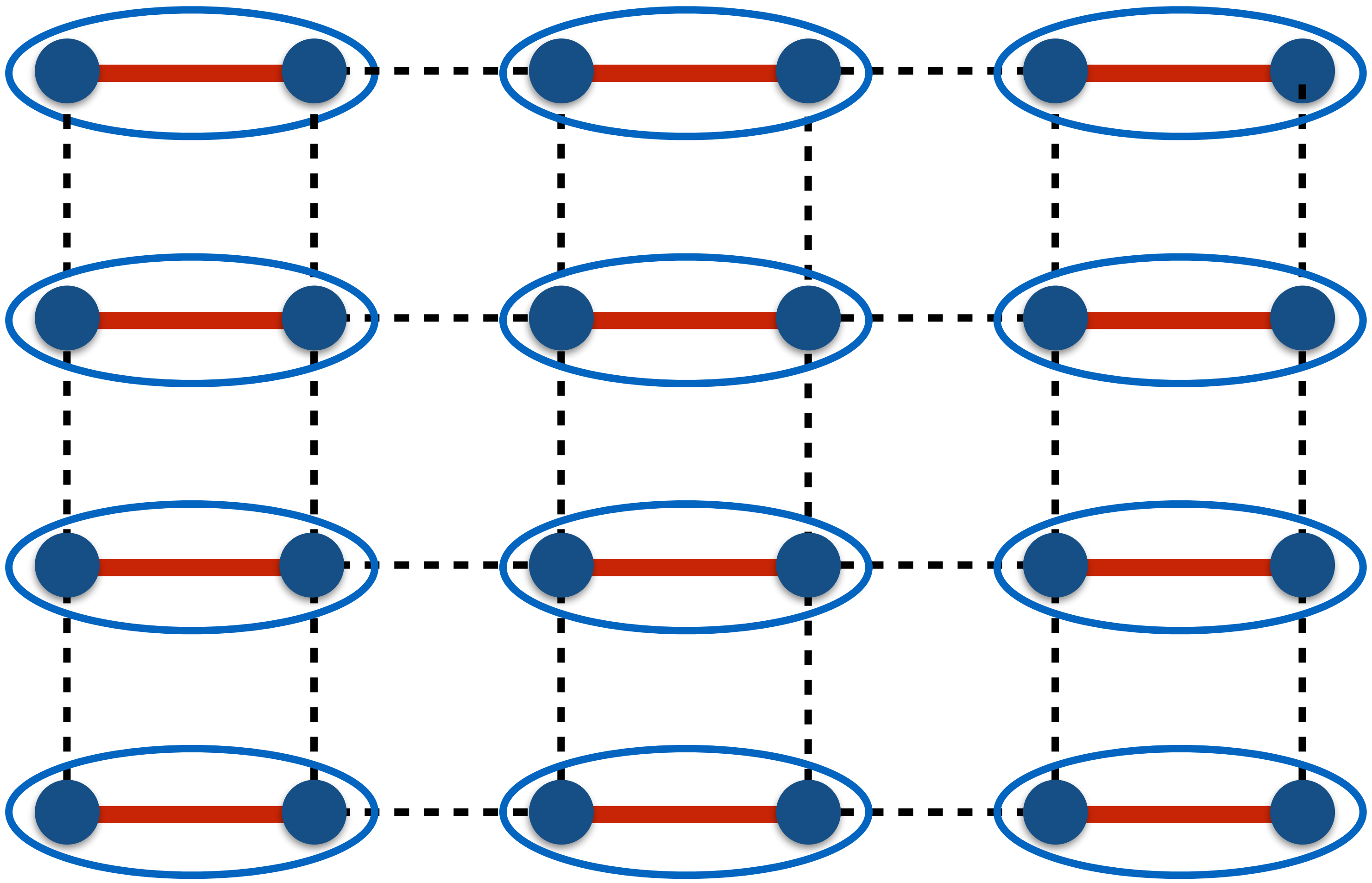


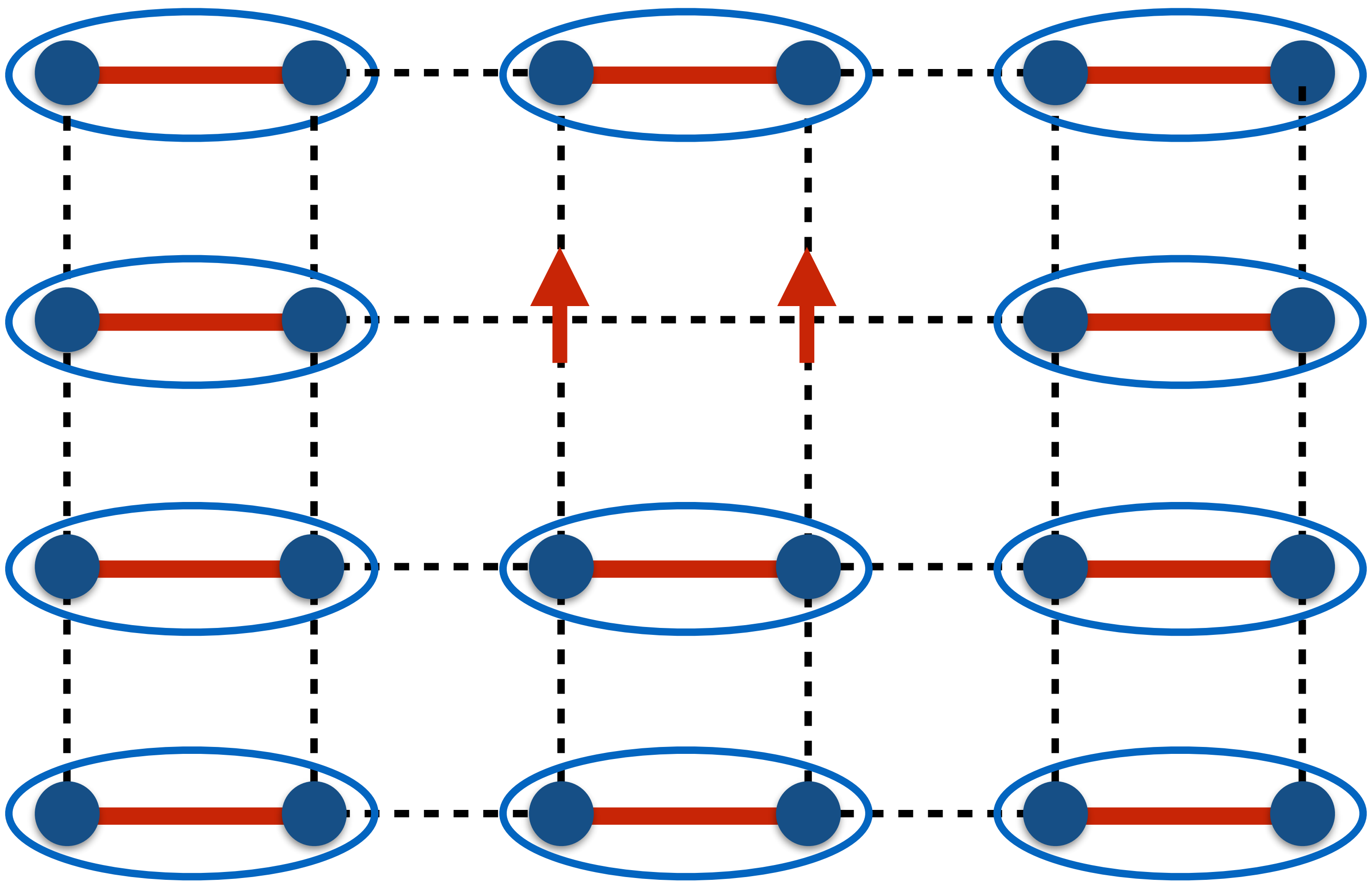
Effective theory for the quantum phase transitions

groundstate for $H < H_{c1}$



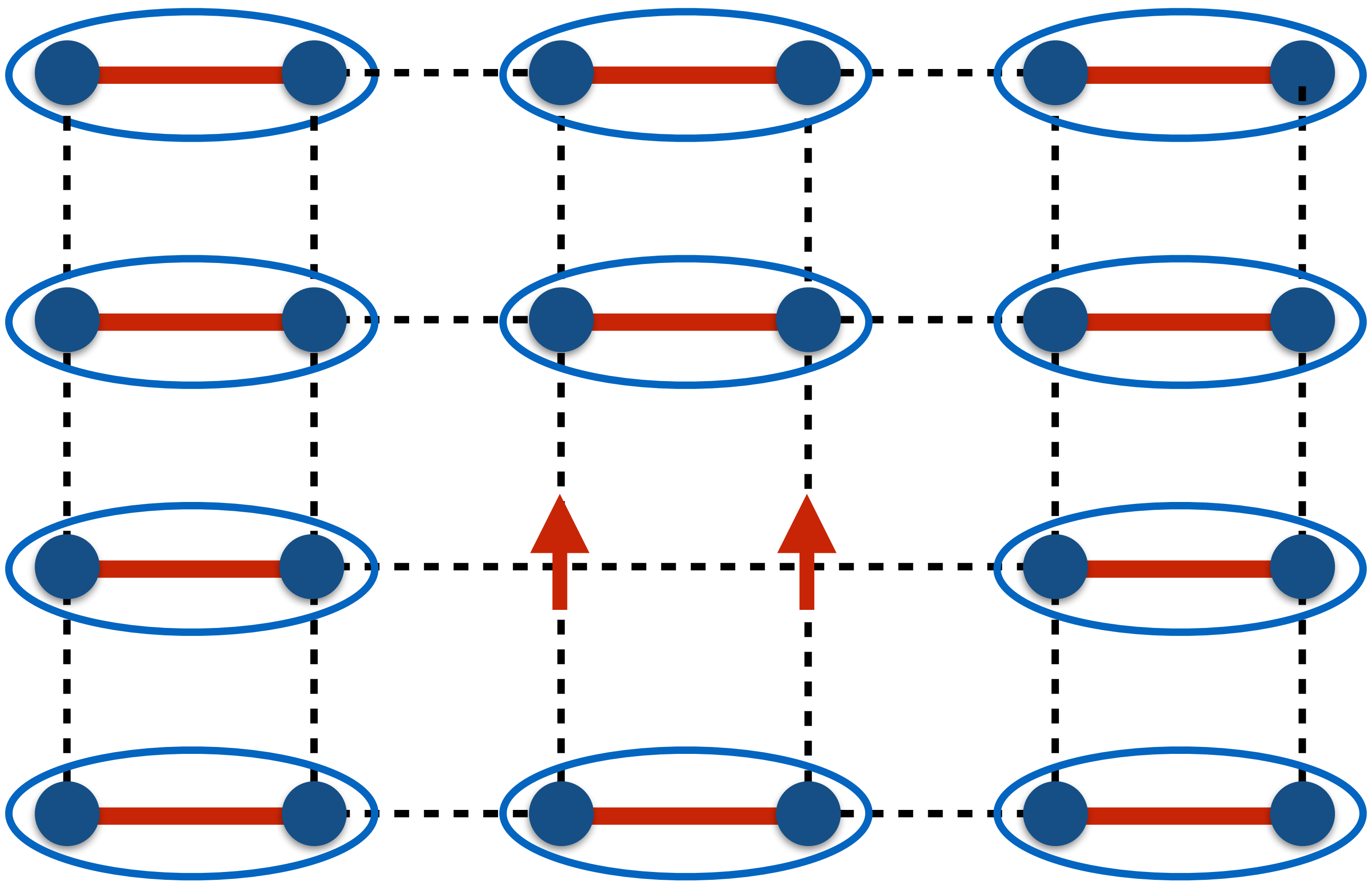
Effective theory for the quantum phase transitions

single triplet excitation



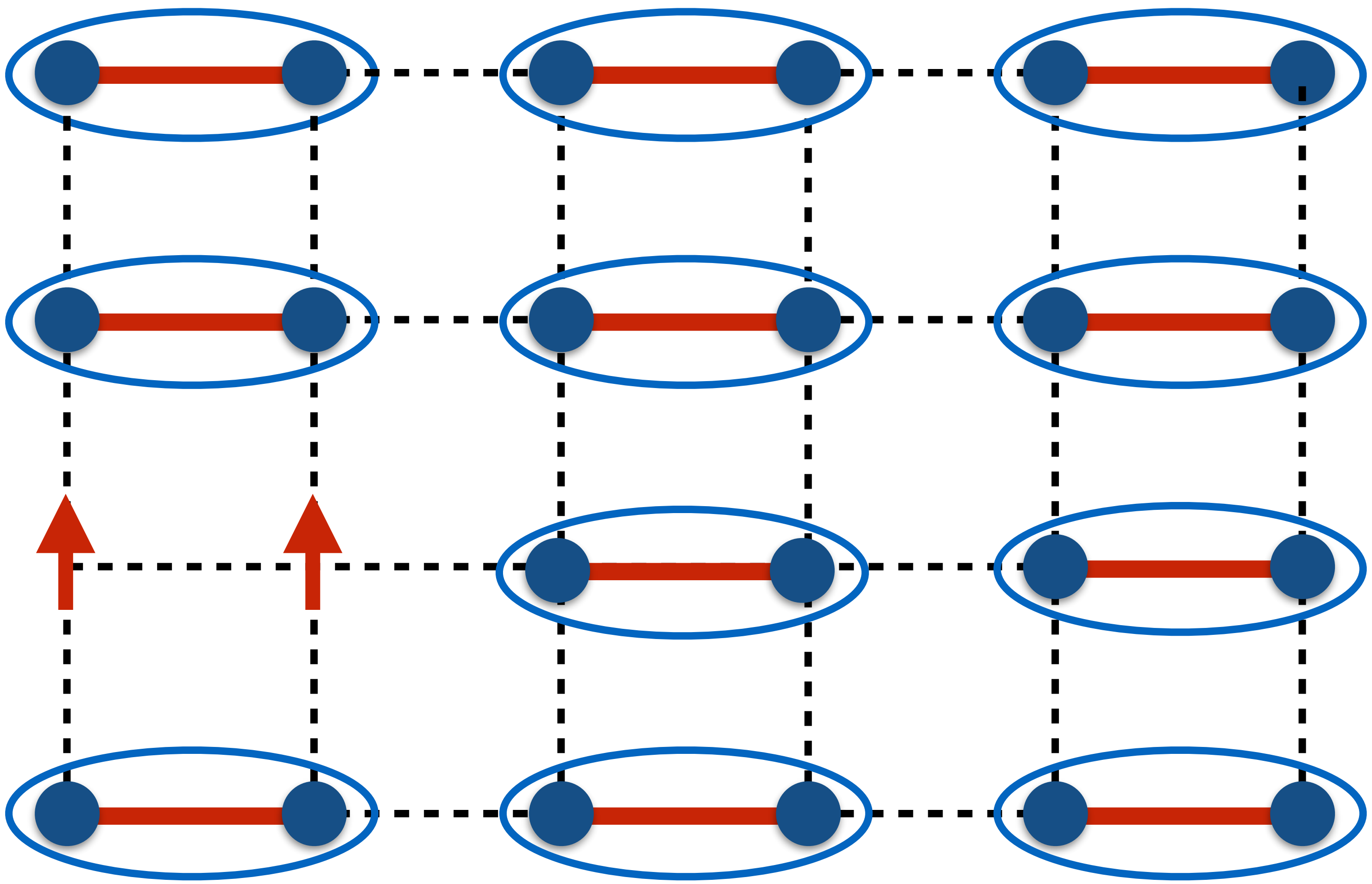
Effective theory for the quantum phase transitions

single triplet excitation



Effective theory for the quantum phase transitions

single triplet excitation

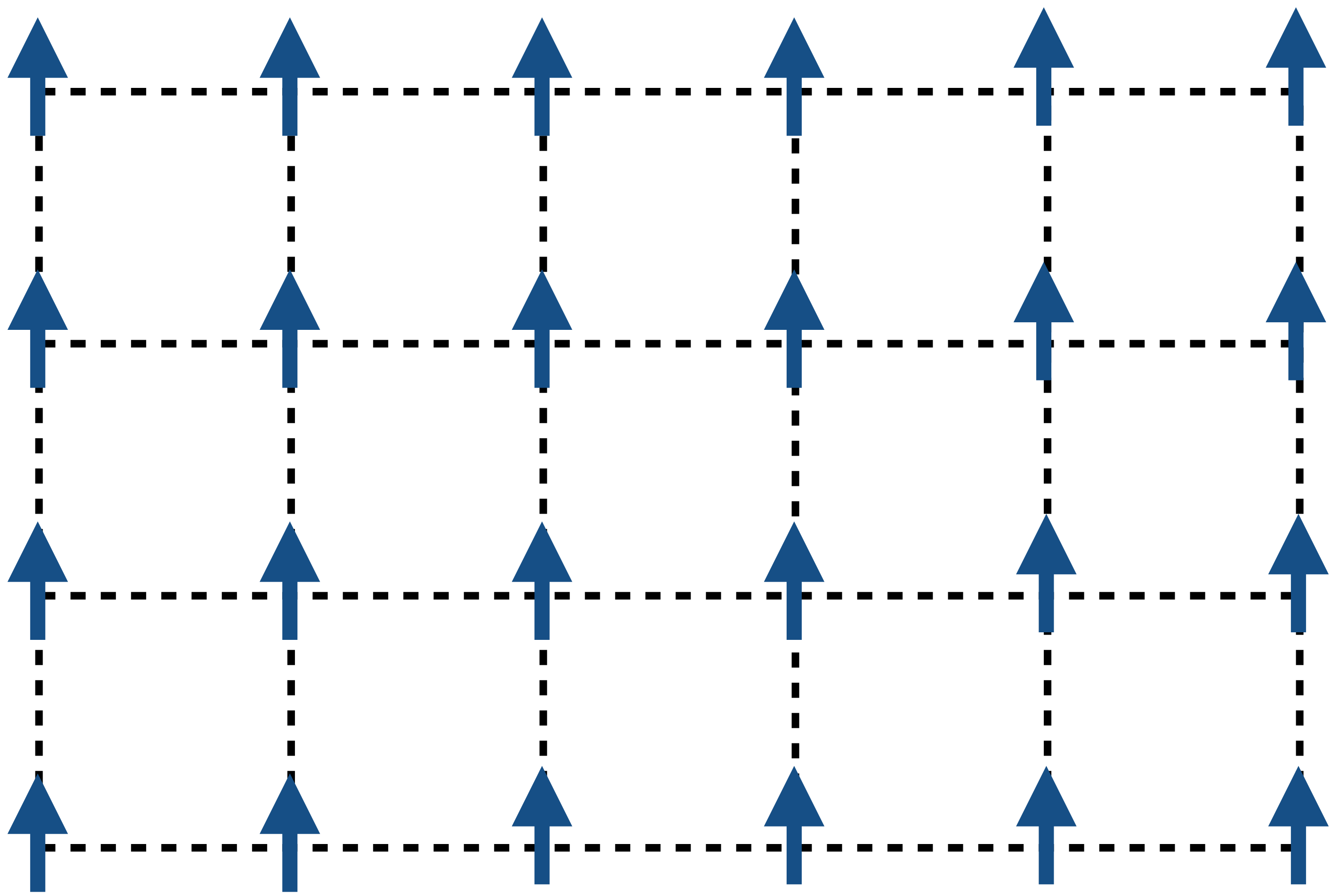


boson with kinetic energy $\frac{p^2}{2m}$ and chemical potential $\mu \propto H - H_{c1}$

⇨ Bose-Einstein condensation of triplons

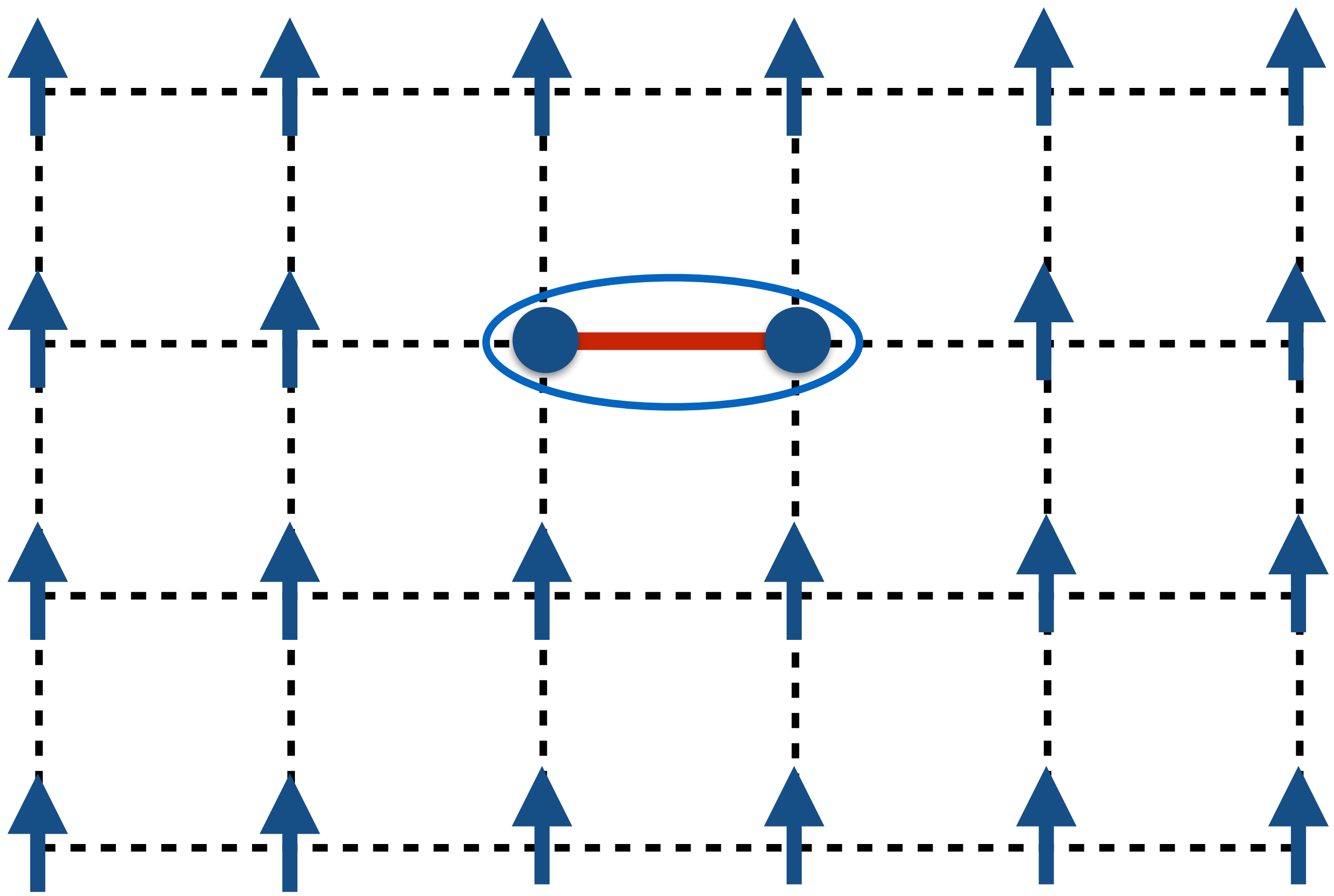
Effective theory for the quantum phase transitions

groundstate for $H > H_{c2}$



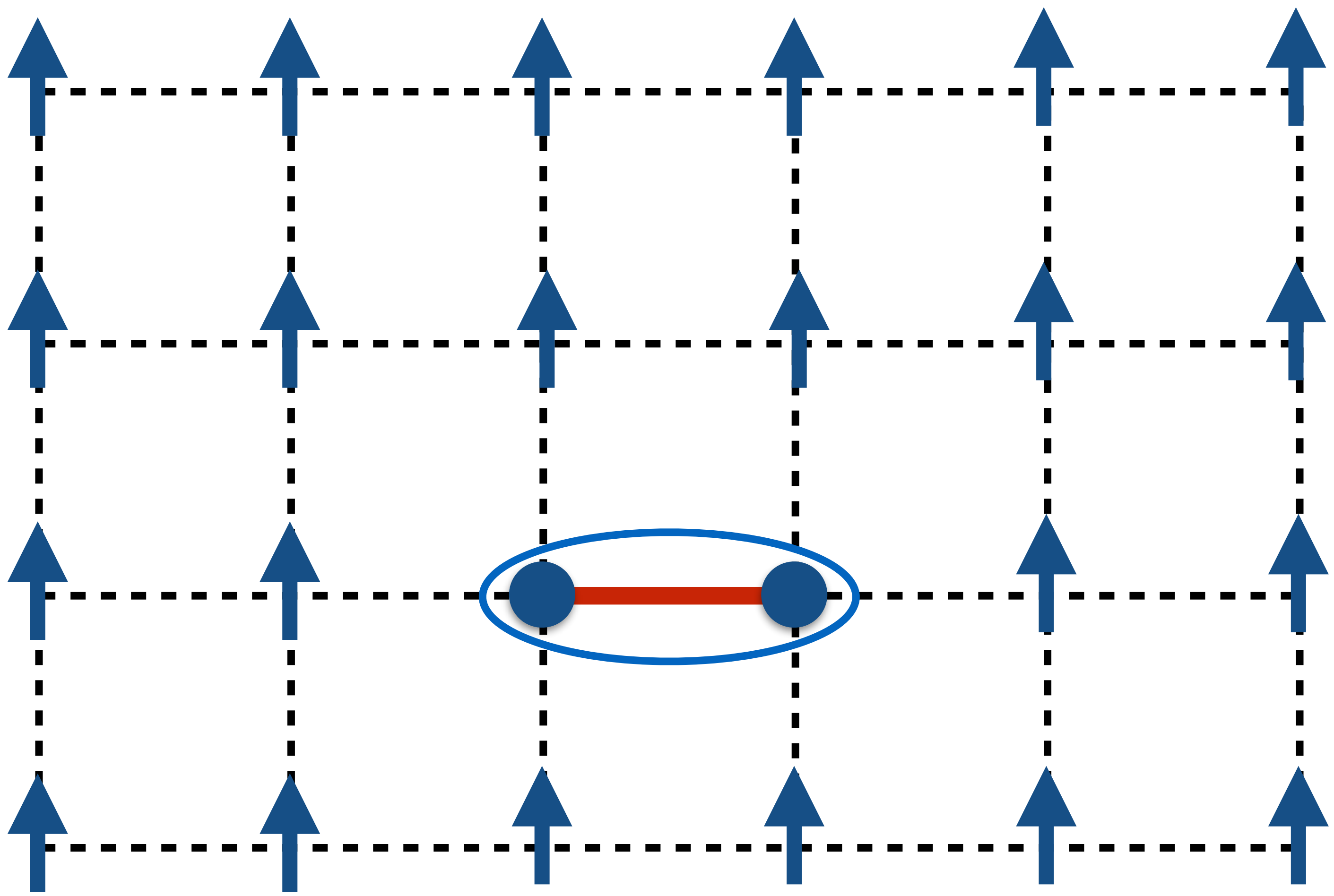
Effective theory for the quantum phase transitions

magnon = spin-flip excitation forming a dimer



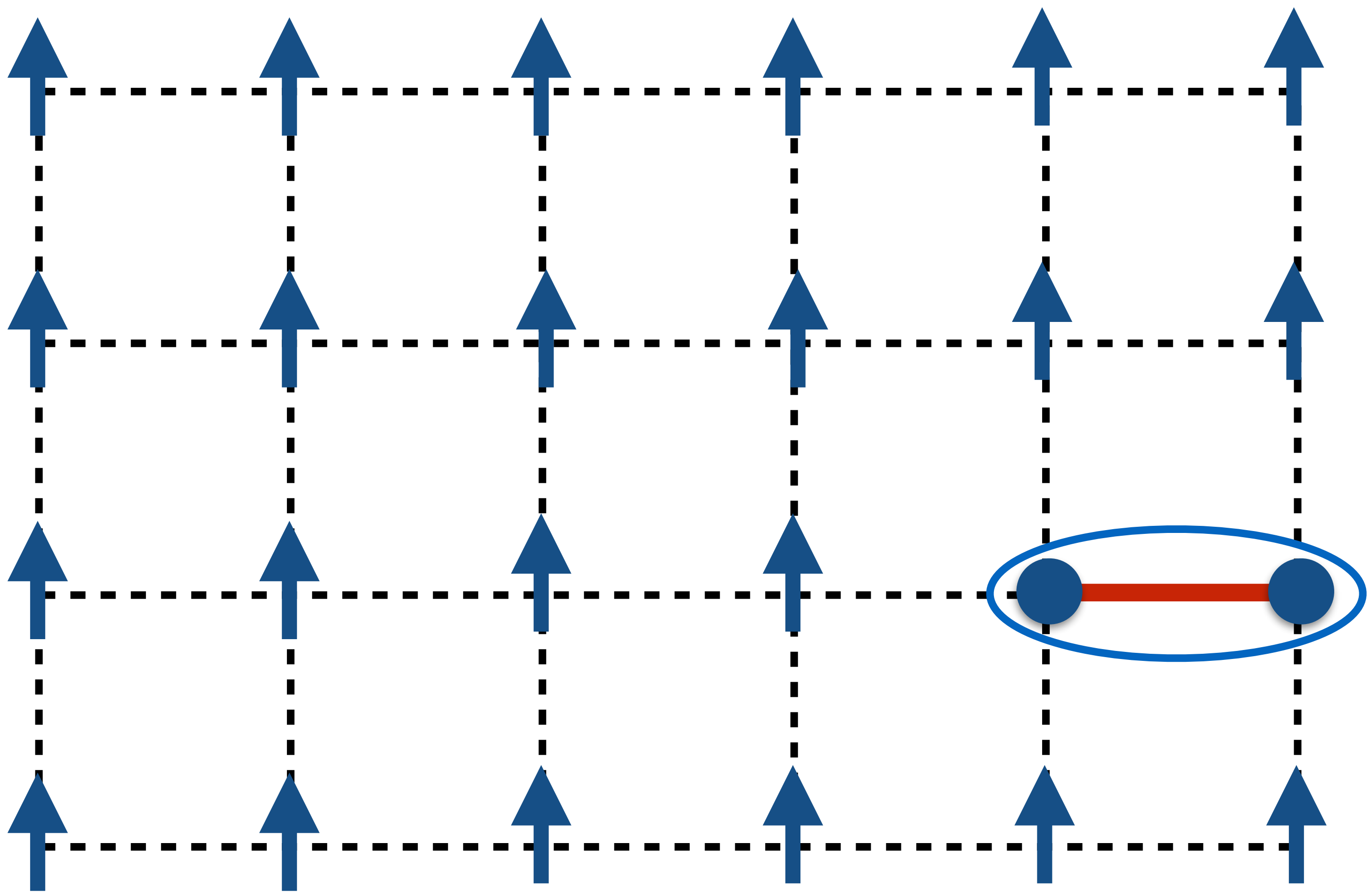
Effective theory for the quantum phase transitions

magnon = spin-flip excitation forming a dimer



Effective theory for the quantum phase transitions

magnon = spin-flip excitation forming a dimer



boson with kinetic energy $\frac{p^2}{2m}$ and chemical potential $\mu \propto H_{c2} - H$

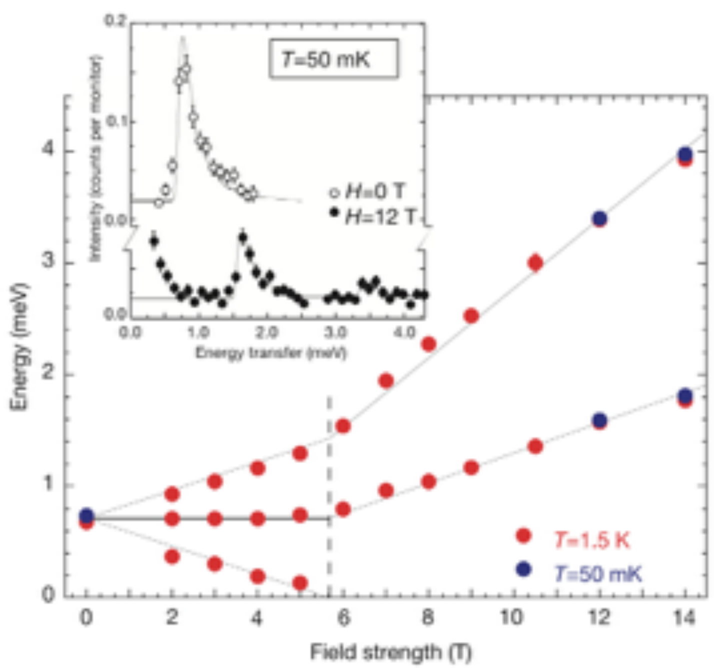
⇨ Bose-Einstein condensation of magnons

Experiments: $TlCuCl_3$

Bose–Einstein condensation of the triplet states in the magnetic insulator $TlCuCl_3$

Ch. Rüegg*, N. Cavadini*, A. Furrer*, H.-U. Güdel†, K. Krämer†, H. Mutka‡, A. Wildes‡, K. Habicht§ & P. Vorderwisch§

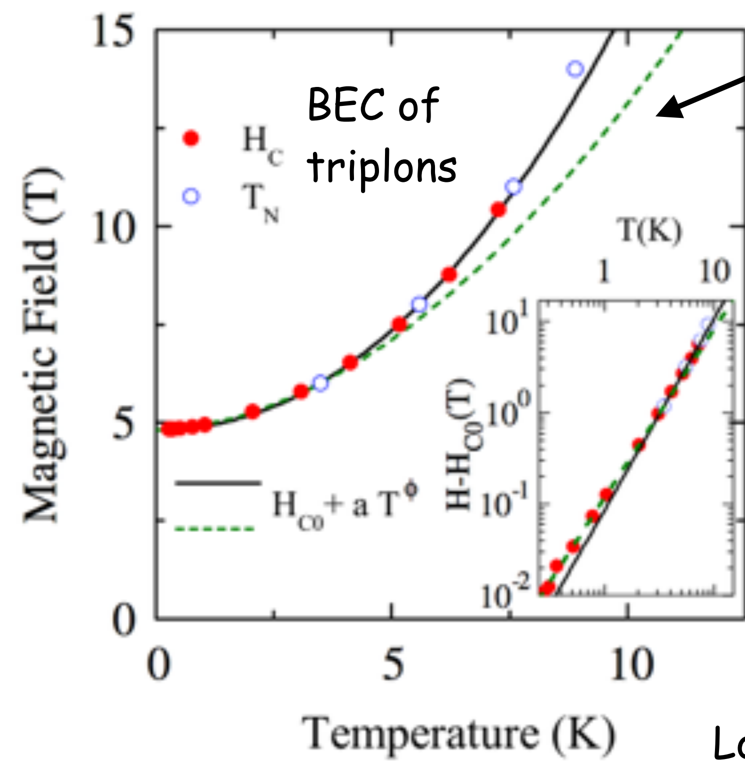
Nature 2003



triplet spectrum obtained by neutron scattering

phase diagram

QPT at ~5 Tesla →

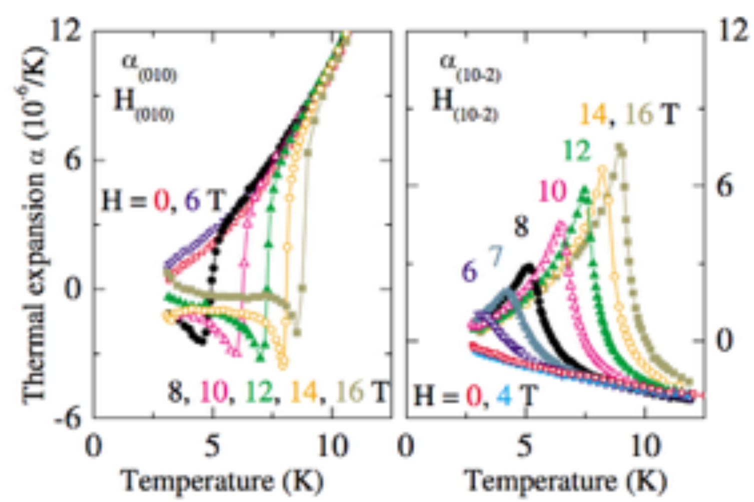


fit to the phase boundary yields $\phi = 1.8$

expected for BEC at lowest T: $\phi = 3/2$

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

Lorenz et al. JMMM (2007)



thermal expansion with characteristic sign changes at the classical transition = entropy accumulation

Johannsen et al. PRL (2005)

Experiments: $Sr_3Cr_2O_8$

Field-induced Bose-Einstein Condensation of triplons up to 8 K in $Sr_3Cr_2O_8$

A. A. Aczel,[1] Y. Kohama,[2] C. Marcenat,[3] F. Weickert,[4] M. Jaime,[2] O. E. Ayala-Valenzuela,[2]
R. D. McDonald,[2] S. D. Selesnic,[1] H. A. Dabkowska,[5] and G. M. Luke[1,5,6]

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[4]*Max Planck Institute for Chemical Physics of Solids, Dresden, Germany*
[5]*Brockhouse Institute for Materials Research, McMaster University, Hamilton, Ontario, Canada, L8S 4M1*
[6]*Canadian Institute of Advanced Research, Toronto, Ontario, Canada, M5G 1Z8*

(Dated: October 26, 2009)

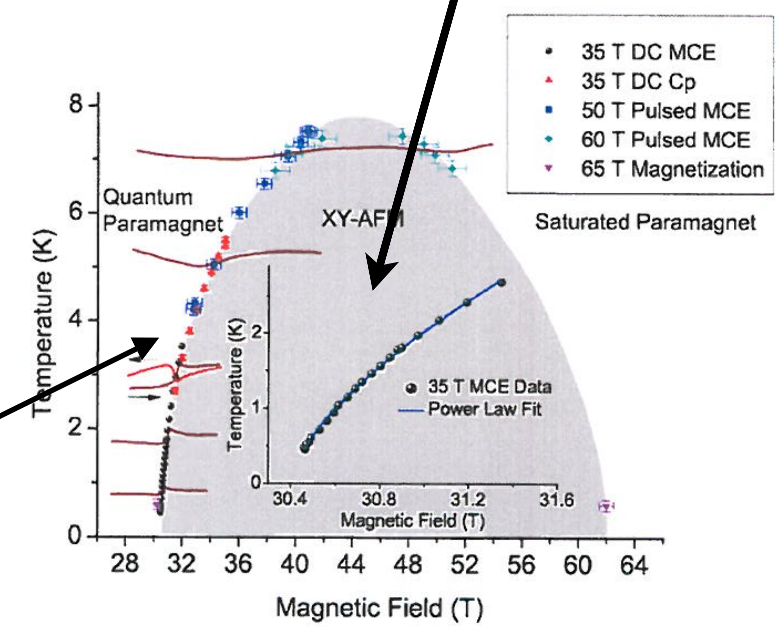
Single crystals of the spin dimer system $Sr_3Cr_2O_8$ have been grown for the first time. Magnetization, heat capacity, and magnetocaloric effect data up to 65 T reveal magnetic order between applied fields of $H_{c1} \sim 30.4$ T and $H_{c2} \sim 62$ T. This field-induced order persists up to $T_c^{max} \sim 8$ K at $H \sim 44$ T, the highest observed in any quantum magnet where H_{c2} is experimentally-accessible. We fit the temperature-field phase diagram boundary close to H_{c1} using the expression $T_c = A(H-H_{c1})^{\nu}$. The exponent $\nu = 0.65(2)$, obtained at temperatures much smaller than T_c^{max}, is that of the 3D Bose-Einstein condensate (BEC) universality class. This finding strongly suggests that $Sr_3Cr_2O_8$ is a new realization of a triplon BEC where the universal regimes corresponding to both H_{c1} and H_{c2} are accessible at ^{4}He temperatures.

PACS numbers: 73.43.Nq, 75.30.Kz, 75.30.Sg, 75.40.Cx

PRL 2009

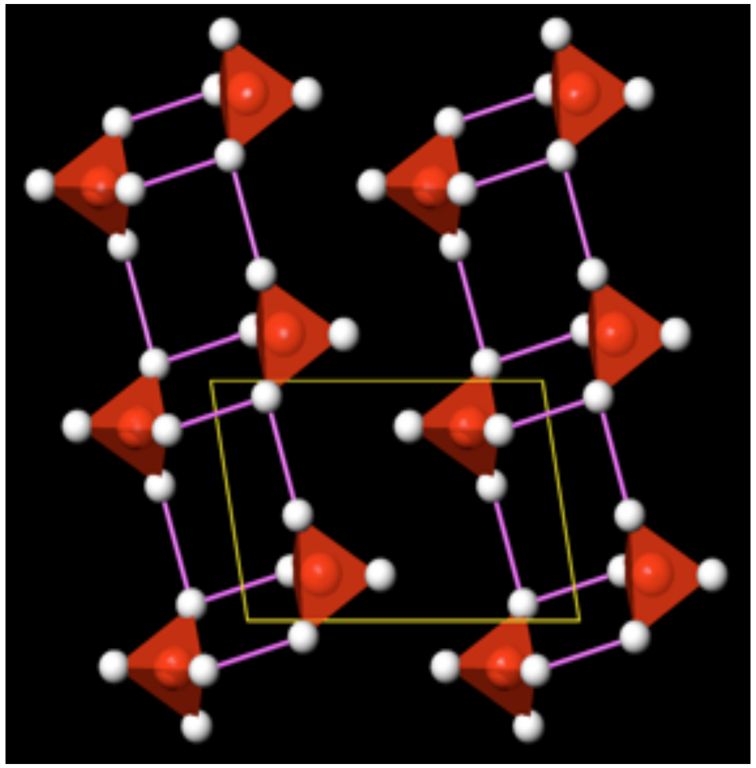
$$T_c \sim \left(\frac{\mu}{u}\right)^{2/3}$$

magnetic long-range order (XY-AFM)



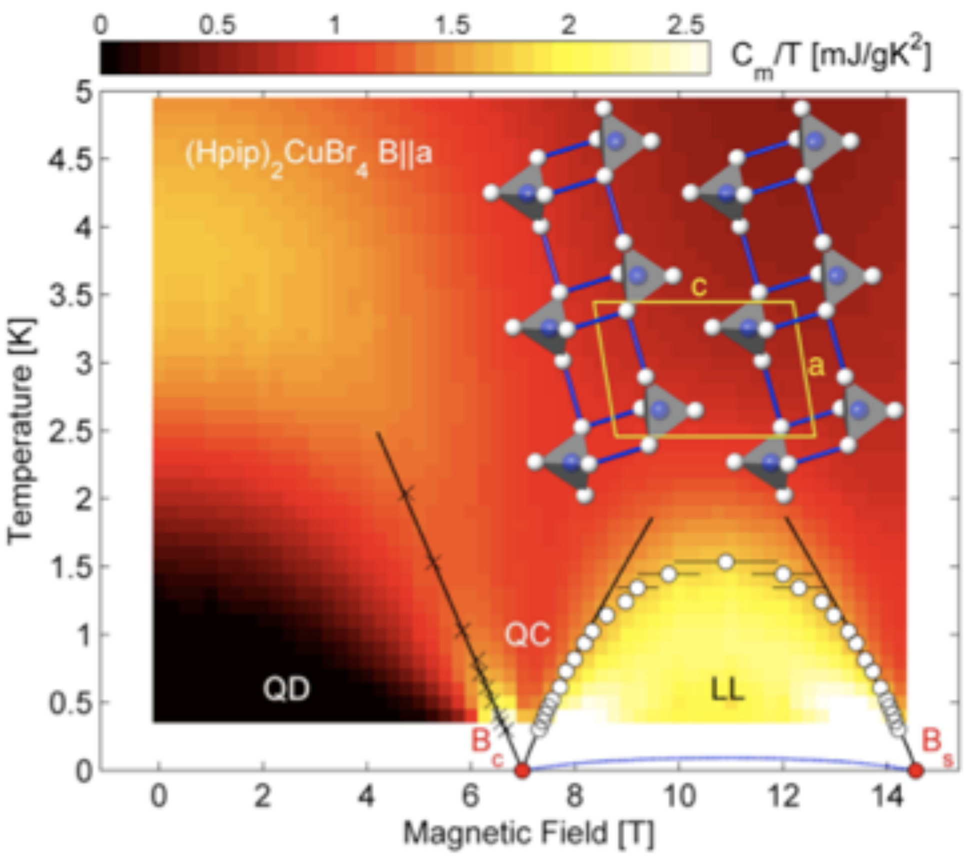
two quantum critical points

Experiments: spin-ladder compound $(C_5H_{12}N)_2CuBr_4$



Patyal et al. (1990)
Watson et al. (2001)
Lorenz et al (2008)
Anfuso et al (2008)
Klanjsek et al. (2008)
Thielemann et al. (2008)
Rüegg et al. (2008)
Bouillot et al (2011)

Phase diagram:



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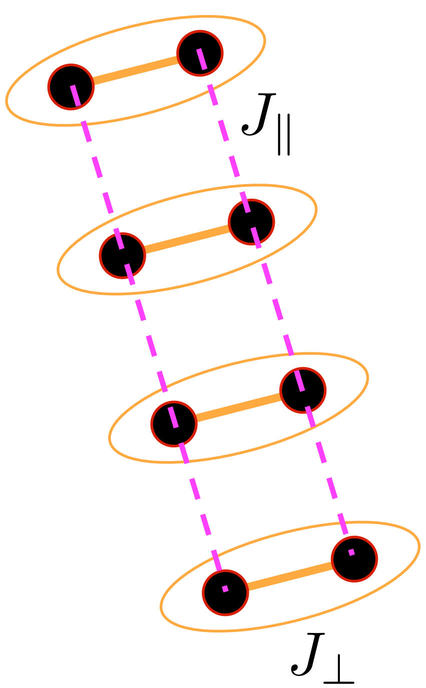


$CuBr_4$ cluster

spin-1/2 ladder

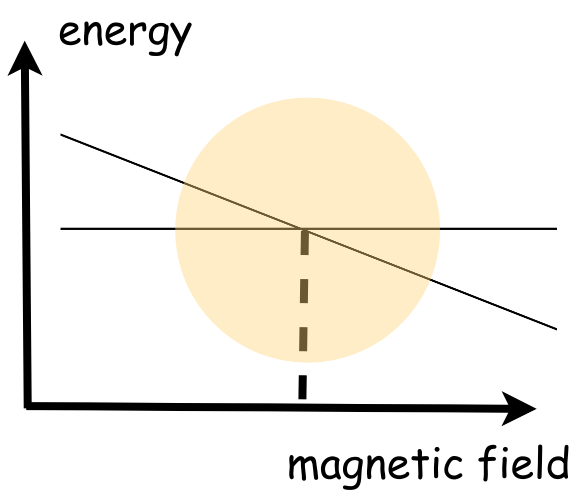
strong rung coupling $J_\perp/k_B = 12.9$ Kelvin

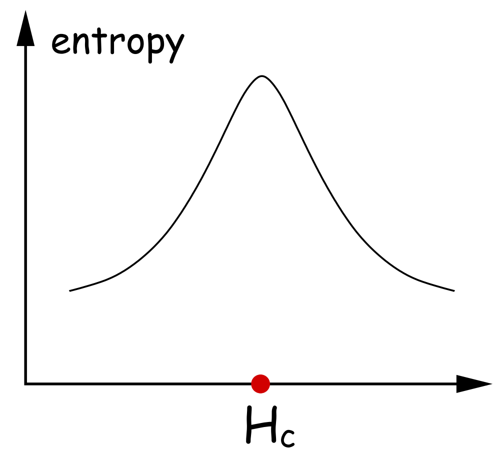
leg coupling $J_\parallel/k_B = 3.6$ Kelvin

Dimensional crossover from 0d to 1d:

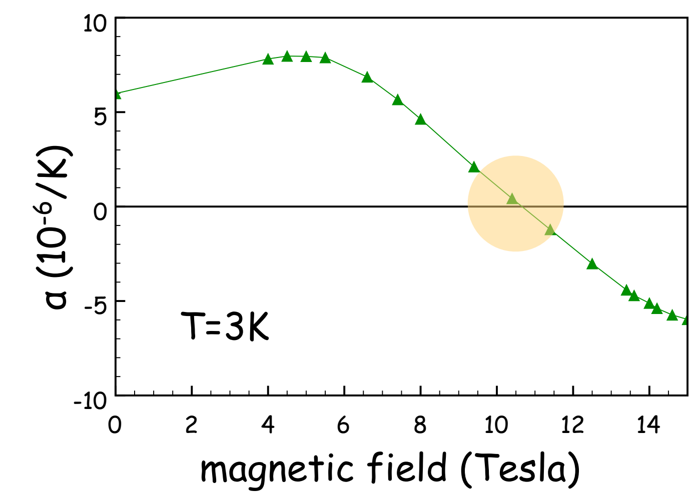
high temperatures

triplet bandwidth
not resolved
-> single entropy peak





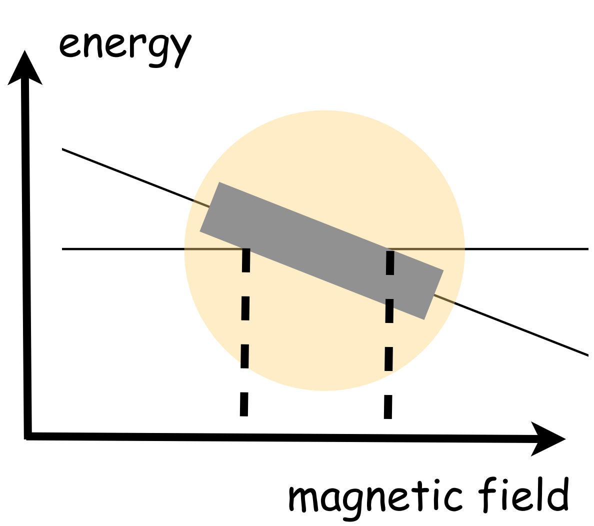
thermal expansion

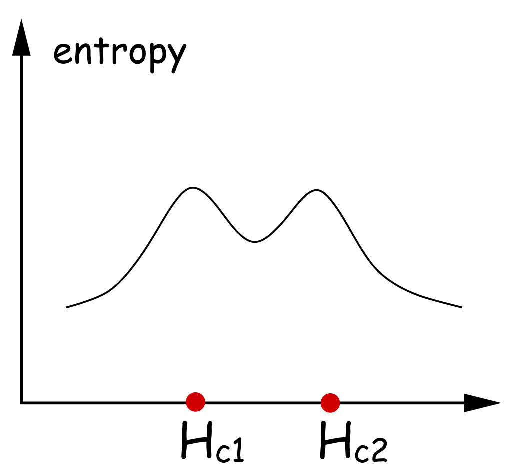


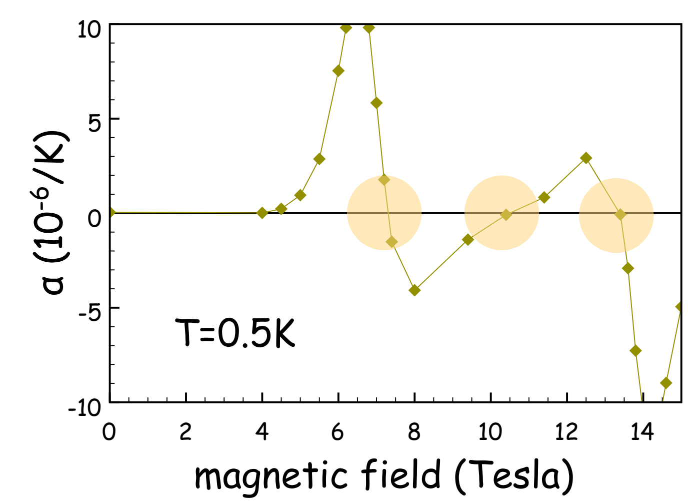
low temperatures

splitting of
entropy peak

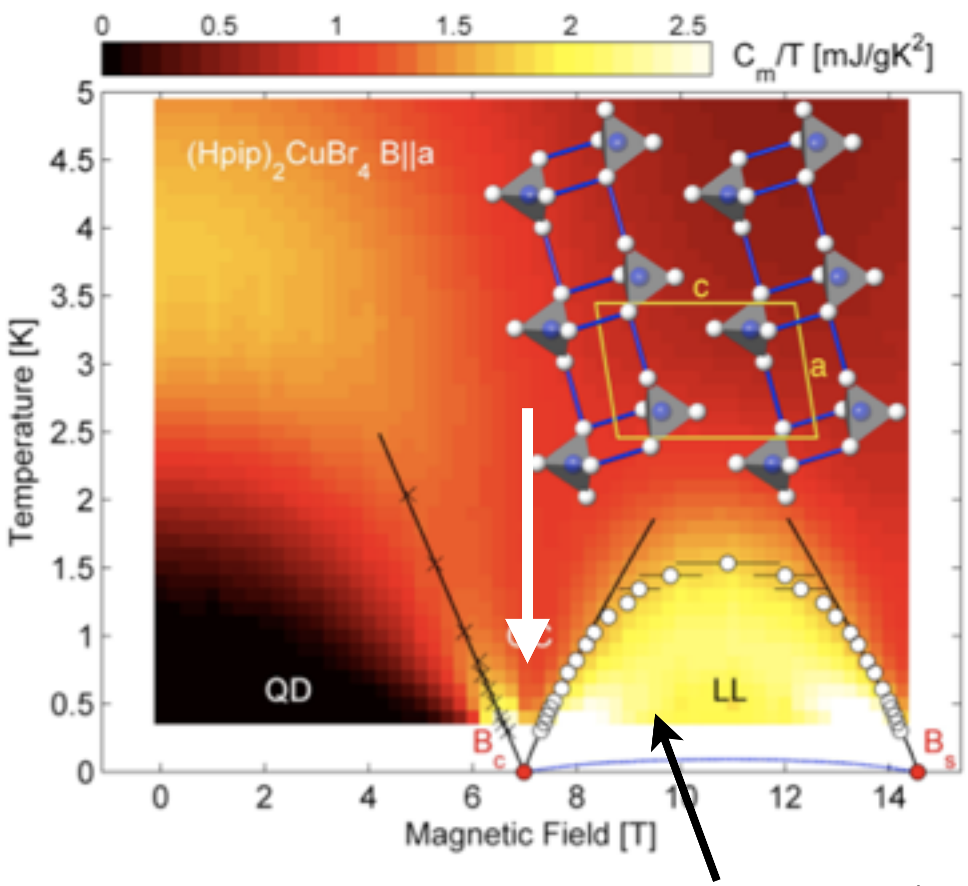
three sign
changes





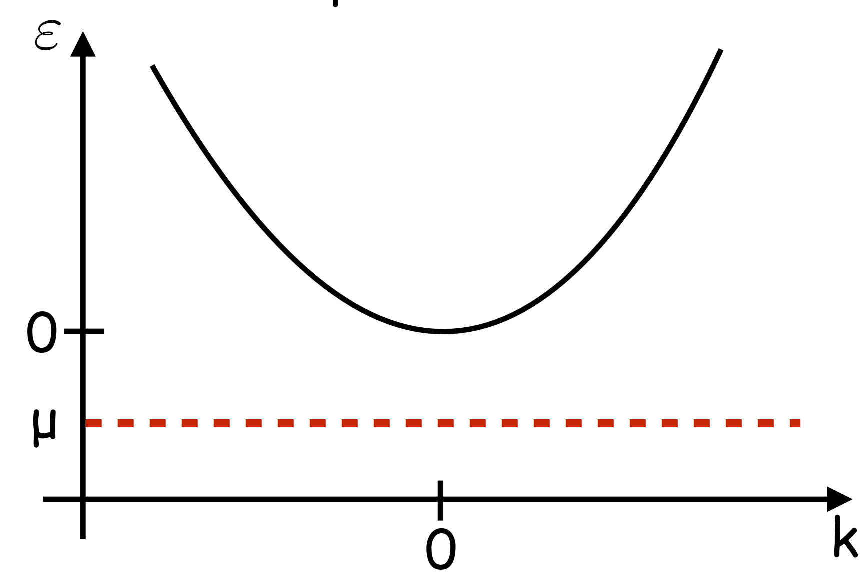


Lifshitz transition and singular thermal expansion



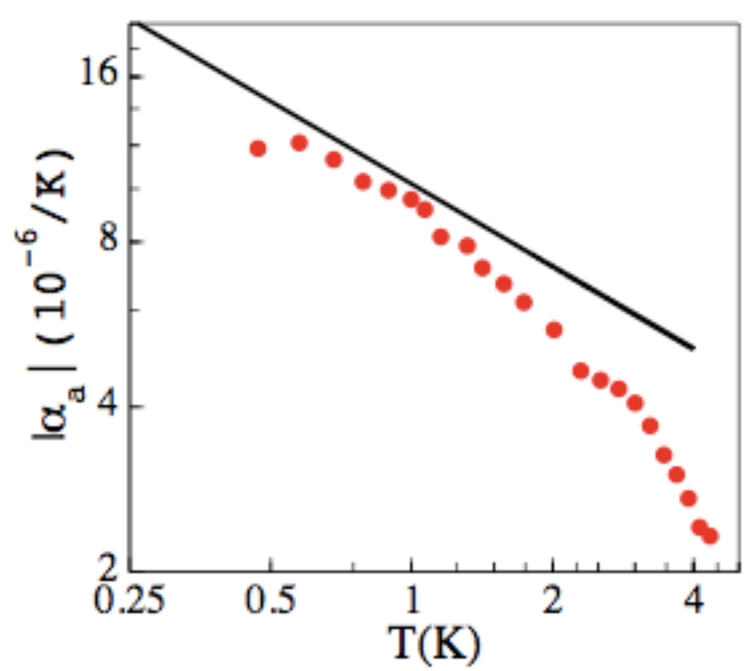
Lifshitz transition:

fermions at the bottom of a parabolic band



➡ divergent thermal expansion at the quantum critical points

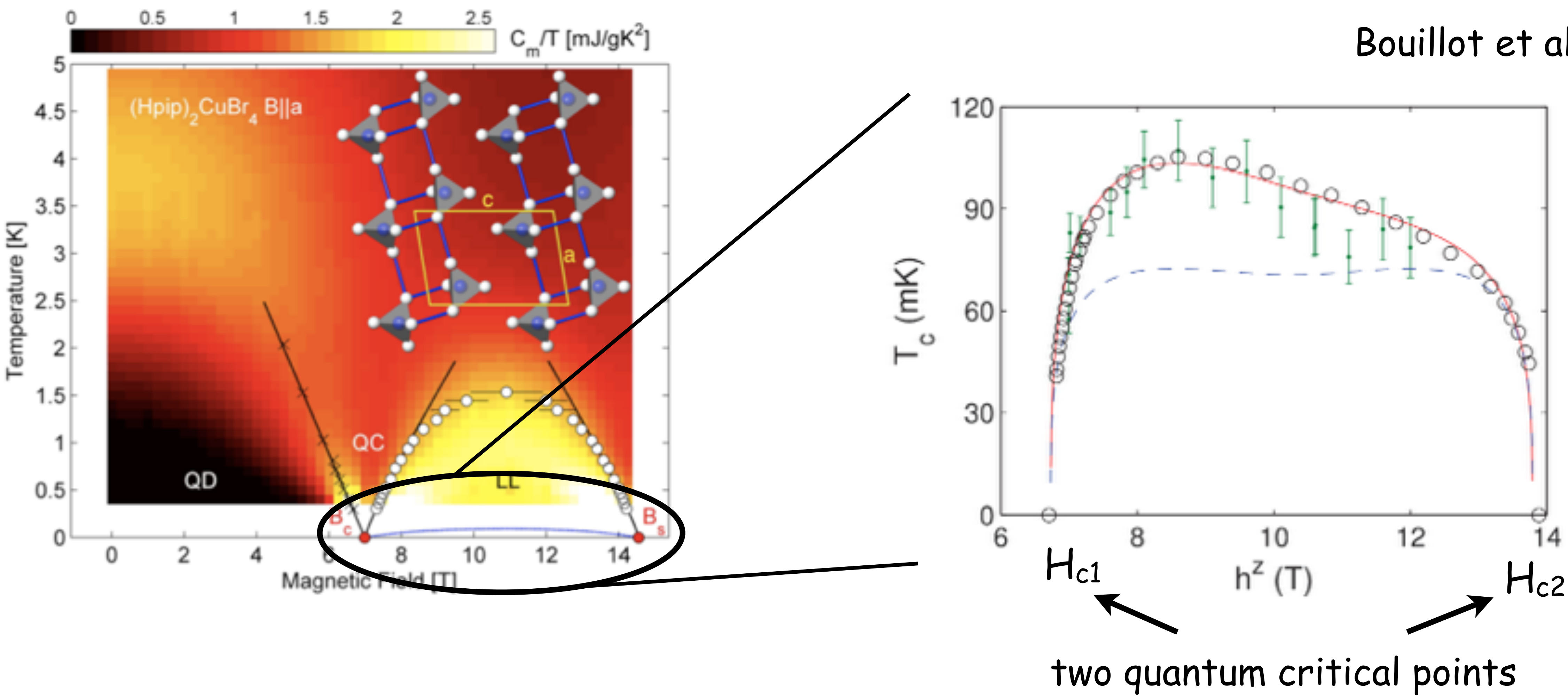
$$\alpha \sim \frac{1}{\sqrt{T}}$$



Anfuso et al. PRB (2008)

Dimensional crossover from 1d to 3d

Bouillot et al. PRB (2011)



Weak coupling between the spin ladders becomes important at lowest energies

⇨ Bose-Einstein condensation of magnons and development of long-range magnetic order at finite $T_c \sim 100$ mK

General theme common in physics:
Hierarchy of energy scales and corresponding effective theoretical description

1d Heisenberg model in a field

1d Heisenberg model in a magnetic field

Heisenberg Hamiltonian

$$H = J \sum_i \vec{S}_i \vec{S}_{i+1} + h \sum_i S^z_i$$

Jordan-Wigner transformation

$$S^+_i = S^x_i + i S^y_i = c^\dagger_i e^{i\pi \sum_{j<i} c^\dagger_j c_j}$$

$$S^-_i = S^x_i - i S^y_i = c_i e^{-i\pi \sum_{j<i} c^\dagger_j c_j}$$

Jordan-Wigner string

$$S^z_i = c^\dagger_i c_i - \frac{1}{2}$$

fermionic operators

$$\Rightarrow \quad H = \sum_i \Big(J (c^\dagger_i c_{i+1} + (c^\dagger_i c_i - \frac{1}{2})(c^\dagger_{i+1} c_{i+1} - \frac{1}{2})) + h (c^\dagger_i c_i - \frac{1}{2})$$

string cancels out in the Hamiltonian

Conserves fermionic particle number $\Leftrightarrow$ spin-rotation symmetry around the magnetic field z-axis

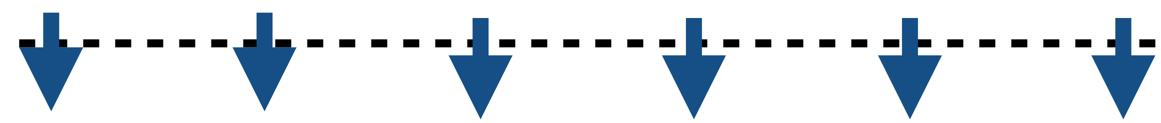
1d Heisenberg model in a magnetic field

$$H = \sum_i \left(J(c_i^\dagger c_{i+1} + (c_i^\dagger c_i - \frac{1}{2})(c_{i+1}^\dagger c_{i+1} - \frac{1}{2})) + h(c_i^\dagger c_i - \frac{1}{2}\right)$$

penalizes the presence of particles

ground state for large fields h >> J:

vacuum $|0\rangle$ with no particles = fully polarised spin chain



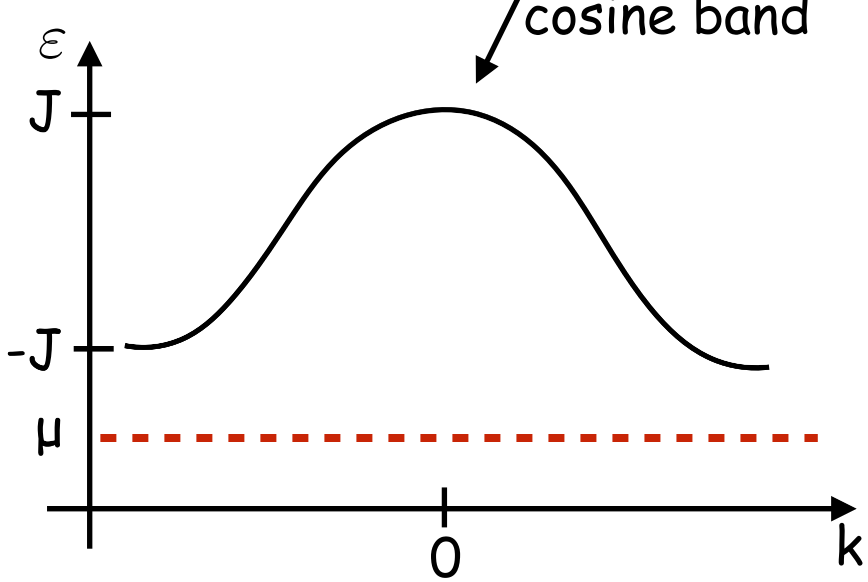
effective Hamiltonian in the dilute limit

$$H_{\text{eff}} = \sum_i \left(J c_i^\dagger c_{i+1} + (h - J) c_i^\dagger c_i \right) + H_{\text{int}}$$

residual interaction can be neglected in the dilute, low-energy limit, Pauli principle!

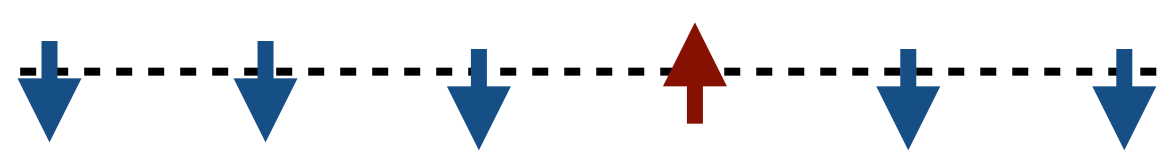
chemical potential μ = J-h

cosine band



Lifshitz transition at $h_c = 2J$

"condensation" of spin-flips



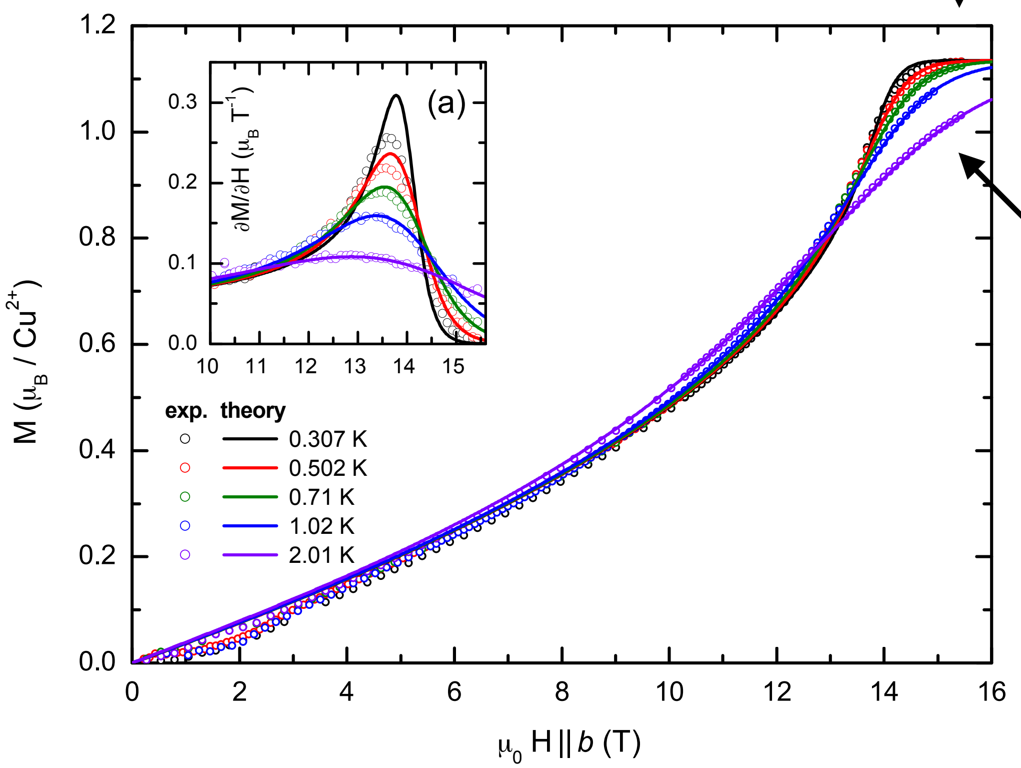
Experiments

remember:

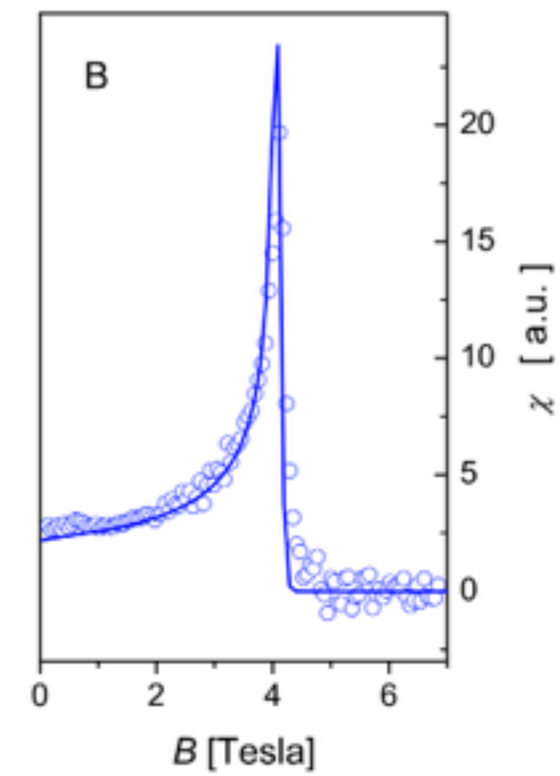
$$F \sim T^{3/2}\Psi\left(\frac{\mu}{T}\right)$$

fully polarised, perfect vacuum magnetization plateau!

$\frac{1}{\sqrt{H-H_c}}$ divergence of the susceptibility reflecting 1d DOS



develops a sharp kink ~ $\sqrt{H-H_c}$



Copper pyrazine dinitrate CuPzN

Breunig et al. (unpublished)

copper-containing coordination polymer
[Cu(μ-C2O4)(4-aminopyridine)2(H2O)]n

Wolf et al, PNAS (2011)

1d Ising model in a transverse field

1d Ising model in a transverse field

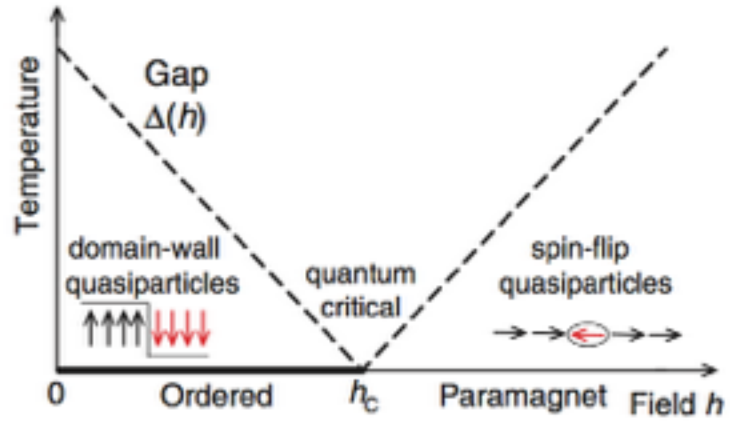
Heisenberg Hamiltonian

$$H = J\sum_i S_i^x S_{i+1}^x - h\sum_i S_i^z$$

Jordan-Wigner transformation

$$S_i^+ = S_i^x + iS_i^y = c_i^\dagger e^{i\pi\sum_{j<i} c_j^\dagger c_j} \qquad S_i^z = c_i^\dagger c_i - \frac{1}{2}$$

$$S_i^- = S_i^x - iS_i^y = c_i e^{-i\pi\sum_{j<i} c_j^\dagger c_j}$$



$$\Rightarrow \quad H = \frac{J}{4}\sum_i (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) - h\sum_i (c_i^\dagger c_i - \frac{1}{2})$$

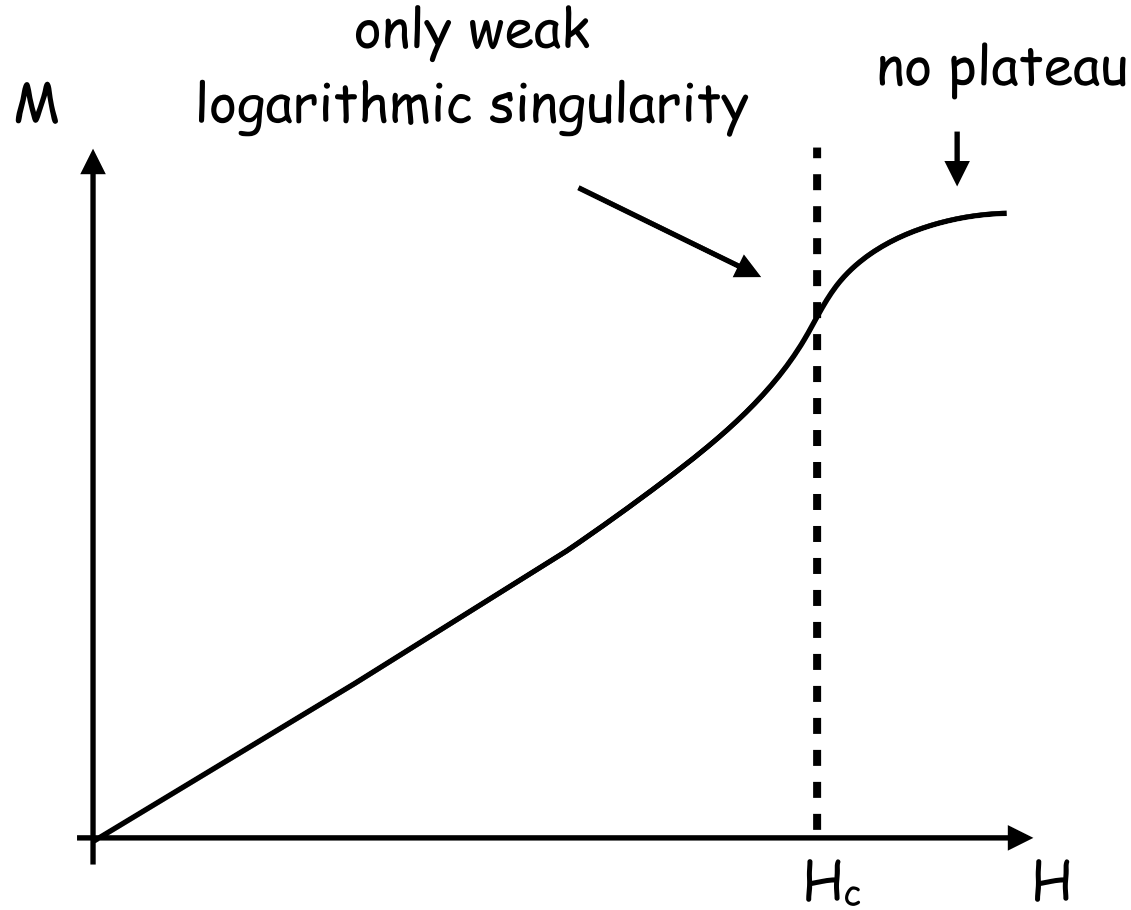
$$= \frac{J}{4}\sum_i (c_i^\dagger c_{i+1}^\dagger - c_i c_{i+1} + c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger) - h\sum_i (c_i^\dagger c_i - \frac{1}{2})$$

anomalous terms

fermionic particle number not conserved ⟺ spin-rotation symmetry broken

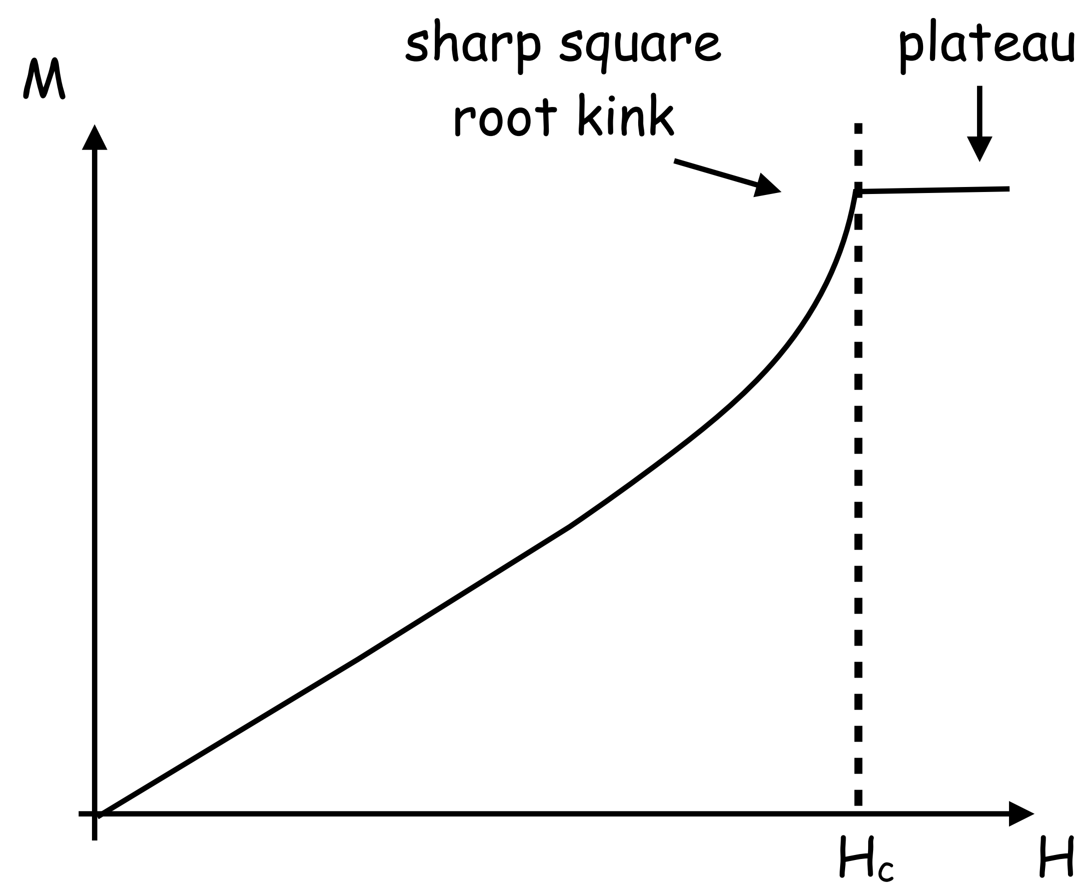
Comparison: magnetization curves

1d Ising model in a transverse field



Ising quantum phase transition

1d Heisenberg model in a magnetic field



Lifshitz quantum phase transition

Experiments: $CoNb_2O_6$

Cobalt niobate approximately realizes the Ising chain in a transverse field

BUT: in addition small longitudinal field h_x probably due to interchange coupling

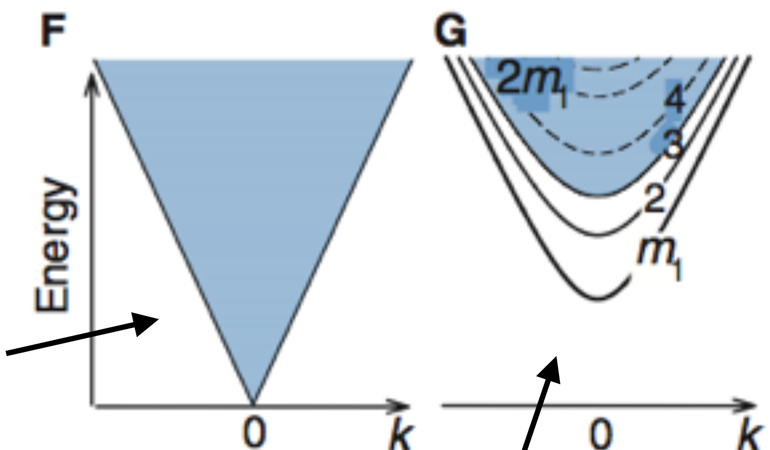
$$H = J \sum_i S_i^x S_{i+1}^x - h_z \sum_i S_i^z - h_x \sum_i S_i^z$$

Quantum Criticality in an Ising Chain: Experimental Evidence for Emergent E_8 Symmetry

R. Coldea,[1*] D. A. Tennant,[2] E. M. Wheeler,[1†] E. Wawrzynska,[3] D. Prabhakaran,[1] M. Telling,[4] K. Habicht,[2] P. Smeibidl,[2] K. Kiefer[2]

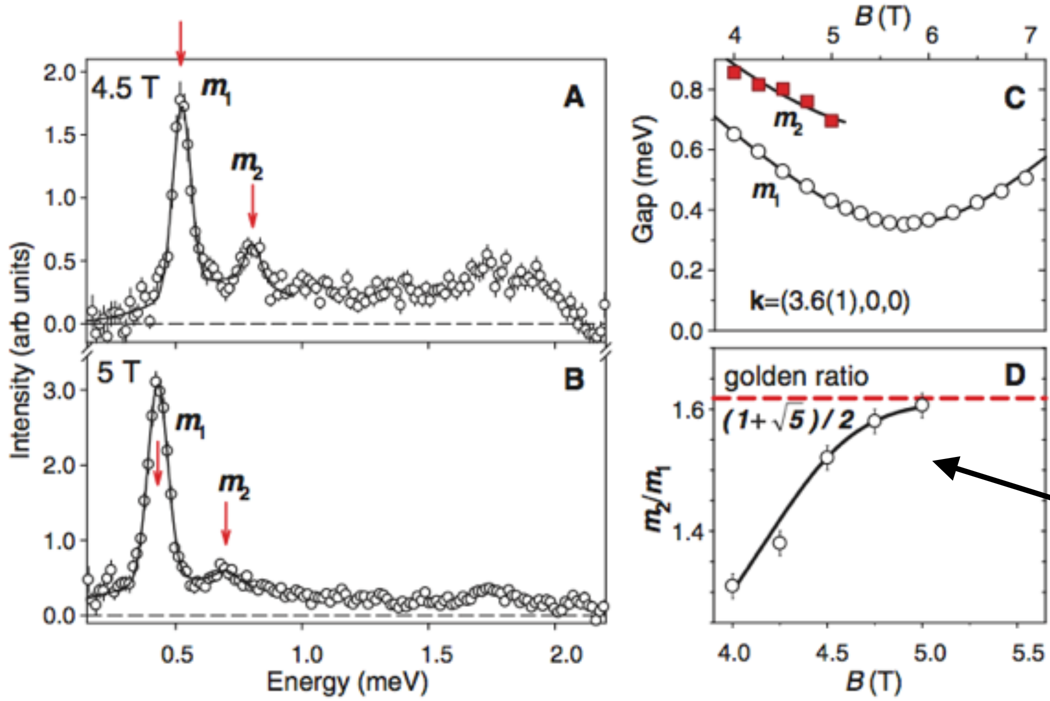
Science (2010)

critical spectrum for h_x=0



in the presence of a small longitudinal field emergence of 8 levels

mathematically described by the E_8 Lie group

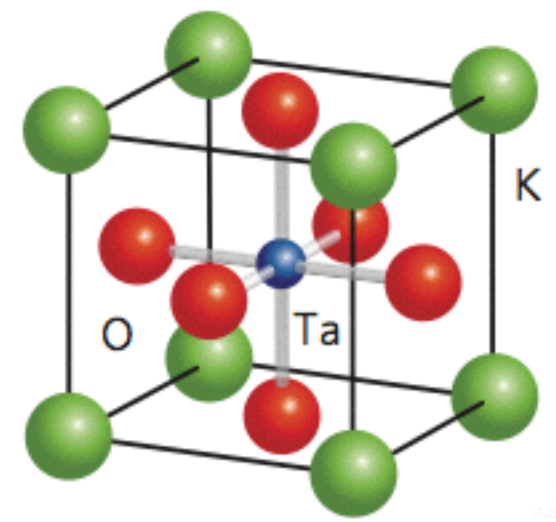


mass of the first and second particle obey Golden ratio

Quantum critical ferroelectrics

Displacive ferroelectrics

Change of the crystal structure by rearrangement, i.e. displacement of atoms



At a 2nd order displace transition at T=0:
optical phonon become soft

if accompanied by emergence of a finite electric polarisation

⇨ quantum critical ferroelectrics

effective theory for electric polarisation P:

couples linearly to electric field (→ PE)

$$\mathcal{L} = \frac{1}{2} P(\partial_t^2 - \nabla^2 - r)P - \frac{u}{4!}P^4 - PE$$

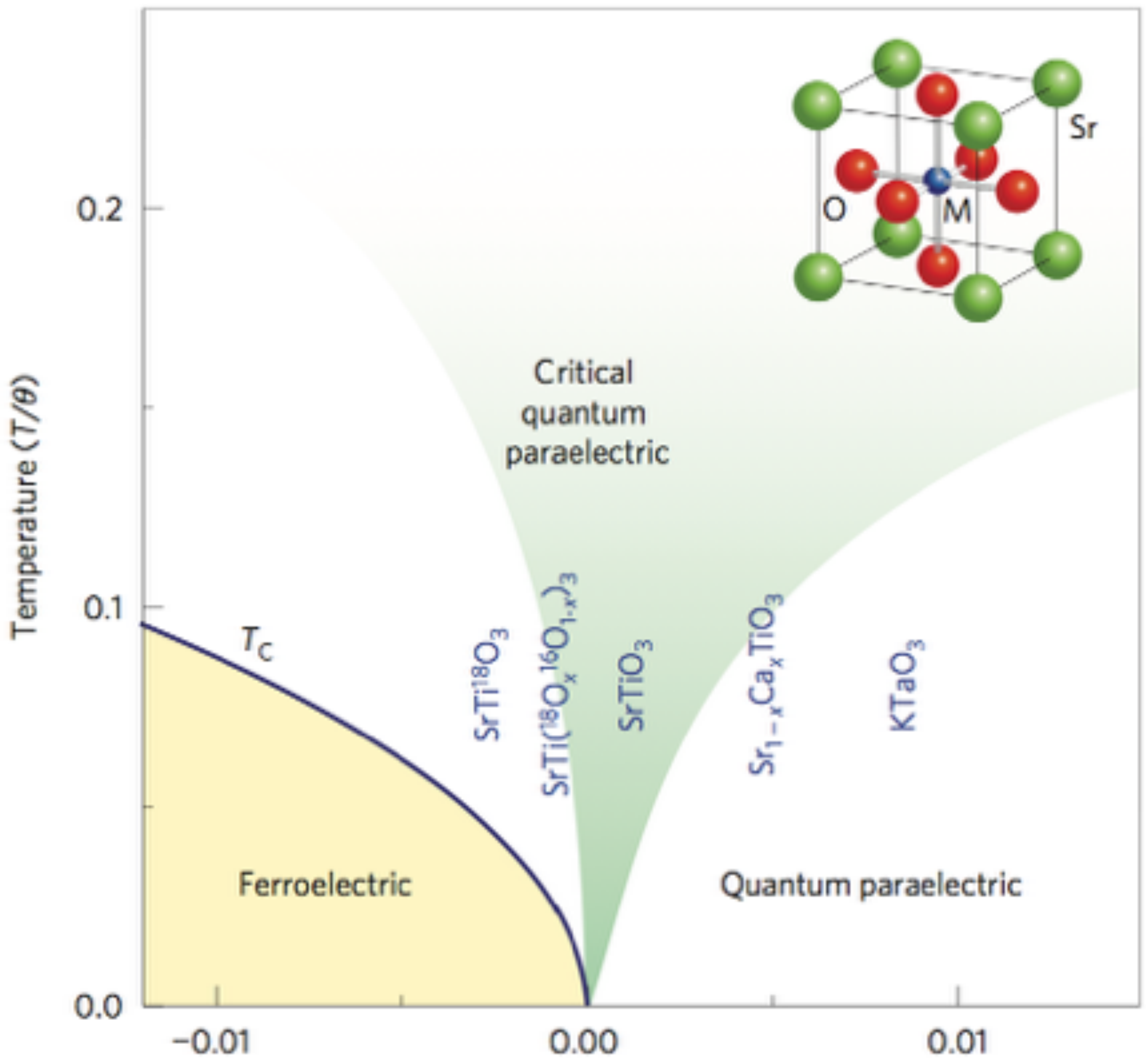
spectrum: $\omega^2 = r + k^2$ optical phonon becomes soft at r-> 0

mean-field exponents:

$$\nu = \frac{1}{2} \quad \text{and} \quad z = 1$$

⇨ d=3 is at the upper critical dimension as d+z = 4 for d=3

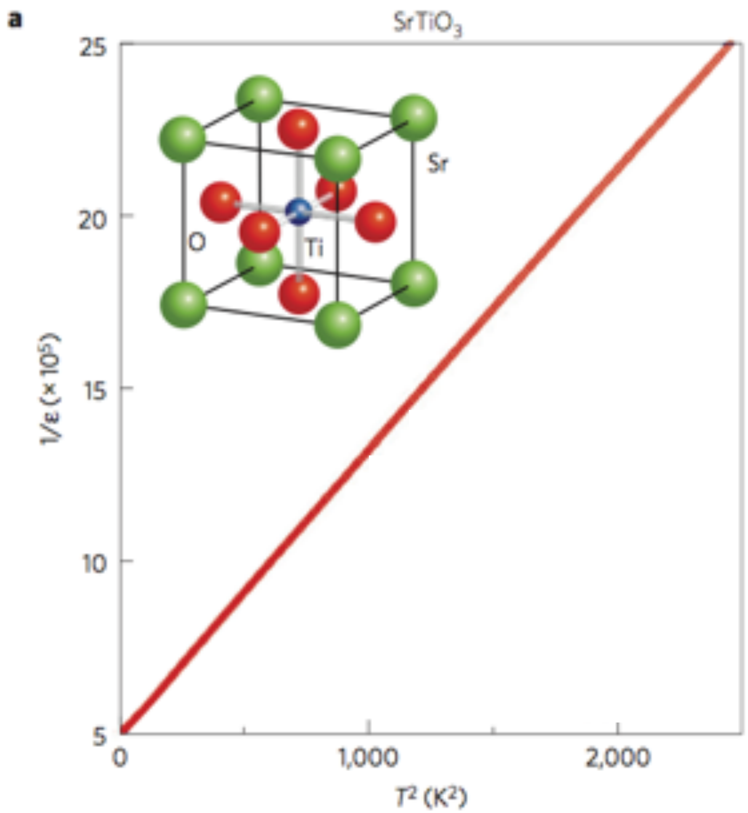
Quantum critical paraelectrics



tuning parameter r

Rowley et al. Nature Physics (2014)

$SrTiO_3$ practically quantum critical:



anomalous T dependence of the dielectric constant $1/\varepsilon \sim T^2$

Hartree-Fock renormalization of the tuning parameter:

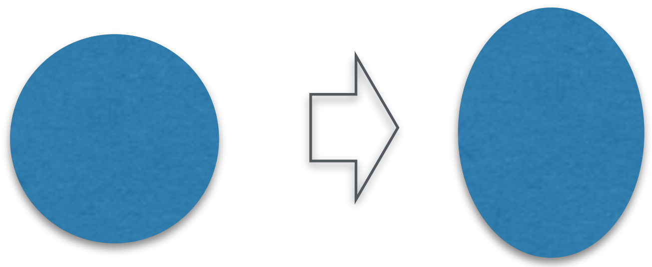
$$1/\varepsilon = r + c\,uT^{\frac{d+z-2}{z}} = r + c\,uT^2$$

Quantum critical metals

Quantum critical metals

Metals are characterised by a Fermi surface

Fermi surface can change at a quantum phase transition



⇨ in general difficult problem and only partly understood (especially in low spatial dimension d=2)

Model:

$$\mathcal{L} = \Psi^\dagger_\sigma (i\partial_t - \varepsilon(-i\nabla))\Psi_\sigma - U \Psi^\dagger_\uparrow \Psi^\dagger_\downarrow \Psi_\downarrow \Psi_\uparrow$$

fermionic operators

interaction that drives some instability like ferromagnetism, antiferromagnetism, nematicity, etc.

Standard procedure:

1. introduce local order parameter Φ by Hubbard-Stratonovich transformation
2. integrate out fermionic degree of freedom
3. expand the action in the order parameter Φ and perform gradient expansion

step 3 dangerous and in certain cases not controlled!

Hertz-Millis theory (e.g. for incommensurate antiferromagnetism)

Ginzburg-Landau theory for the order parameter field Φ = incommensurate AFM

$$\mathcal{L}_{\text{eff}} = \frac{1}{2}\Phi^* \Big(-\gamma\partial_t + \nabla^2 - r \Big)\Phi - \frac{u}{2}|\Phi|^4$$

similar to BEC but with dissipative dynamics

Landau damping of the order parameter due to the excitation of particle-hole pairs in the metal

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Landau damping of the order parameter due to the excitation of particle-hole pairs in the metal

critical exponents

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

renormalization of the tuning parameter: (Hartree-Fock calculation similar to BEC)

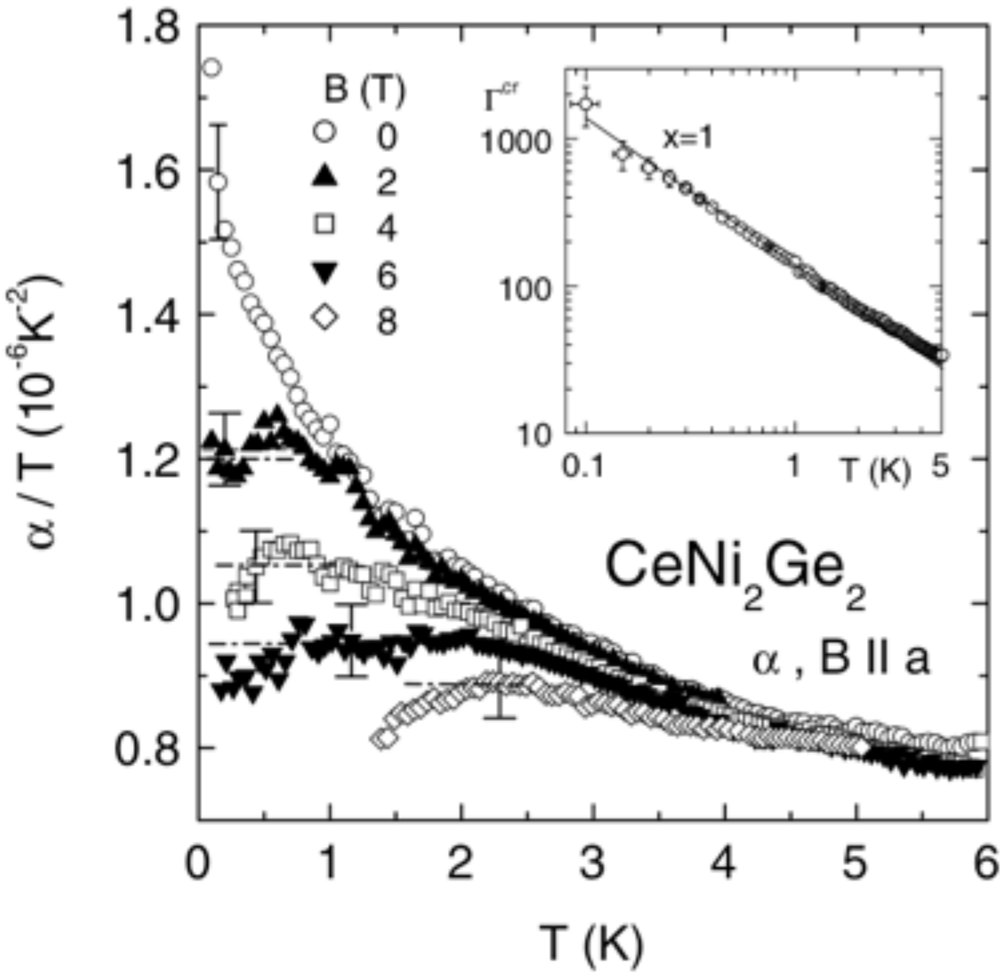
$$R = r + c\,uT^{\frac{d+z-2}{z}} = r + c\,uT^{\frac{3}{2}}$$

for z=2 and d=3

Sometimes it works…

heavy-fermion compound $CeNi_2Ge_2$

is close to a AFM QCP



Küchler et al. PRL (2003)

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

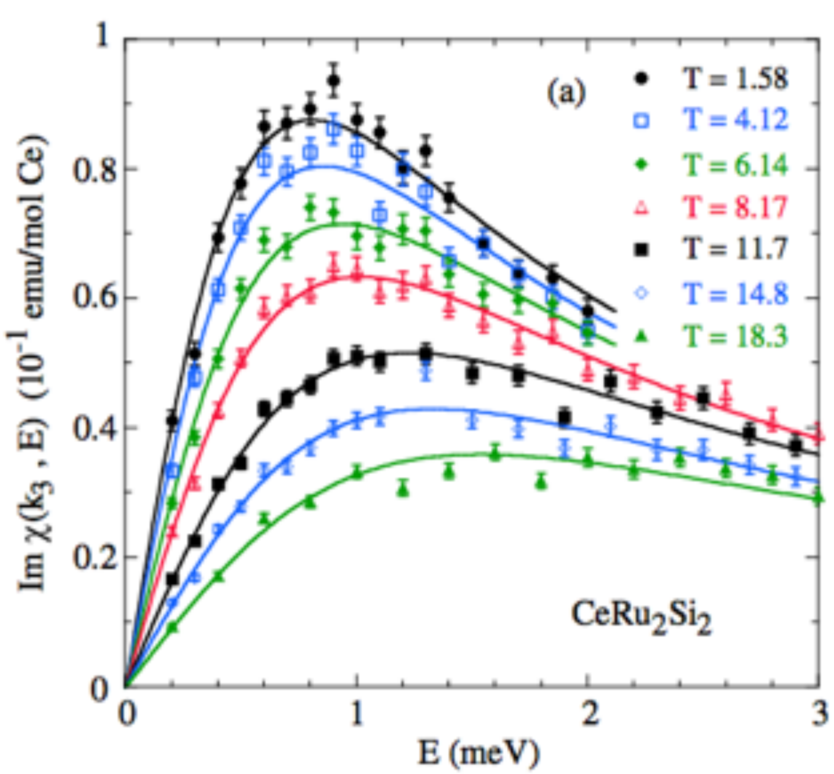
expected power-law for the Grüneisen parameter experimentally observed

Sometimes it works…

Quantum Critical Point of an Itinerant Antiferromagnet in a Heavy Fermion

Hiroaki Kadowaki,[1] Yoshikazu Tabata,[2] Masugu Sato,[3] Naofumi Aso,[4] Stephane Raymond,[5] and Shuzo Kawarazaki[2]
[1]*Department of Physics, Tokyo Metropolitan University, Hachioji-shi, Tokyo 192-0397, Japan*
[2]*Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan*
[3]*MSD, JASRI, 1-1-1 Kouto Mikazuki-cho Sayo-gun, Hyogo 679-5198, Japan*
[4]*NSL, Institute for Solid State Physics, University of Tokyo, Tokai, Ibaraki 319-1106, Japan*
[5]*CEA-Grenoble, DSM/DRFMC/SPSMS, 38054 Grenoble, France*
(Received 23 April 2005; published 3 January 2006)

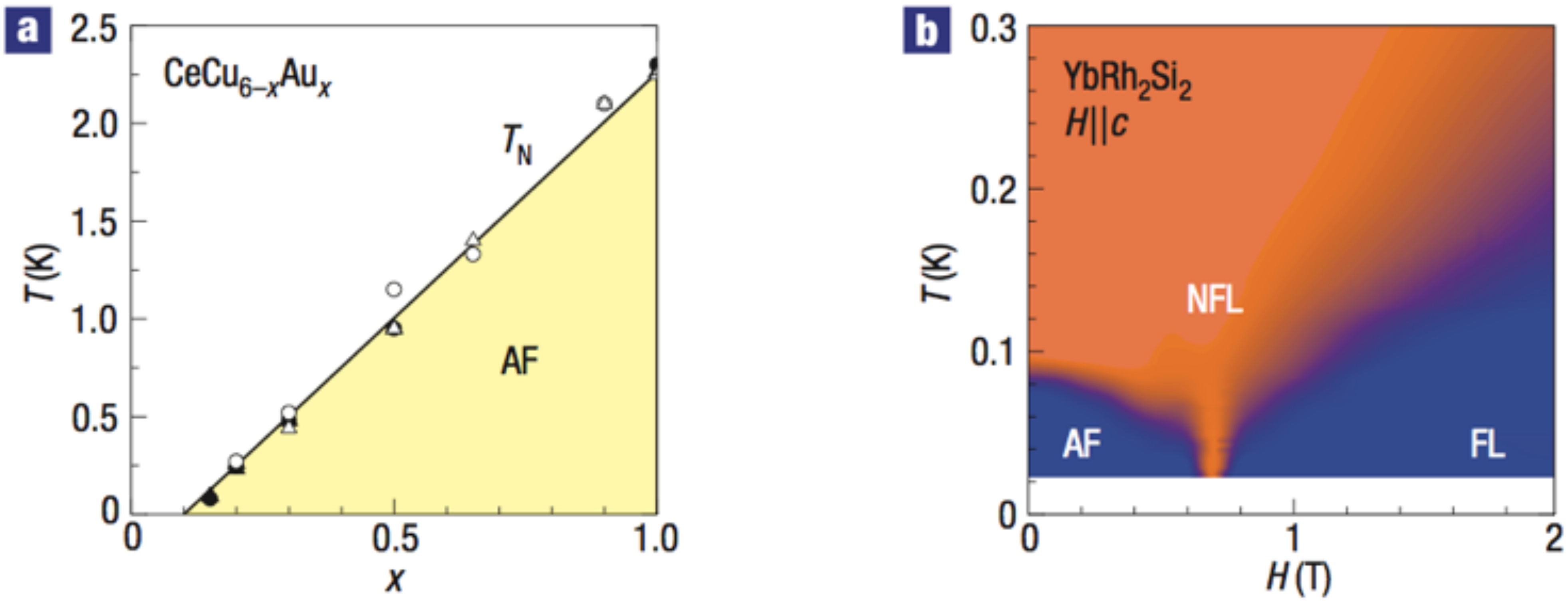
A quantum critical point of the heavy fermion $Ce(Ru_{1-x}Rh_x)_2Si_2$, ($x = 0, 0.03$) has been studied by single-crystalline neutron scattering. By accurately measuring the dynamical susceptibility at the antiferromagnetic wave vector $\boldsymbol{k}_3 = 0.35\boldsymbol{c}^*$, we have shown that the inverse energy width $\Gamma(\boldsymbol{k}_3)$, i.e., the inverse correlation time, depends on temperature as $\Gamma(\boldsymbol{k}_3) = c_1 + c_2 T^{3/2\pm0.1}$, where c_1 and c_2 are x-dependent constants, in a low temperature range. This critical exponent $3/2 \pm 0.1$ proves that the quantum critical point is controlled by that of the itinerant antiferromagnet.



$$R = r + c\,u T^{\frac{d+z-2}{z}} = r + c\,u T^{\frac{3}{2}}$$

Sometimes it doesn't….

Most famous heavy-fermion compounds where Hertz-Millis theory fails



for a review see H. V. Löhneysen, et al. Rev. Mod. Phys. 79, 1015 (2007).

triggered development of alternative theories:
Kondo-breakdown, fractionalized Fermi liquids, AdS/CFT,…

Literature:

- S. Sachdev and B. Keimer, Phys. Today 64, 29 (2011).
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- 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)
- …