Quantum Phase Transitions in Magnetic Systems

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Outline

- Quantum vs. Thermal Phase Transitions
    - Critical phenomena
    - Quantum criticality
    - Example: Transverse-field Ising model

- Quantum Magnetism
    - Quantum Heisenberg model
    - Spin dimers and spin liquids
    - Magnetic-field-induced BEC of triplons
    - Pressure-induced QPT
    - Impurity effects

- Exotic Phases and Criticality
    - Frustration
    - Exotic quantum phases
    - Deconfined quantum critical points

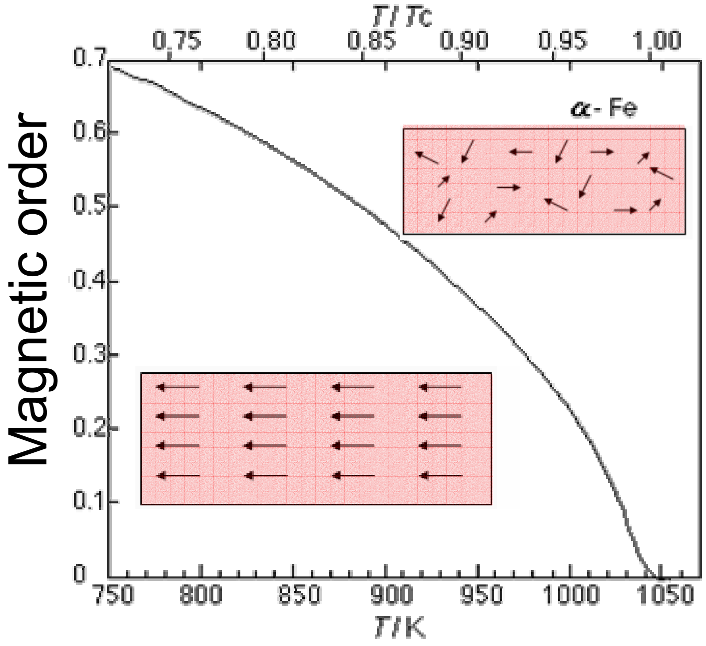
Thermal Phase Transitions

First-Order Transitions

- Coexistence of phases at transition temperature T_C

Second-Order Transitions

- Ex: ferromagnetism in iron
- Order vanishes continuously



Order Parameter Fluctuations

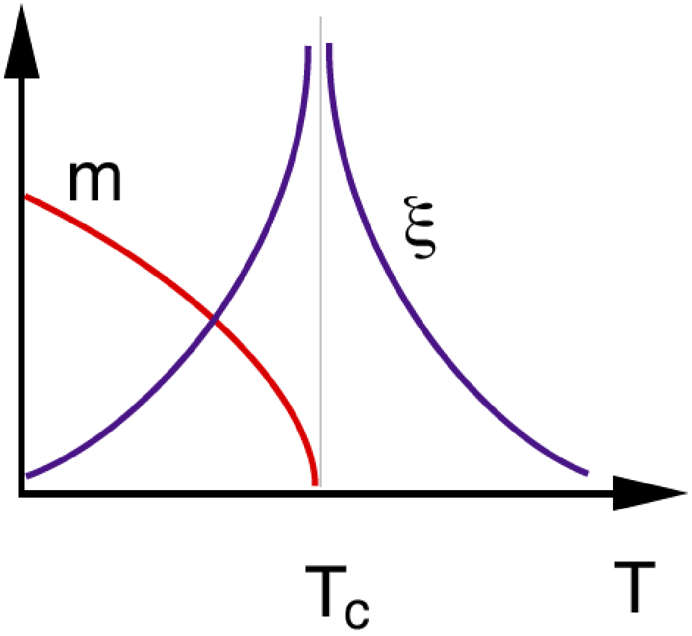
Thermodynamic quantity to identify phases

- Ferromagnet: magnetization *m*

Phenomenological description

- Ginzburg-Landau theory

Correlation length of local order parameter fluctuations around its mean value: ξ

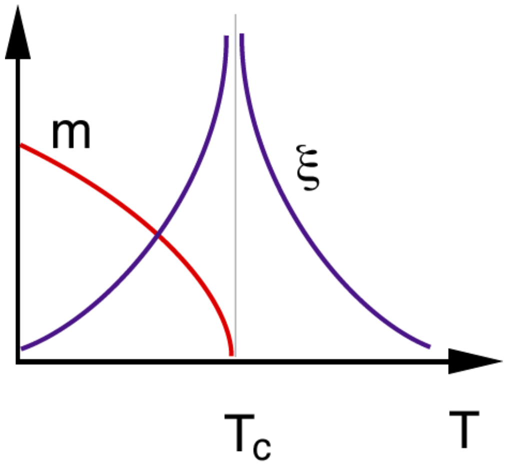


Critical Phenomena

Long ranged spatial correlations at T_C

$$\xi \propto |t|^{-\nu}$$

$$t = (T - T_C) / T_C$$



Characteristic timescale of the fluctuations

$$\tau \propto \xi^{\boxed{z}} \propto |t|^{-\nu z}$$

dynamical critical exponent

Correlations on all length- and time-scales

Scale Invariance

Power-law behavior of observables

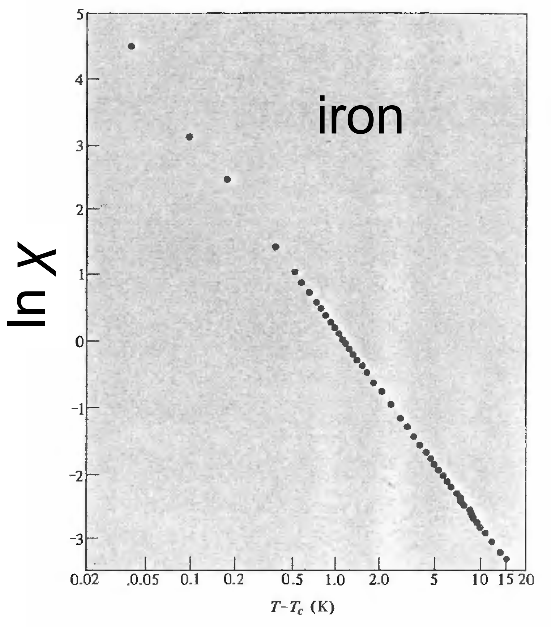
Critical exponents – depend on

- symmetry of the order parameter
- dimensionality of the system
- interaction range

Universality classes

Renormalization group approach

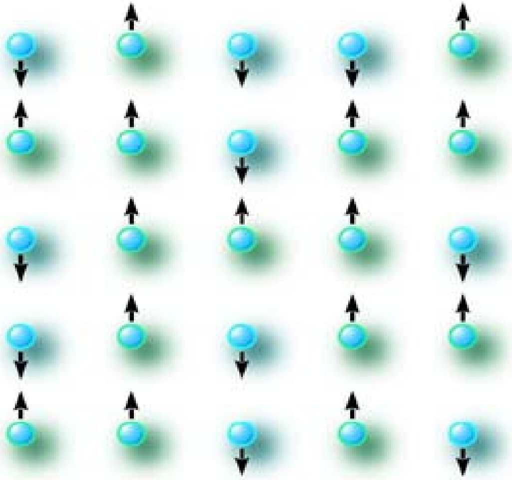
	Exponent	Definition	Conditions
Specific heat	α	$C \propto \|t\|^{-\alpha}$	$t \to 0, B = 0$
Order parameter	β	$m \propto (-t)^{\beta}$	$t \to 0$ from below, $B = 0$
Susceptibility	γ	$\chi \propto \|t\|^{-\gamma}$	$t \to 0, B = 0$
Critical isotherm	δ	$B \propto \|m\|^{\delta}\mathrm{sign}(m)$	$B \to 0, t = 0$
Correlation length	ν	$\xi \propto \|t\|^{-\nu}$	$t \to 0, B = 0$
Correlation function	η	$G(r) \propto \|r\|^{-d+2-\eta}$	$t = 0, B = 0$
Dynamic	z	$\tau_c \propto \xi^{z}$	$t \to 0, B = 0$



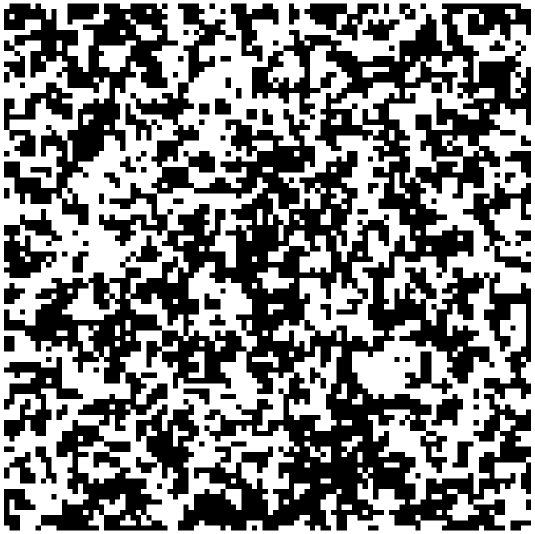
Ising Model

Z_2 symmetry universality class

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j , \quad \sigma_i = \pm 1$$



Critical fluctuations



$T = T_C = 2.269\, J / k_B$

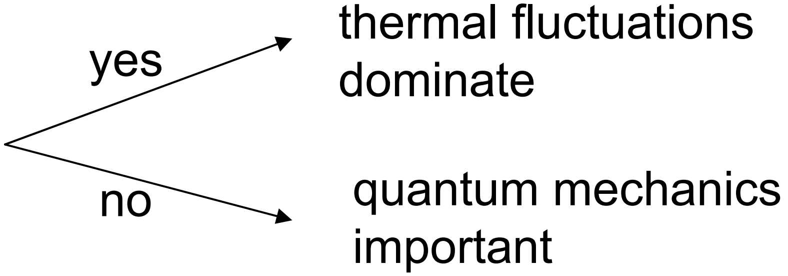
2D: $\alpha = 0 \quad \beta = 1/8 \quad \gamma = 7/4 \quad \delta = 15 \quad \nu = 1 \quad \eta = 1/4$

Relevance of Quantum Mechanics Near Thermal Transitions

Characteristic energy of large-scale order parameter fluctuations

$$\hbar\omega_C \propto 1/\tau \propto |t|^{\nu z} \xrightarrow{t\to 0} 0$$

$$\hbar\omega_C << k_B T \ ?$$



yes

thermal fluctuations dominate

no

quantum mechanics important

Critical fluctuations behave classical close to T_C

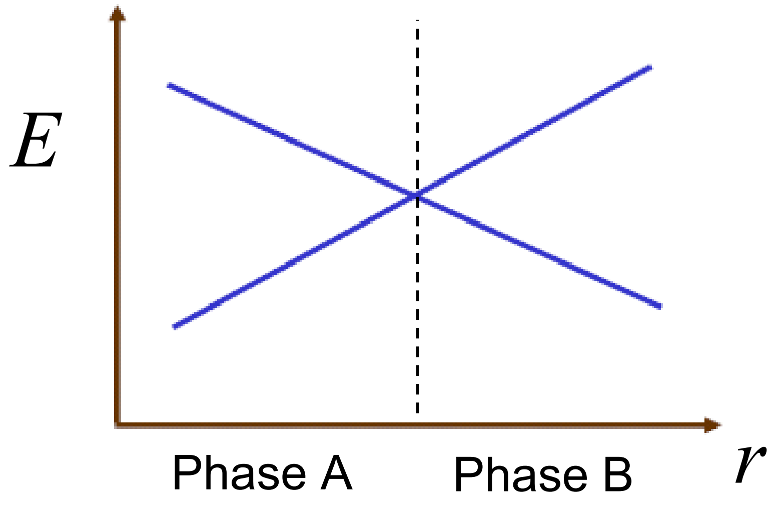
Critical behavior is of purely classical nature

Quantum Phase Transitions

Varying a non-thermal control parameter r

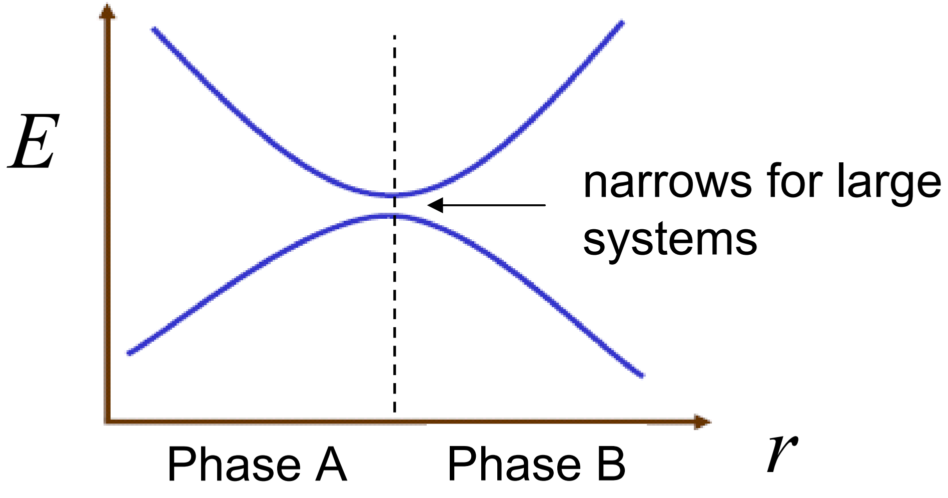
- magnetic field, pressure, composition

level crossing:



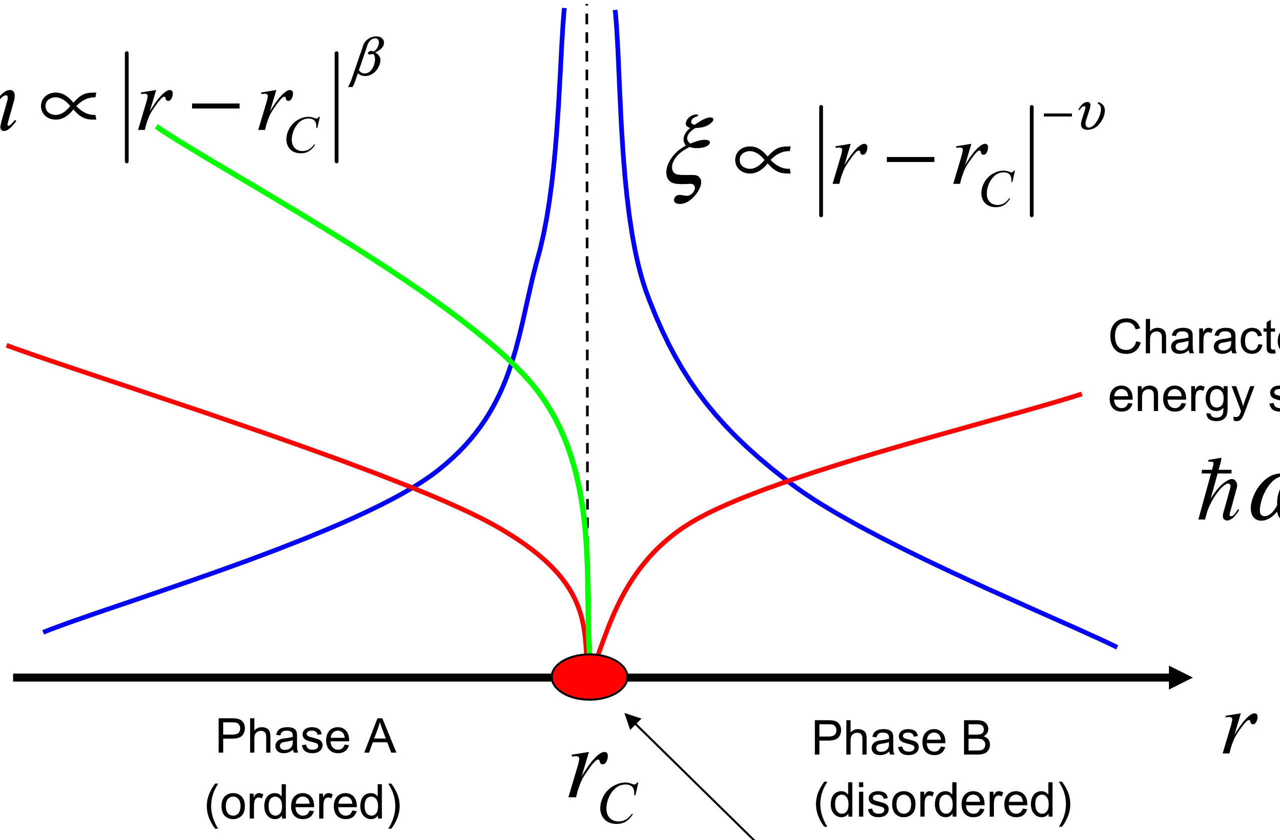
discontinuous transition

avoided level crossing:



continuous transition

Continuous QPT



$m \propto |r - r_C|^{\beta}$

$\xi \propto |r - r_C|^{-\upsilon}$

Characteristic
energy scale (e.g. gap)

$\hbar\omega_C \propto \xi^{-z}$

Phase A
(ordered)

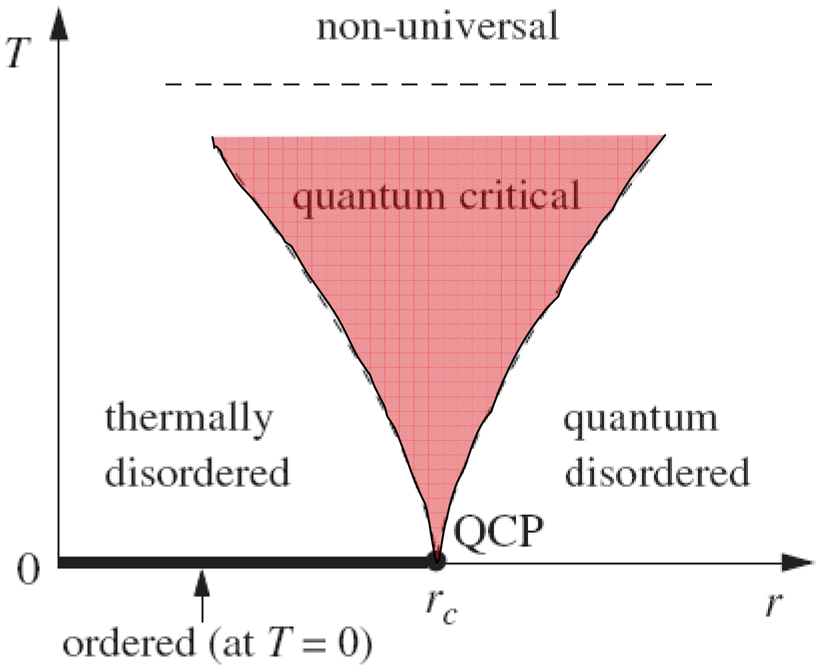
r_C

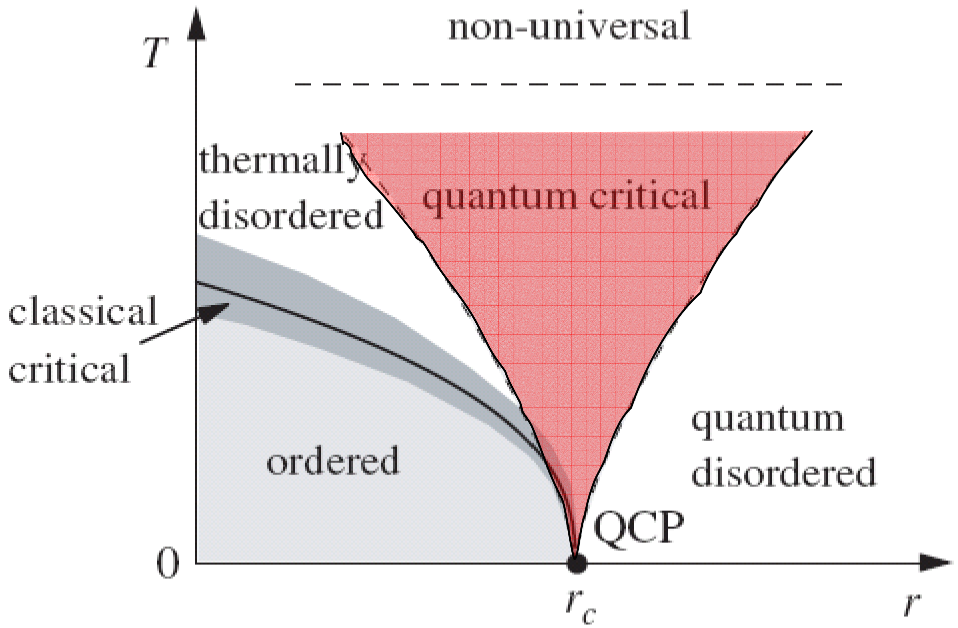
Phase B
(disordered)

r

quantum critical point

Phase Diagram near a QCP



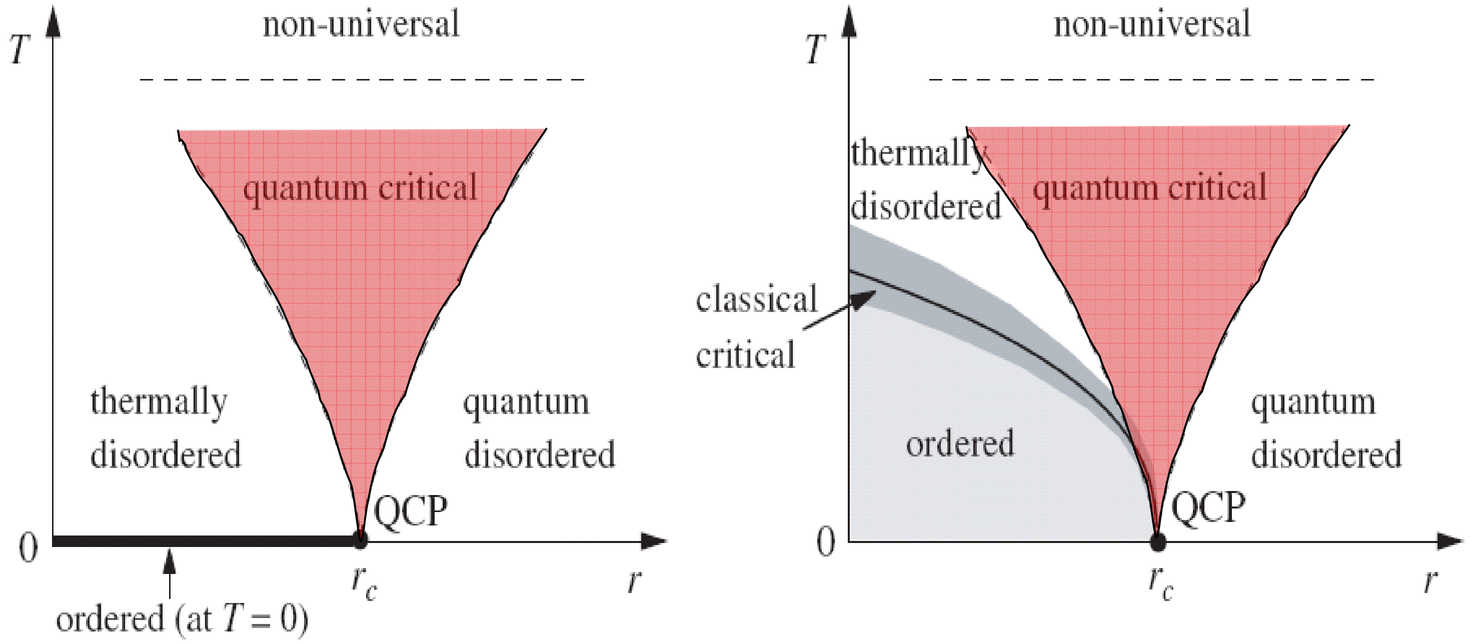


crossover to the quantum critical regime:

$$k_B T \approx \hbar \omega_C \propto |r - r_C|^{\nu z}$$

Quantum Critical Regime

Extends up to high temperatures



Ex.: Magnetic exchange in cuprates: $J \approx 100\ \text{meV}$

$$k_B T \approx J \quad \Rightarrow \quad T \approx 1000 K$$

Quantum-Classical Mapping

d-dimensional
quantum system

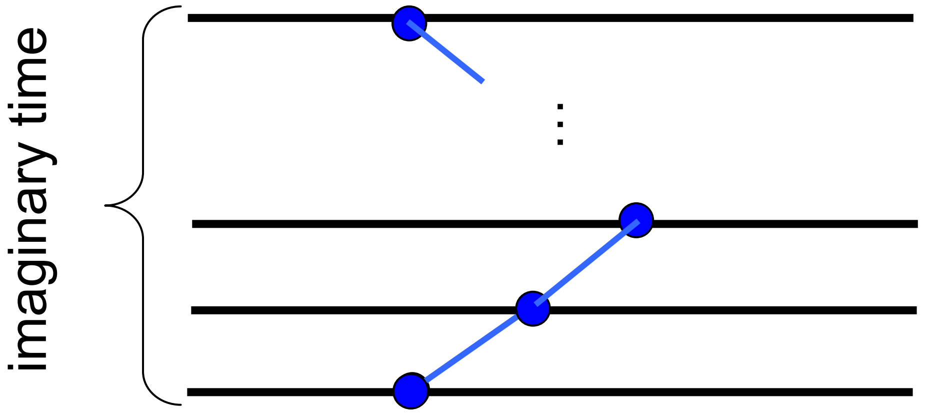
Temperature T

(d+1)-dimensional
classical system

additional dimension of extend
$\beta = 1/k_B T$

$$Z_Q = \mathrm{Tr}\left(e^{-H/k_B T}\right)$$

$$Z_C = \sum_C W(C)$$



$\beta = 1/k_B T$

$e^{-\varepsilon H} = e^{-i\tau H},\ \tau = -i\varepsilon$

imaginary
time-step

What makes QPT special?

- Non-standard effective classical models
  - topological effects e.g. from Berry-phases
  - effects to disorder

- Dynamical critical properties cannot directly be extract from the quantum-classical mapping

- No quasi-classical particle description of the excitations inside the quantum critical regime

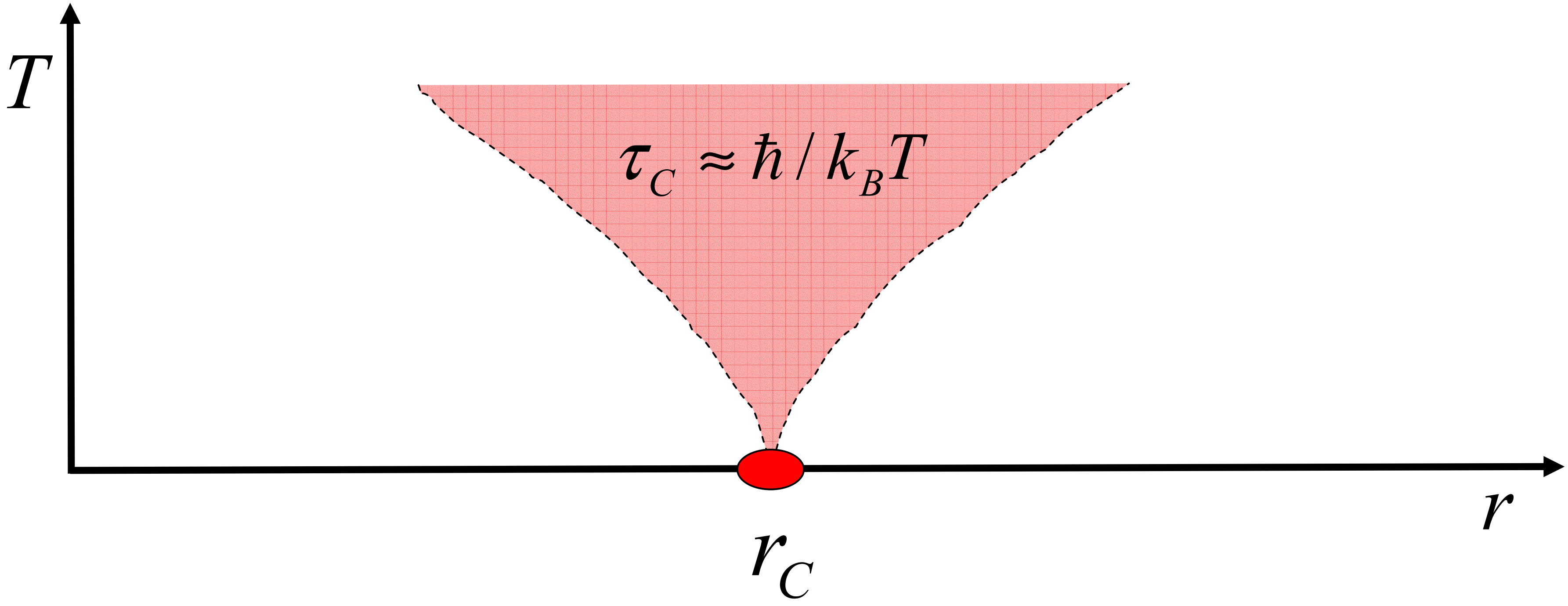
- New states of matter with strong quantum and thermal fluctuations inside the broad quantum critical temperature regime (e.g. non-Fermi liquids)
  → Talk by A. Muramatsu

- Genuine new time-scale: quantum phase-coherence time τ_C

Phase Coherence Time

Time scale over which the system retains phase coherence

- quantum effects relevant on scales below τ_C



Example: Ising Chain in a Transverse Field

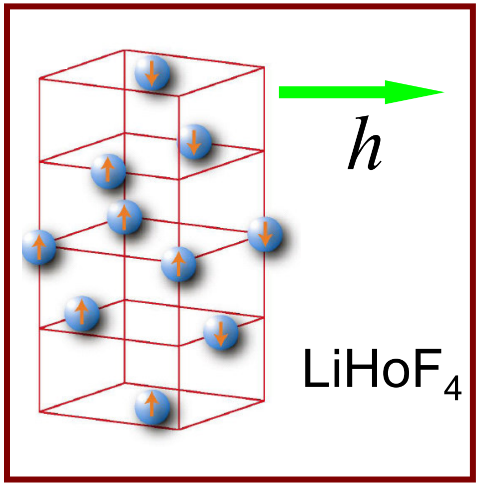
Chain of (many) coupled qbits

$$H = -J\sum_{\langle i,j\rangle} S_i^z S_j^z - h\sum_i S_i^x$$

align neighbors

quantum tunneling

$$|\uparrow\rangle_i \leftrightarrow |\downarrow\rangle_i$$



$$S_i^x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Ground states in simple limits:

$$J >> h: \quad |\uparrow\rangle_0 \otimes |\uparrow\rangle_1 \otimes \ldots \otimes |\uparrow\rangle_N, \quad \text{or} \quad |\downarrow\rangle_0 \otimes |\downarrow\rangle_1 \otimes \ldots \otimes |\downarrow\rangle_N$$

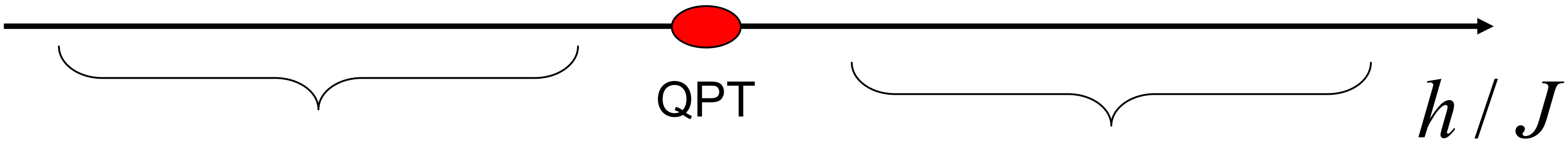
$$h >> J: \quad |\rightarrow\rangle_0 \otimes |\rightarrow\rangle_1 \otimes \ldots \otimes |\rightarrow\rangle_N, \qquad |\rightarrow\rangle_i = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_i + |\downarrow\rangle_i\right)$$

Ground State Phase Diagram

$$H = -J\sum_{\langle i,j\rangle} S_i^z S_j^z - h\sum_i S_i^x$$

$$|\uparrow\rangle_0 \otimes |\uparrow\rangle_1 \otimes \ldots \otimes |\uparrow\rangle_N ,$$
$$|\downarrow\rangle_0 \otimes |\downarrow\rangle_1 \otimes \ldots \otimes |\downarrow\rangle_N$$

$$|\rightarrow\rangle_0 \otimes |\rightarrow\rangle_1 \otimes \ldots \otimes |\rightarrow\rangle_N$$



long ranged order
Z_2 symmetry breaking

$$\begin{cases} S_i^x \rightarrow S_i^x \\ S_i^z \rightarrow -S_i^z \end{cases}$$

exponential decay
of the correlation function

$$\left\langle S_i^z S_j^z \right\rangle \propto e^{-|x_i - x_j|/\xi}$$

Quantum Critical Point

Critical decay of the correlation function

$$J = h: \ \left\langle S_i^z S_j^z \right\rangle \approx \frac{1}{\left| x_i - x_j \right|^{1/4}}$$

Quantum-classical mapping

→ 2D Ising universality class ($z = 1$)

Low-Energy Excitations

Quasi-classical particle description

$$h >> J: \quad |\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rangle \quad \rightarrow \quad |\rightarrow\rightarrow\rightarrow\rightarrow\leftarrow\rightarrow\rightarrow\rightarrow\rangle$$

Flipped spin
Mobile for finite *J*

$$|\leftarrow\rangle_i = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_i - |\downarrow\rangle_i\right)$$

Dispersing quasi-particle excitations

Many flipped spin states

$$|\rightarrow\leftarrow\rightarrow\rightarrow\leftarrow\rightarrow\rightarrow\rightarrow\rangle$$

Low-Energy Excitations

A different quasi-particle description

$$J >> h: \quad \left|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\ \uparrow\uparrow\right\rangle \rightarrow \quad \left|\uparrow\uparrow\uparrow\uparrow\uparrow|\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\right\rangle$$

$$\left|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow|\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\right\rangle$$

$$\left|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow|\downarrow\downarrow\downarrow\downarrow\downarrow\right\rangle$$

$$\left|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow|\downarrow\downarrow\downarrow\downarrow\right\rangle$$

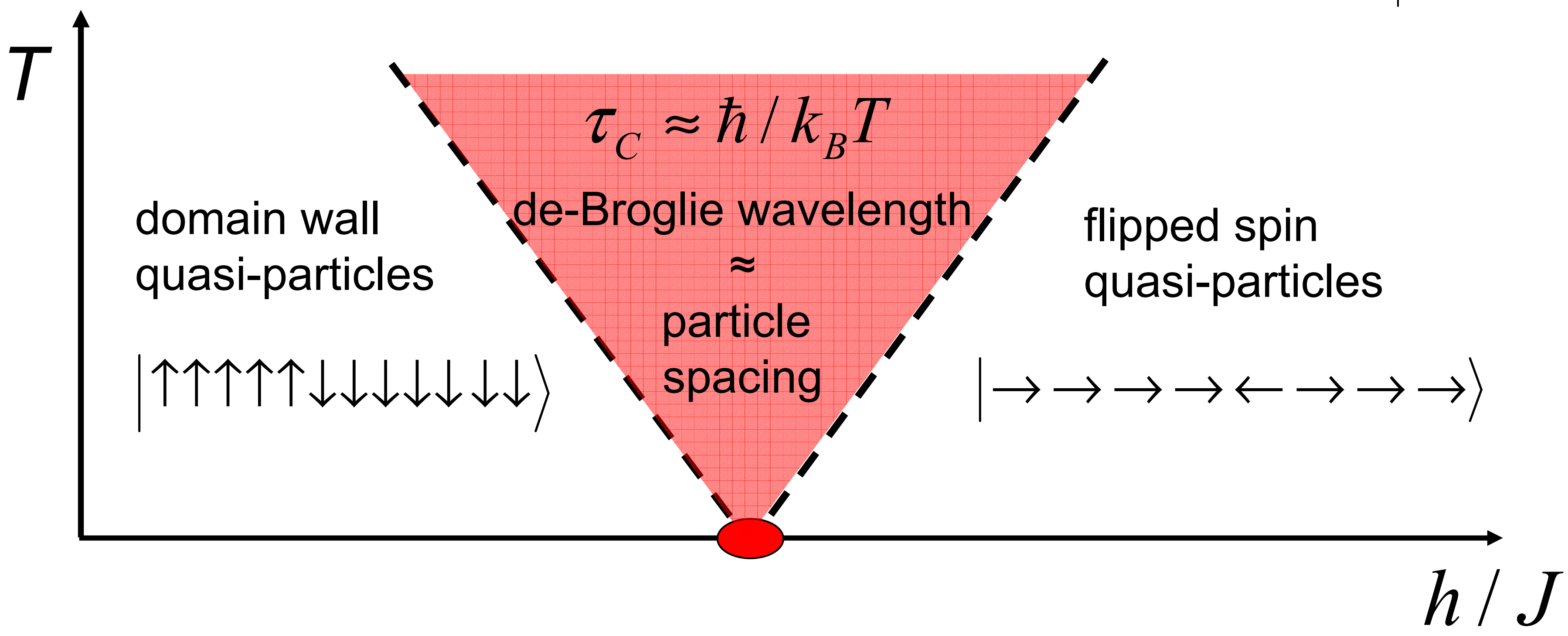
Domain wall
Mobile for finite *h*

Dispersing quasi-particle excitations

Many domain wall states

$$\left|\uparrow\uparrow\uparrow\uparrow\uparrow|\downarrow\downarrow\downarrow\downarrow|\uparrow\uparrow\uparrow\uparrow\right\rangle$$

Phase Diagram



$\tau_C \approx \hbar / k_B T$

de-Broglie wavelength
≈
particle
spacing

domain wall
quasi-particles

$|\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle$

flipped spin
quasi-particles

$|\rightarrow\rightarrow\rightarrow\rightarrow\leftarrow\rightarrow\rightarrow\rightarrow\rangle$

Universal response function inside the quantum critical regime

$$\chi(k=0,\omega) = T^{-7/4}\Phi(\hbar\omega / k_B T)$$

ω / T scaling

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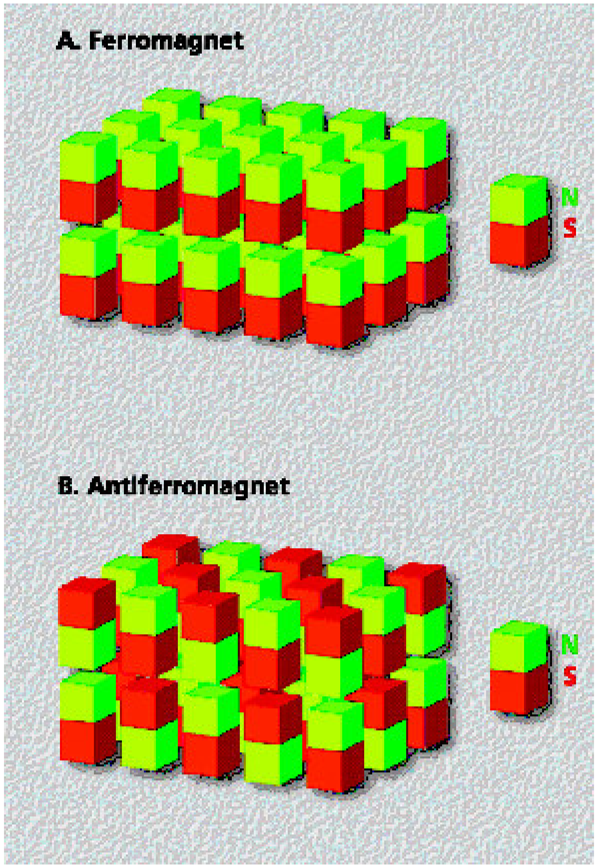
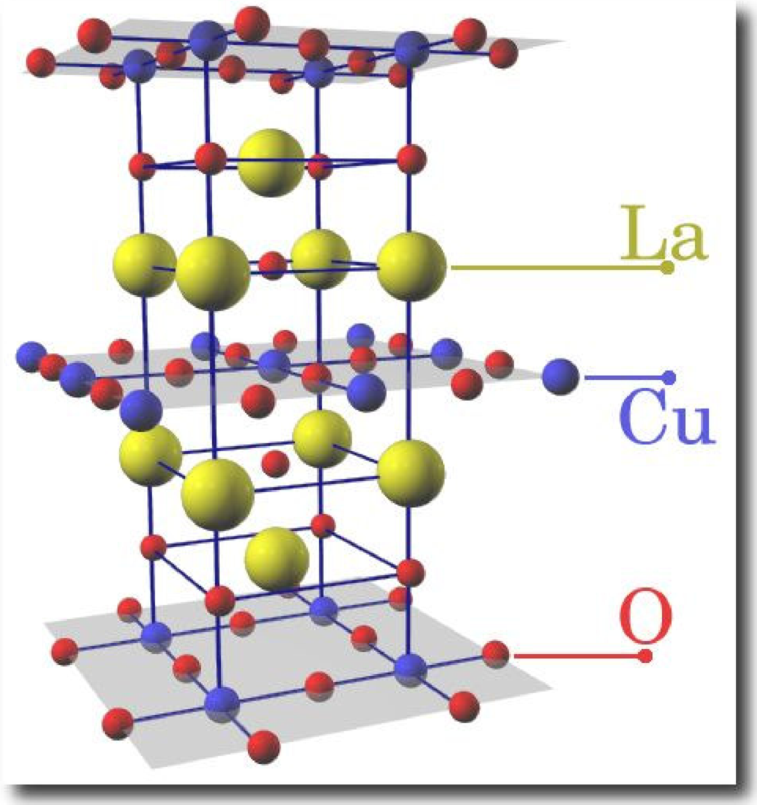
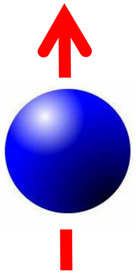


Quantum Antiferromagnet
La_2CuO_4



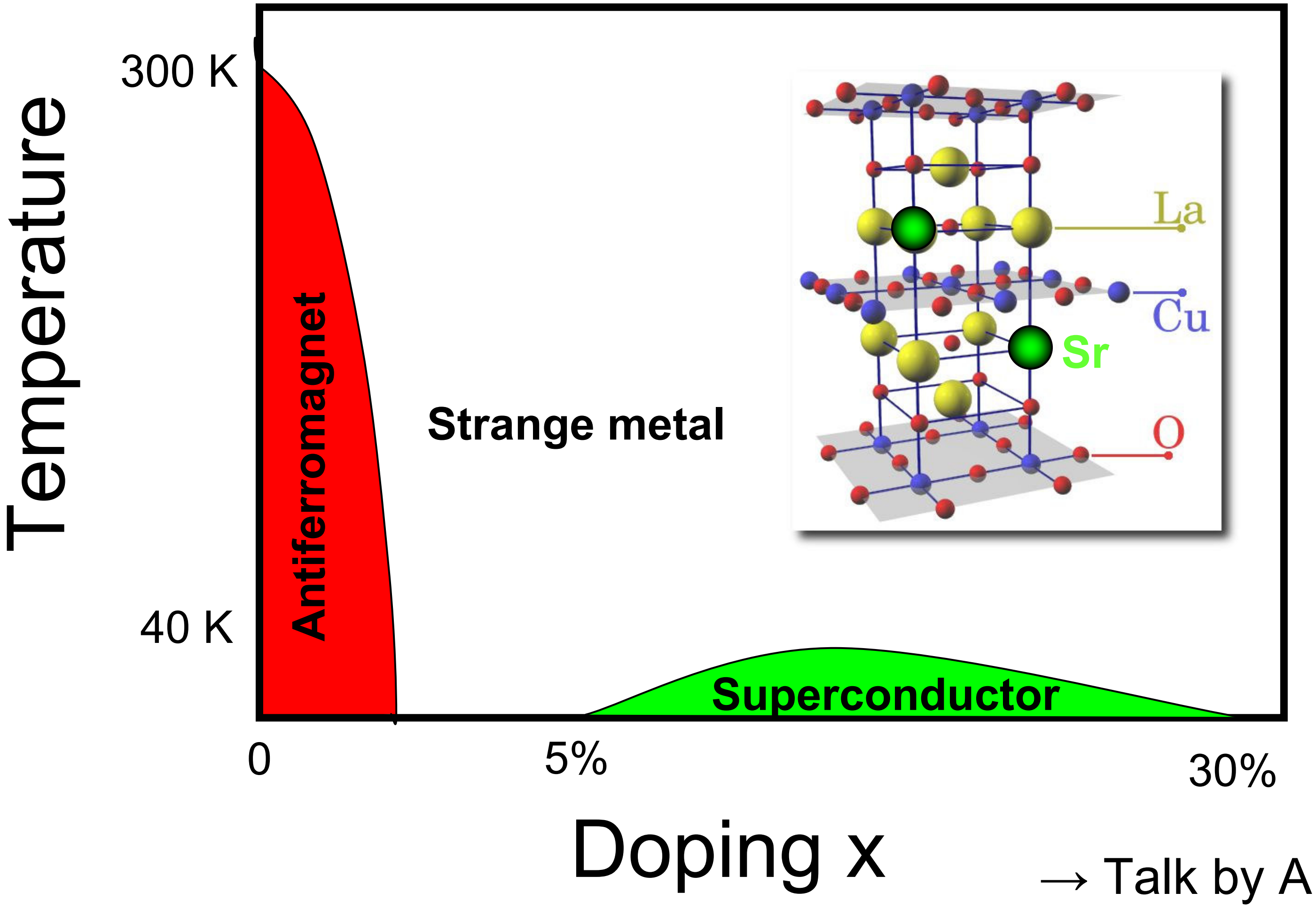


Cu^{2+}

spin-1/2

Band theorie: half filling → metall

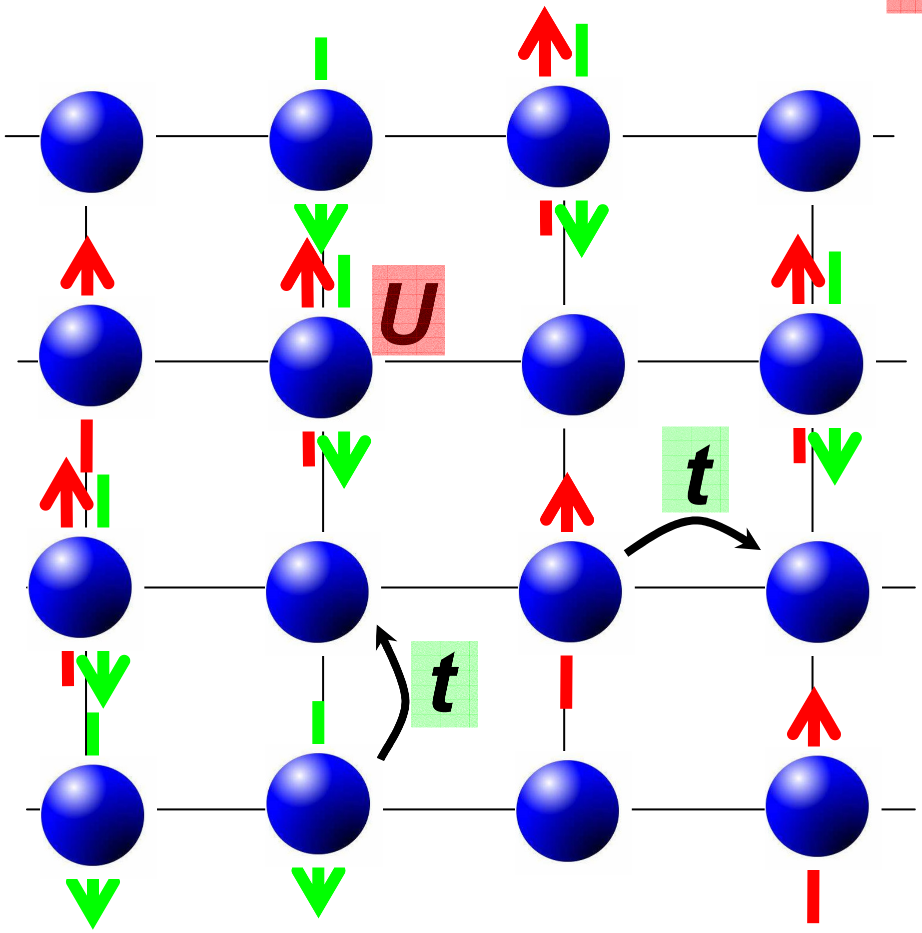
High-TC Superconductor $La_{2-x}Sr_xCuO_4$

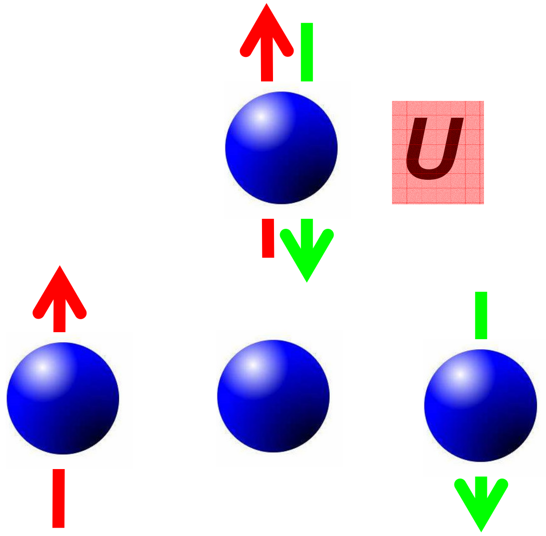


→ Talk by A. Muramatsu

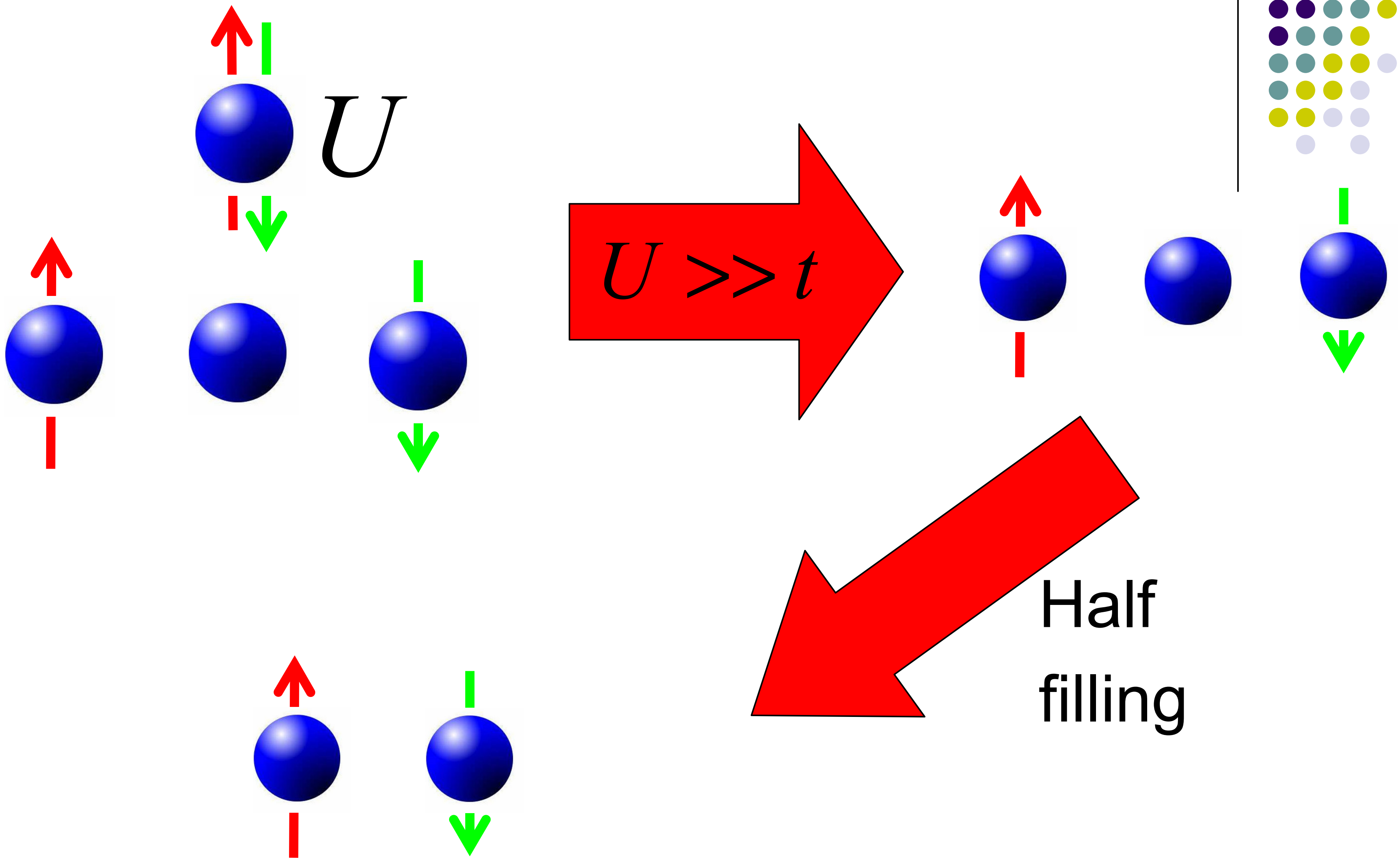
Hubbard Model

Mobile electrons + Screened coulomb repulsion





Bosonic version
→ Talk by HP. Büchler



U

$U >> t$

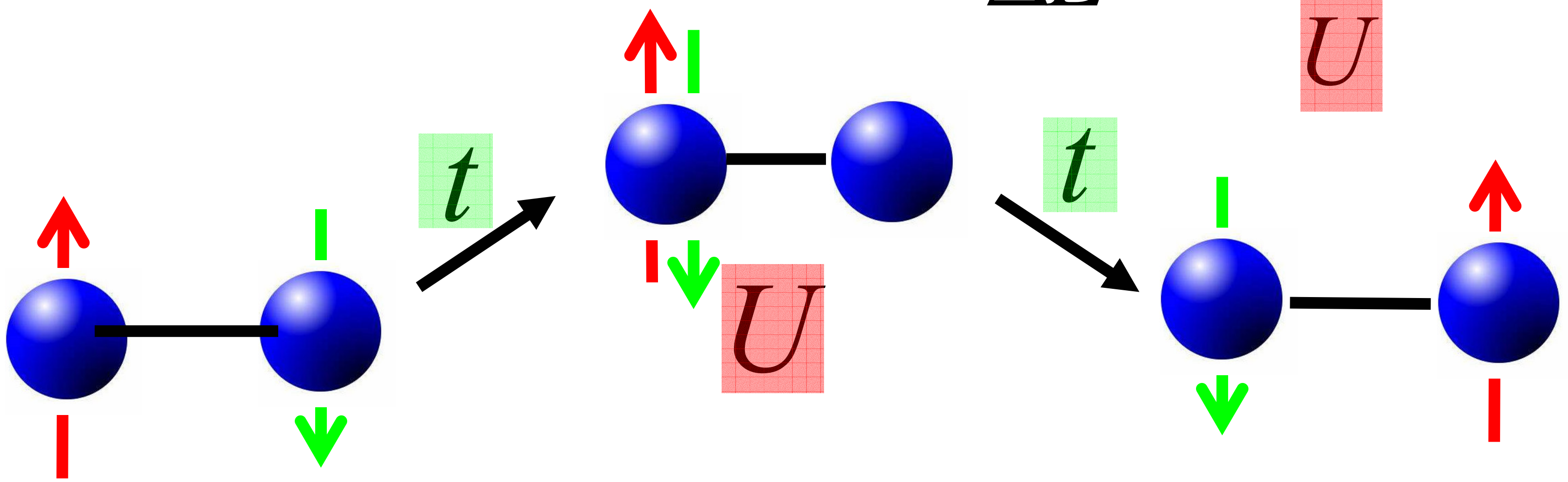
Half filling

Effective spin model ?

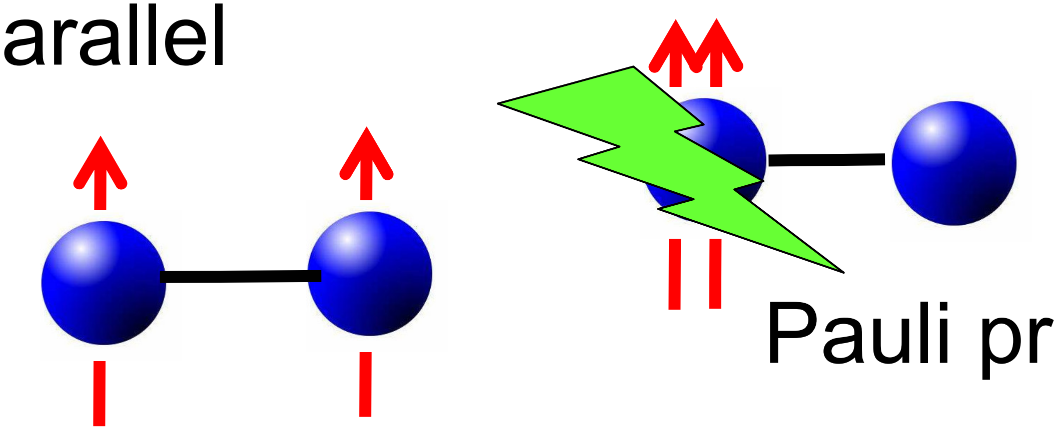
Kinetic Exchange

Anti-parallel → energy gain

$$\Delta E \propto -\frac{t^2}{U}$$



Parallel



Pauli principle

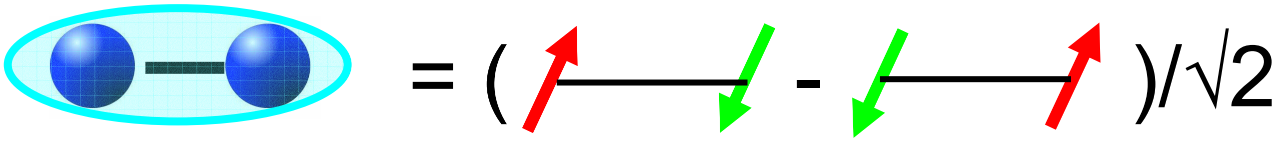
blocked

Quantum Heisenberg Antiferromagnet

$$\mathcal{H} = \boxed{J} \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j$$

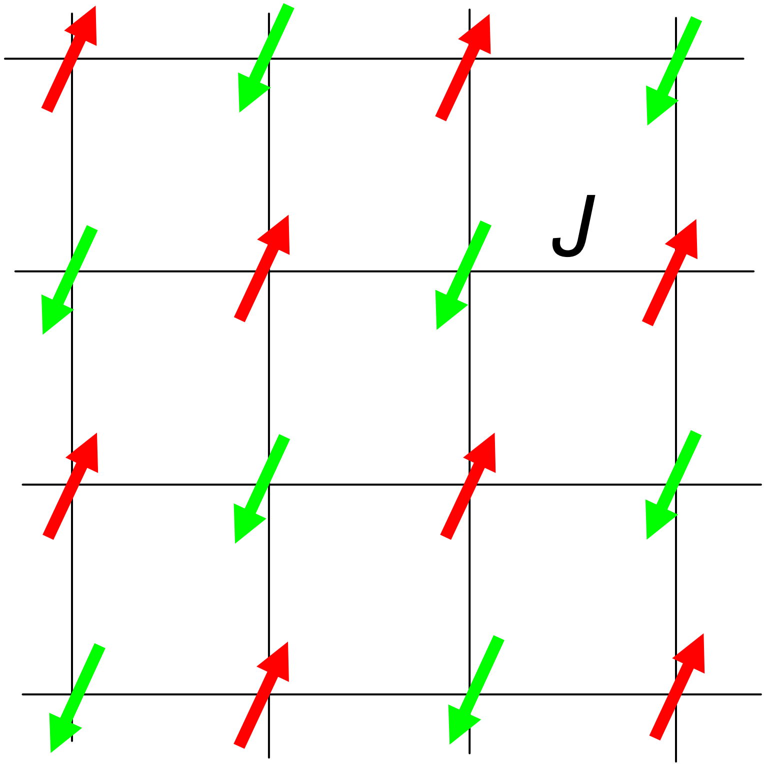
$$\boxed{J = \frac{4t^2}{U} > 0}$$

Antiferromagnetic exchange



Two spins bound in a spin singlet state

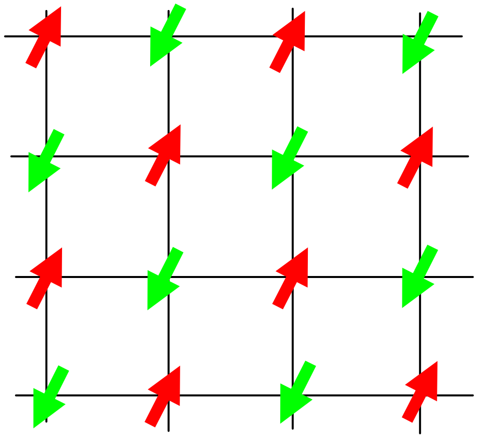
Antiferromagnetic order…



…at low temperaturs?

Mermin-Wagner Theorem

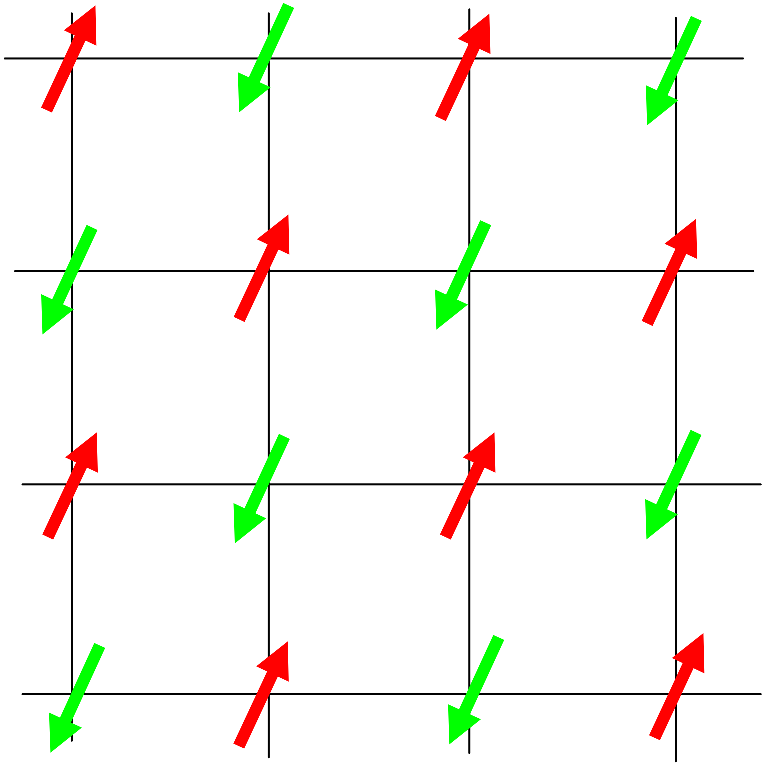
No spontaneous breaking of
a continuous symmetry
at finite temperatures



spin-rotation symmetry
broken

→ order only in the ground state (T= 0)

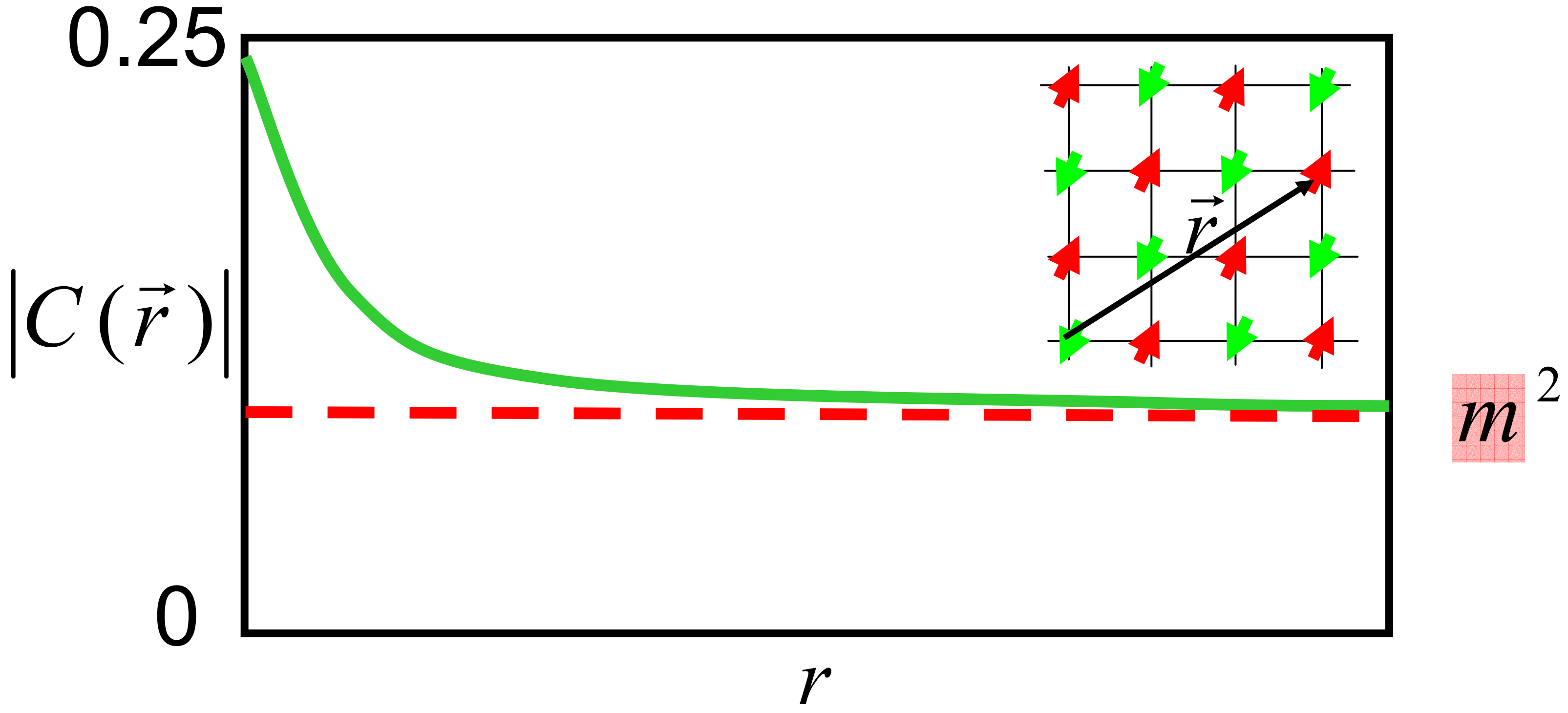
Not An Eigenstate



$$H\left|N\acute{e}el\right\rangle \neq E_0\left|N\acute{e}el\right\rangle$$

Staggered Moment

Correlation function $C(\vec{r}) = \left\langle \vec{S}(\vec{r}) \cdot \vec{S}(0) \right\rangle$

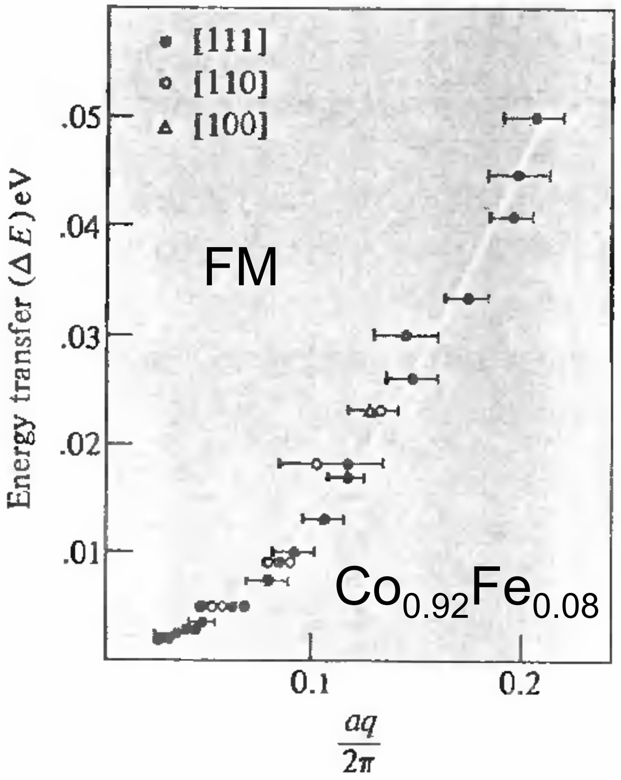


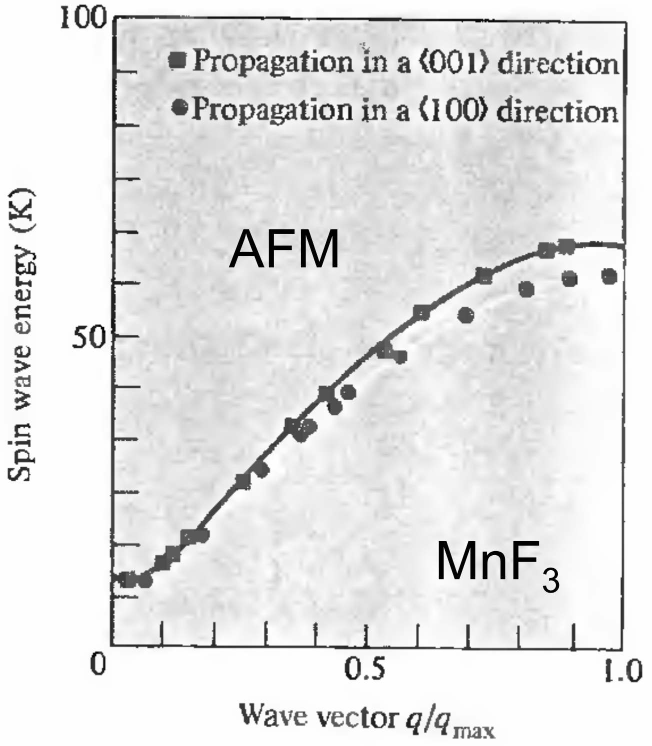
quantum fluctuations→ $m \approx 0.3$

Excitations

Spin waves (Goldstone modes)

Spectrum accessible via neutron scattering



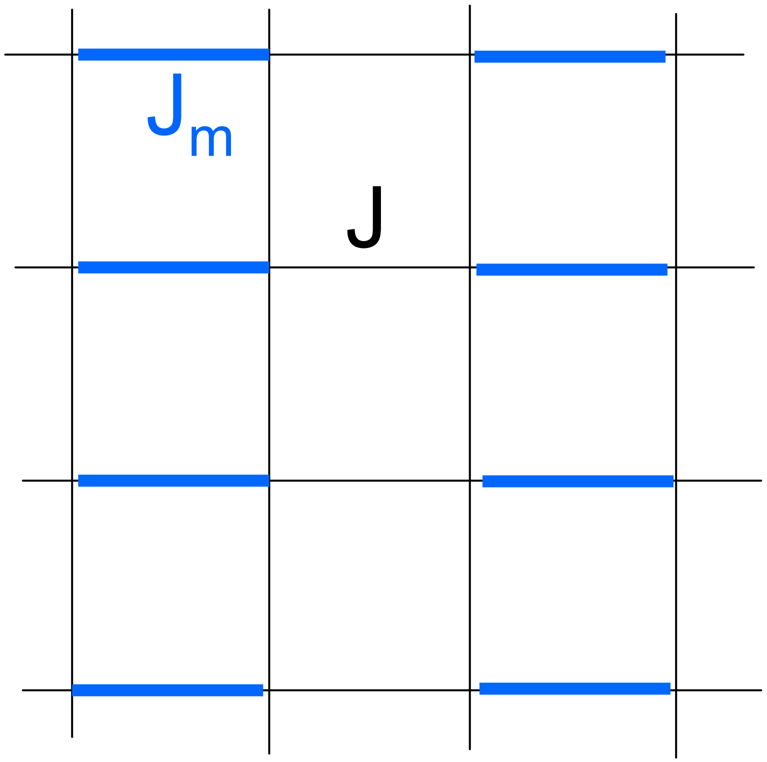


How to destroy the AF order?

- Enhance quantum fluctuations
- Frustration
- Both !

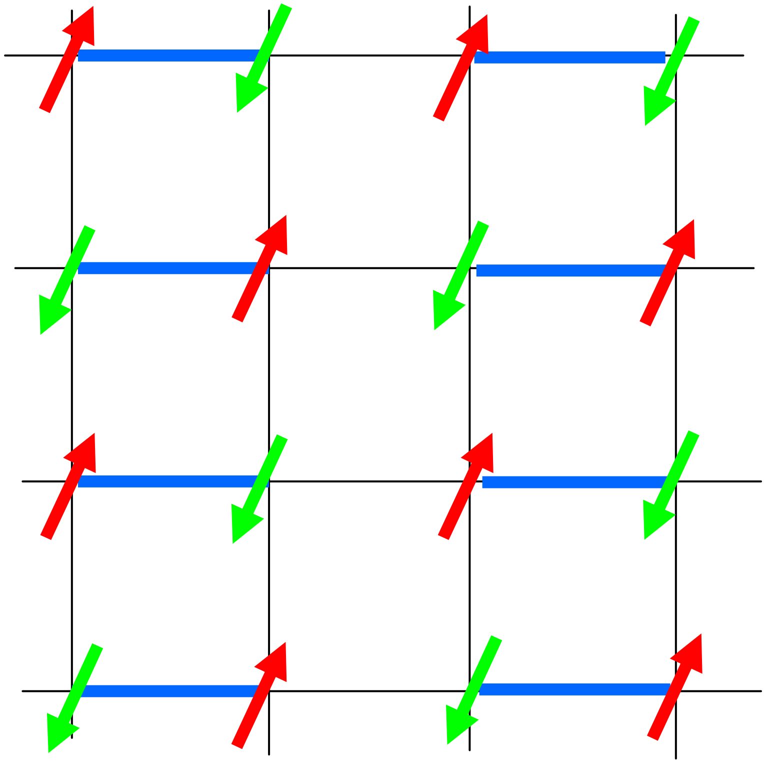
Bond Modulations

$J_m \geq J$



Weak Modulations

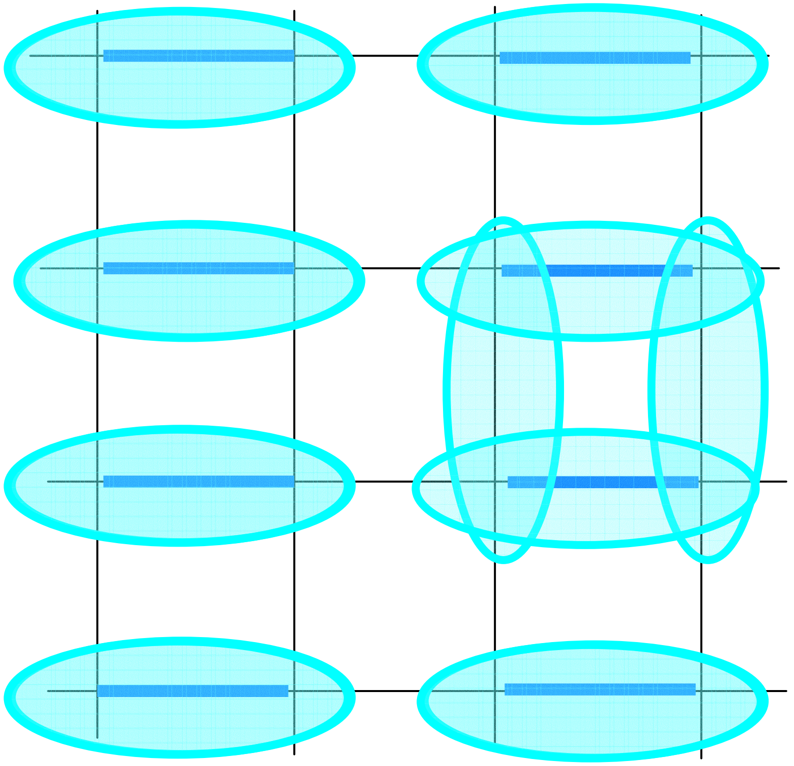
$J_m \approx J$

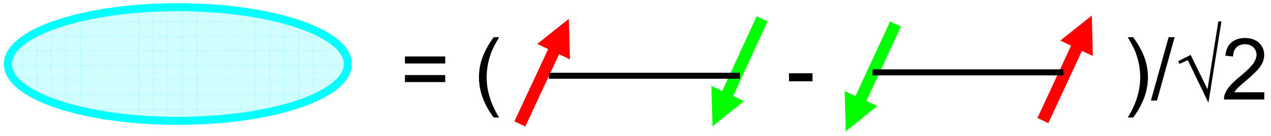


antiferromagnetic order

Strong Modulations→ Singlets

$J_m » J$



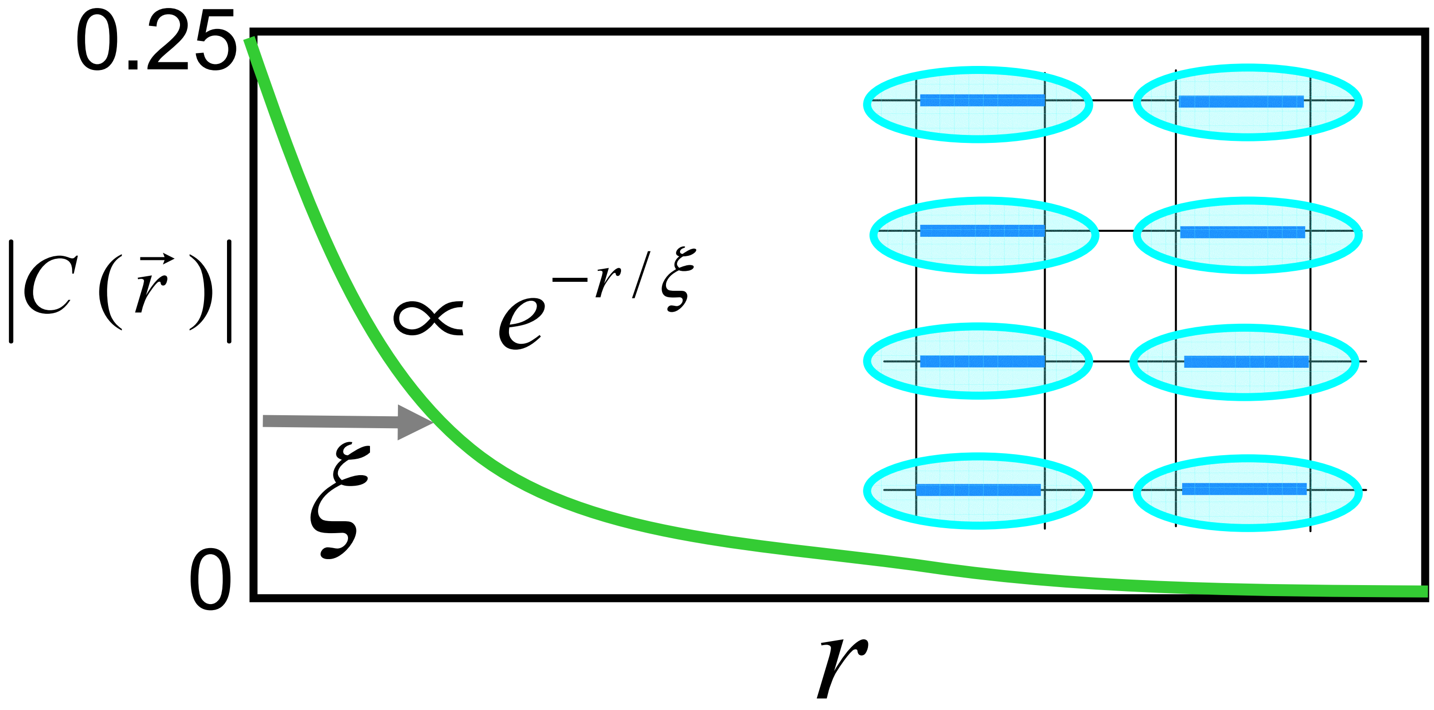


Spin Liquid

No long range magnetic order

Finite correlation length

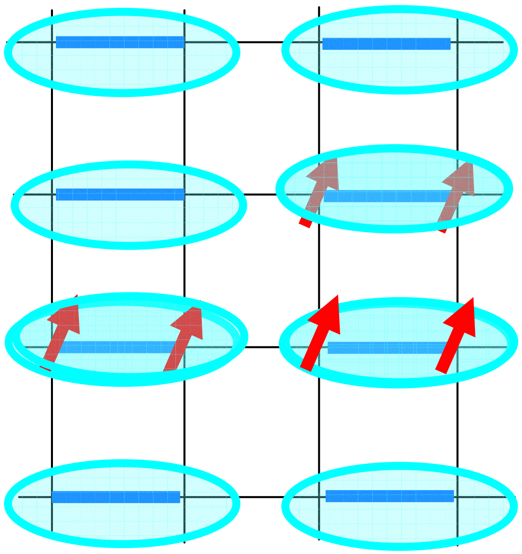
$$C(\vec{r}) = \left\langle \vec{S}(\vec{r}) \cdot \vec{S}(0) \right\rangle$$



Spin Liquid

Finite energy gap to magnetic excitations (spin gap)

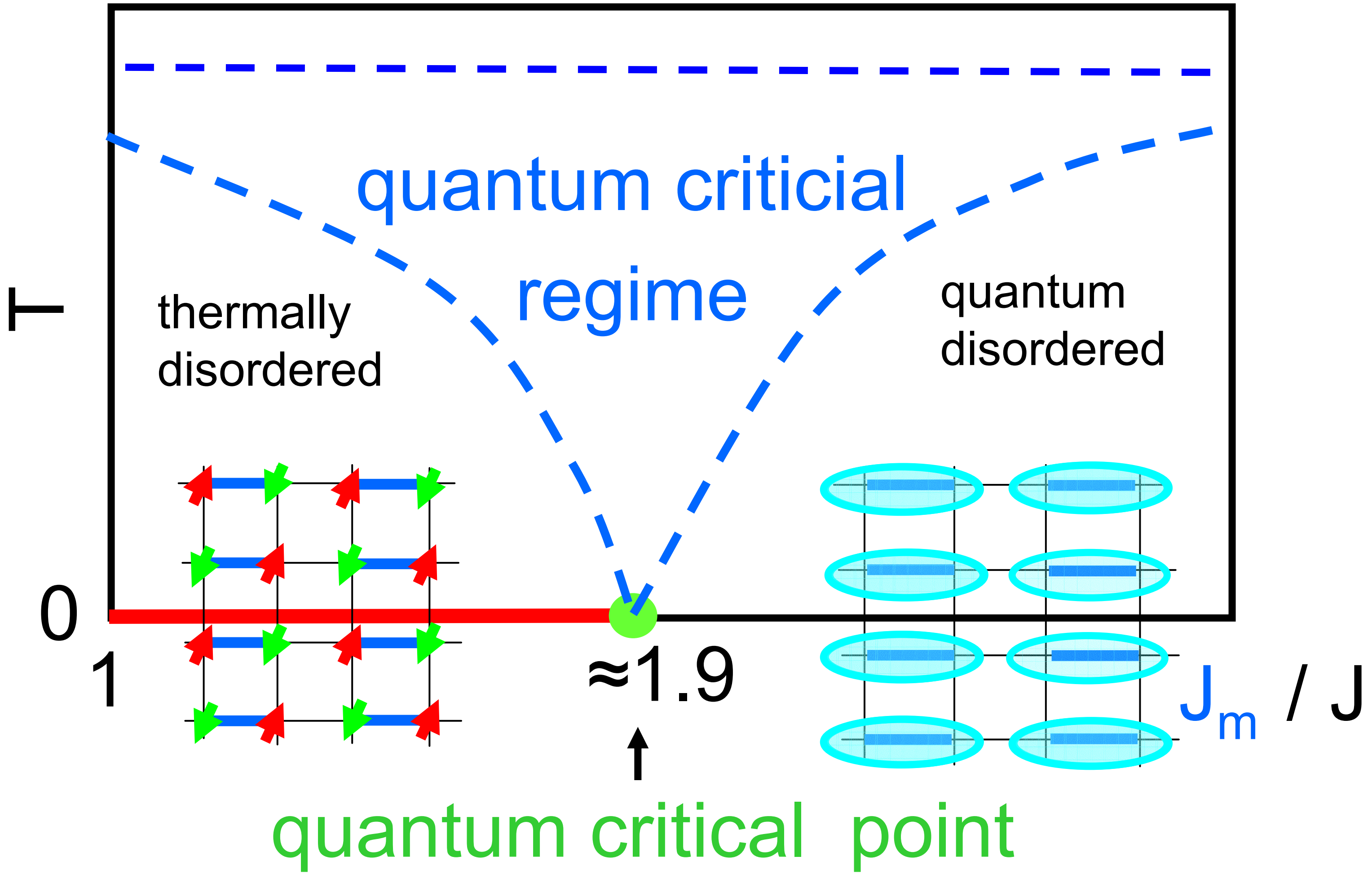
- breaking up a singlet



triplet

→ triplons

Phase Diagram



quantum criticial regime

T

thermally disordered

quantum disordered

0

1

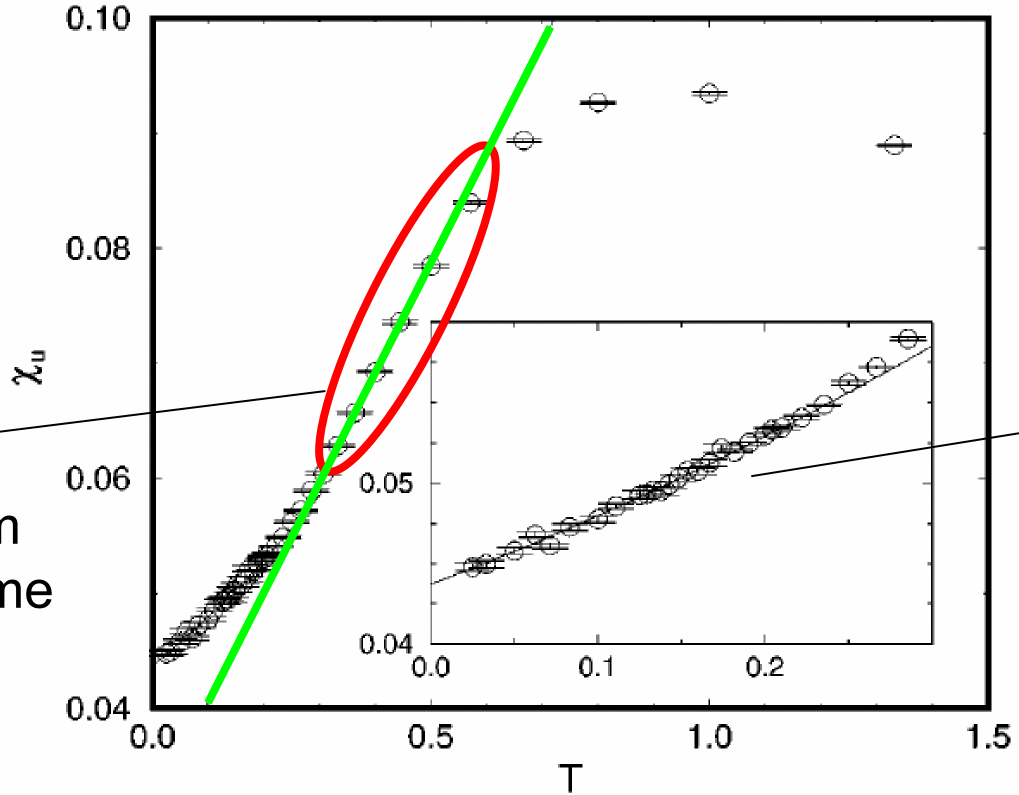
≈1.9

J_m / J

quantum critical point

Quantum Critical Scaling

Uniform susceptibility of the uniform Heisenberg model



T-linear scaling in the quantum critical regime

Scaling in the low-T thermally disordered regime

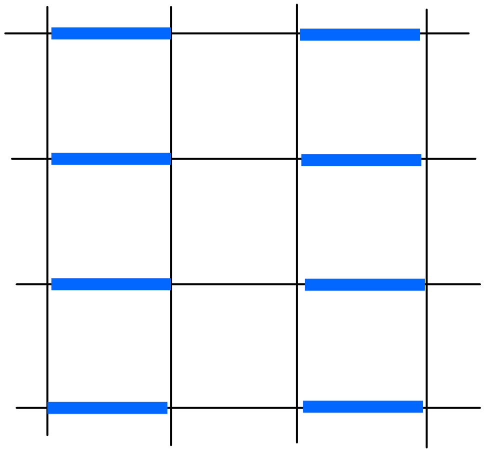
Kim, Troyer PRL (98)

Universality Class of the QCP

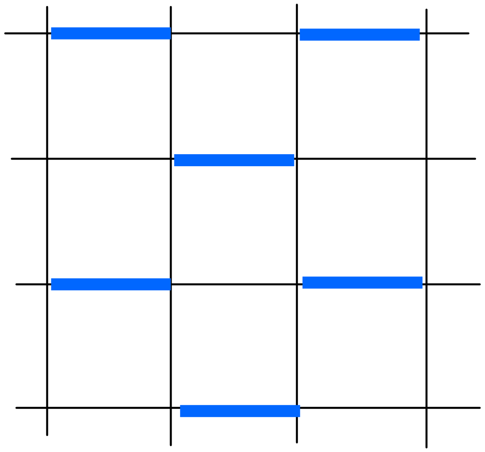
Quantum-classical mapping:

QPT is in the 3D O(3) universality class

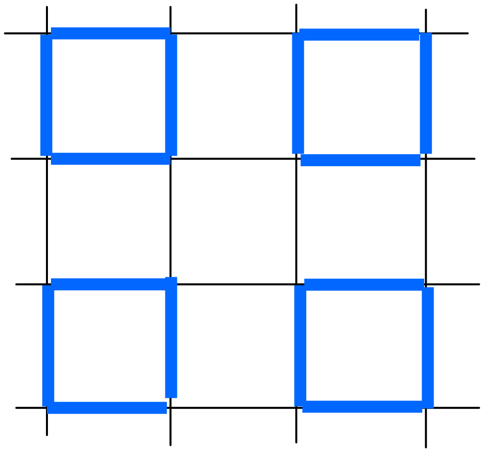
Recent Quantum Monte Carlo results call this into question:



3D O(3)



????

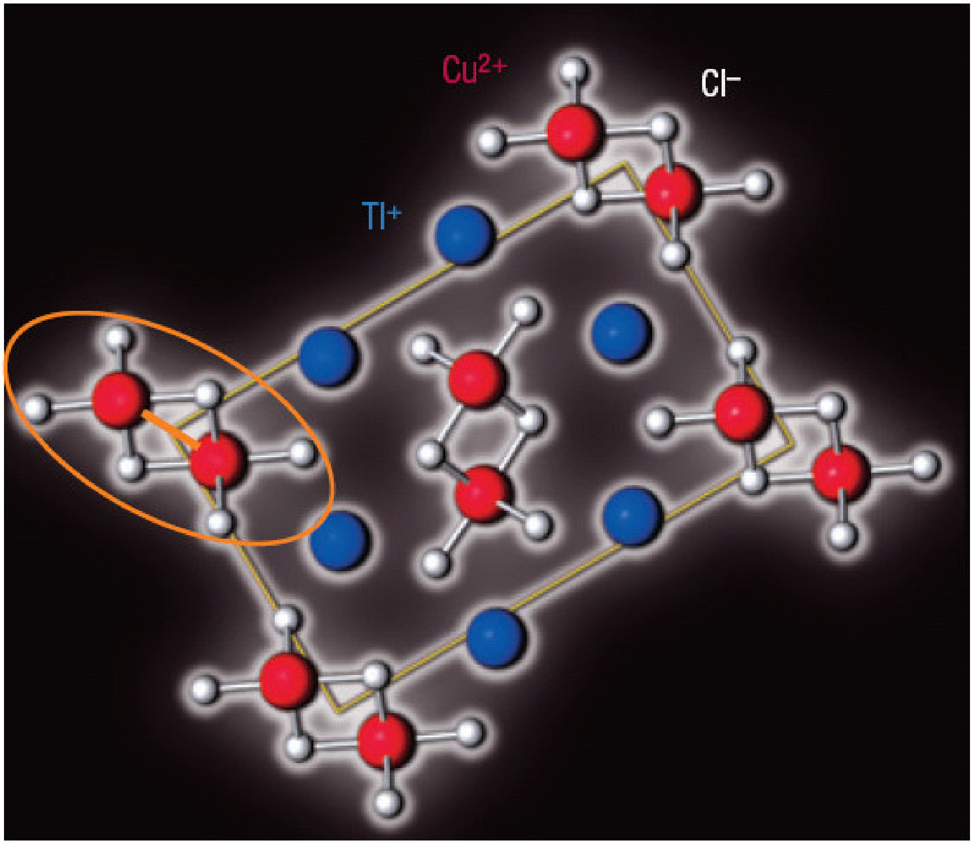


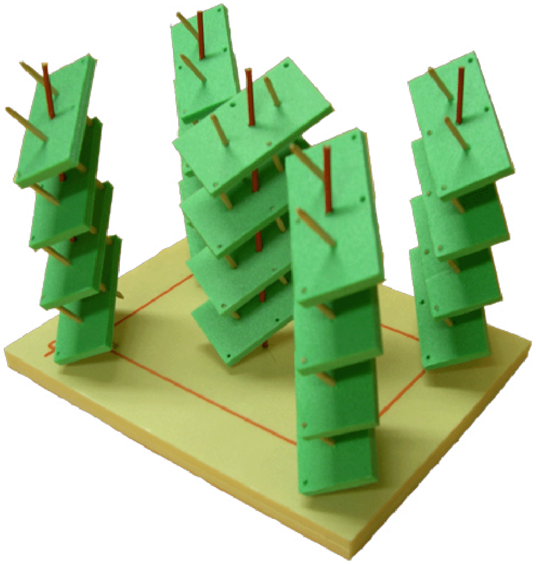
3D O(3)

Topological effect from Berry-phases in the quantum action?

Experimental Realization

$TlCuCl_3$ – a 3D array of coupled spin dimers

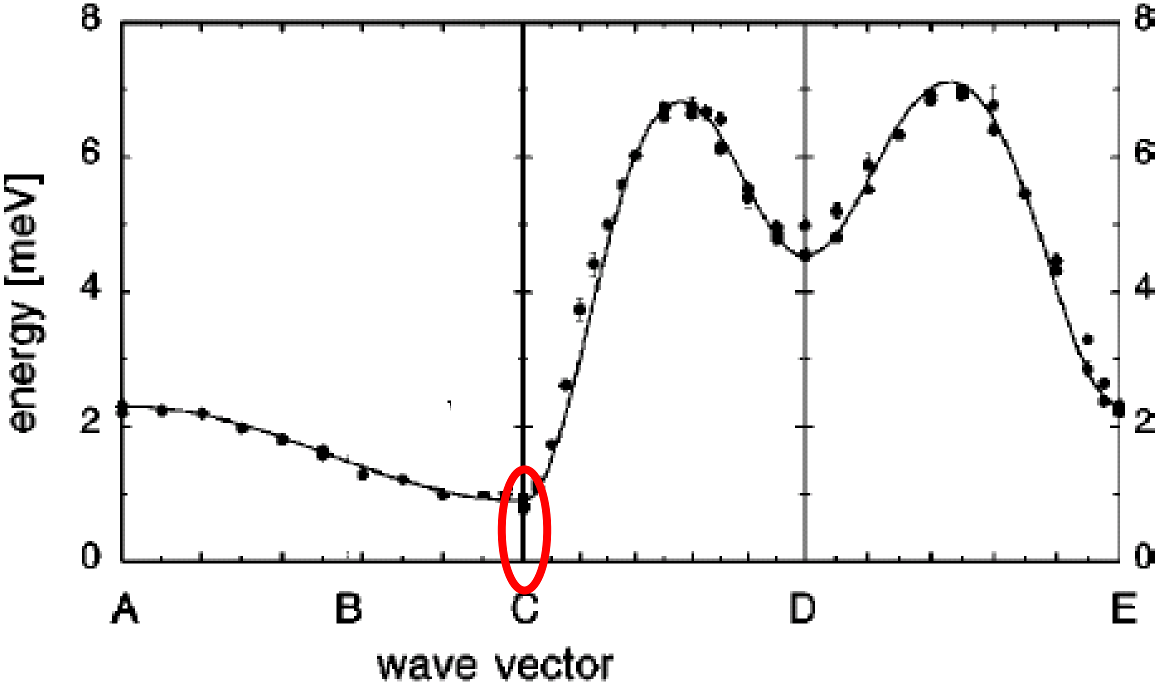


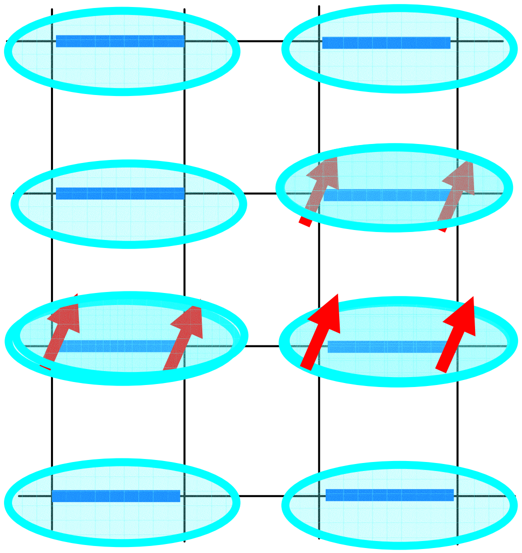


Spin gap ≈ 0.8 meV ≈ 8 K

Triplon Excitations

Neutron scattering

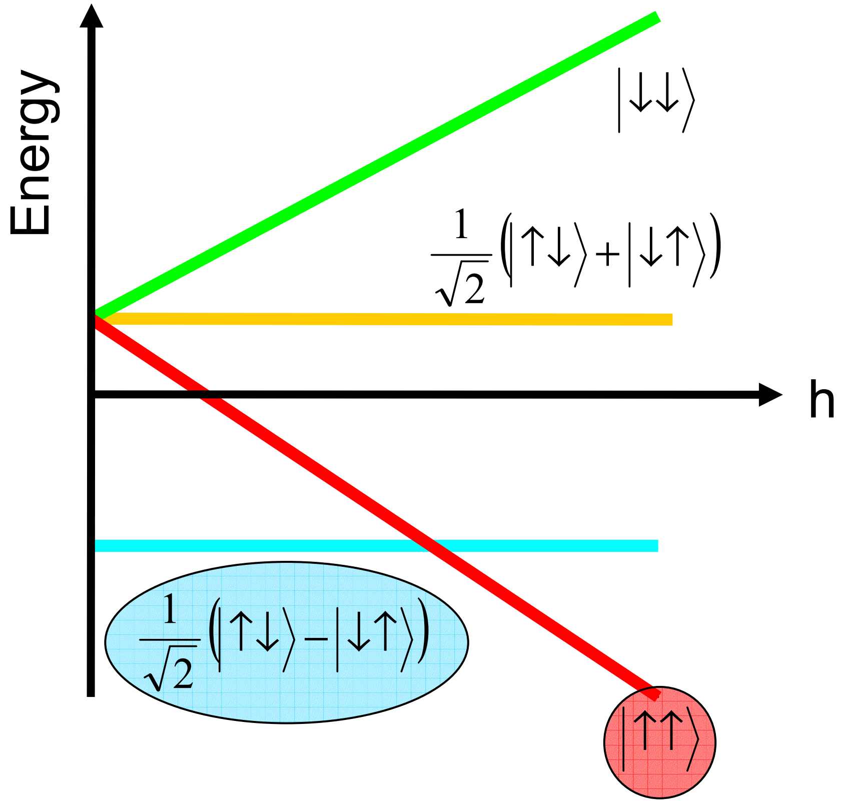


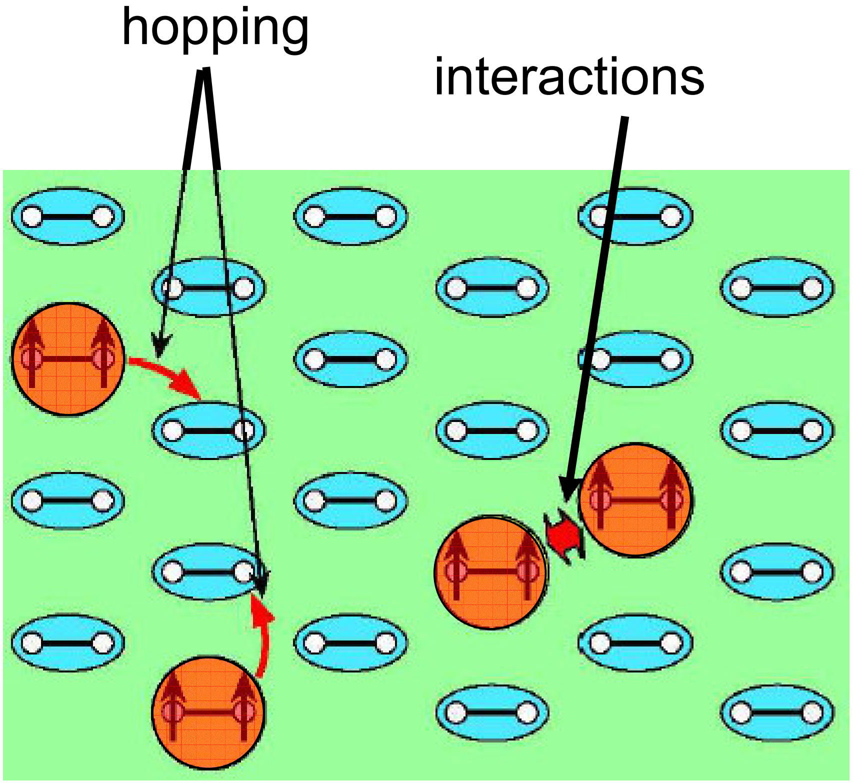


N. Cavadini et al., PRB 2001

Magnetic Field Driven QPT

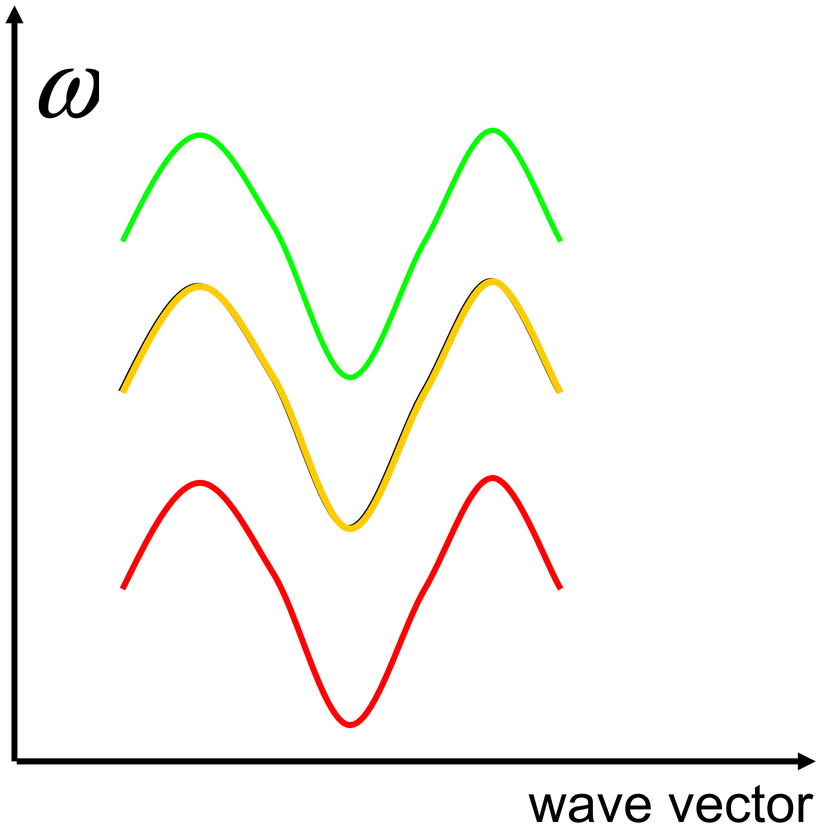
Coupled dimers

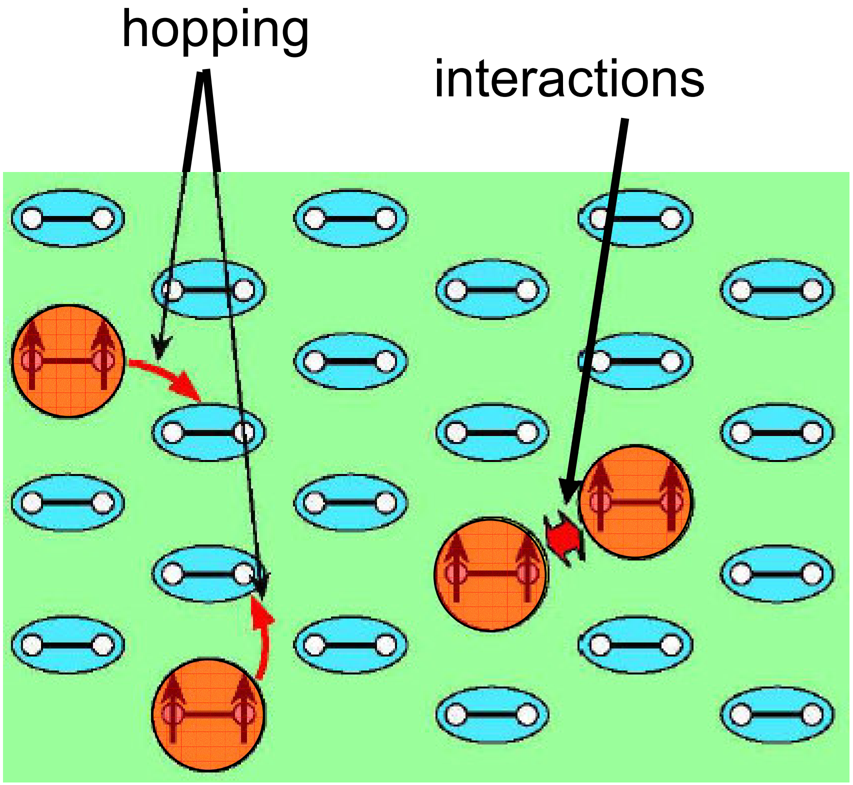




Magnetic Field Driven QPT

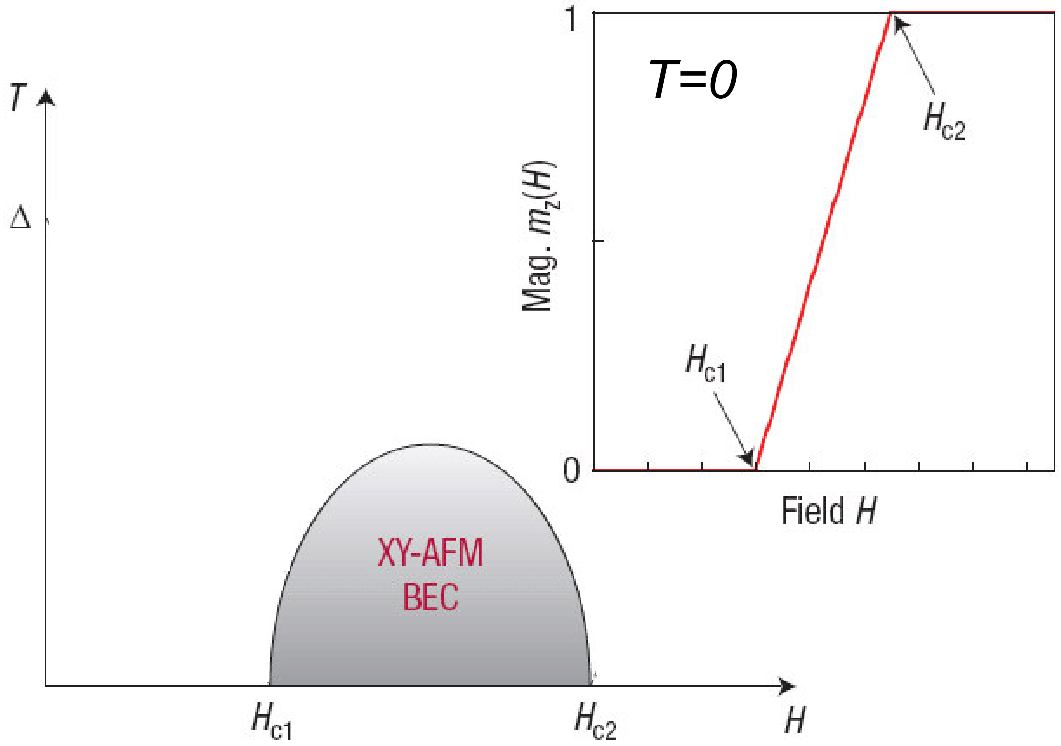
Coupled dimers



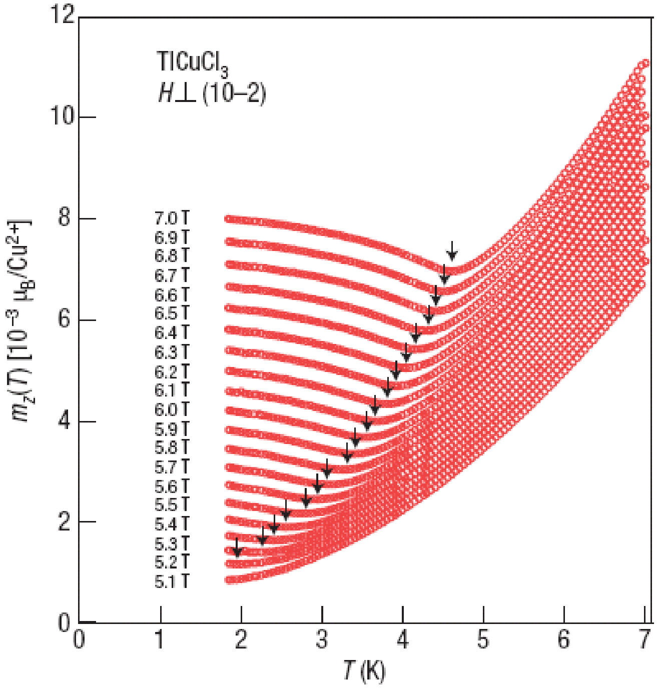


Magnetic Phase Diagram

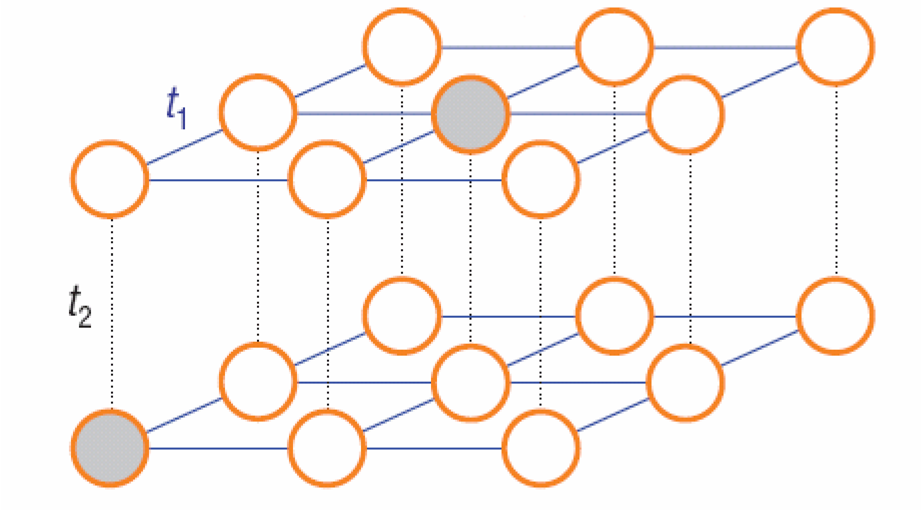
BEC of Triplons

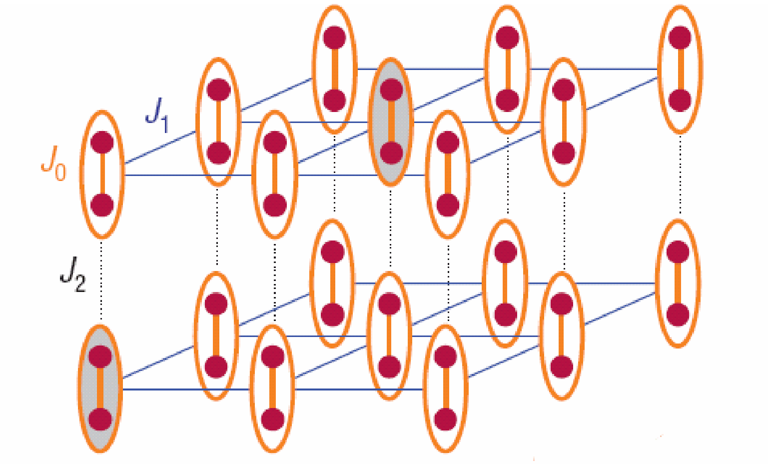


Magnetization curves



BEC of Triplons

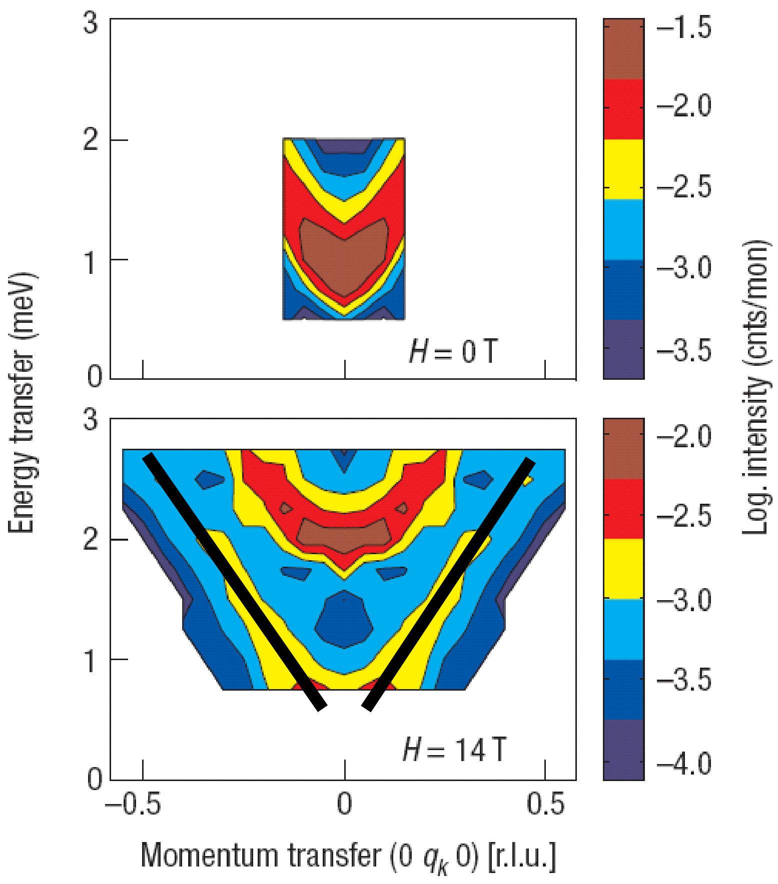


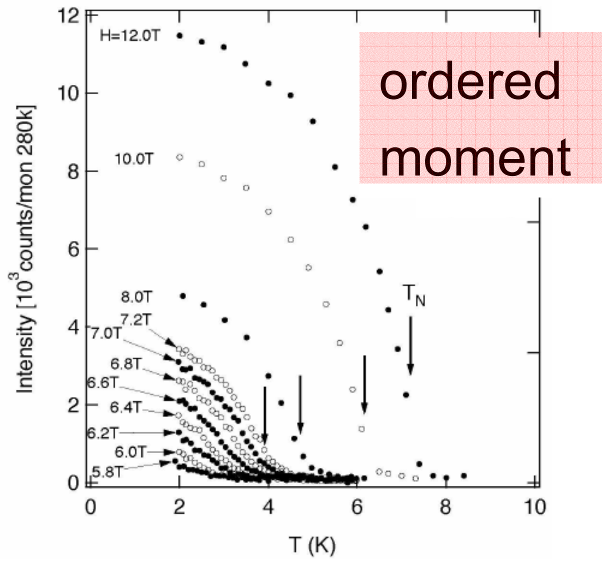


Bose gas	Antiferromagnet
Particles	Spin excitations ($S=1$ quasiparticles)
Boson number N	Spin component S^z
Charge conservation $U(1)$	Rotational invariance $O(2)$
Condensate wavefunction $\langle \psi(\mathbf{r}) \rangle$	Transverse magnetic order $\langle S_i^x + iS_i^y \rangle$
Chemical potential μ	Magnetic field H
Superfluid density ρ_s	Transverse spin stiffness
Mott insulating state	Magnetization plateau

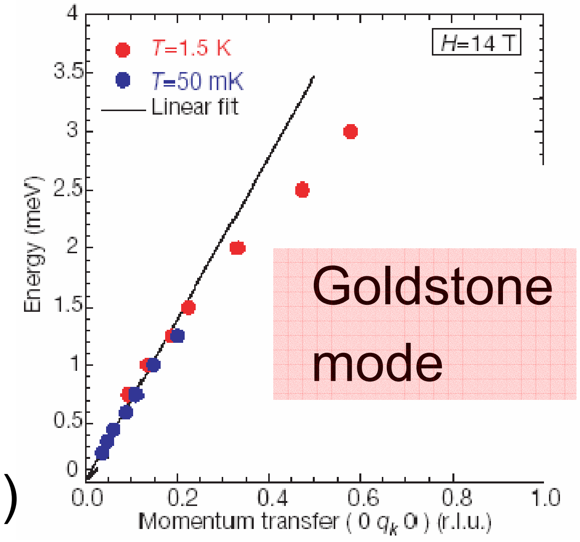
Magnetic Order and Excitations

Neutron scattering





ordered moment



Goldstone mode

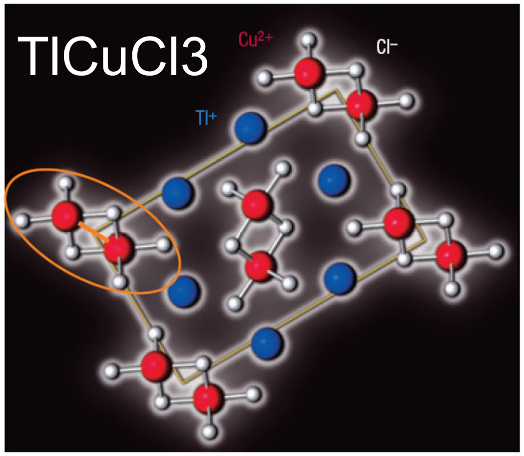
C. Ruegg et al., Nature (2003)

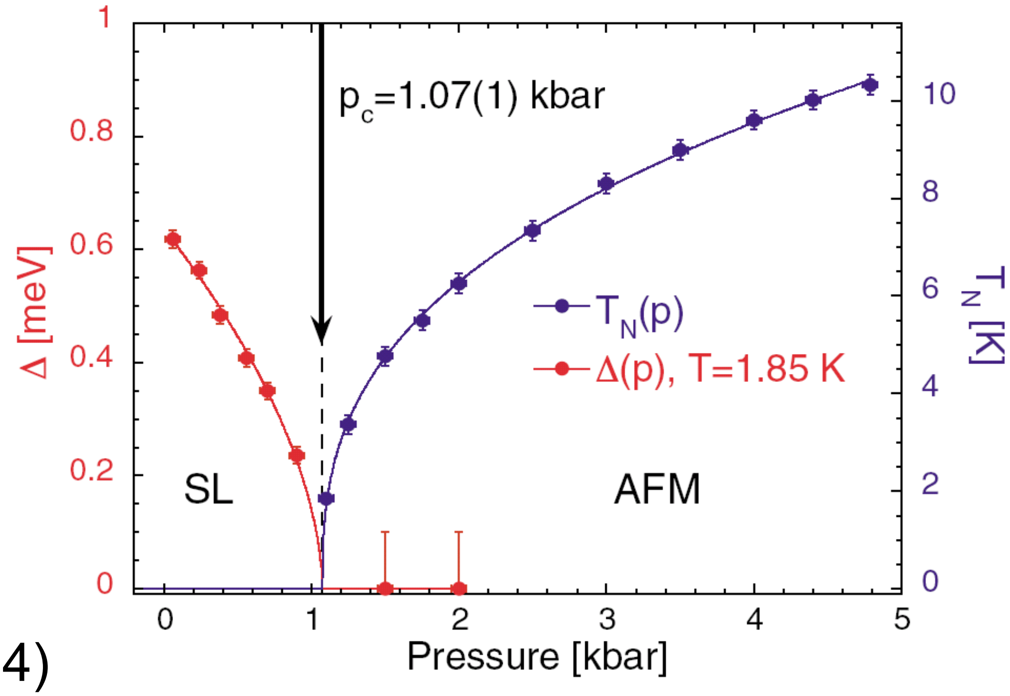
Pressure Driven QPT

- Pressure modifies the exchange constants

  Inter-dimer exchange enhanced

- Can drive a pressure induced QPT to an ordered state

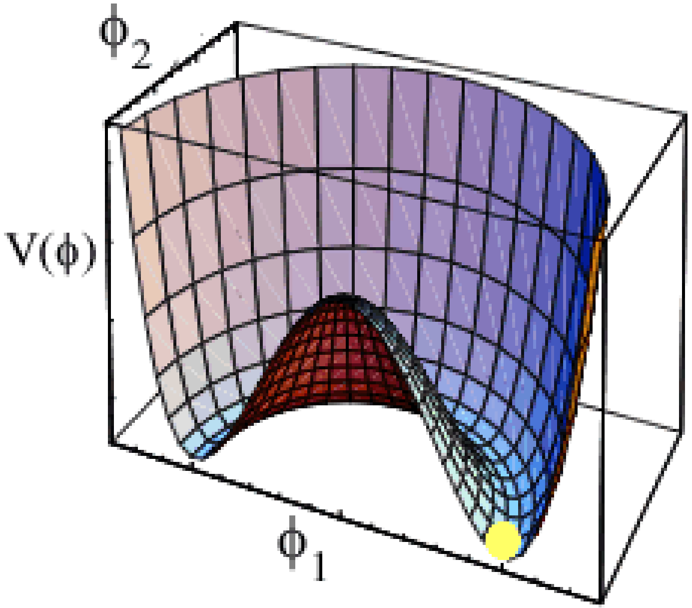


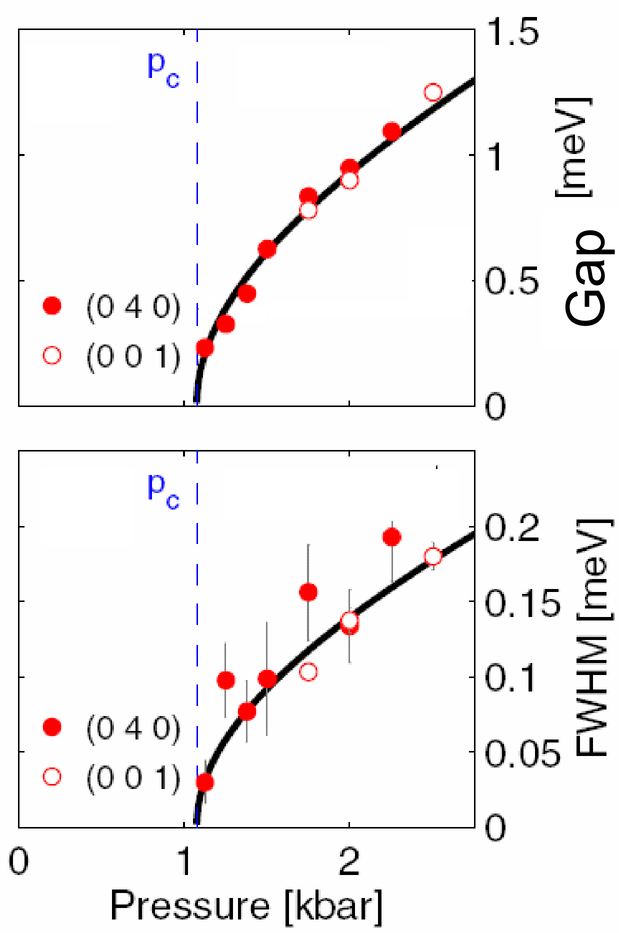


C. Ruegg et al., PRL (2004)

Excitations

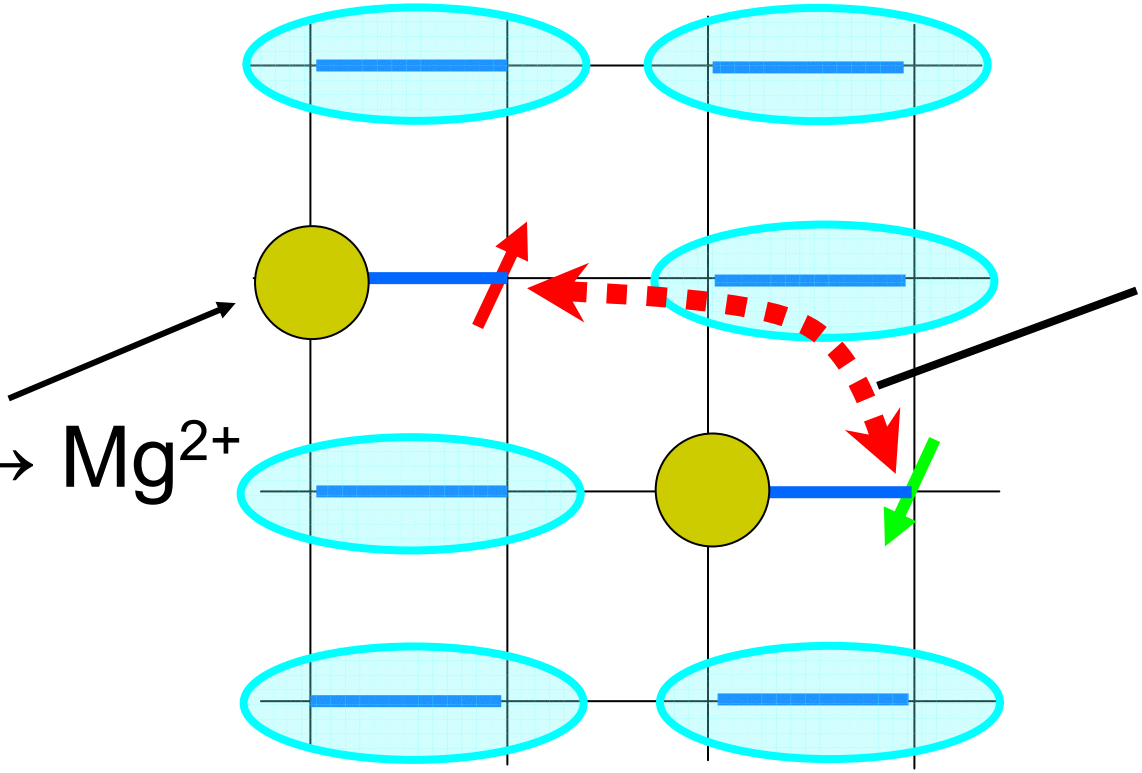
- Gapped longitudinal mode emerges in the ordered phase
  - Amplitude modulations





C. Ruegg et al., PRL (2008)

Impurities in Spin Liquids

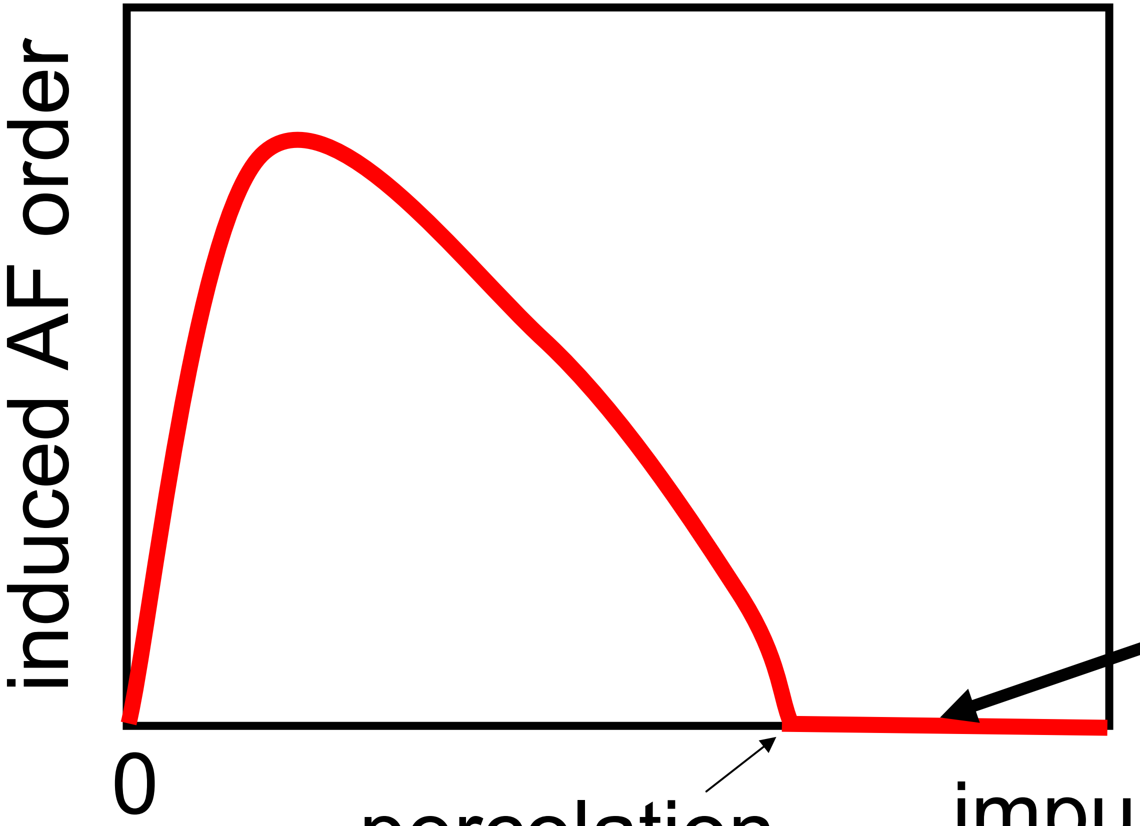


weak
coupling

$Cu^{2+} \rightarrow Mg^{2+}$

„dangling spins“

Order by Disorder



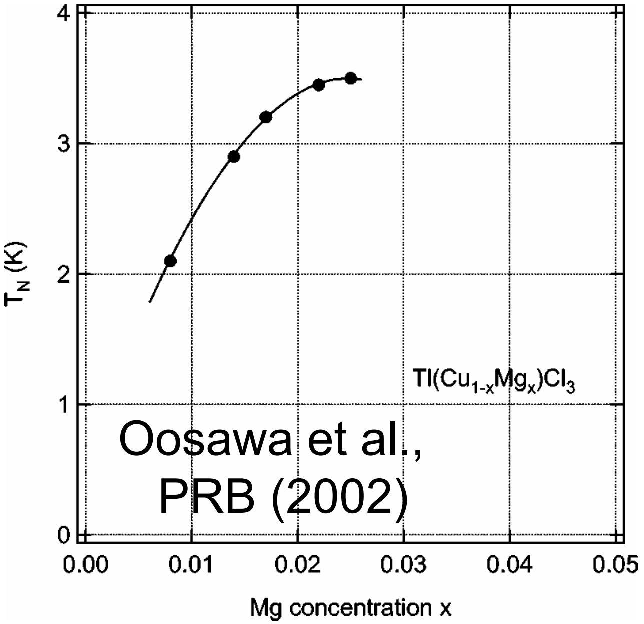
induced AF order

0

percolation treshold

impurity concentration

only finite clusters



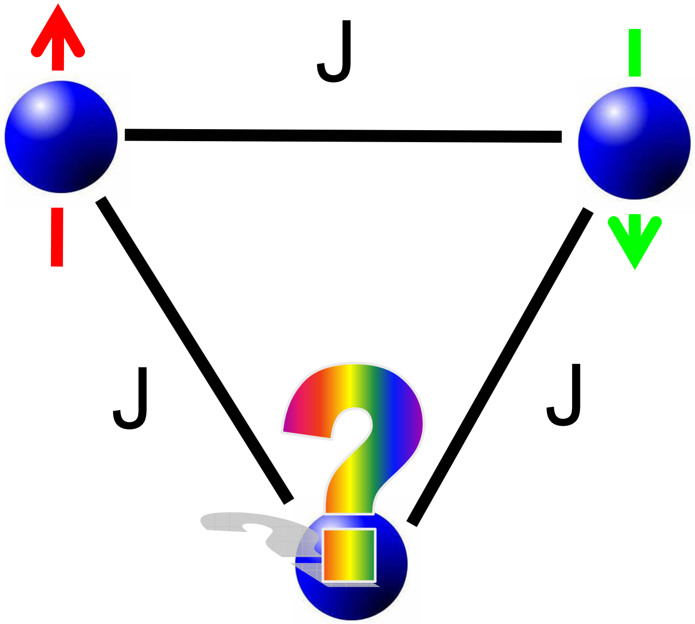
Oosawa et al., PRB (2002)

Outline

- Quantum vs. Thermal Phase Transitions
  - Critical phenomena
  - Quantum criticality
  - Example: Transverse-field Ising model

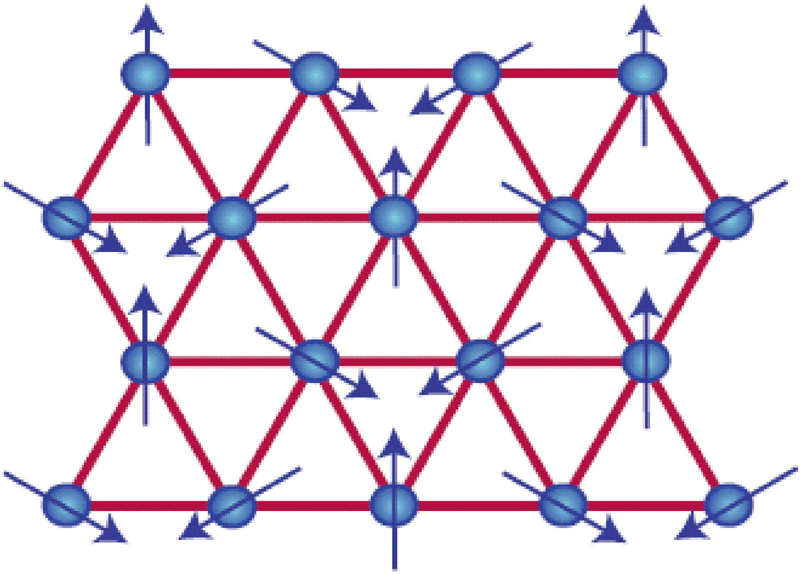
- Quantum Magnetism
  - Quantum Heisenberg model
  - Spin dimers and spin liquids
  - Magnetic-field-induced BEC of triplons
  - Pressure-induced QPT
  - Impurity effects

- Exotic Phases and Criticality
  - Frustration
  - Exotic quantum phases
  - Deconfined quantum critical points



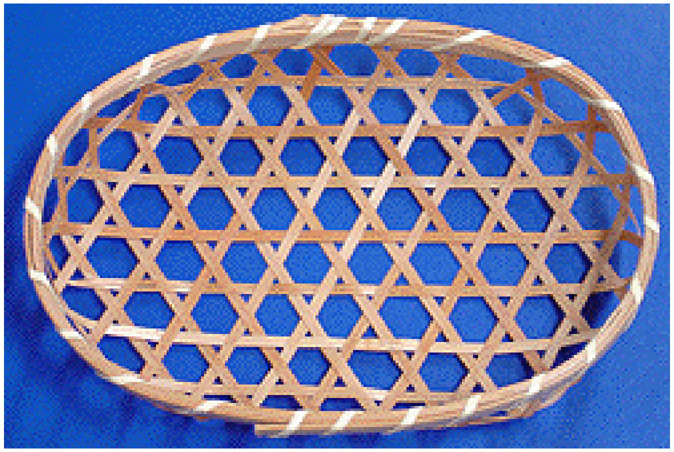
Frustrated Quantum Spins

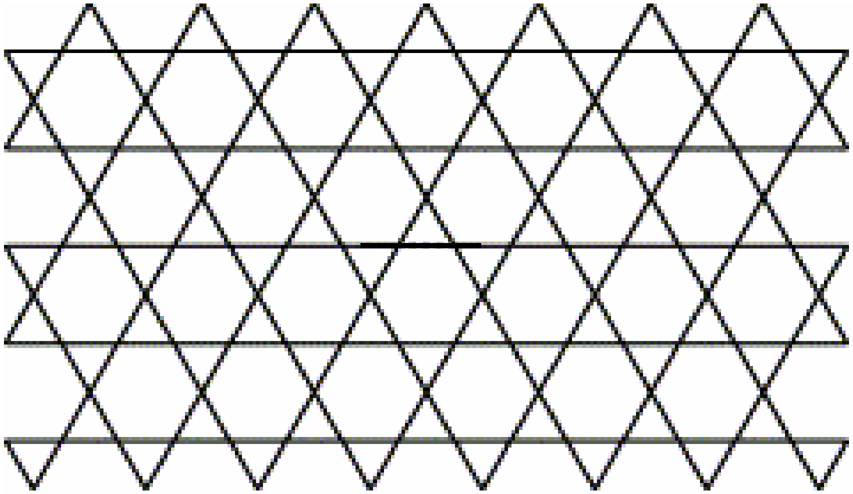
- Triangular lattice: Long range order survives quantum fluctuations (in theory…)



κ-$(ET)_2Cu_2(CN)_3$: no long range order down to 5mK

Kagome Lattice





No long-range order
No apparent spin gap

What is the nature of the magnetic ground state?

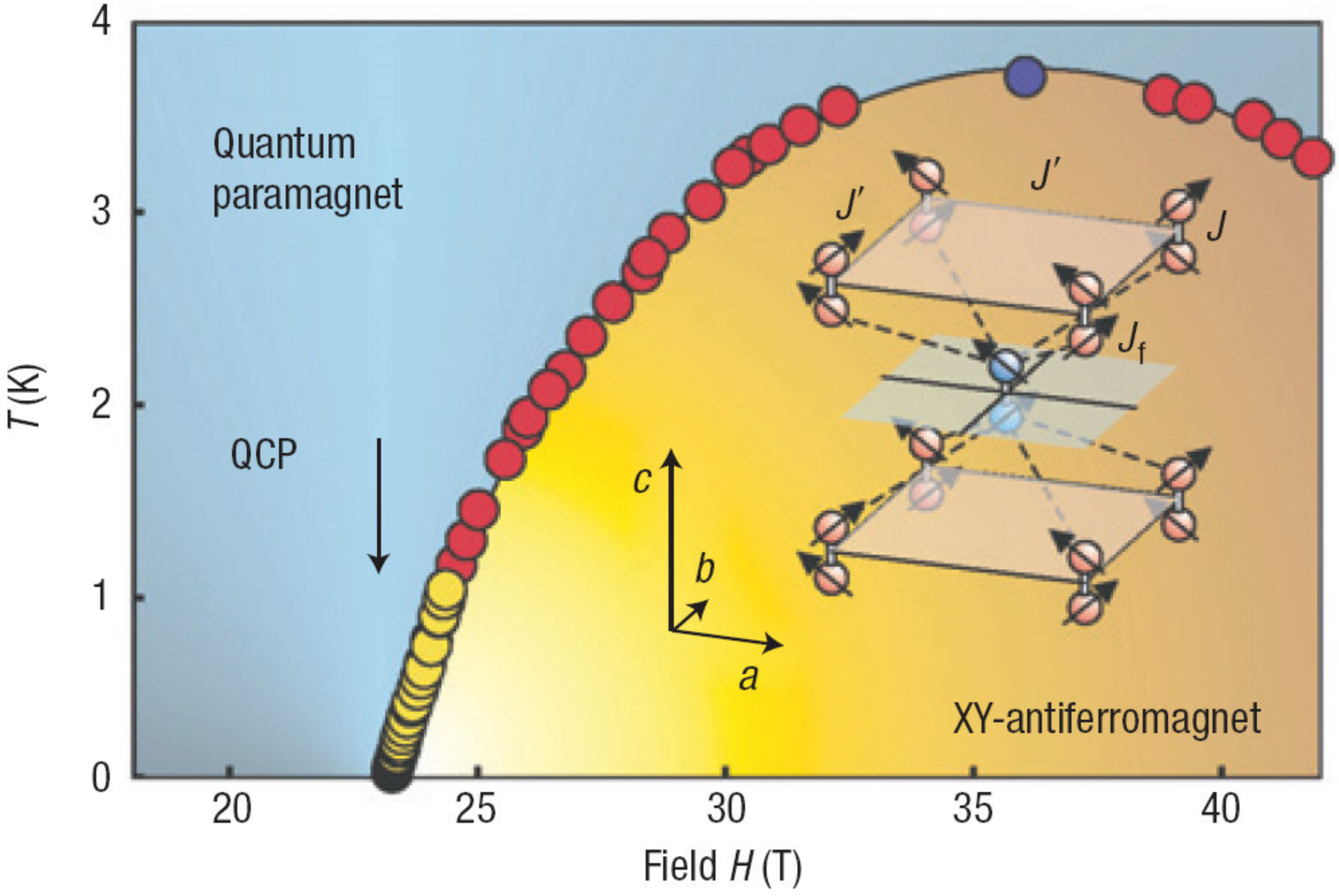
$ZnCu_3(OH)_6Cl_2$

Dimensional Reduction

at a QCP - driven by frustration

$BaCuSi_2O_6$

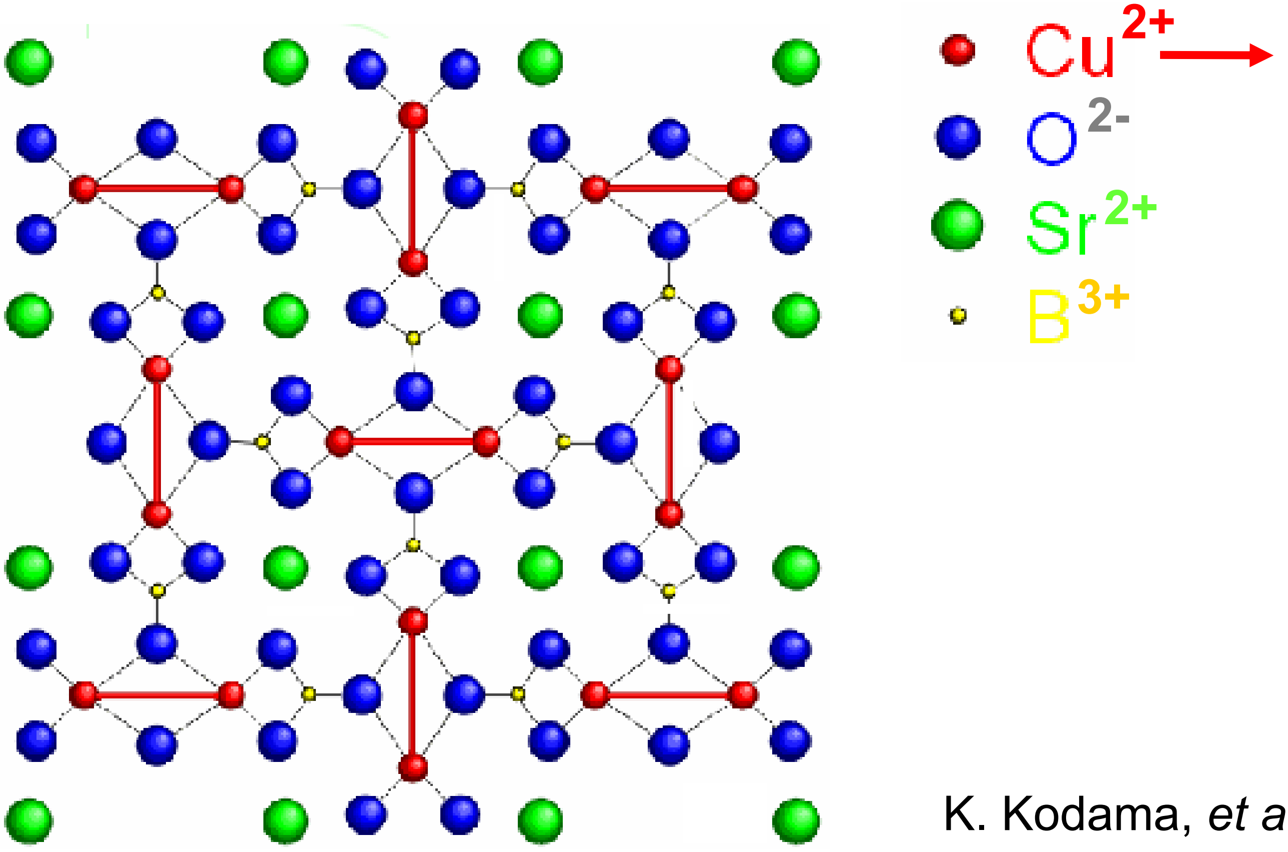
Han purple pigment



S. Sebastian et al., Nature 2006

Another Prominent Example

$SrCu_2(BO_3)_2$

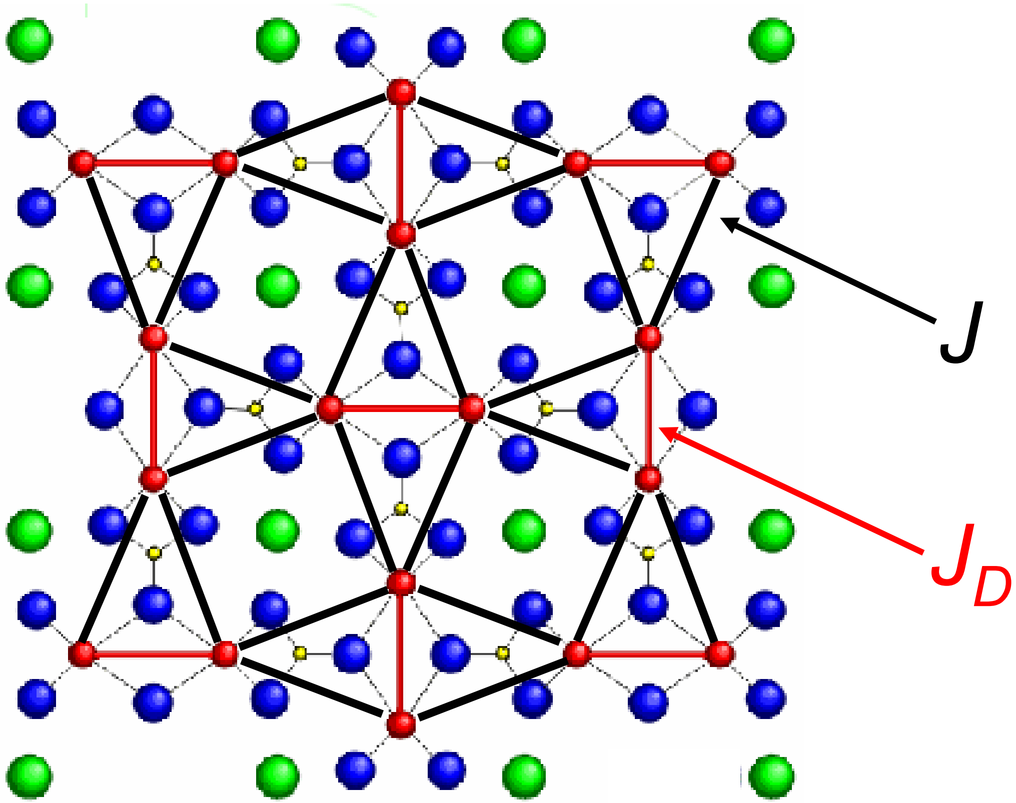


spin-1/2

K. Kodama, *et al.,* Science (2002)

Orthogonal Spin Dimers

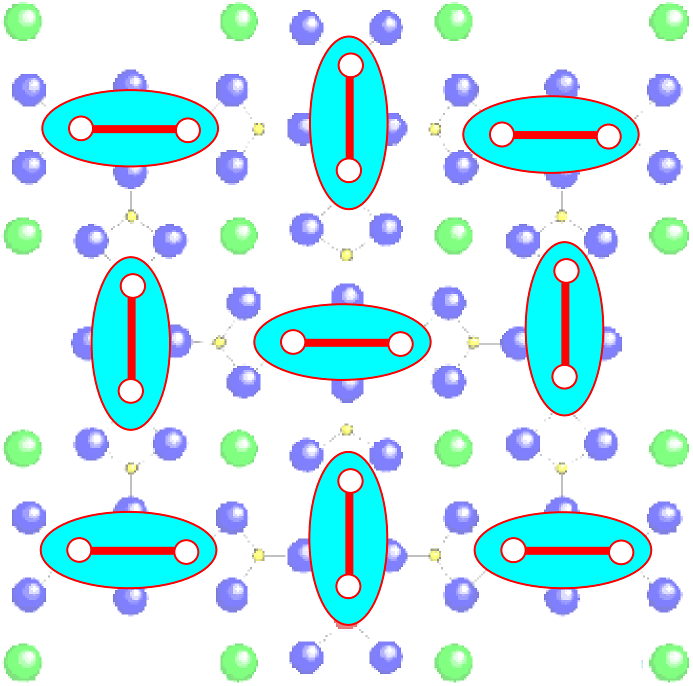
Strong quantum fluctuations + frustration



$J_D / J \approx 1.57$

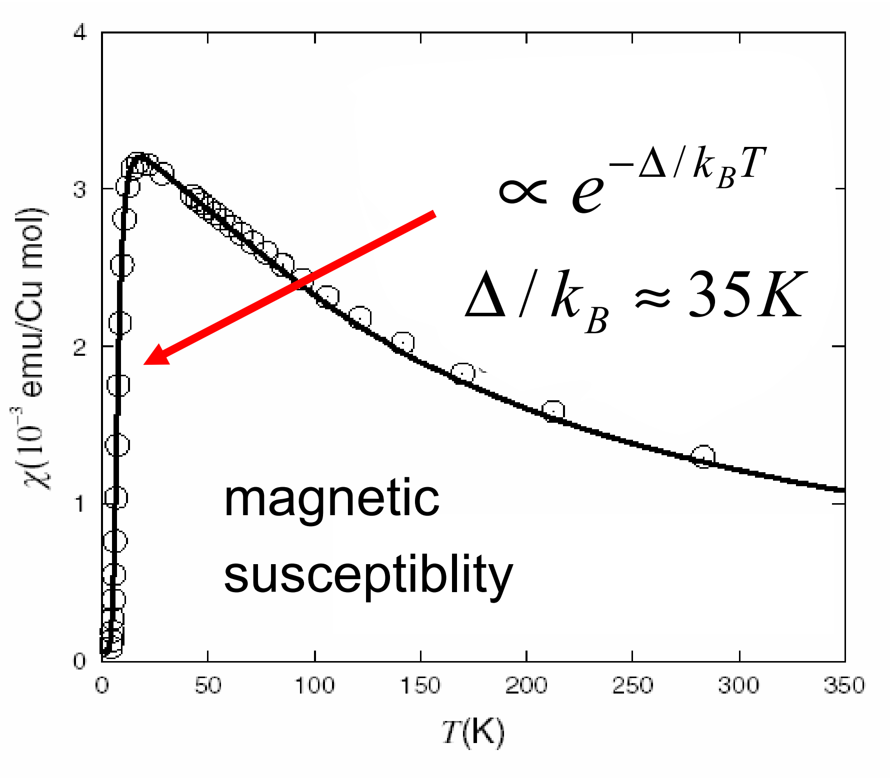
Exact Ground State

Singlet product state: $\left|\Psi_0\right\rangle = \prod_{\text{dimers}} \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$



Magnetic Excitations

spin gap $\approx 3.5\,\mathrm{meV} \approx 35\,\mathrm{K}$

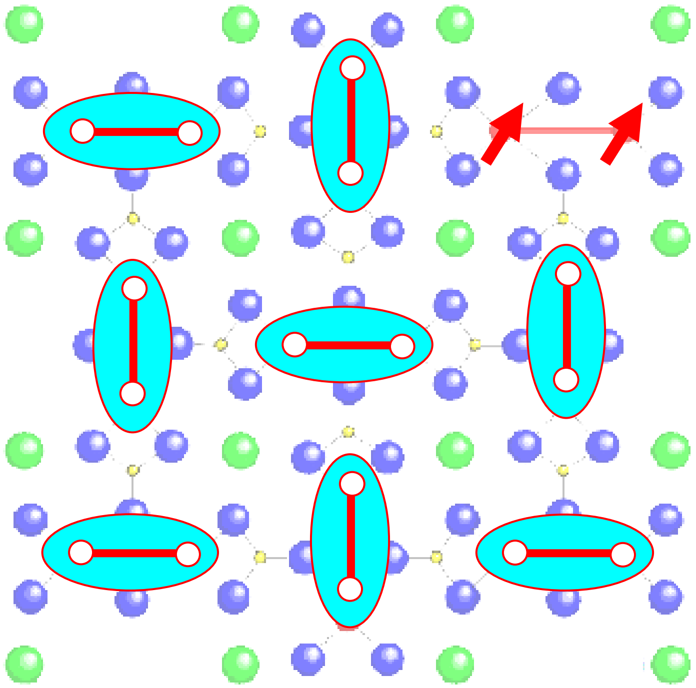


$$\propto e^{-\Delta/k_B T}$$

$$\Delta / k_B \approx 35K$$

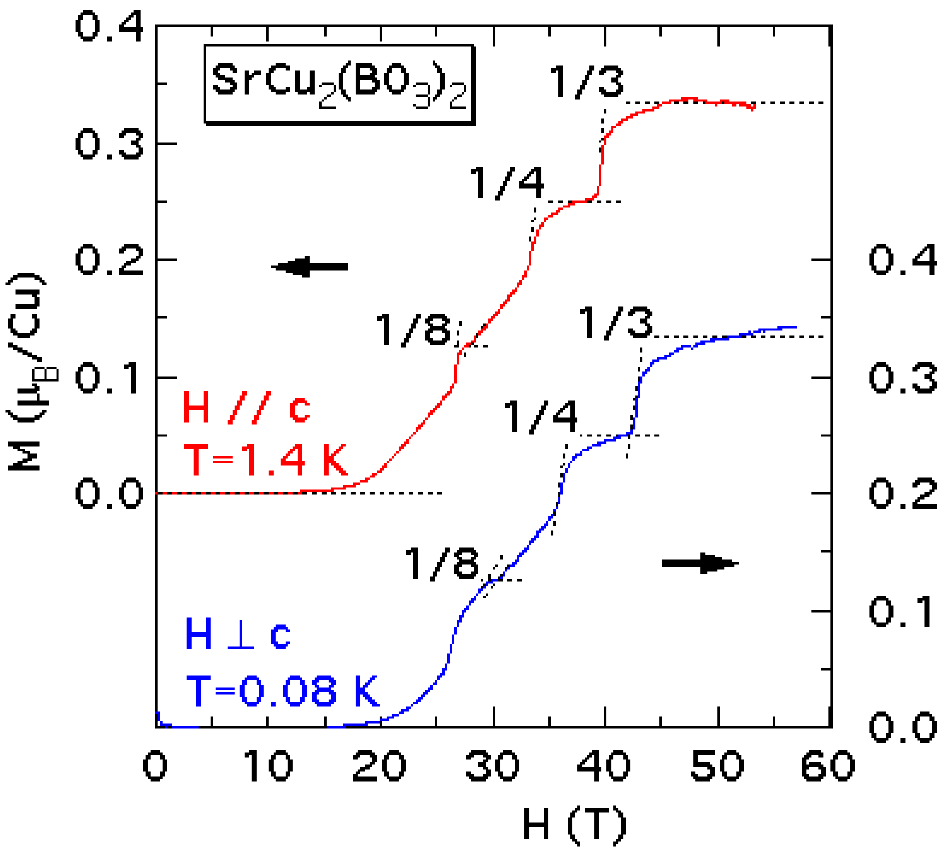
magnetic susceptiblity

lokalized triplets

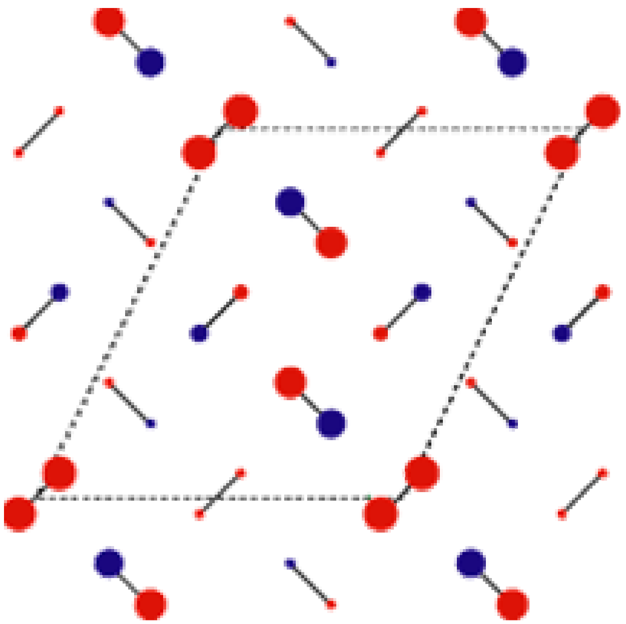


Fractional Magnetization Plateaus

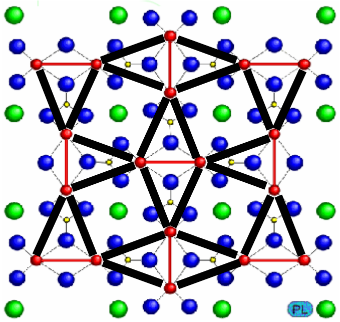
Mott insulator of magnetic excitations



Magnetic super structure at m/m_s=1/8



Quantum Phase Diagram



Maximum frustration

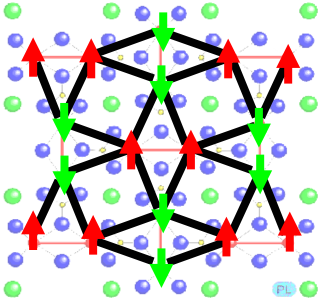
1

?

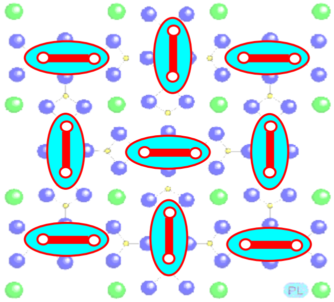
1.5

J_D / J

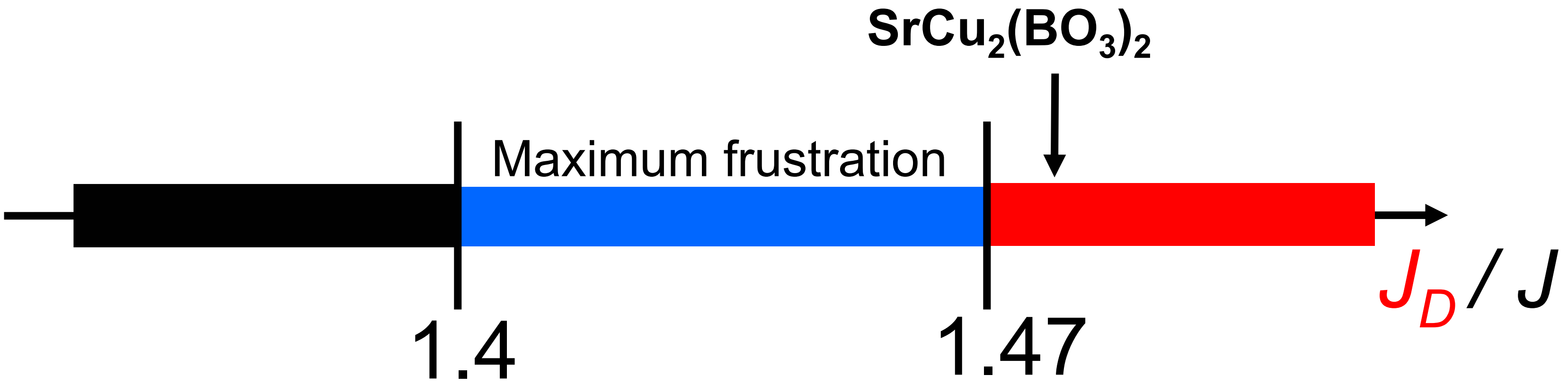
Néel



singlets



New Quantum Phase



$SrCu_2(BO_3)_2$

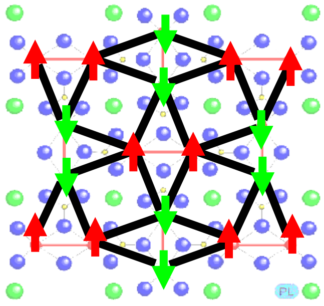
Maximum frustration

1.4

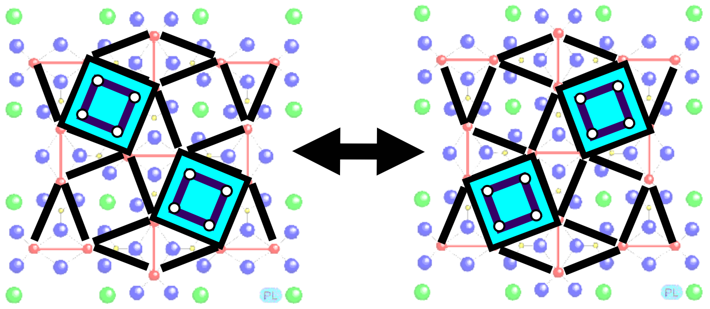
1.47

J_D / J

Néel

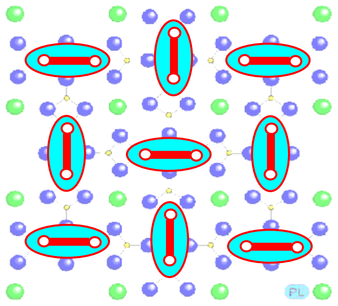


Valence Bond Crystal



Plaquette - ordering

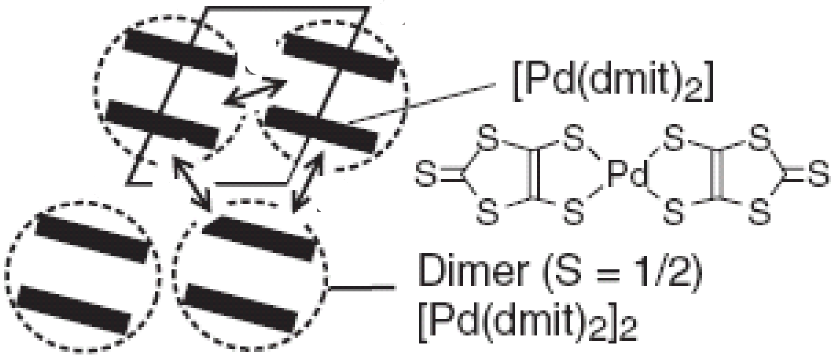
Singlets

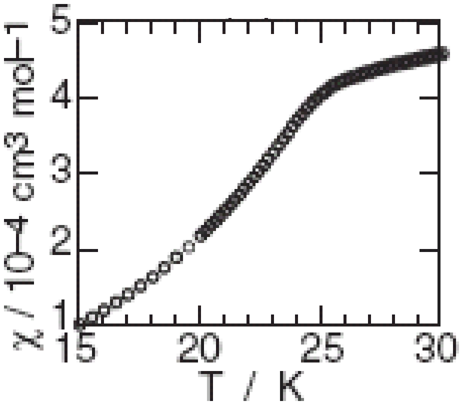


Valence Bond Crystals

- Realized in a number of compounds

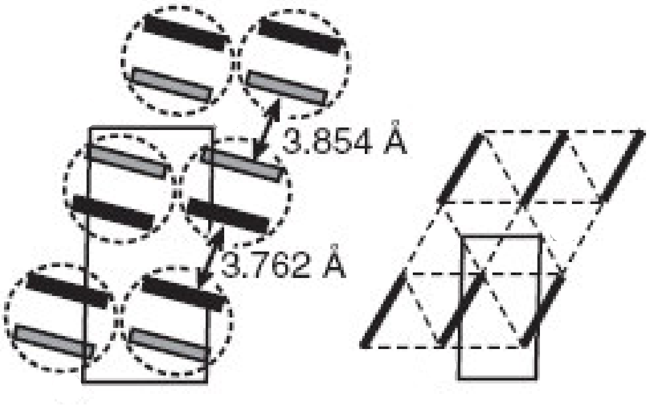
$(C_2H_5)(CH_3)_3P[Pd(dmit)_2]_2$



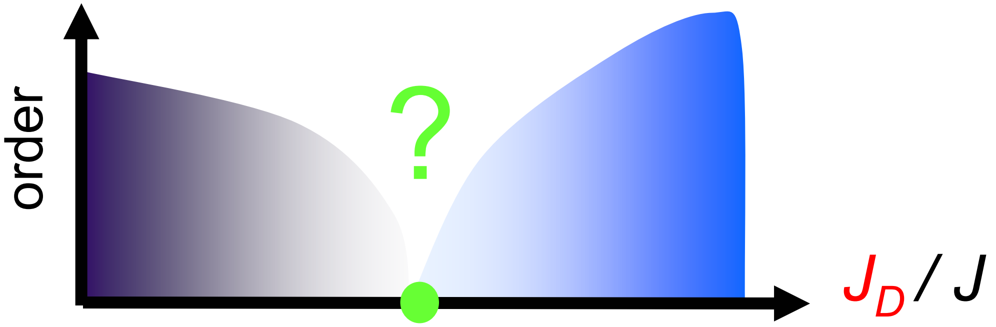


Spontaneous breaking of the lattice symmetry

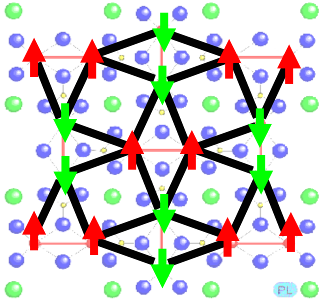
2D Spin-Peierls transition



Continuous Quantum Phase Transition?

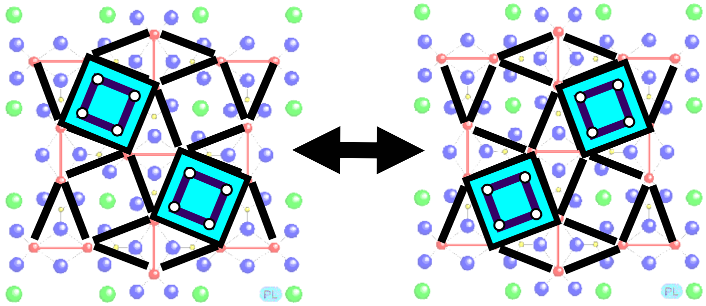


Néel



Spin rotation symmetry spontaneously broken

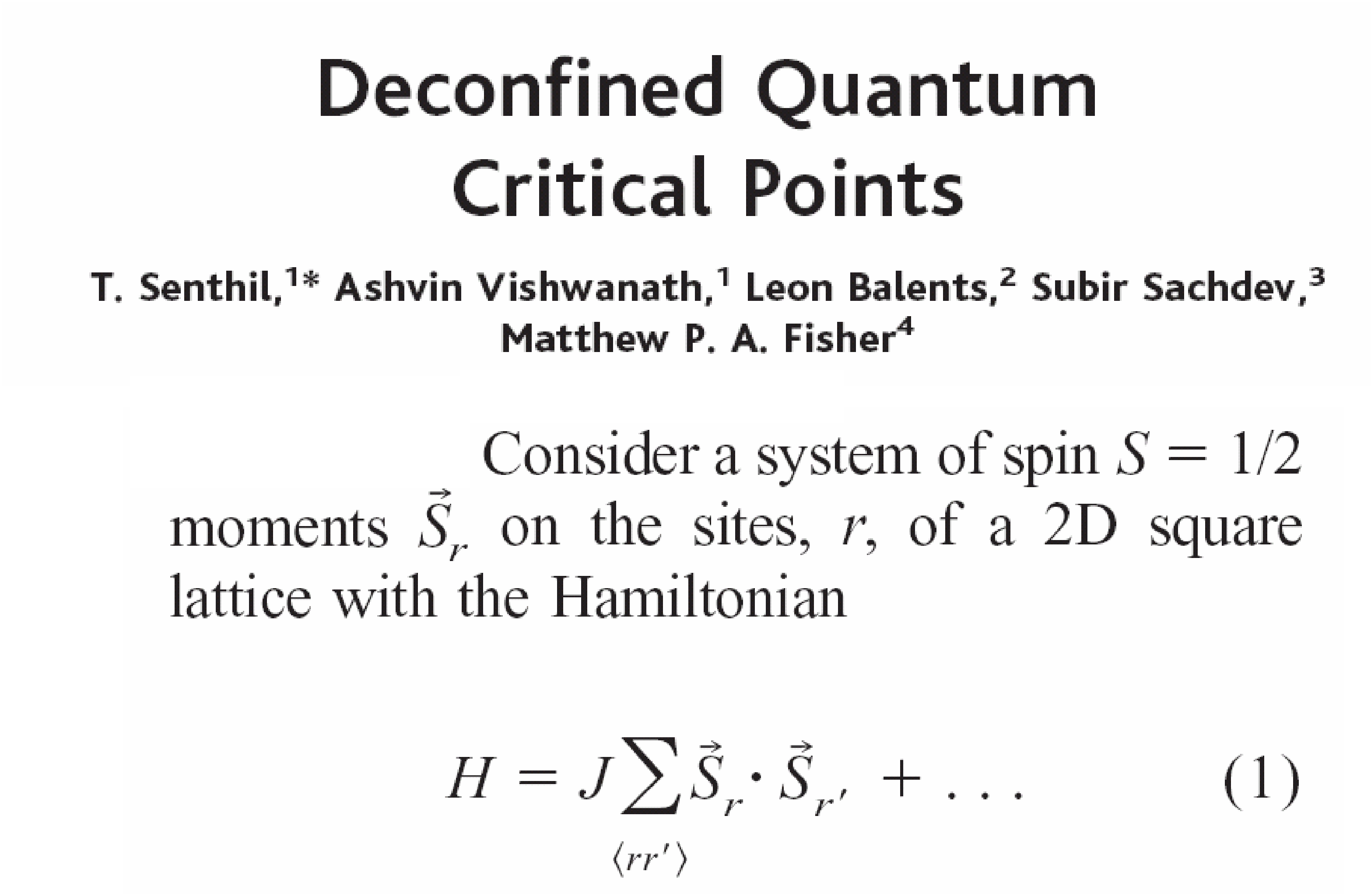
Valence Bond Crystal



Lattice symmetry spontaneously broken

Landau-Ginzburg Theory: generically first-order transition

5 MARCH 2004 VOL 303 SCIENCE www.sciencemag.org



Deconfined Quantum Critical Points

T. Senthil,[1*] Ashvin Vishwanath,[1] Leon Balents,[2] Subir Sachdev,[3] Matthew P. A. Fisher[4]

Consider a system of spin $S = 1/2$ moments $\vec{S}_r$ on the sites, r, of a 2D square lattice with the Hamiltonian

$$H = J \sum_{\langle rr' \rangle} \vec{S}_r \cdot \vec{S}_{r'} + \ldots \qquad (1)$$

Effective Quantum Field Theory

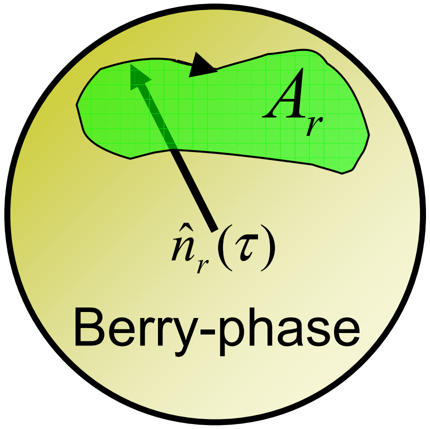
3D Nonlinear sigma-model + Berry-phases

Fluktuations around the Néel-state

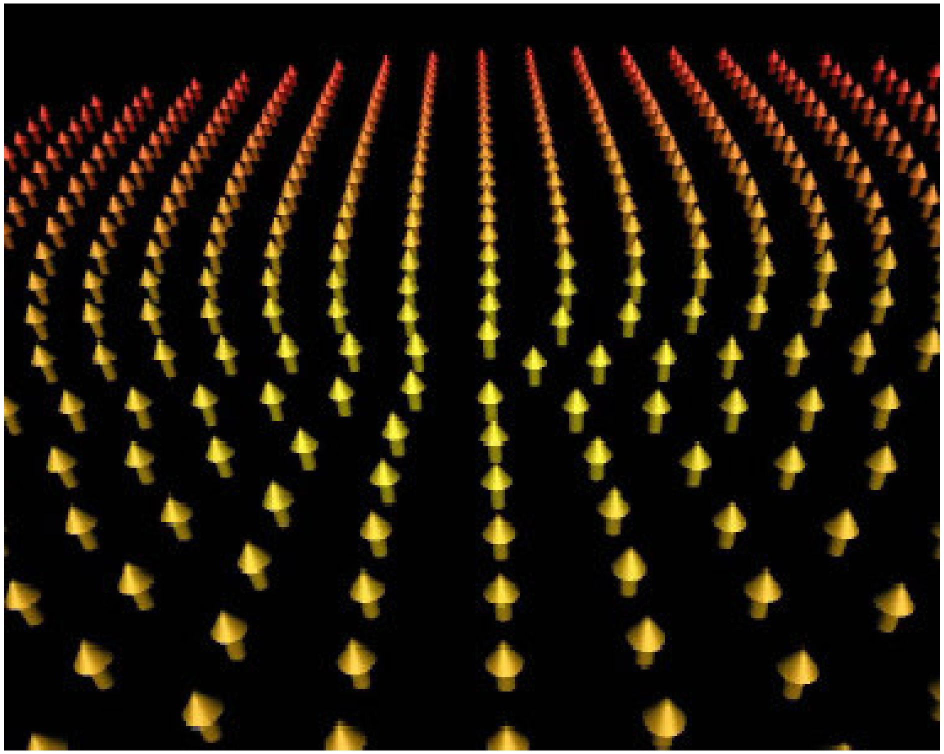
$$S_n = \frac{1}{2g}\int d\tau \int d^2r \left[\left(\frac{\partial \hat{n}}{\partial \tau}\right)^2 + (\nabla_r \hat{n})^2 \right] + iS \sum_r (-1)^r A_r$$

Controlls the strength of the fluctuations

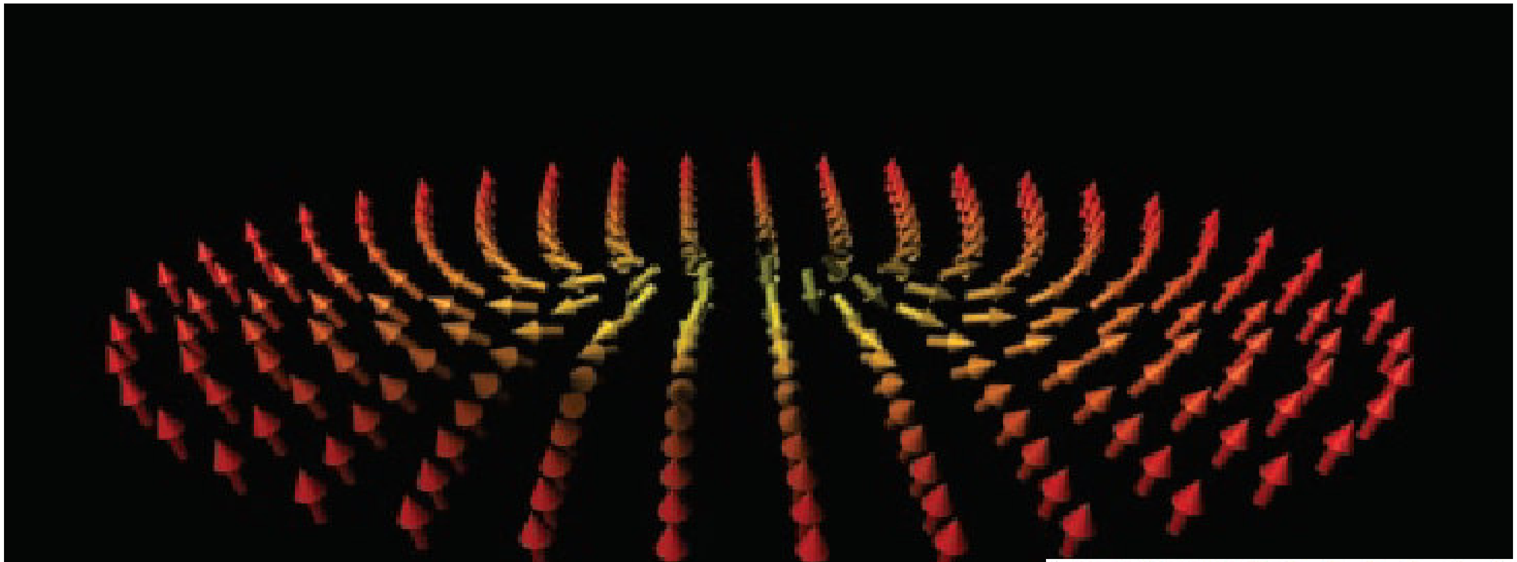
Spin-quantization

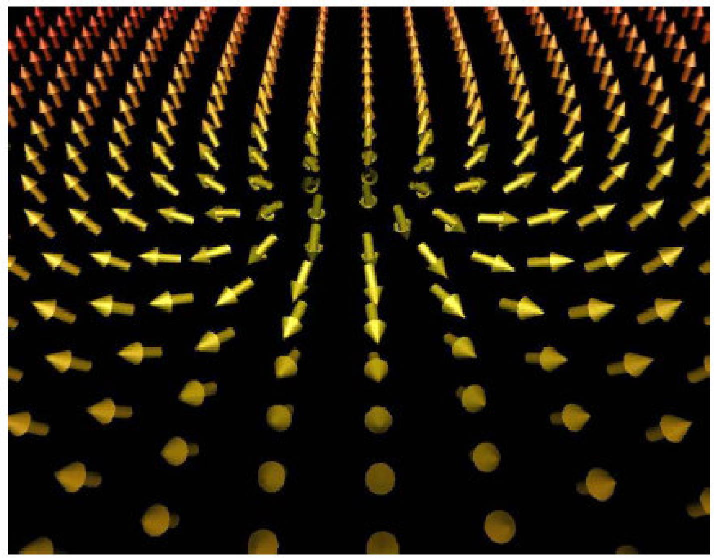


Configuration of the Vector Field



Skyrmion - Configuration

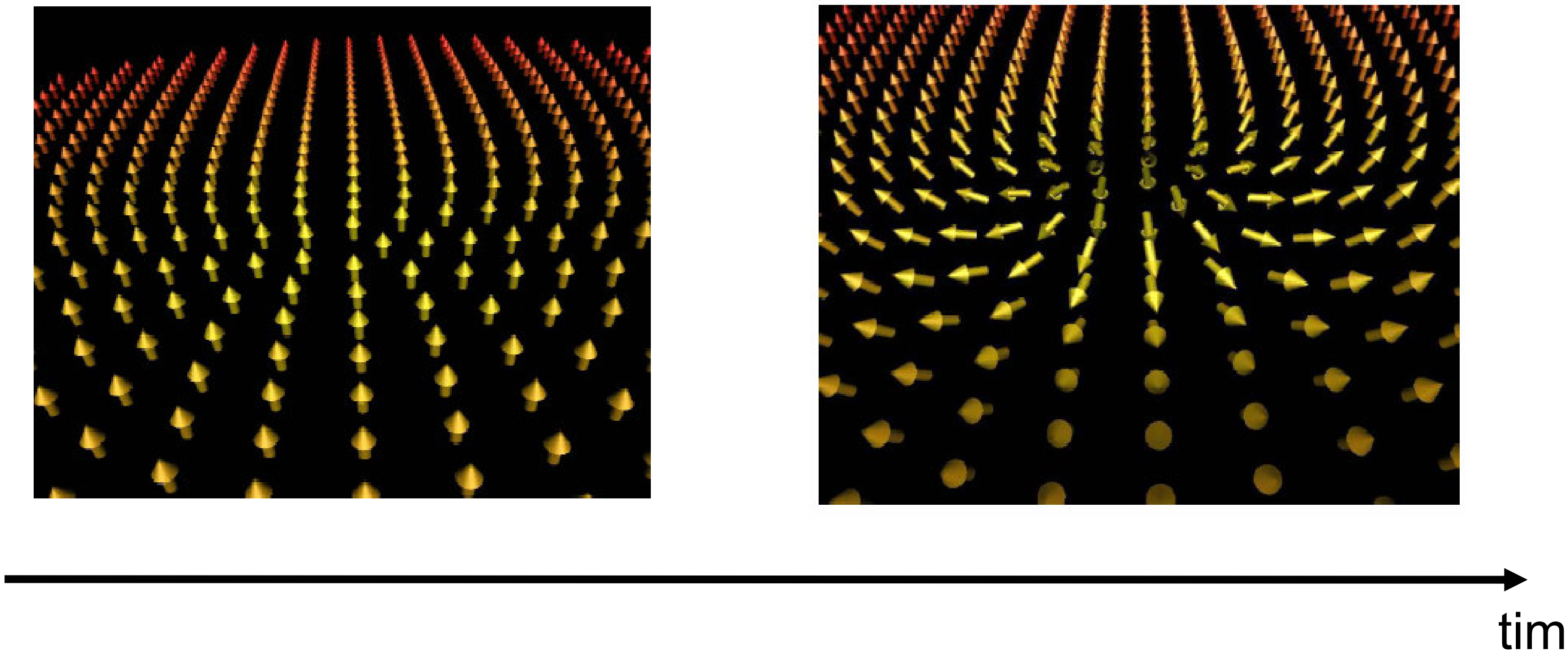




Skyrmion number (topological invariant)

$$Q = \frac{1}{4\pi}\int d^2r\ \hat{n} \cdot \partial_x \hat{n} \times \partial_y \hat{n} = 1$$

Hedgehogs

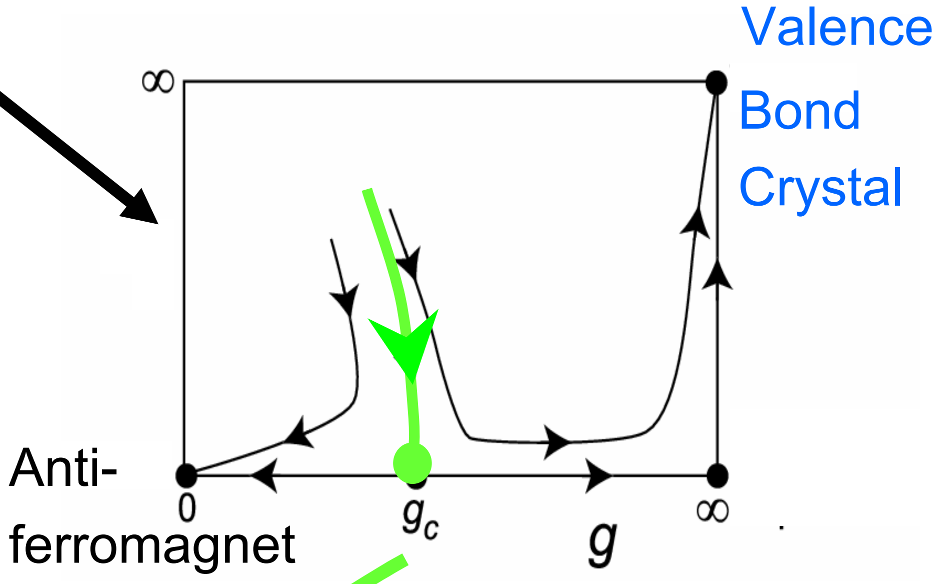


Change the configuration’s skyrmion number

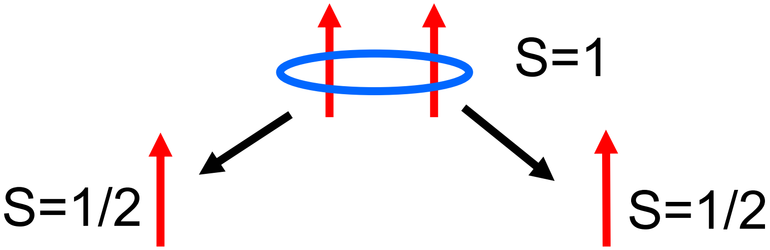
Give rise to the Valence Bond Solid order

Continuous QPT

Relevance of hedgehog excitations



Deconfinement of spin excitations over large scales

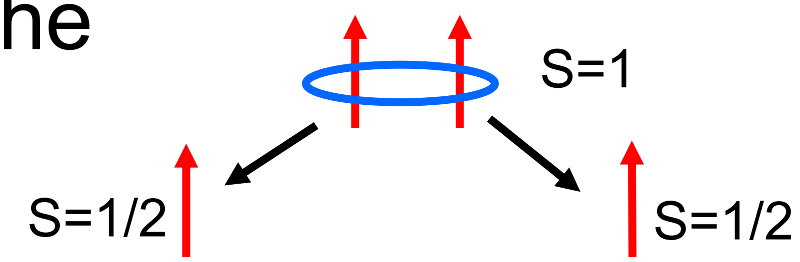


Quantum critical point

Deconfined QCP

Exotic critical exponents

Deconfinement at the critical point

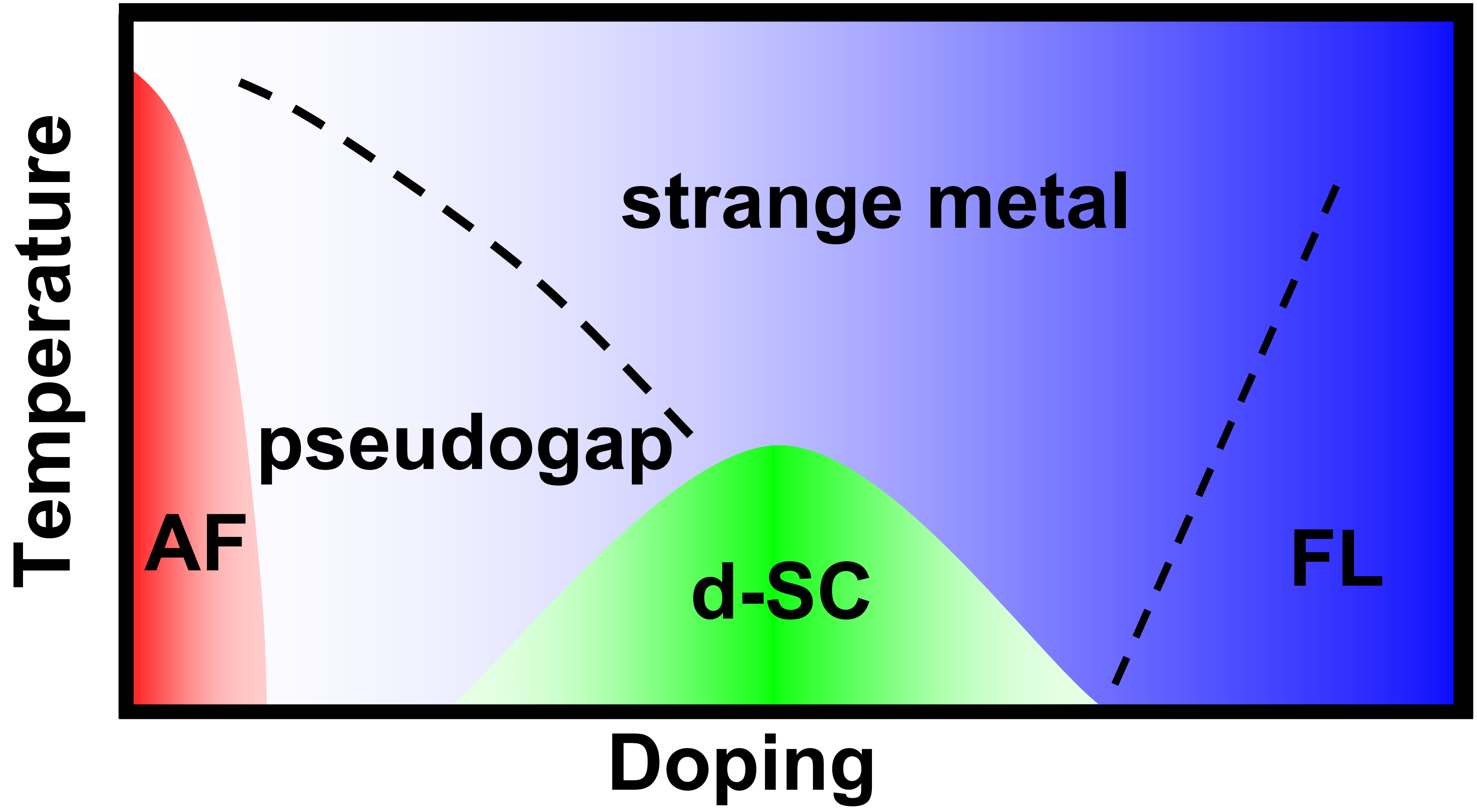


New paradigma for quantum phase transitions?

→ currently being investigated (thus far not conclusive ...)

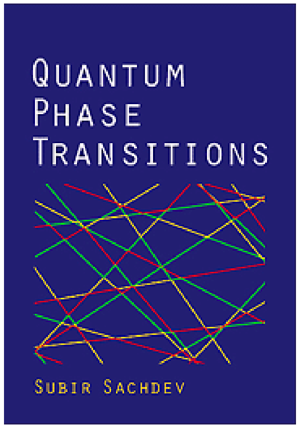
Doping With Mobile Charges

Phase diagram of the High-T_C materials



→ Talk by A. Muramatsu

Further Readings



- S. Sachdev: *Quantum Phase Transitions*
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- M. Voijta: *Quantum Phase Transitions*
  Prep. Prog. Phys. 66 (2003) 2069-2110
- S. Sachdev: *Quantum magnetism and criticality*
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Für das Themenheft