Orbitals, Frustration, and Quantum Criticality

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1. Quantum criticality primer
2. More ingredients: Orbitals, spin-orbit coupling & frustration
3. Exotic quantum criticality in frustrated insulators
4. Beyond insulators: Mott quantum criticality

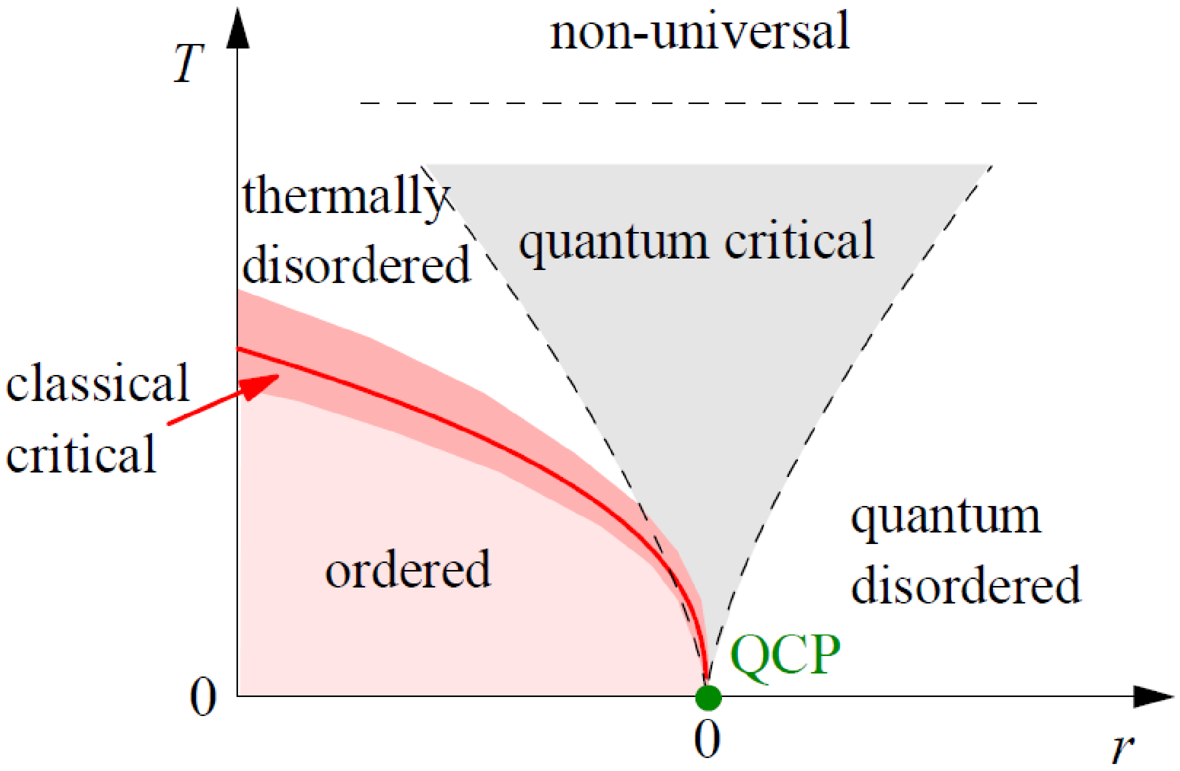
What is a phase transition?

A change in the collective properties of a macroscopic number of atoms.

What is a quantum phase transition?

A phase transition at $T = 0$,
driven by “quantum fluctuations”.

What is a quantum phase transition?



Experimentally observed in many compounds,
e.g. in $TlCuCl_3$ under pressure.

Rüegg *et al.*, PRL **100**, 205701 (2008)

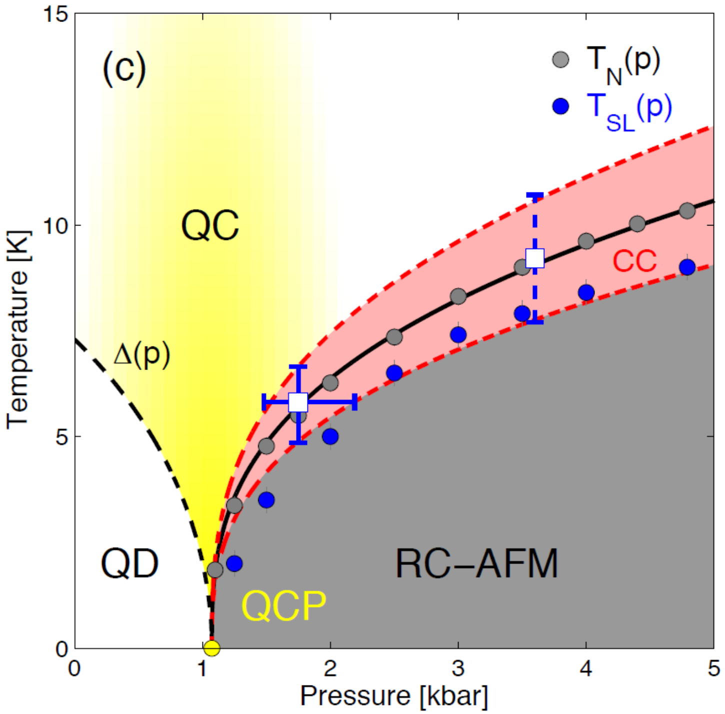
What is „quantum“ about a quantum phase transition?

Fluctuations of the order parameter
follow **quantum** statistical mechanics.

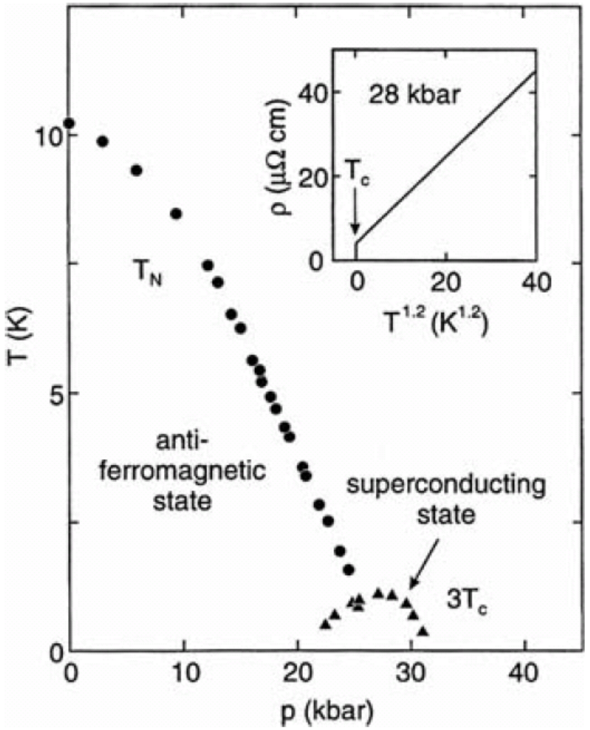
Near a continuous phase transition (both classical and quantum)
fluctuations become slow ($\omega_{typ} \to 0$).

Sufficiently close to a finite-temperature transition,
fluctuations can therefore be treated **classically**!
($k_B T >> \hbar\omega_{typ}$)

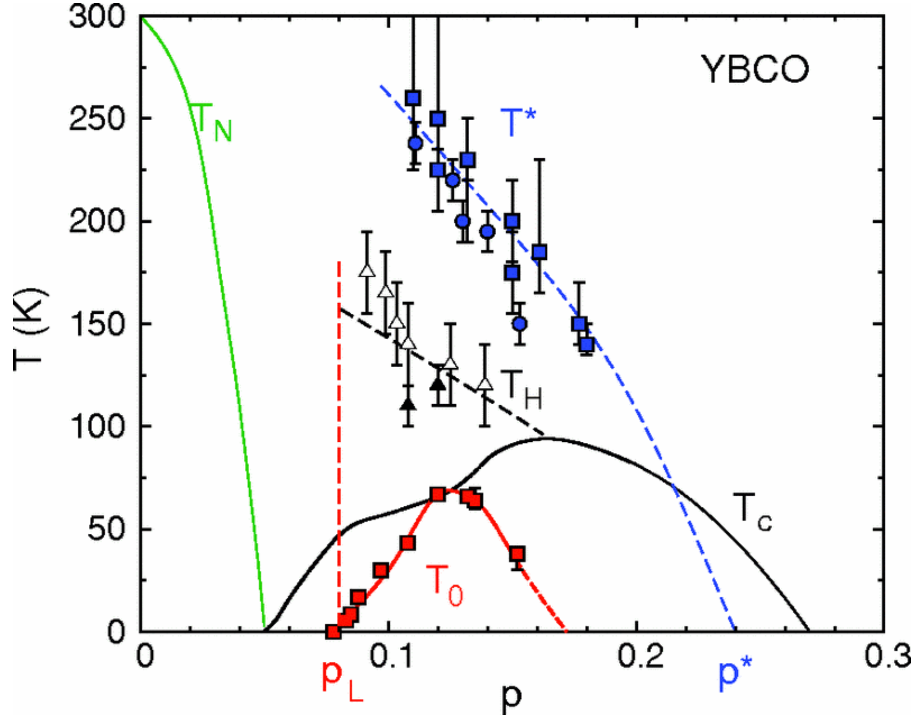
Experimental examples



TlCuCl$_3$
(insulator)



CePd$_2$Si$_2$
(metal)

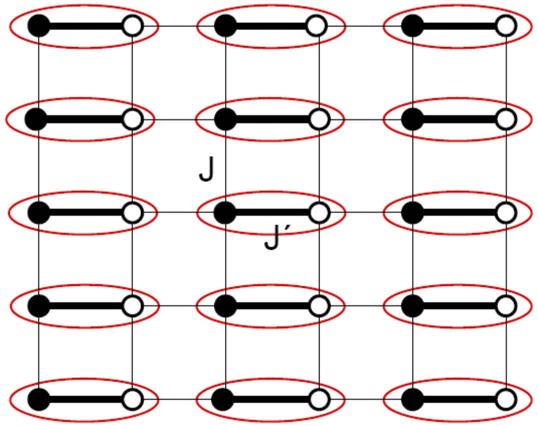


YBa$_2$Cu$_3$O$_{6+x}$
(superconductor)

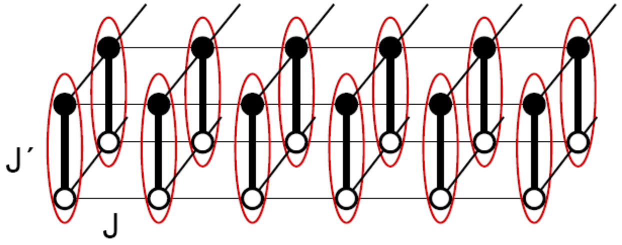
Coupled-dimer antiferromagnets

S=1/2 spins on coupled dimers $\mathcal{H} = \sum_{\langle jj' \rangle} J_{jj'} \vec{S}_j \cdot \vec{S}_{j'}$

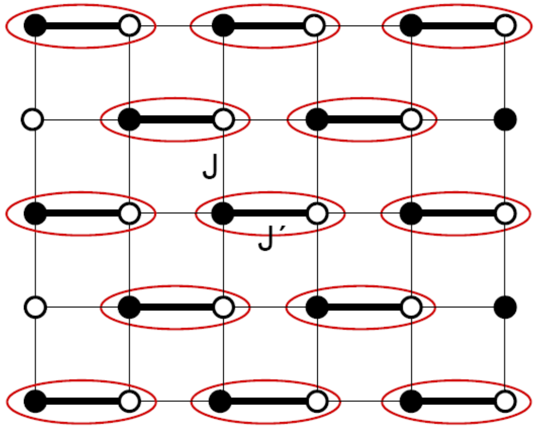
Columnar



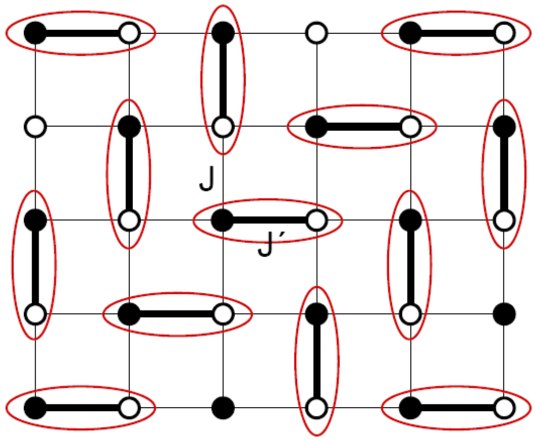
Bilayer



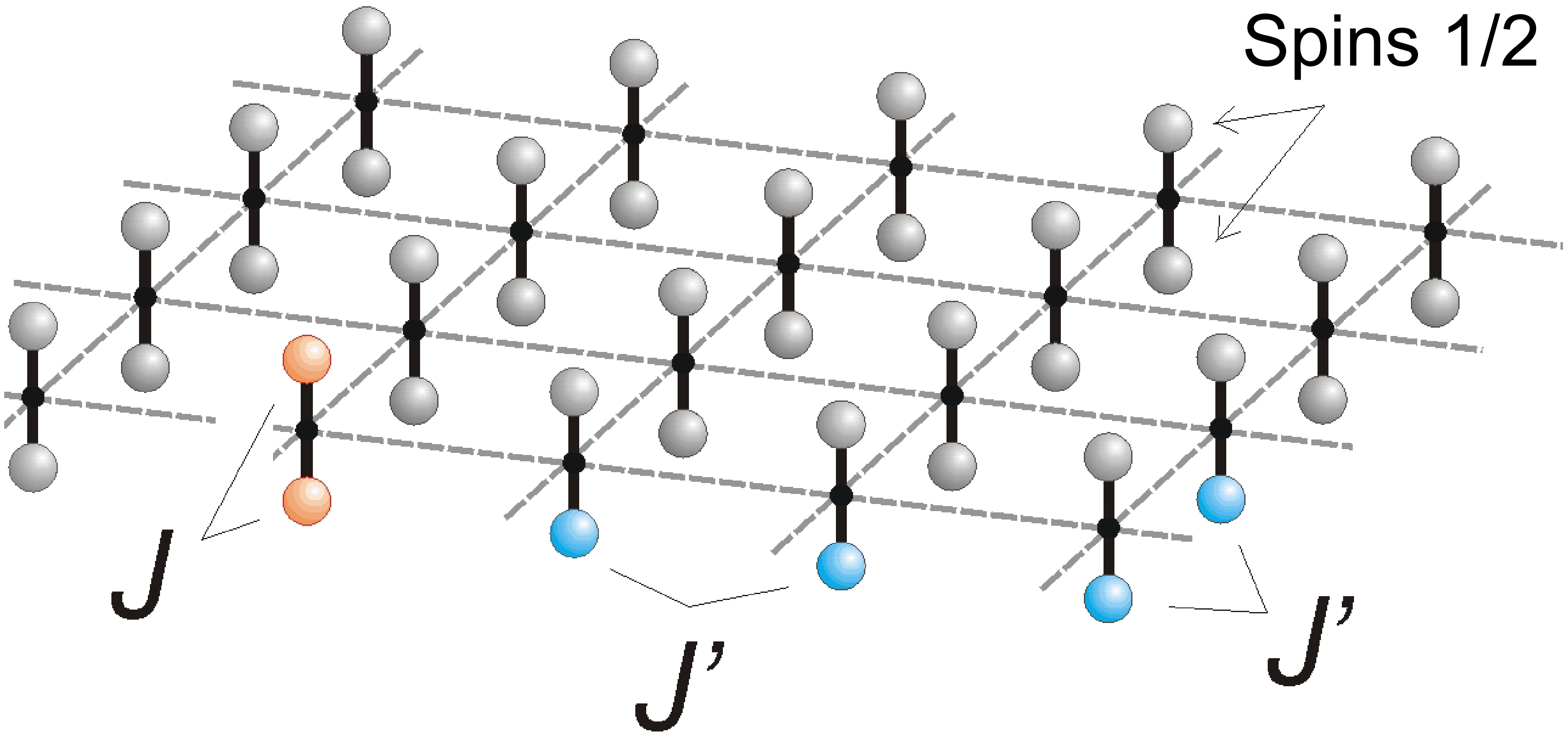
Staggered



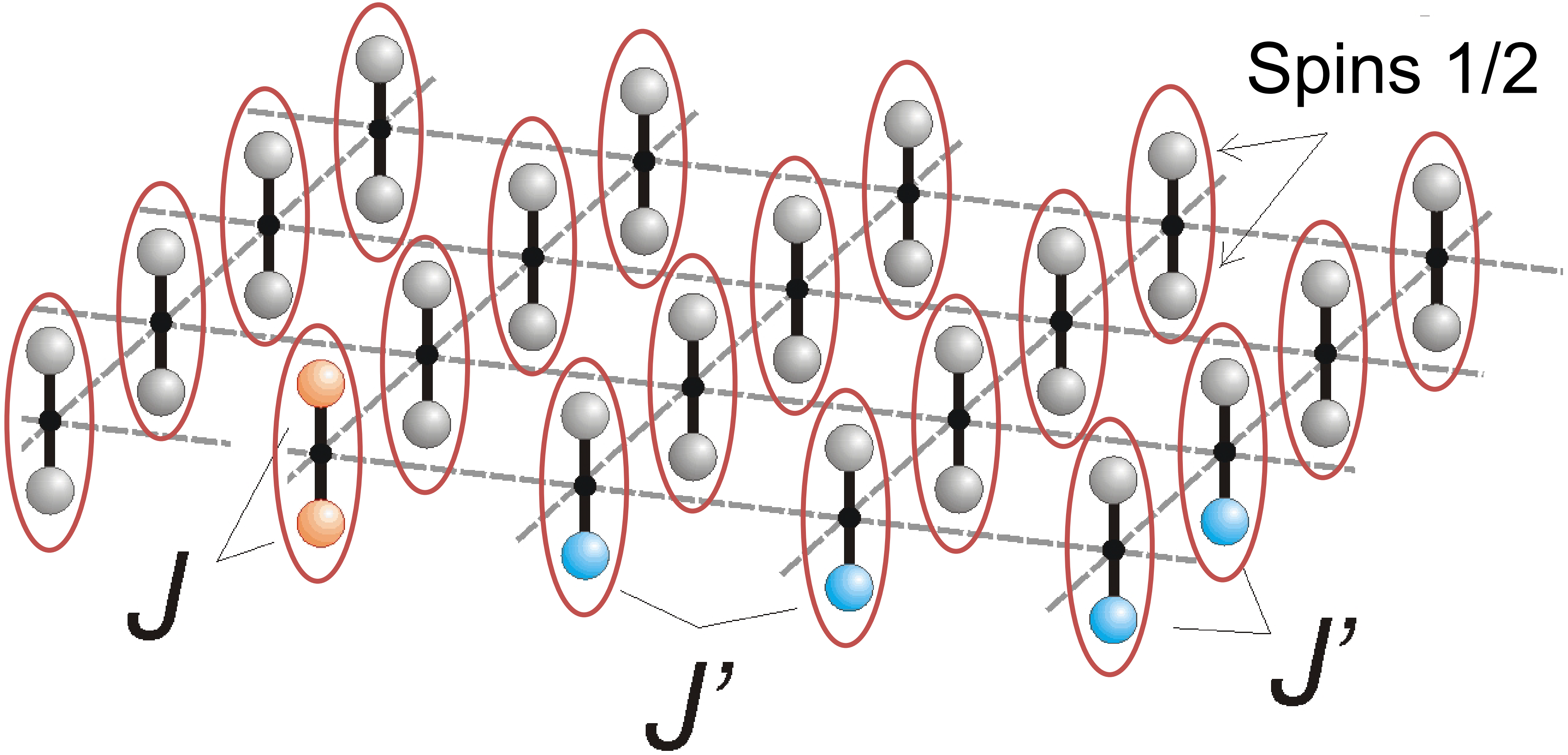
Herringbone

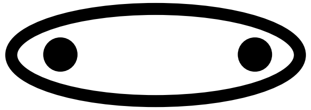


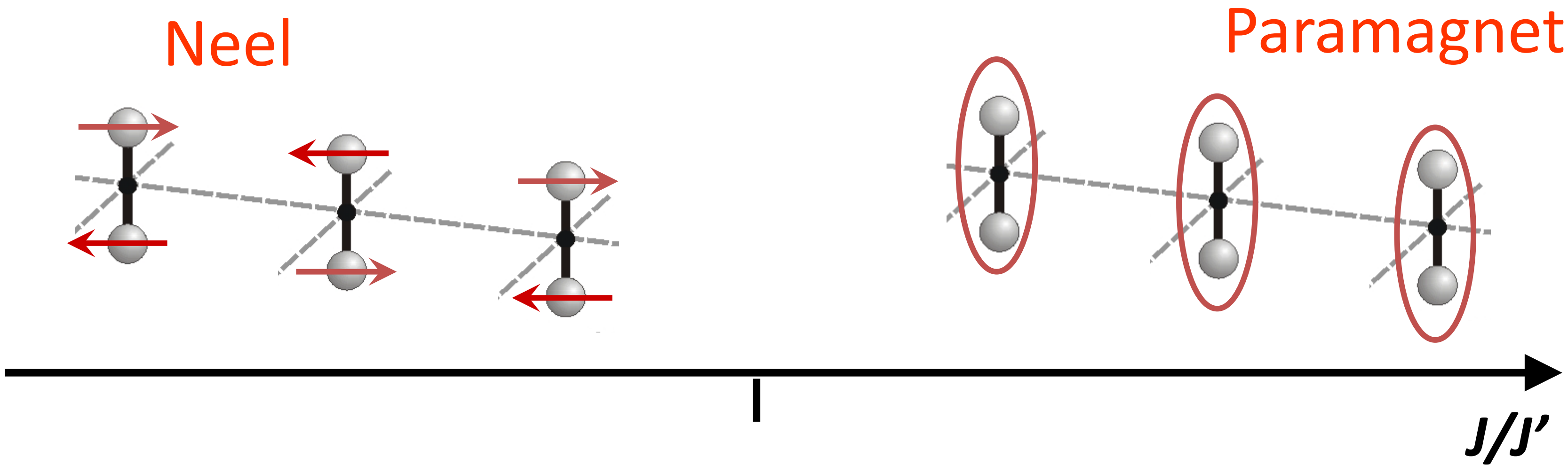
Bilayer Heisenberg antiferromagnet



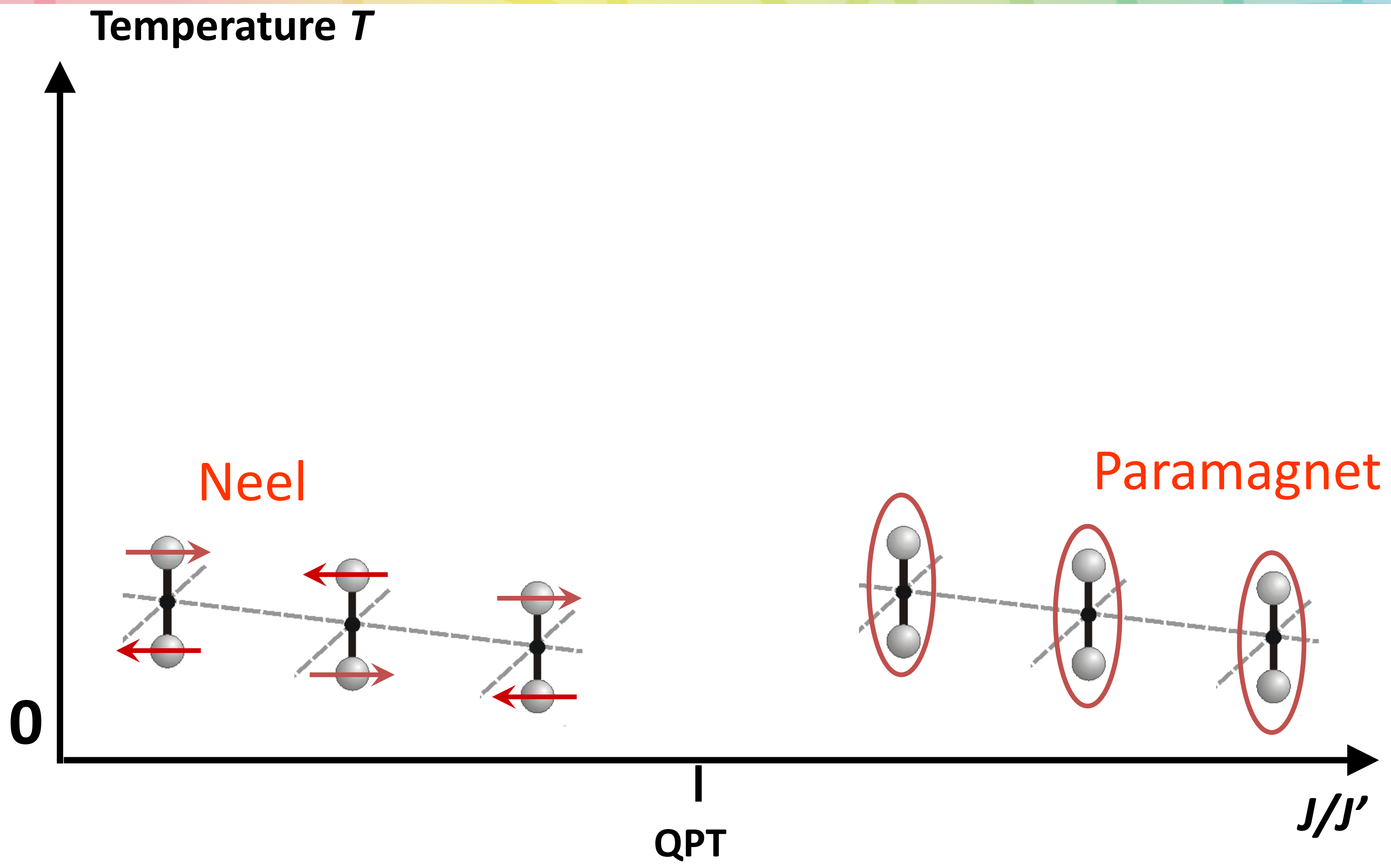
$J \gg J'$: Quantum paramagnet



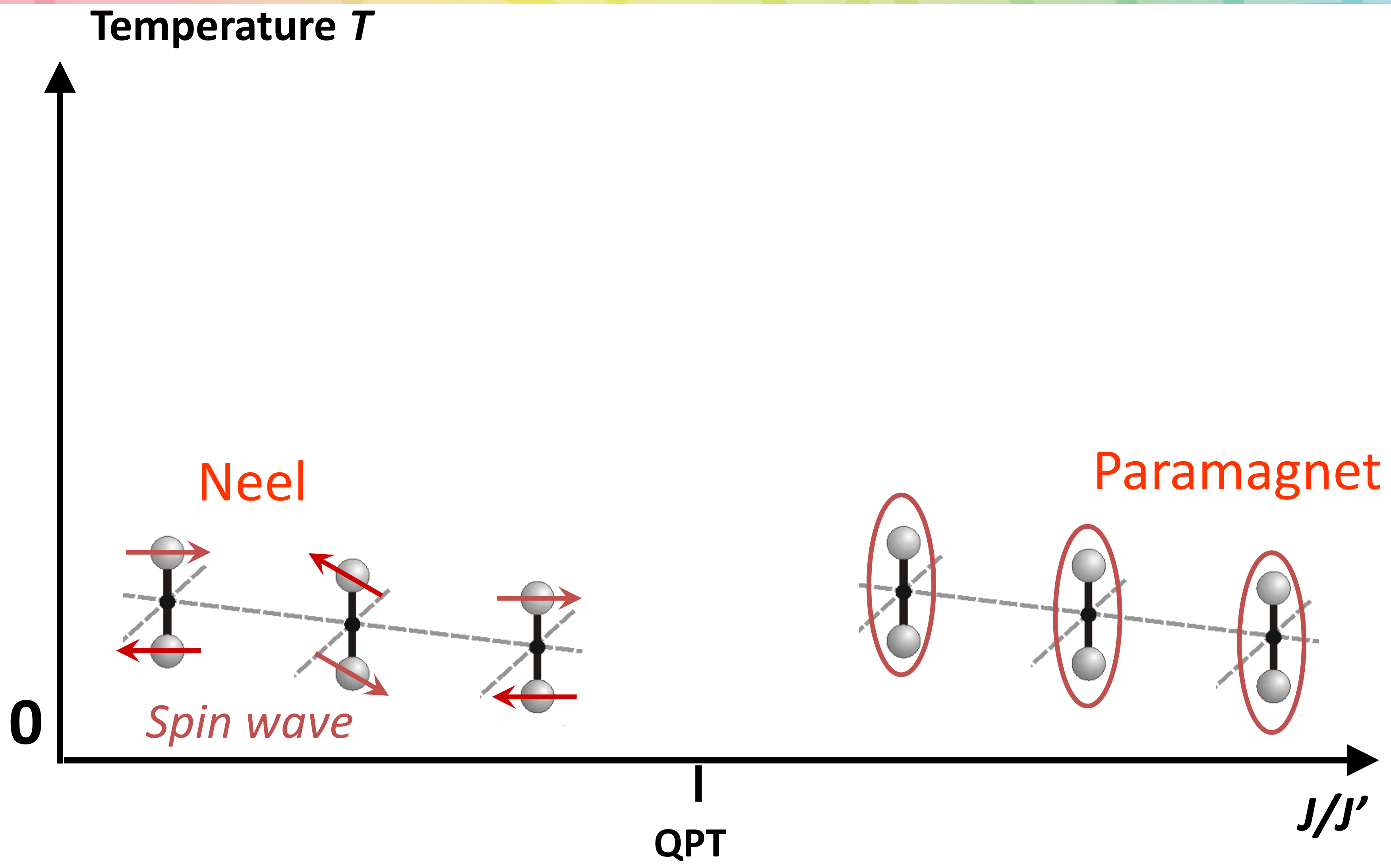
Singlet  $= (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) / \sqrt{2}$

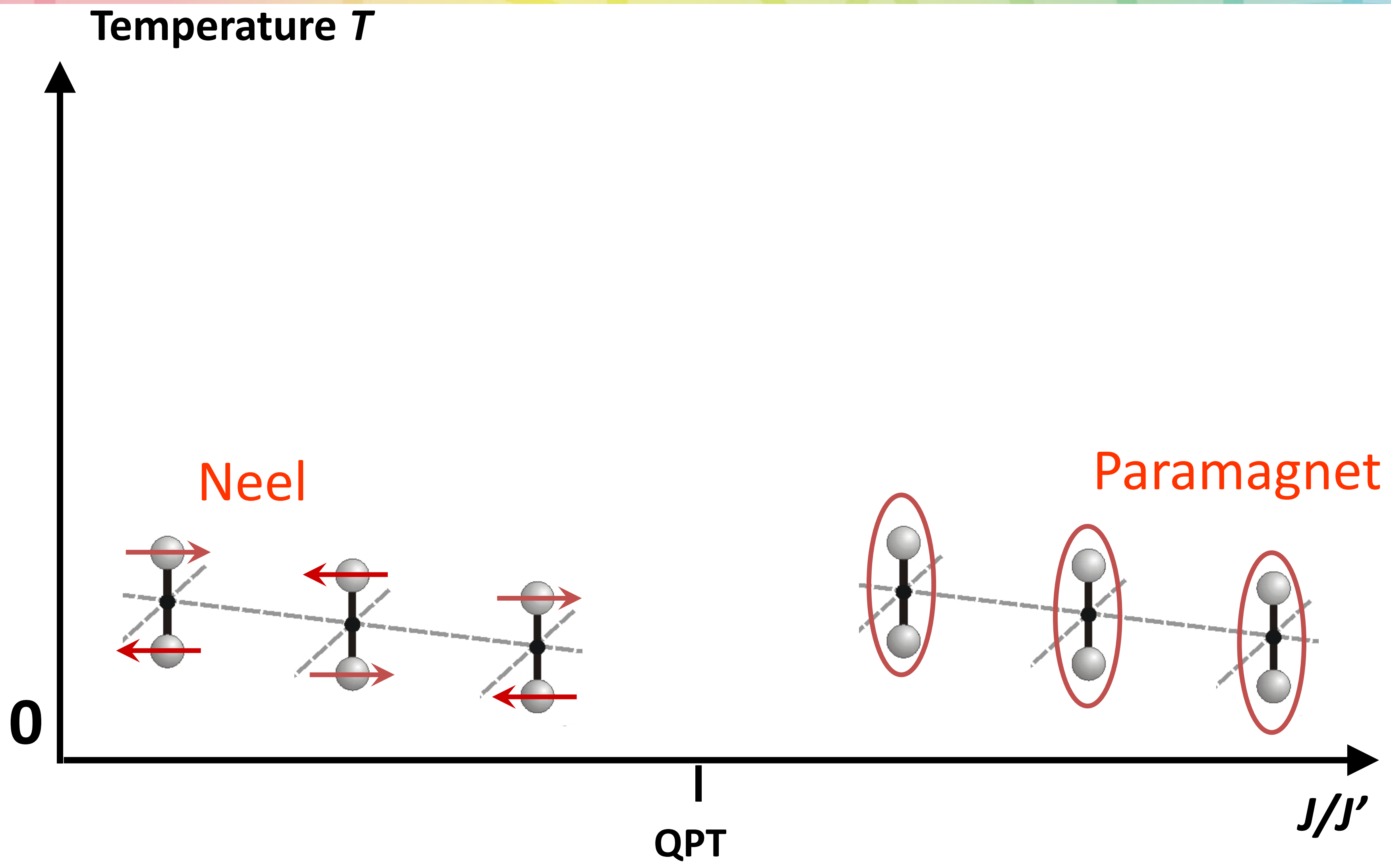


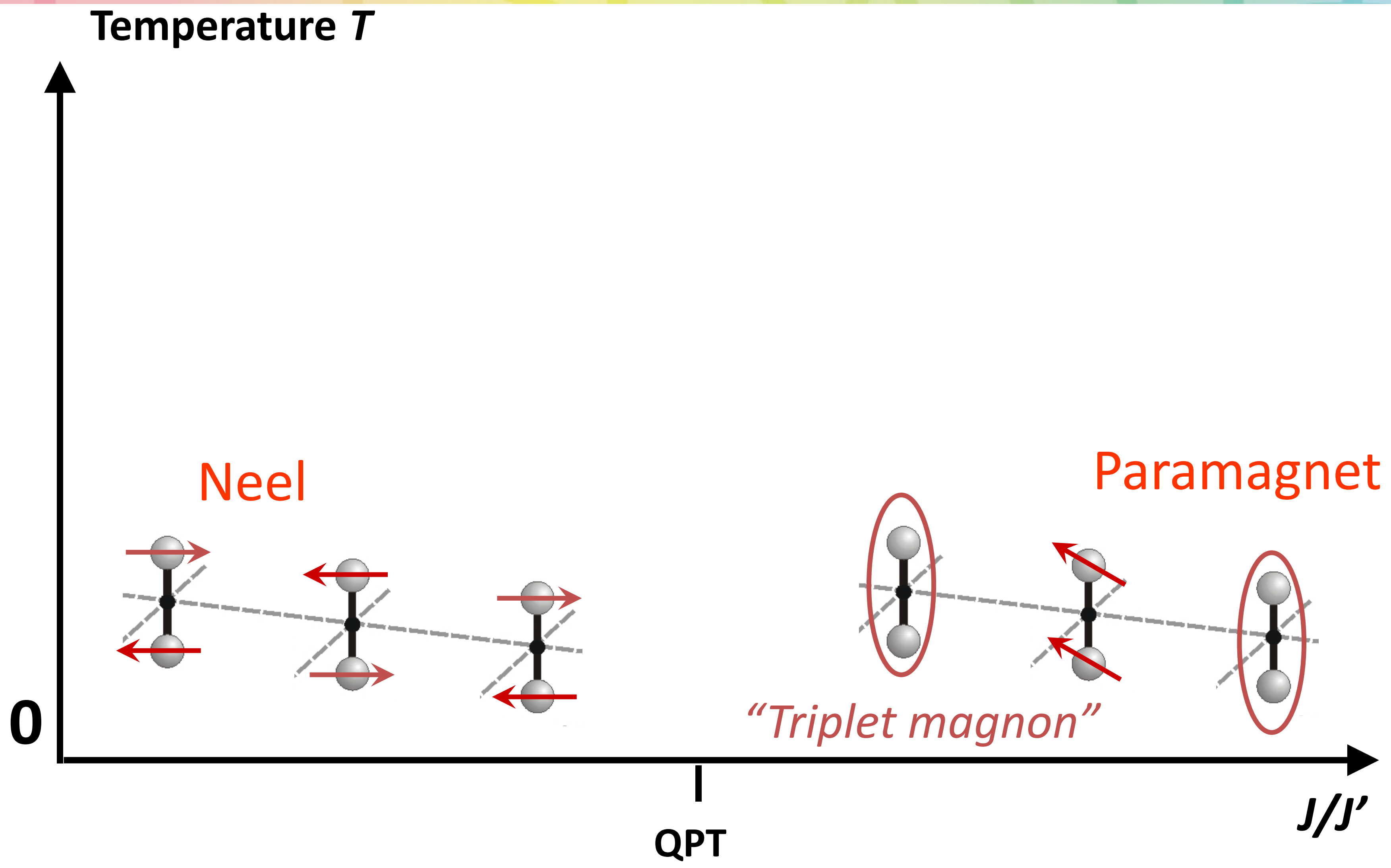
Vary the ratio ***J/J'***

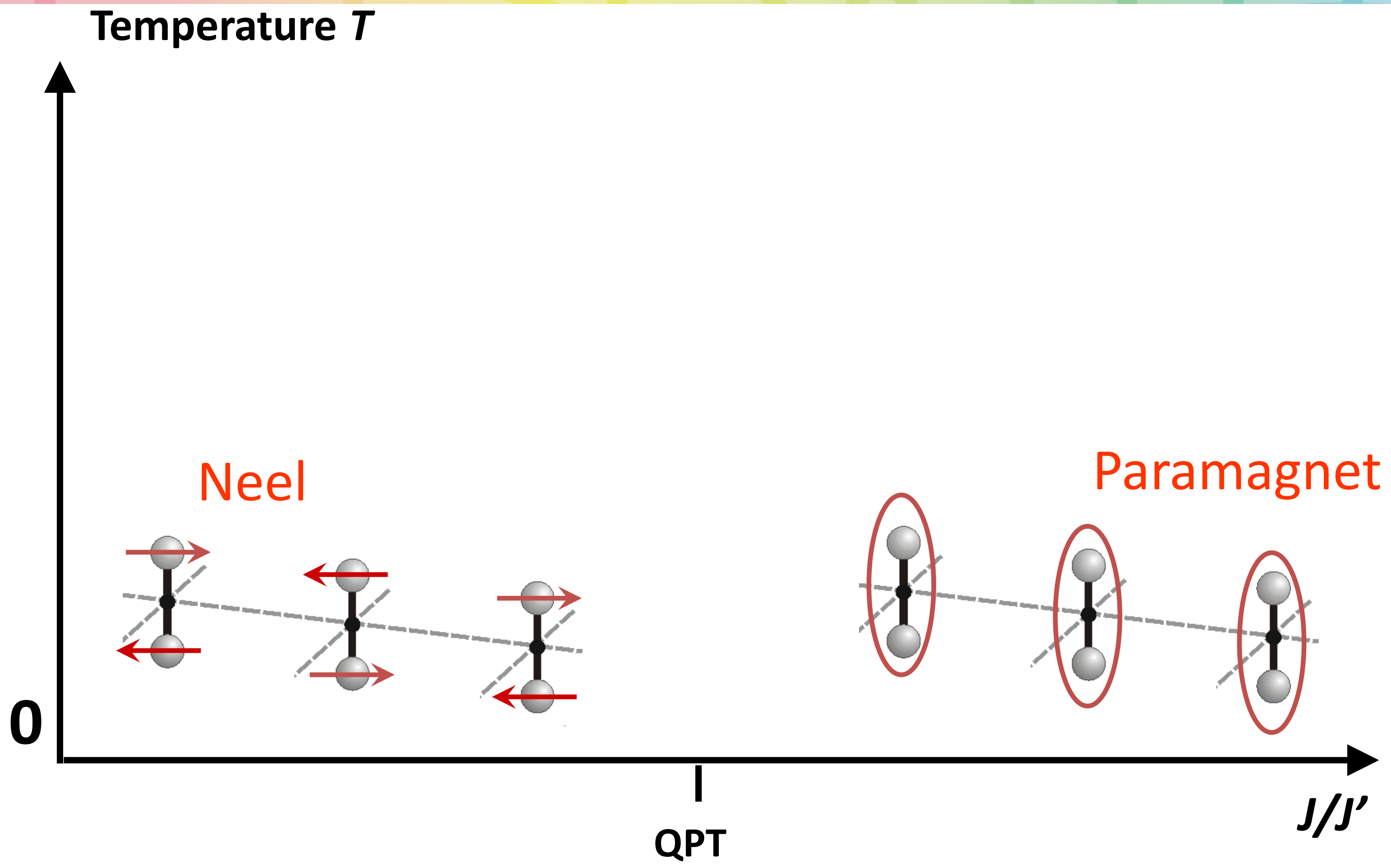


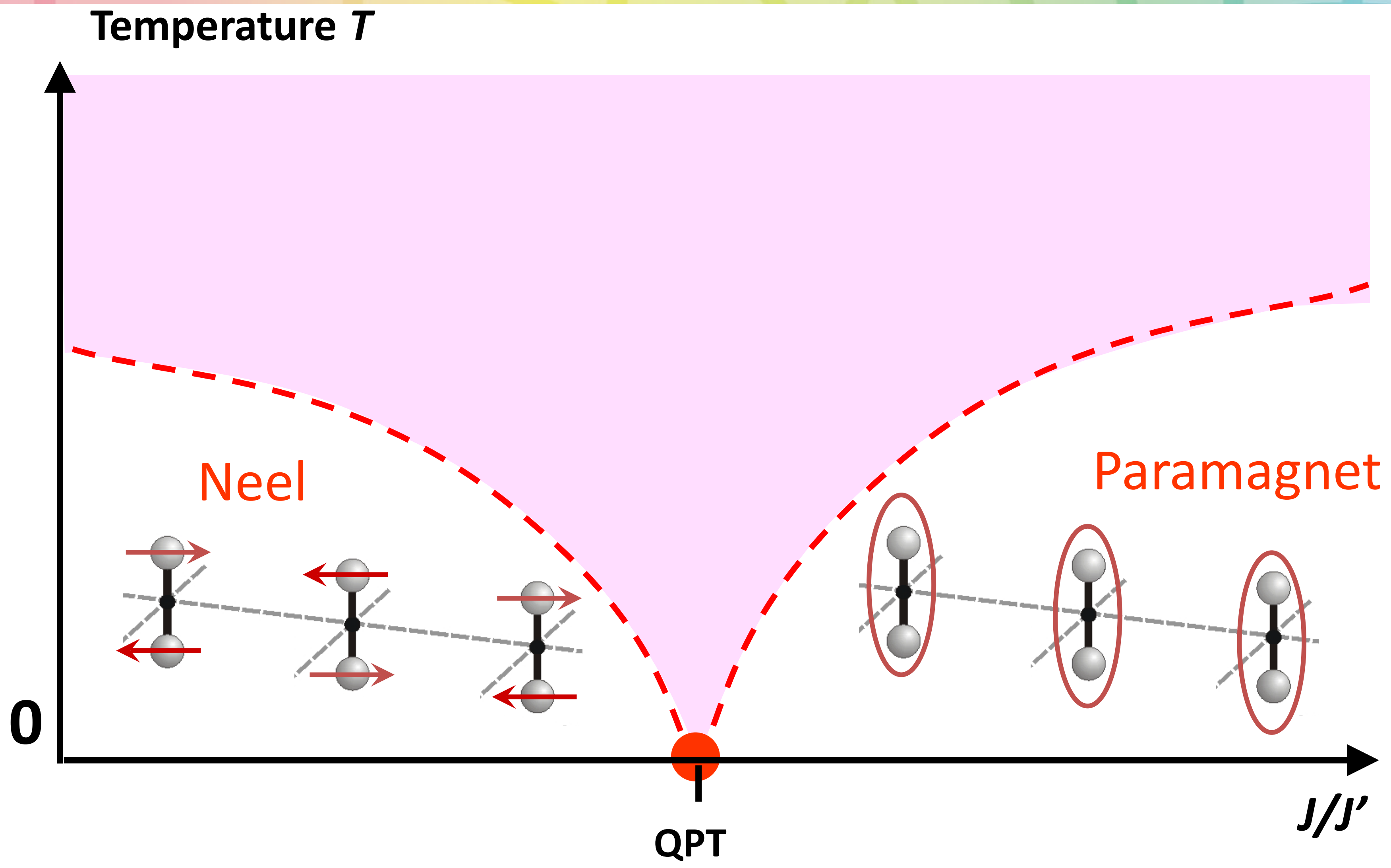
Temperature T
Neel
Paramagnet
0
QPT
J/J'

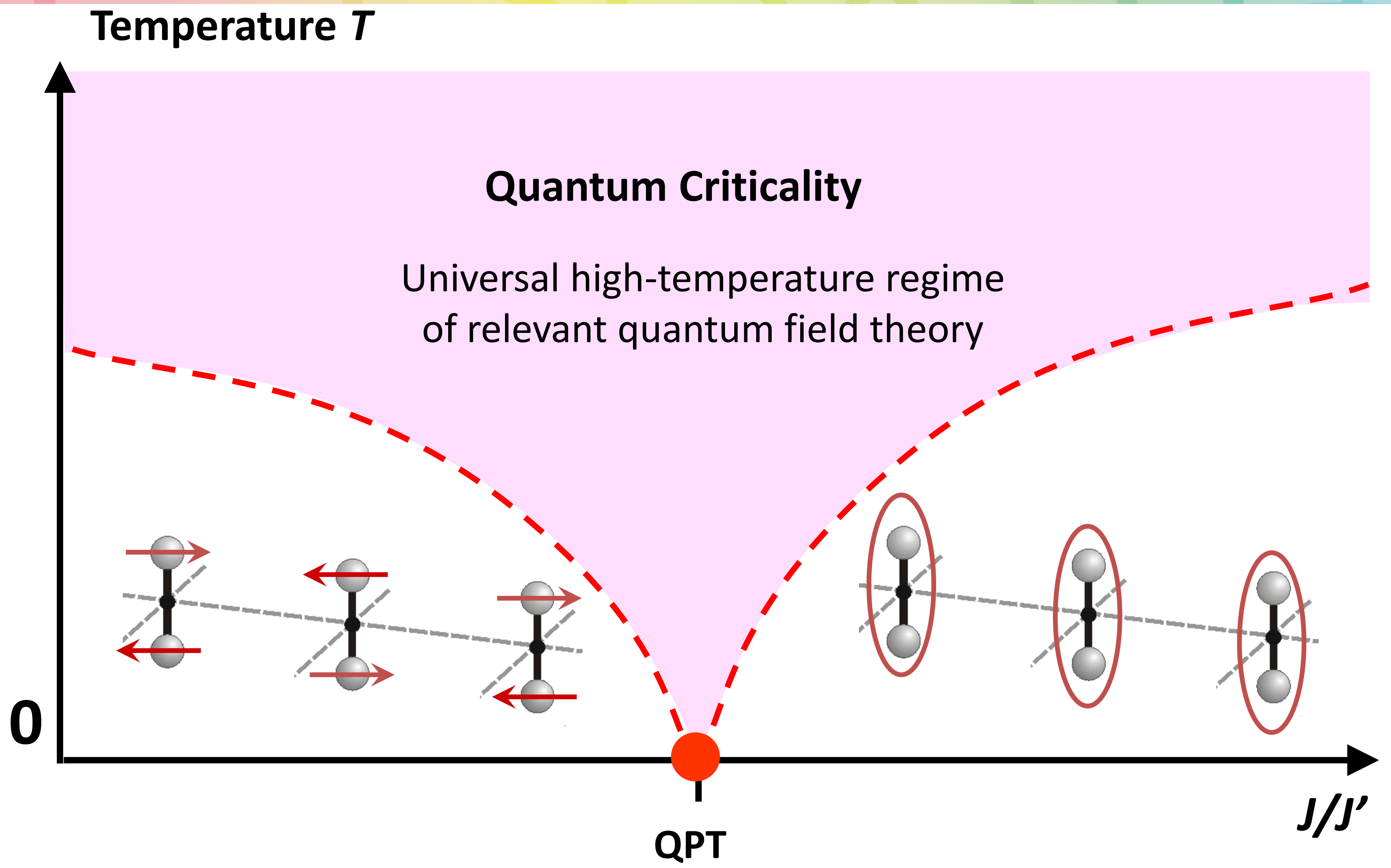

Temperature *T*
Neel
Paramagnet
0
Spin wave
QPT
J/J'


Temperature T
Neel
Paramagnet
0
QPT
J/J'

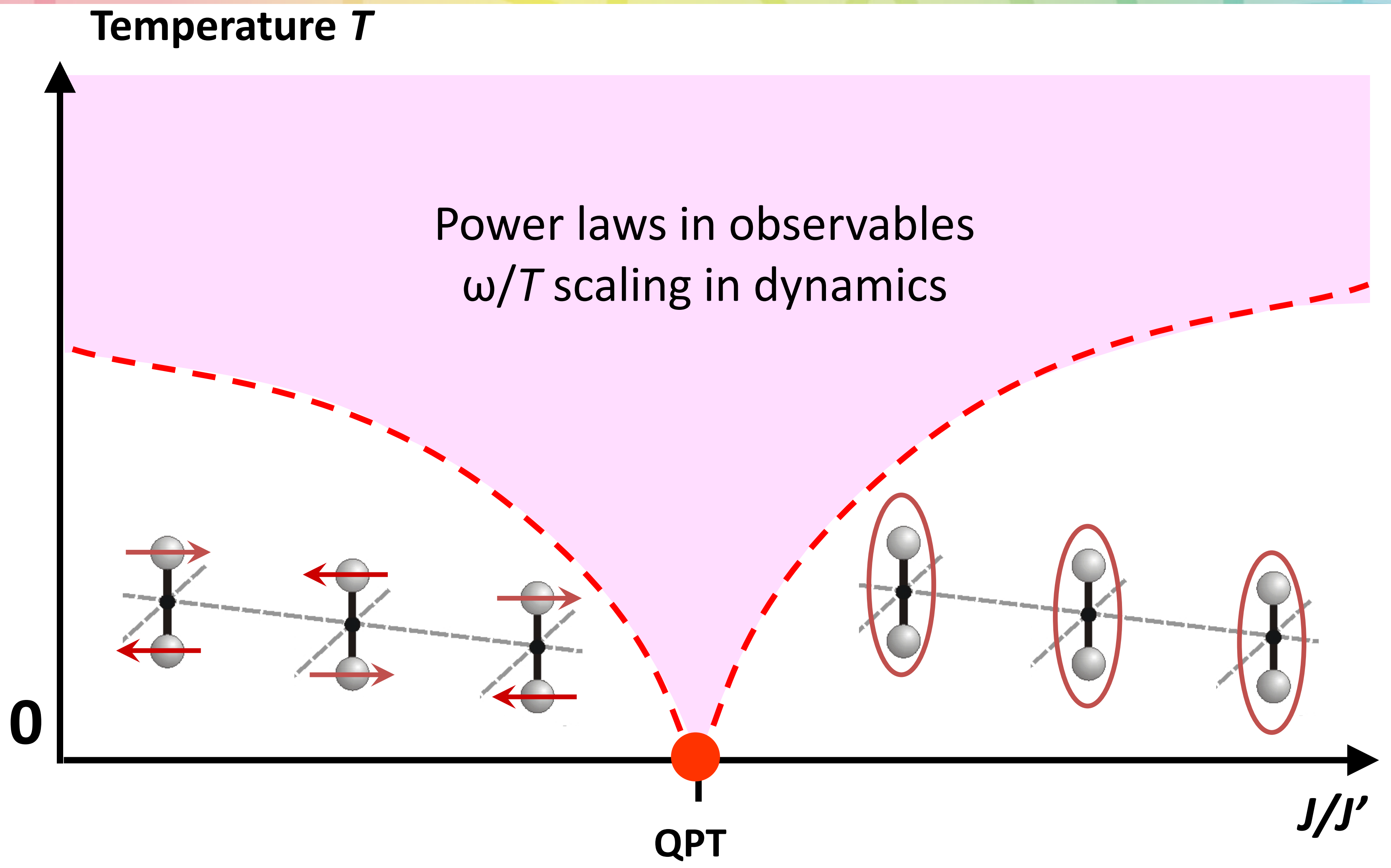

Temperature *T*
0
Neel
Paramagnet
"Triplet magnon"
QPT
J/J'


Temperature T
Neel
Paramagnet
0
QPT
J/J'

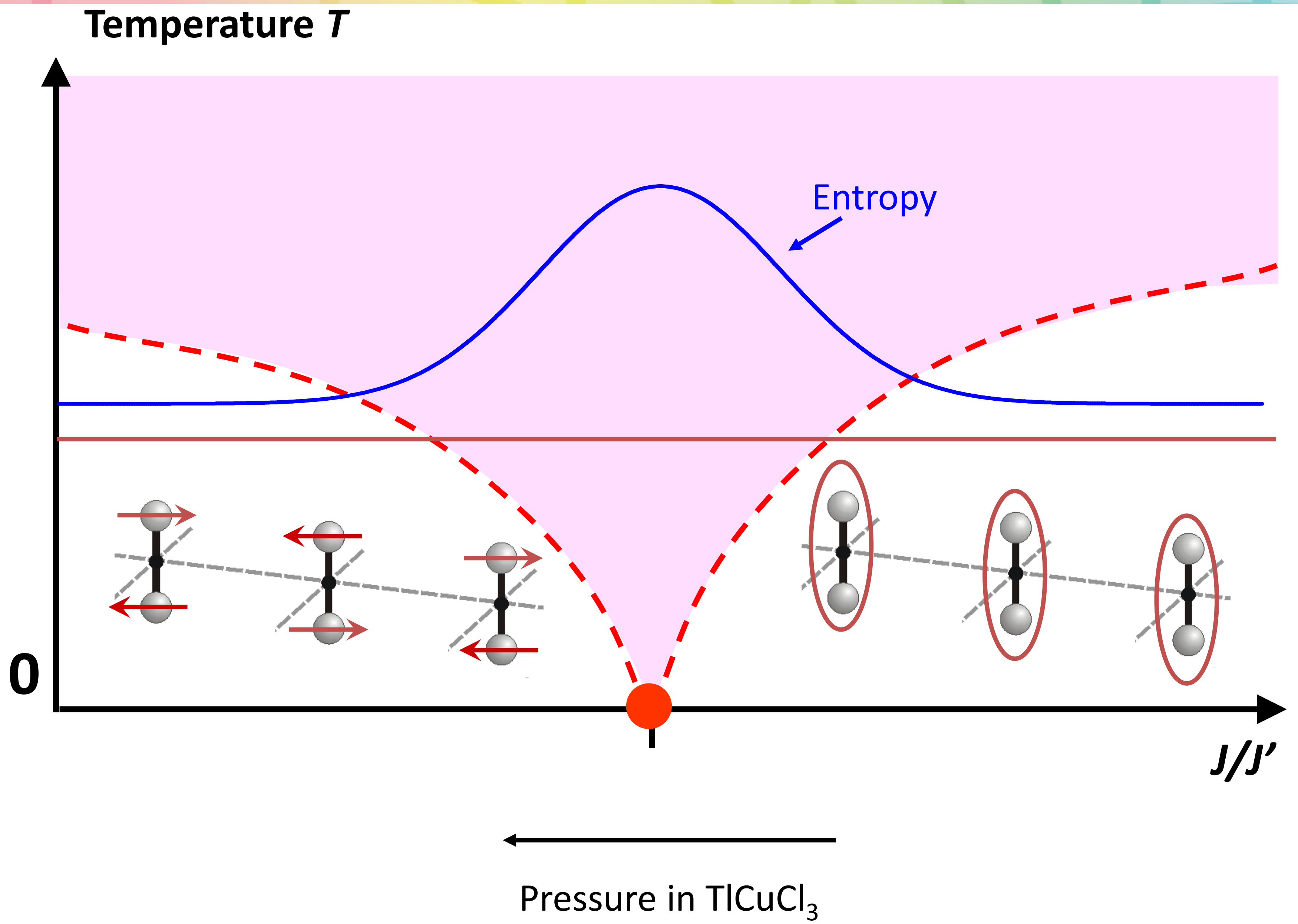

Temperature *T*
0
Neel
Paramagnet
QPT
J/J'

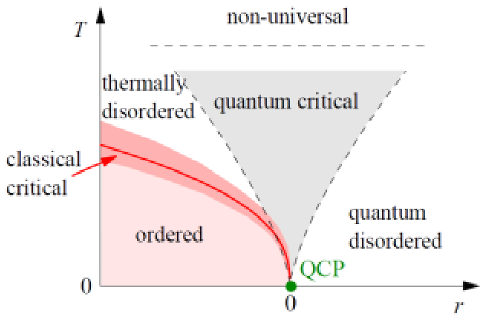


Sachdev / Ye, *Phys. Rev. Lett.* **69**, 2411 (1992)



Temperature *T*
Power laws in observables
ω/*T* scaling in dynamics
0
QPT
J/*J*’


Temperature T
Entropy
0
J/J'
Pressure in $TlCuCl_3$



Landau-Ginzburg-Wilson (LGW) theory:

Write down an effective action for the order parameter
(here staggered magnetization $\varphi_\alpha(\vec{x},\tau)$)
by expanding in powers of φ and its spatial and temporal derivatives,
while preserving all symmetries of the microscopic Hamiltonian

$$S_\varphi = \int d^2x d\tau \left[\frac{1}{2} \left((\nabla_x \vec{\varphi})^2 + \frac{1}{c^2} (\partial_\tau \vec{\varphi})^2 + (\lambda_c - \lambda) \vec{\varphi}^2 \right) + \frac{u}{4!} (\vec{\varphi}^2)^2 \right]$$

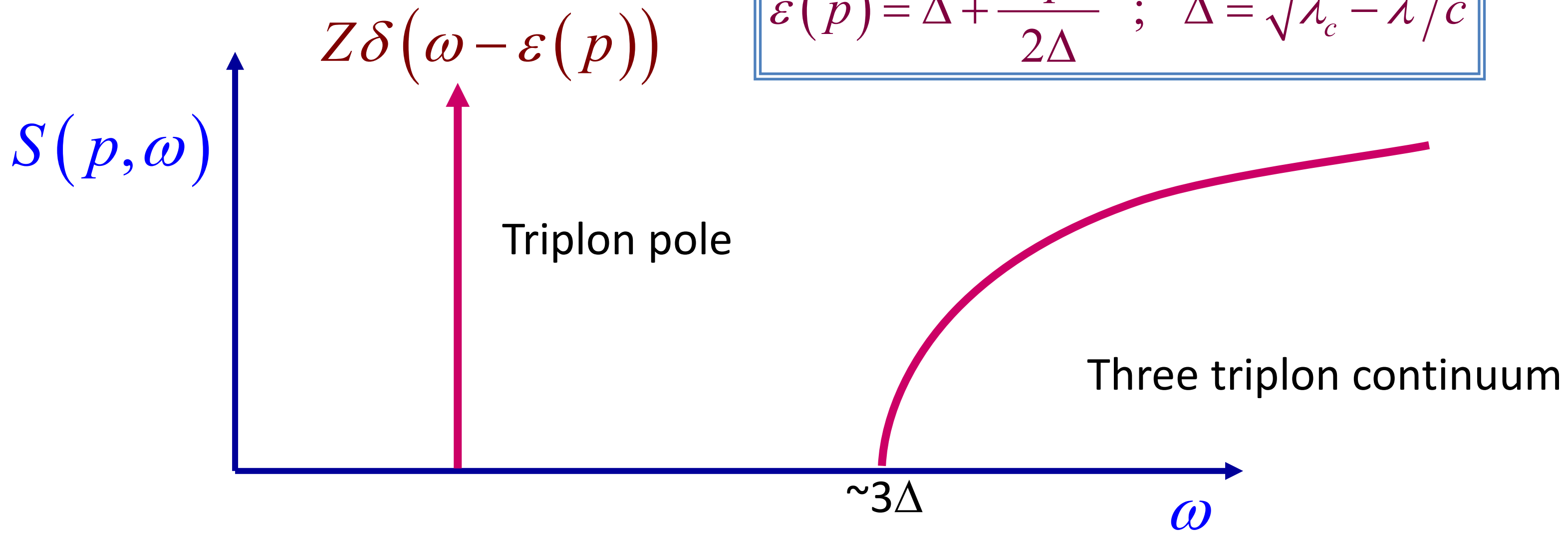
Coarse-grained description of
microscopic (physical or emergent) degrees of freedom

$$S_\varphi = \int d^2x d\tau \left[\frac{1}{2} \left((\nabla_x \vec{\varphi})^2 + \frac{1}{c^2} (\partial_\tau \vec{\varphi})^2 + (\lambda_c - \lambda) \vec{\varphi}^2 \right) + \frac{u}{4!} (\vec{\varphi}^2)^2 \right]$$

φ_α → (N=3)-component antiferromagnetic order parameter

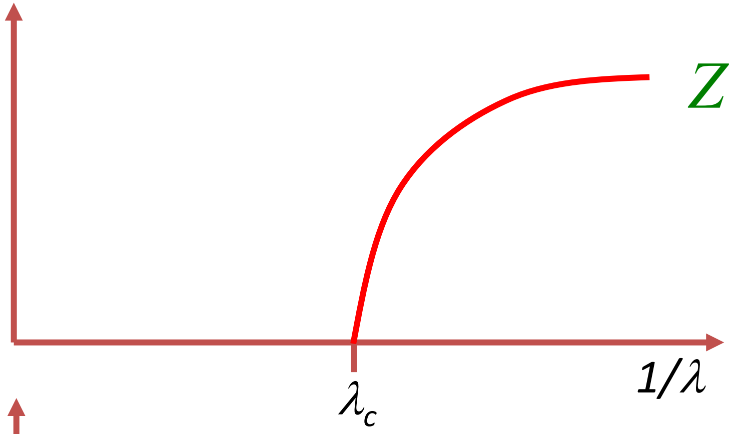
For $\lambda < \lambda_c$ oscillations of φ_α about $\varphi_\alpha = 0$ lead to the following structure in the dynamic structure factor $S(p,\omega)$

$$\varepsilon(p) = \Delta + \frac{c^2 p^2}{2\Delta} \quad ; \quad \Delta = \sqrt{\lambda_c - \lambda}/c$$



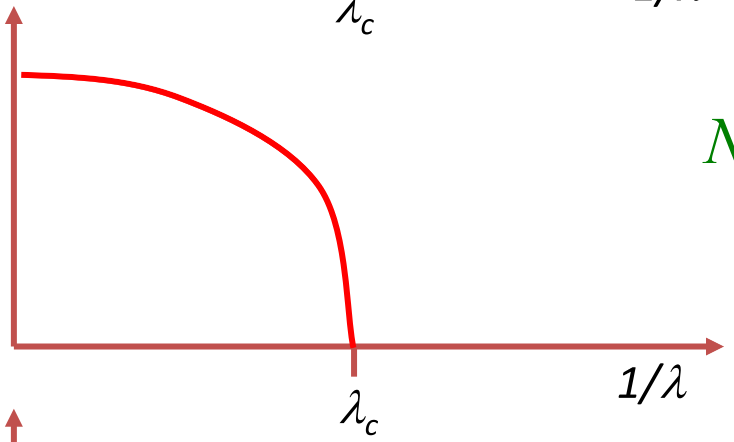
Properties near quantum criticality

Triplon quasiparticle weight Z



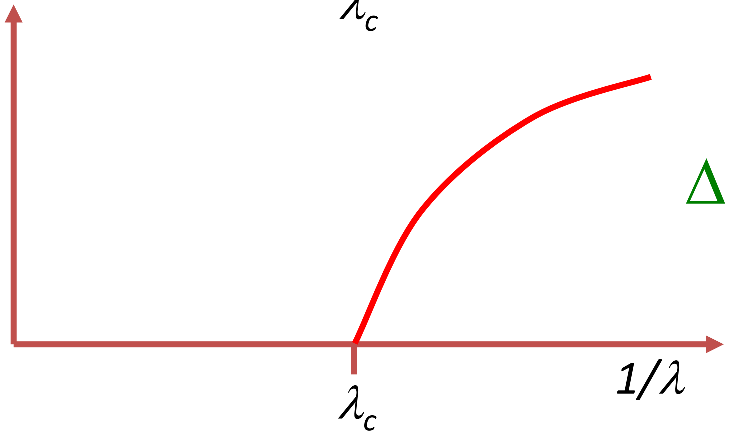
$$Z \sim (\lambda_c - \lambda)^{\eta\nu}$$

Antiferromagnetic moment N_0



$$N_0 \sim (\lambda - \lambda_c)^{\beta}$$

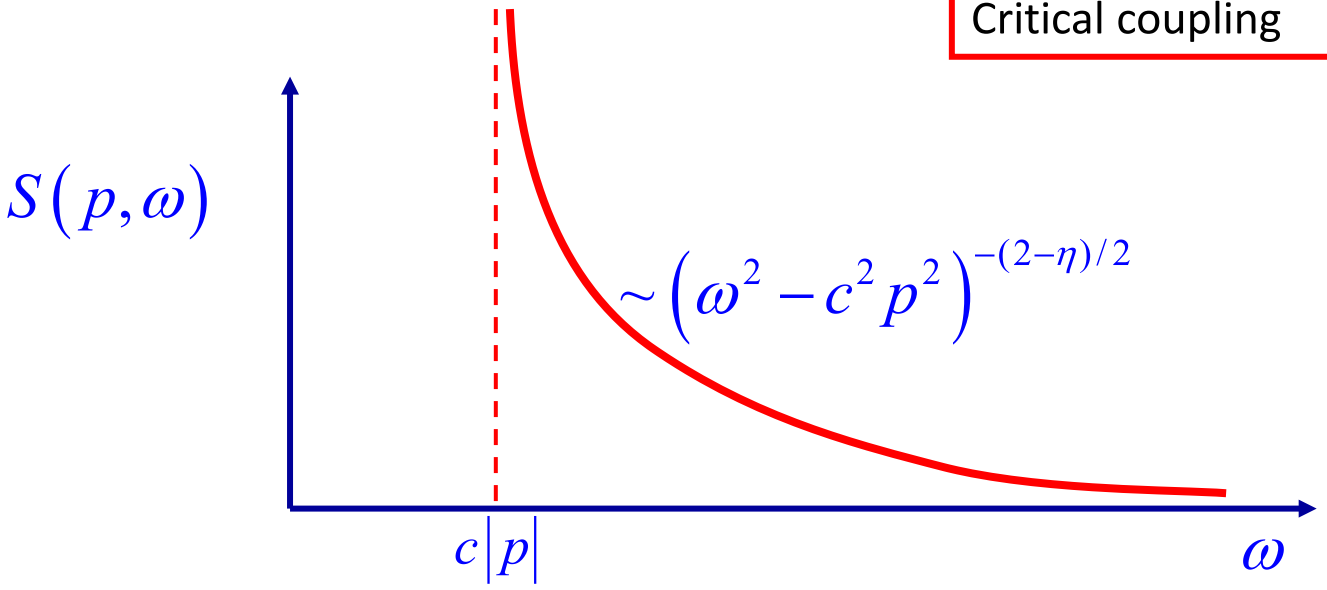
Triplon energy gap Δ



$$\Delta \sim (\lambda_c - \lambda)^{\nu}$$

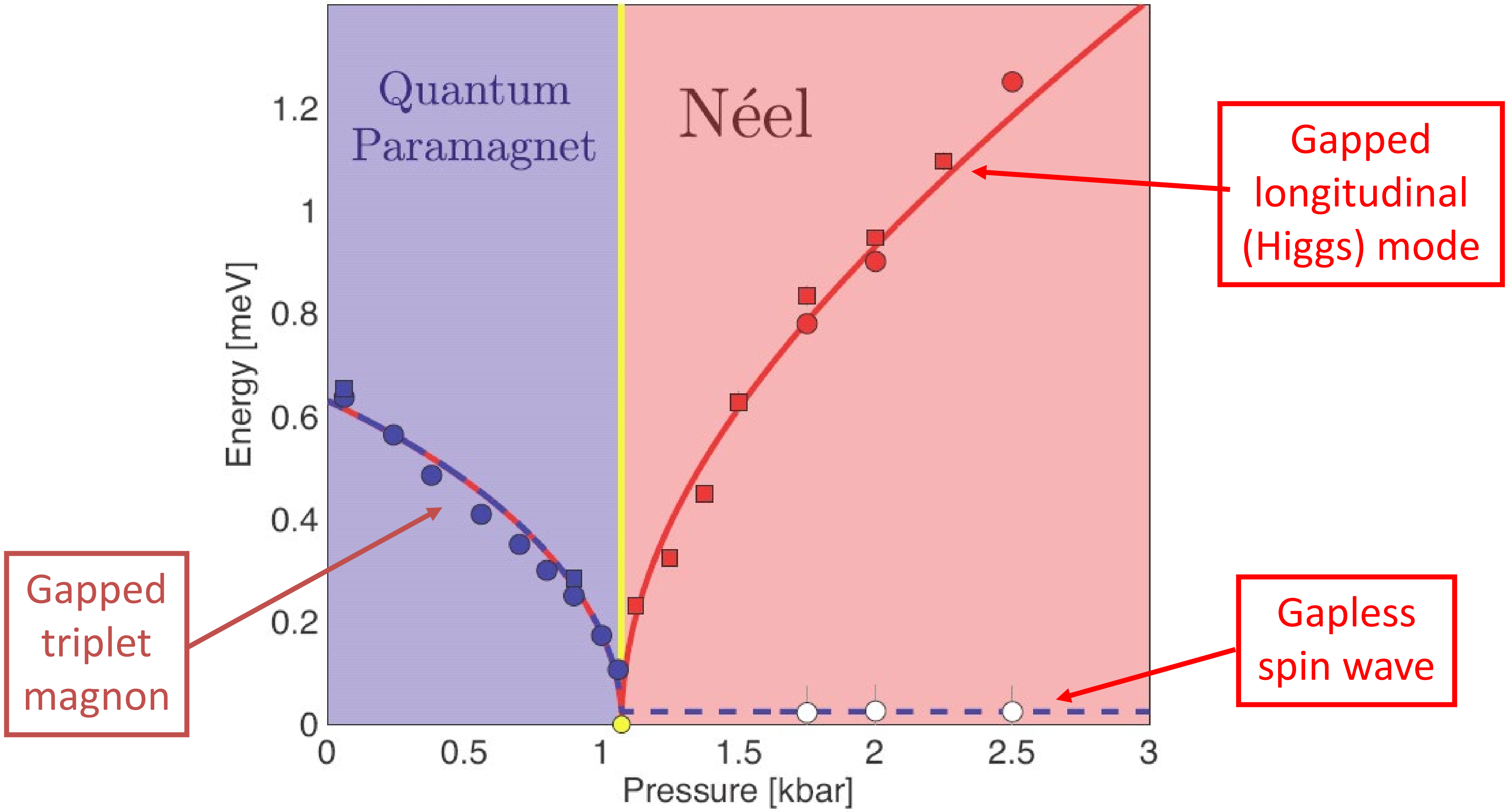
Dynamic spectrum at quantum critical point

Critical coupling $(\lambda = \lambda_c)$



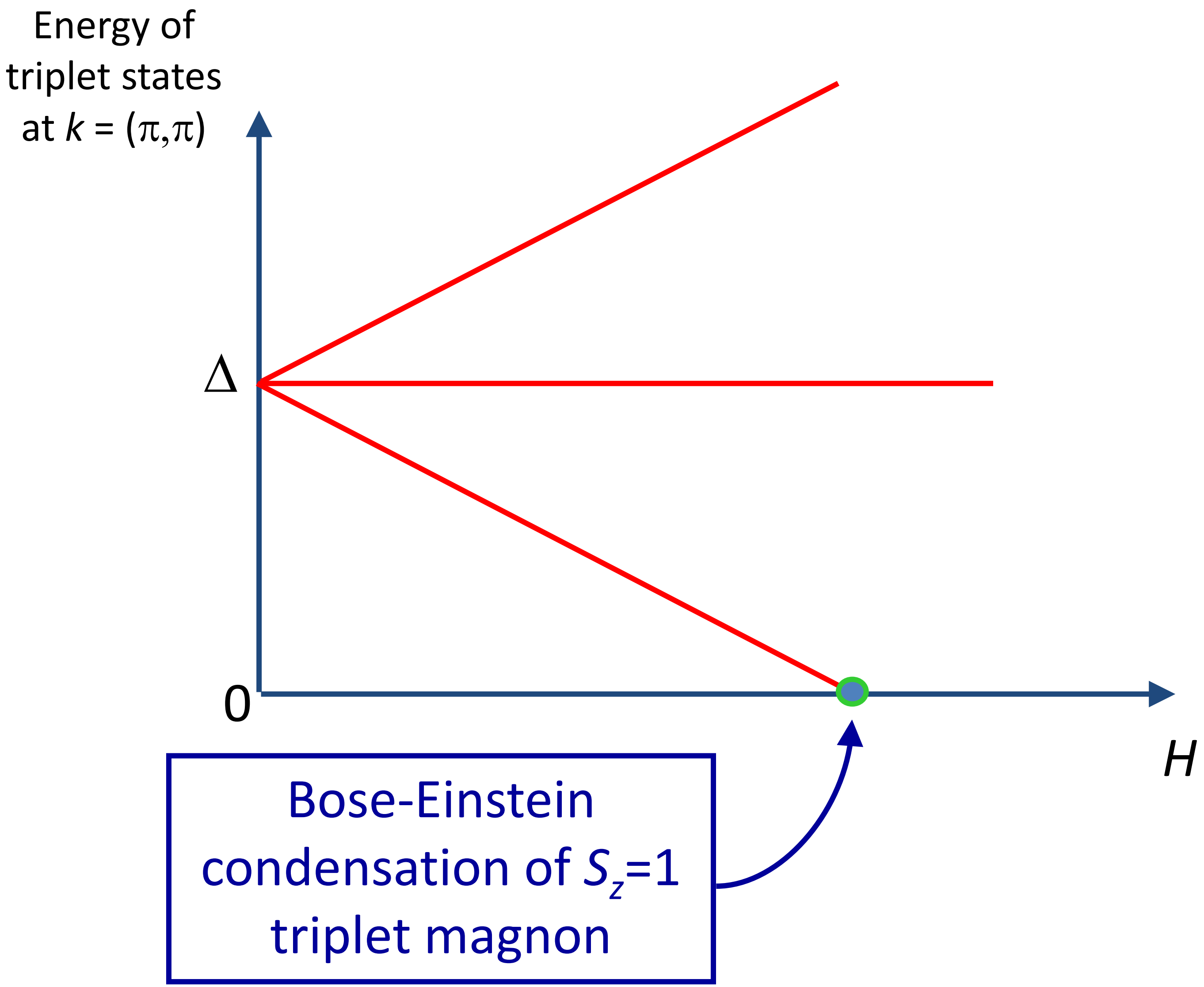
No quasiparticles – dissipative critical continuum

Pressure-driven QPT in $TlCuCl_3$: Neutron scattering

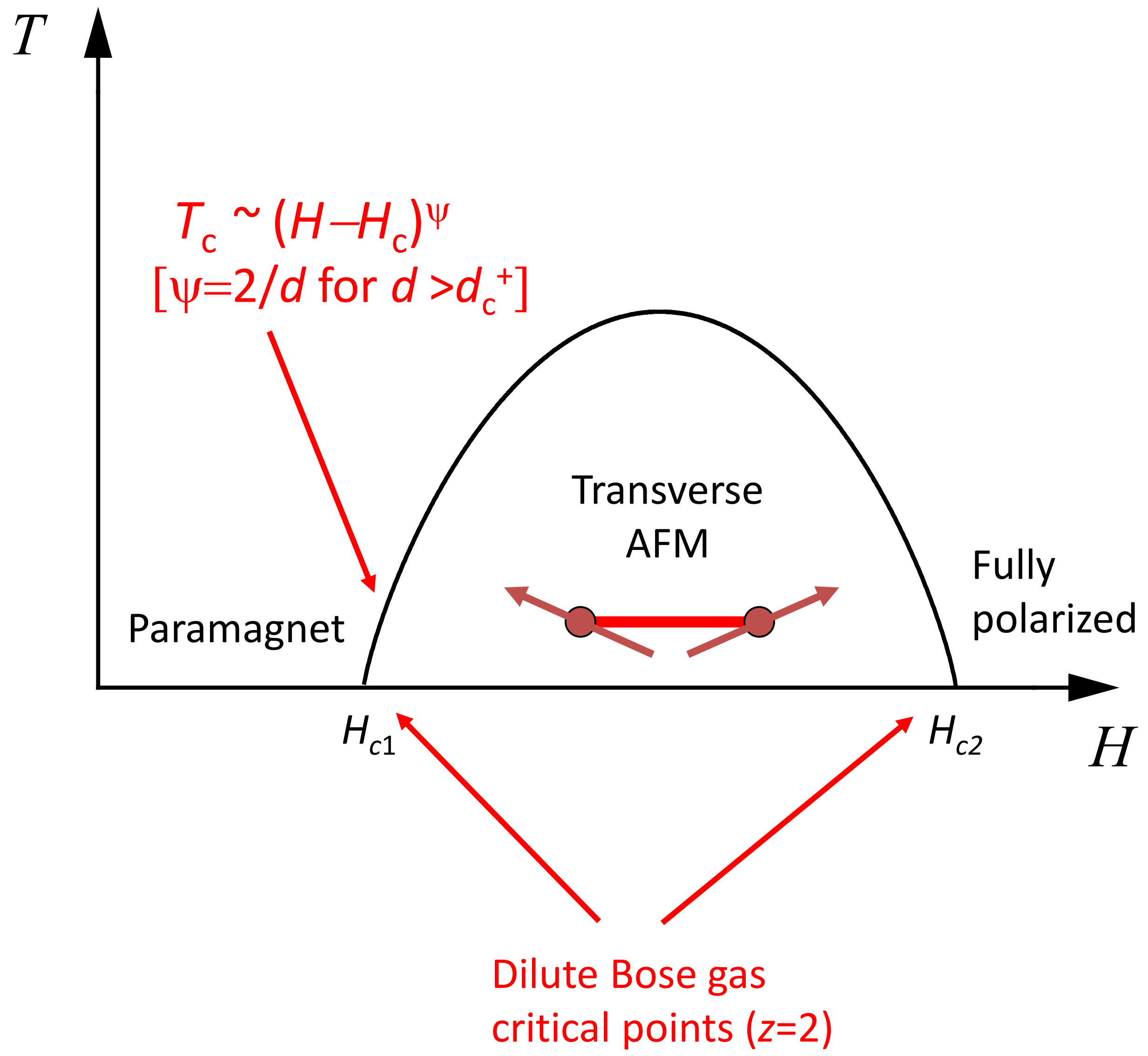


Rüegg *et al.*, PRL **100**, 205701 (2008)

Effect of field on paramagnet



Phase diagram in a magnetic field



Quantum criticality in living matter?

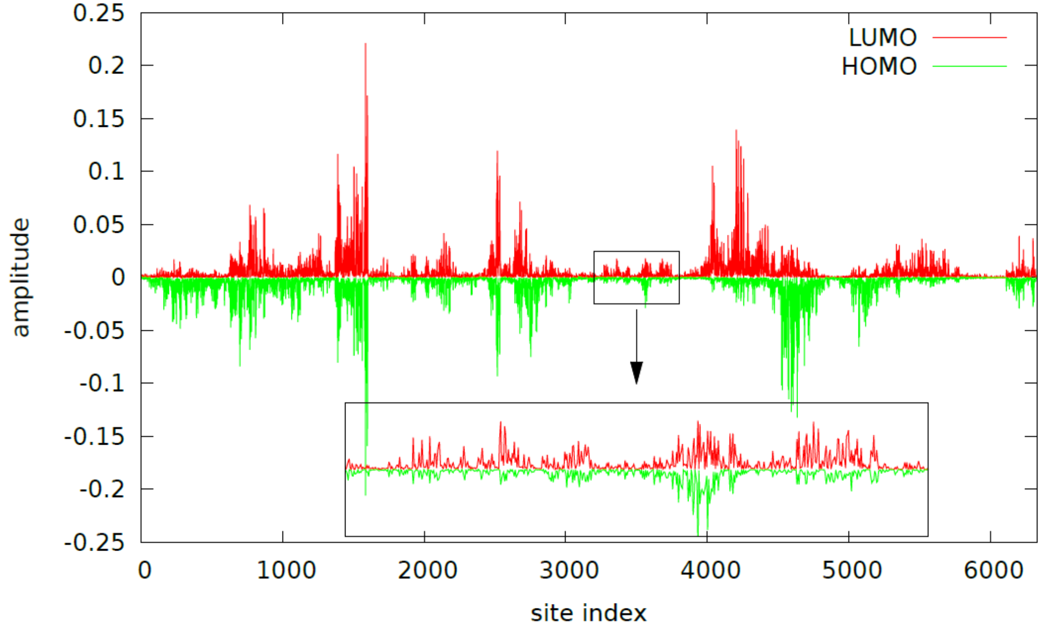
7th International Workshop DICE2014 Spacetime – Matter – Quantum Mechanics IOP Publishing
Journal of Physics: Conference Series **626** (2015) 012023 doi:10.1088/1742-6596/626/1/012023

Quantum criticality at the origin of life

Gábor Vattay[1], Dennis Salahub[2], István Csabai[1], Ali Nassimi[2,3] and Stuart A Kaufmann[2,4]

Claim:

Electronic wavefunctions in certain biomolecules display characteristics of Anderson metal-insulator transition (multifractality, critical level statistics)



Interpretation:

Charge transport in biological systems is environment-assisted (decoherence!); this is most effective near Anderson transition.

Since criticality requires fine-tuning, evolution must have selected critical molecules!

Orbitals, spin-orbit coupling & frustration:
What‘s different?

Additional degrees of freedom: orbital pseudospins

Need to consider problem of coupled spins and orbitals.
Toy models have enhanced symmetry (e.g. SU(4)).

Higher symmetry usually not present at microscopic level,
but may emerge at criticality.

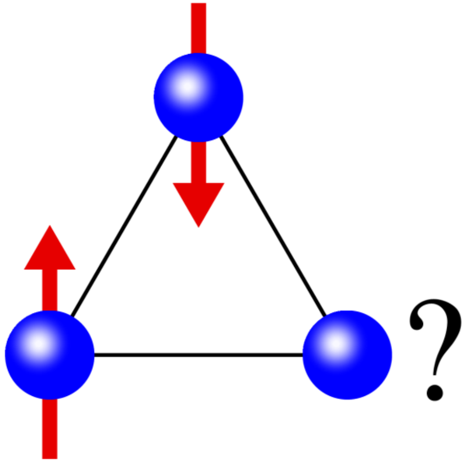
Rotation symmetry in spin space broken:

Lower symmetry for magnetic order parameter
Ising (N=1) or XY (N=2) instead of Heisenberg (N=3).

Spin-orbit coupling enables new physics!

Topological insulators
Exchange frustration → Kitaev spin liquid

Geometric frustration

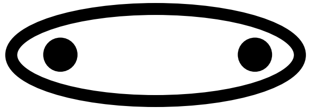


Frustration tends to suppress magnetic order

What is a spin liquid?

A (ground)state of magnetic moments in zero field which does not break any symmetries.

(liquid = short-range order only)

Singlet  $= (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) / \sqrt{2}$

More specifically:

State with half-odd-integer spin per unit cell which does not break any symmetries.

The birth of spin liquids

RESONATING VALENCE BONDS: A NEW KIND OF INSULATOR?*

P. W. Anderson
Bell Laboratories, Murray Hill, New Jersey 07974
and
Cavendish Laboratory, Cambridge, England

(Received December 5, 1972; Invited**)

ABSTRACT

The possibility of a new kind of electronic state is pointed out, corresponding roughly to Pauling's idea of "resonating valence bonds" in metals. As observed by Pauling, a pure state of this type would be insulating; it would represent an alternative state to the Néel antiferromagnetic state for S = 1/2. An estimate of its energy is made in one case.

Anderson, Mater Res Bull **8**, 153 (1973)

On the ground state properties of the anisotropic triangular antiferromagnet

By P. Fazekas† and P. W. Anderson‡
Cavendish Laboratory, Cambridge, England

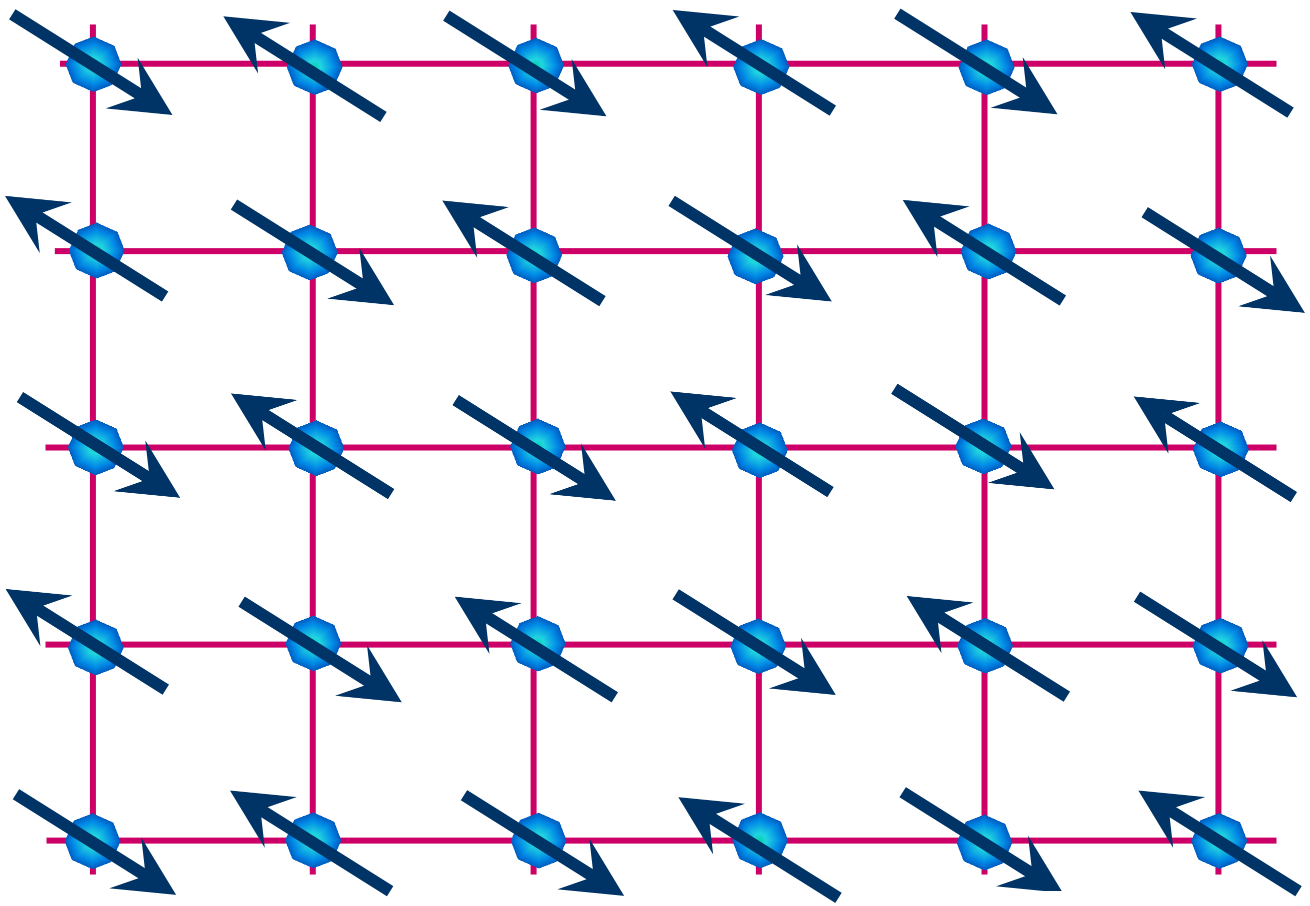
[Received 24 May 1974]

Abstract

Our aim is to present further evidence supporting a recent suggestion by Anderson (1973) that the ground state of the triangular antiferromagnet is different from the conventional three-sublattice Néel state. The anisotropic Heisenberg model is investigated. Near the Ising limit a peculiar, possibly liquid-like state is found to be energetically more favourable than the Néel-state. It seems to be probable that this type of ground state prevails in the anisotropy region between the Ising model and the isotropic Heisenberg model. The implications for the applicability of the resonating valence bond picture to the $S=\frac{1}{2}$ antiferromagnets are also discussed.

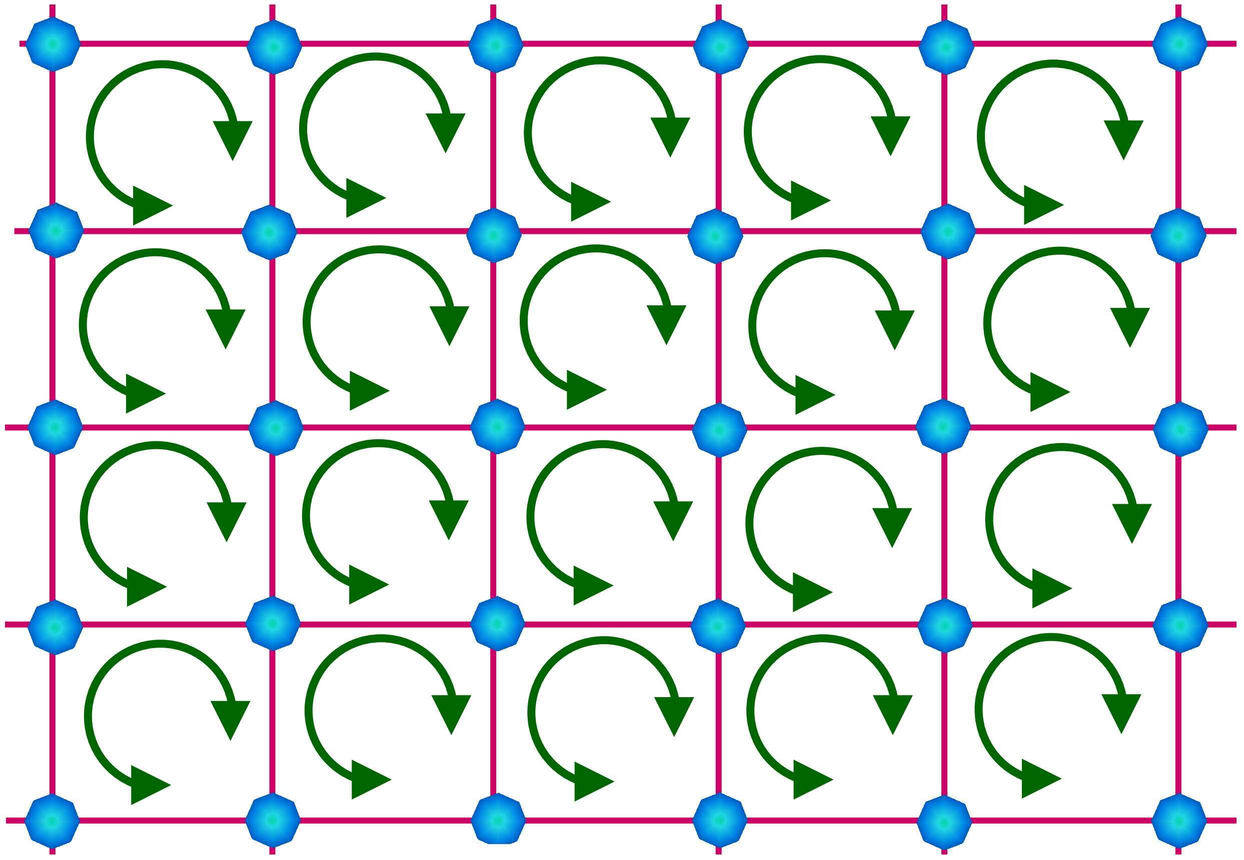
Fazekas /Anderson, Phil Mag **30**, 23 (1974)

Antiferromagnetic Néel order



$$H = J \sum_{\langle ij \rangle} S_i \cdot S_j$$

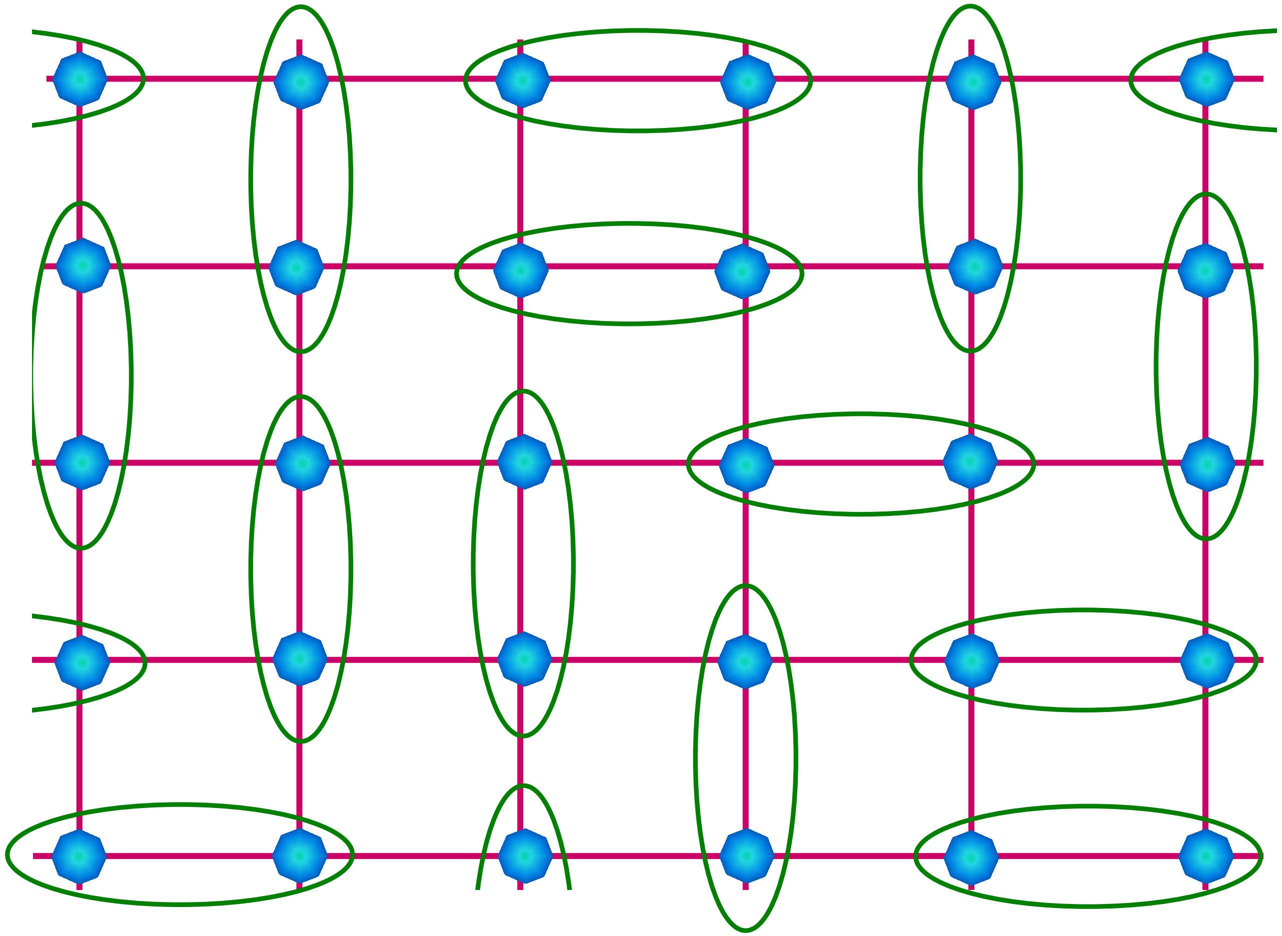
Suppress AF order by frustration

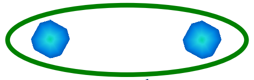


$$H = J\sum_{\langle ij\rangle} S_i \cdot S_j + K\sum_{\square} \text{4-spin exchange}$$

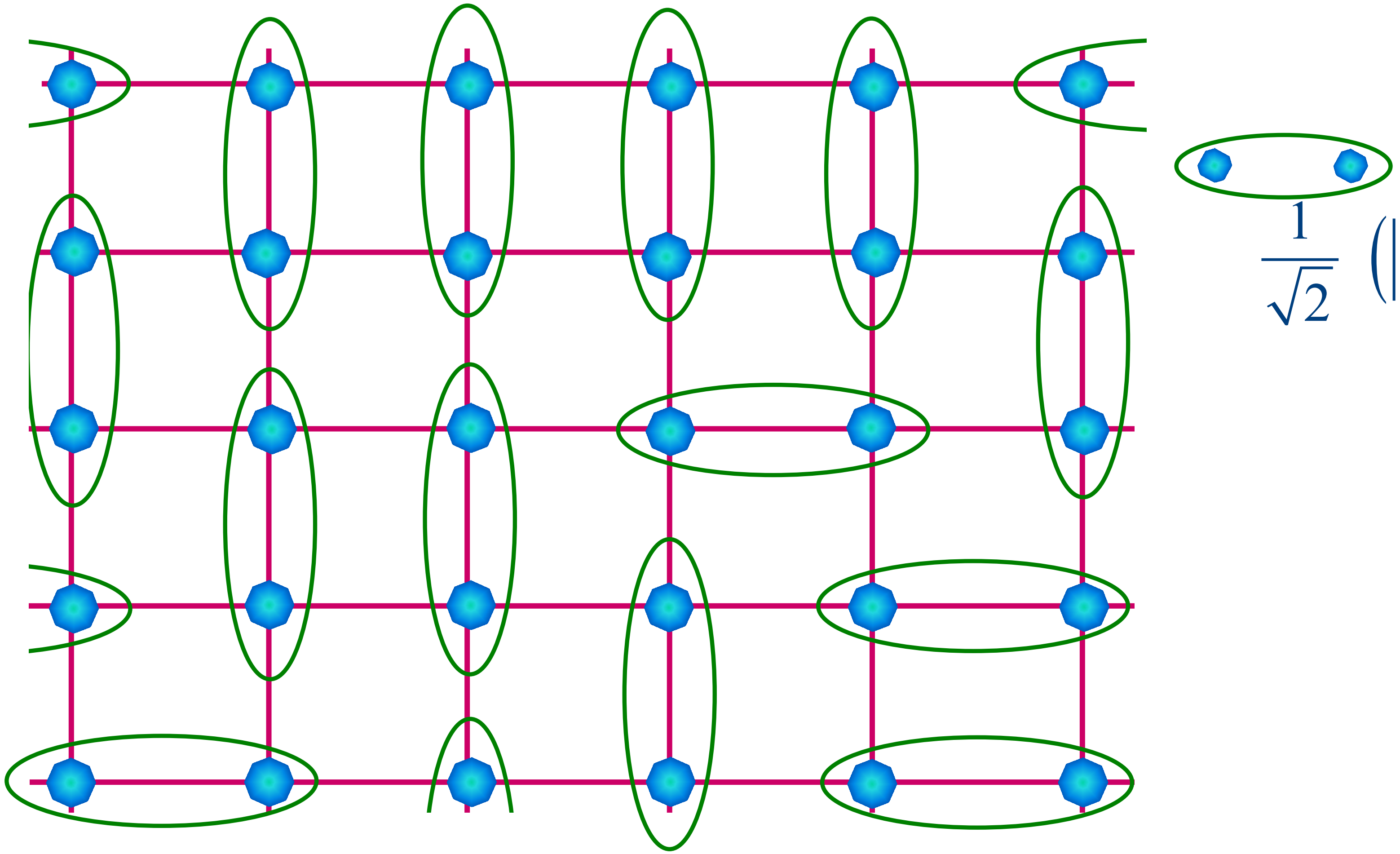
Sandvik, PRL **98**, 227202 (2007)

Paramagnetic phase: Valence bond singlet pairs

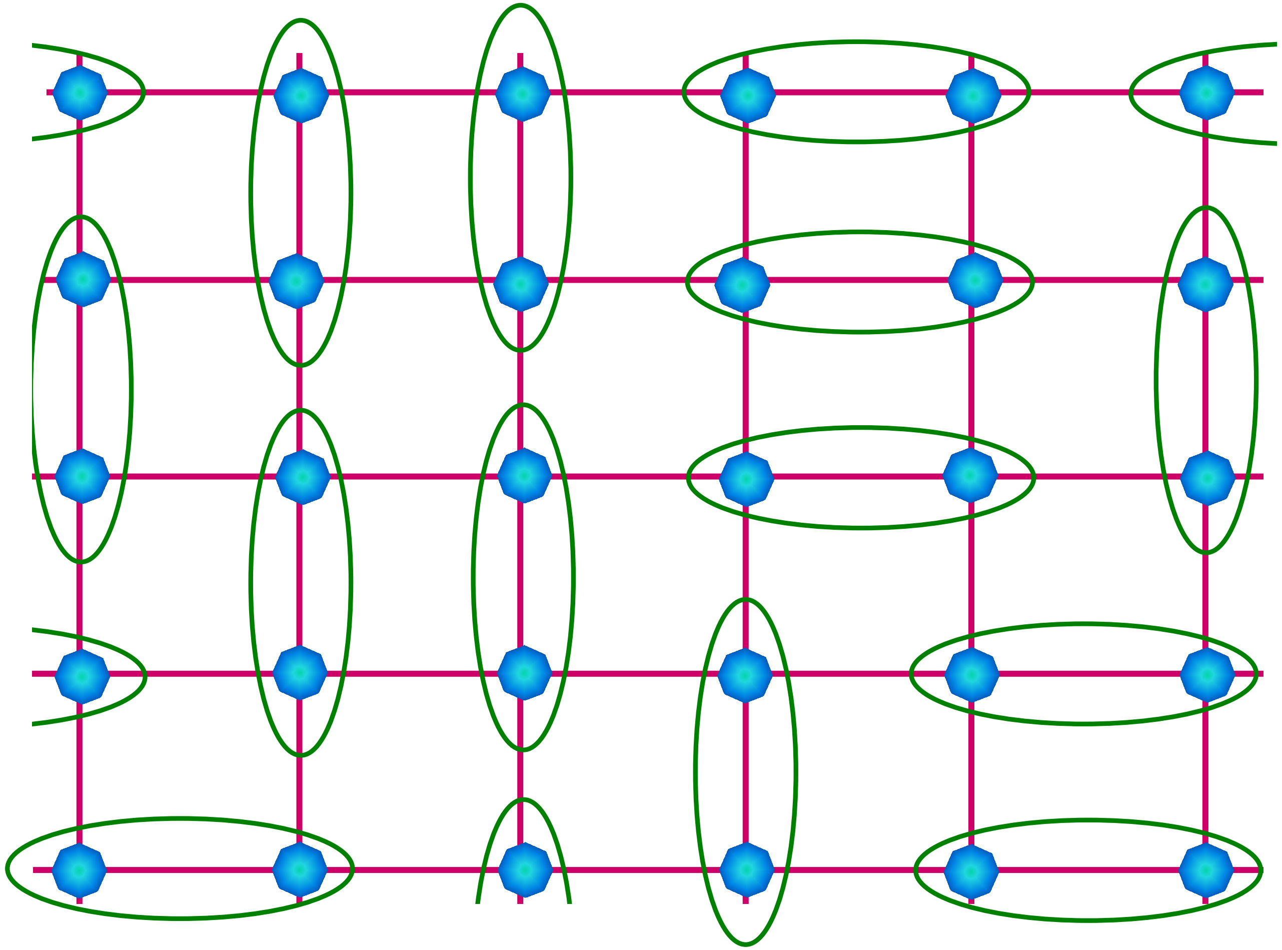


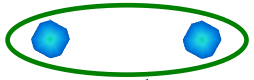


$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

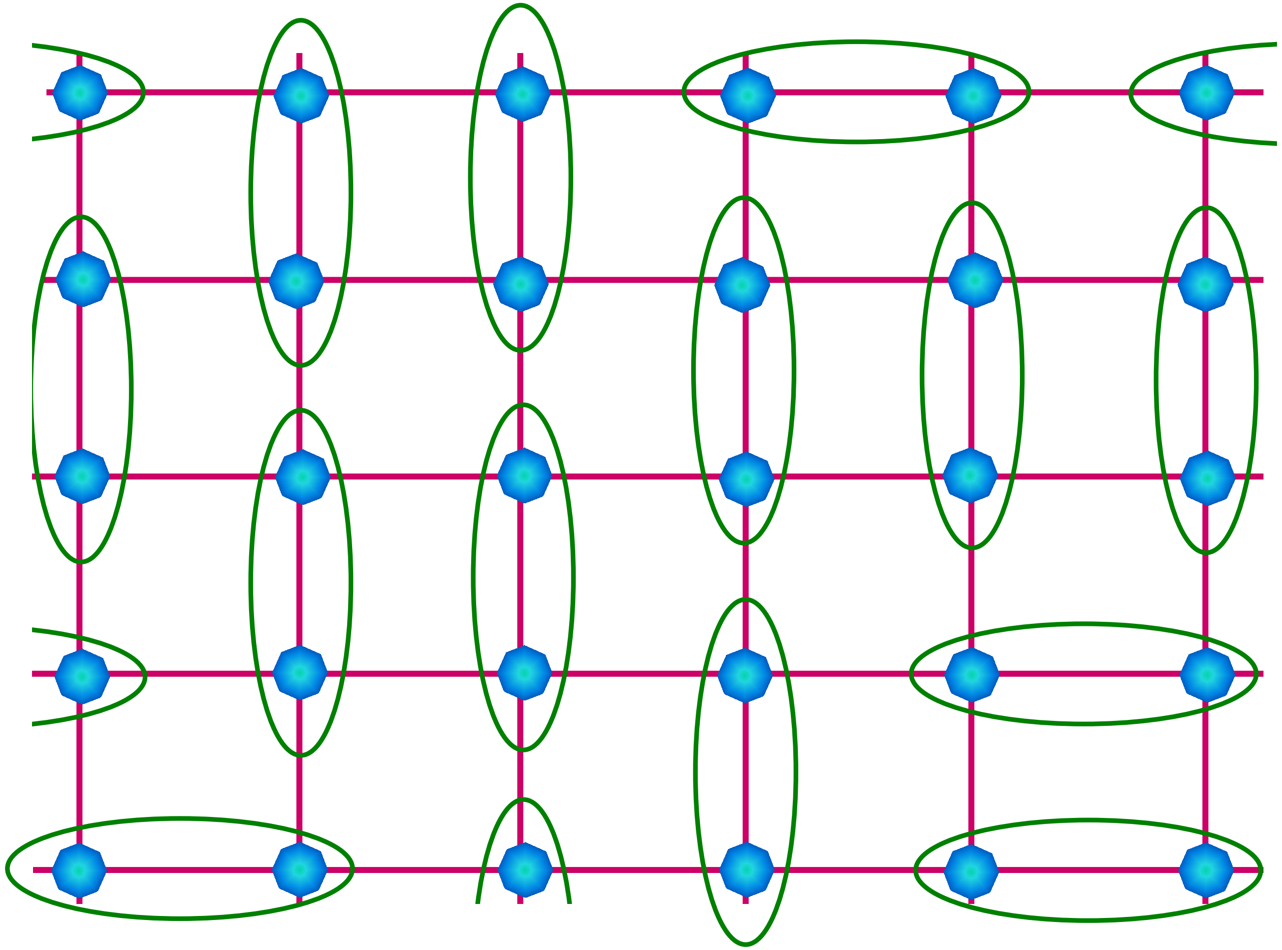


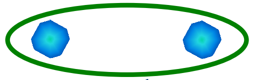
$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$



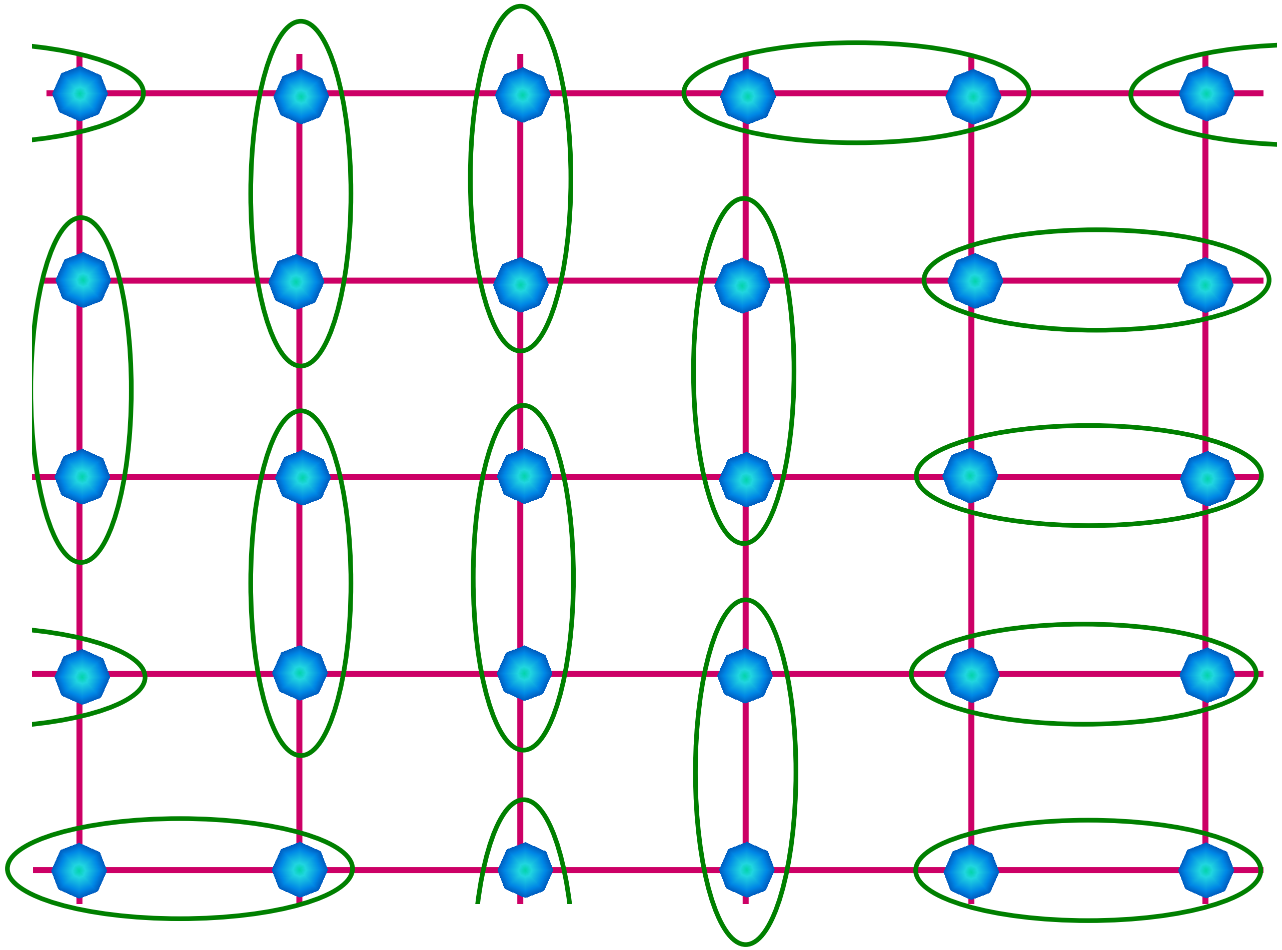


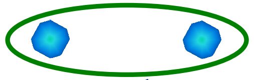
$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$





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

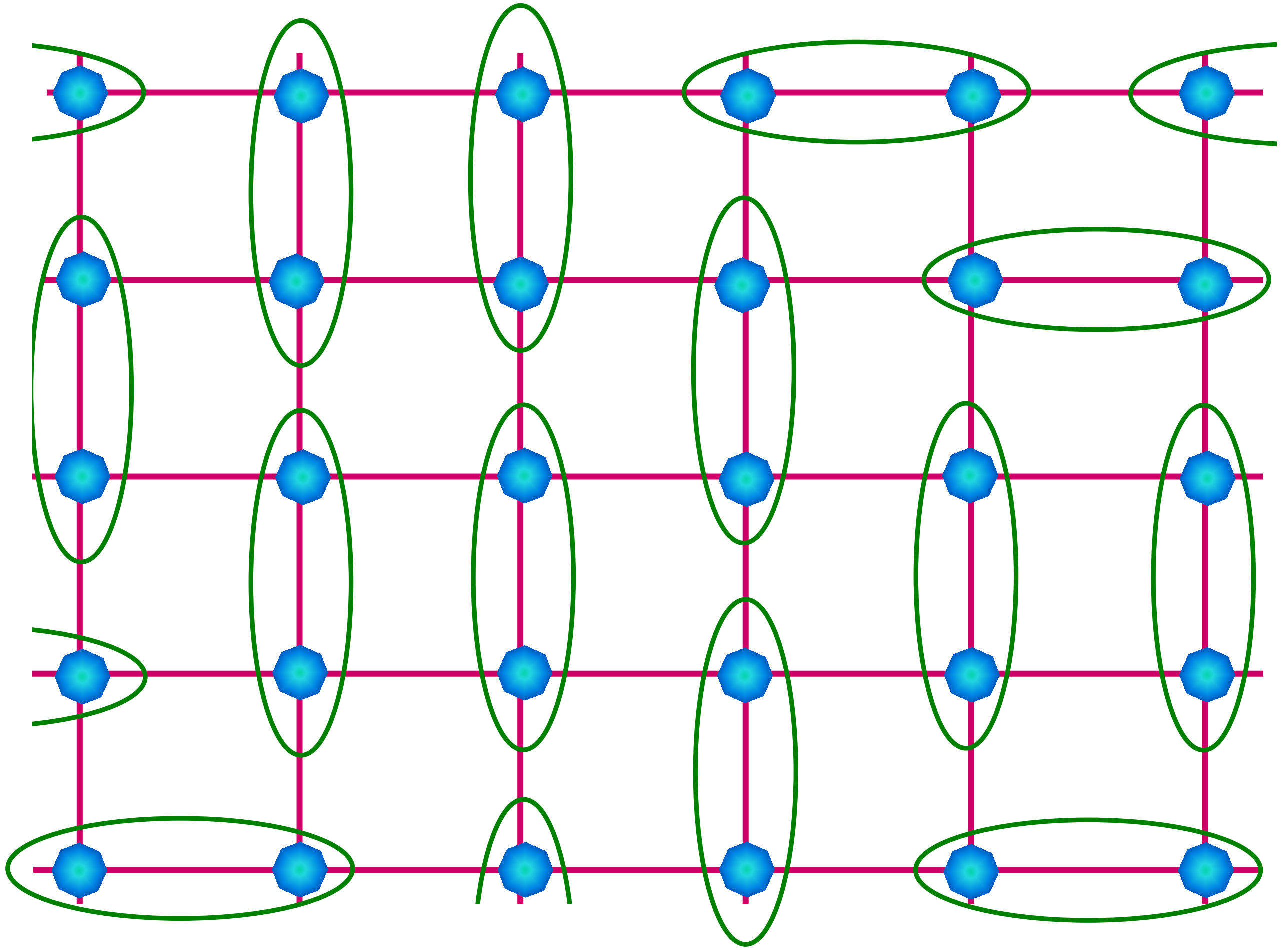


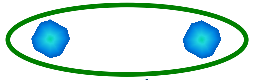


$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Superposition: Entangled liquid of valence bonds

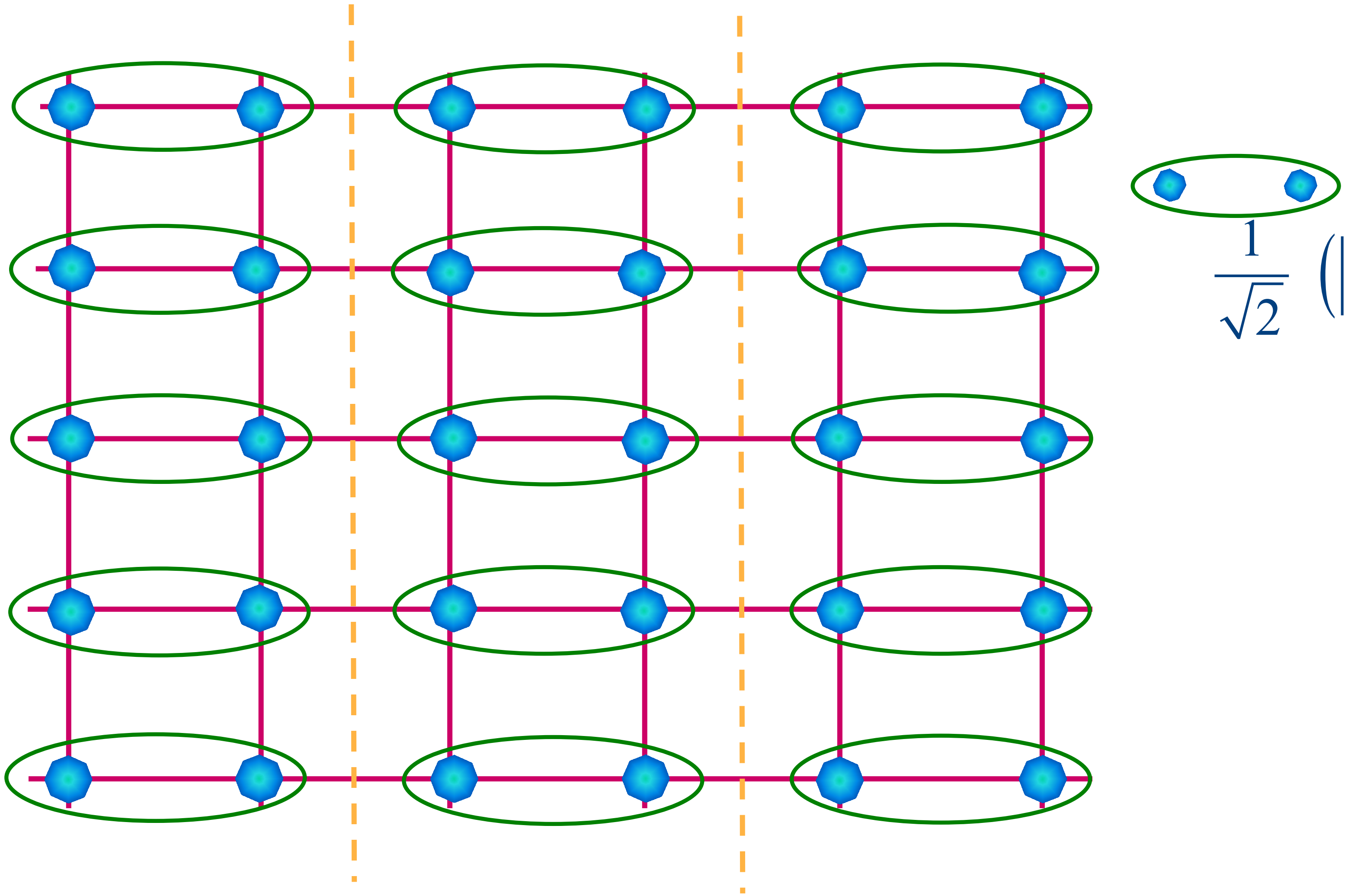
Resonating valence-bond state (technically a Z_2 spin liquid)



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

Fazekas /Anderson, *Phil Mag* **30**, 23 (1974)

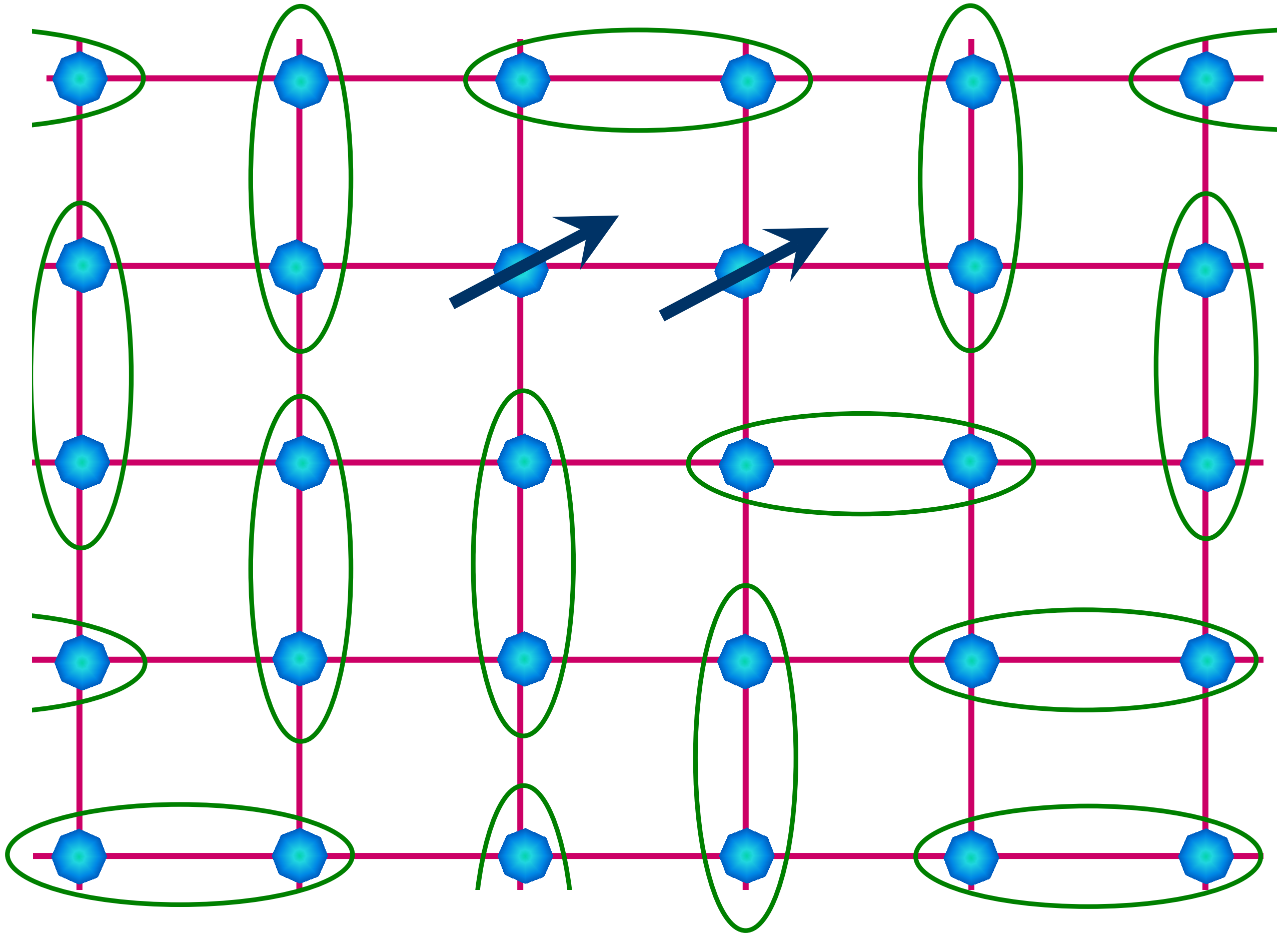
Valence bond solid (VBS)

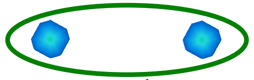


$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Read / Sachdev, PRL **62**, 1694 (1989)
Moessner / Sondhi, PRB **63**, 224401 (2001)

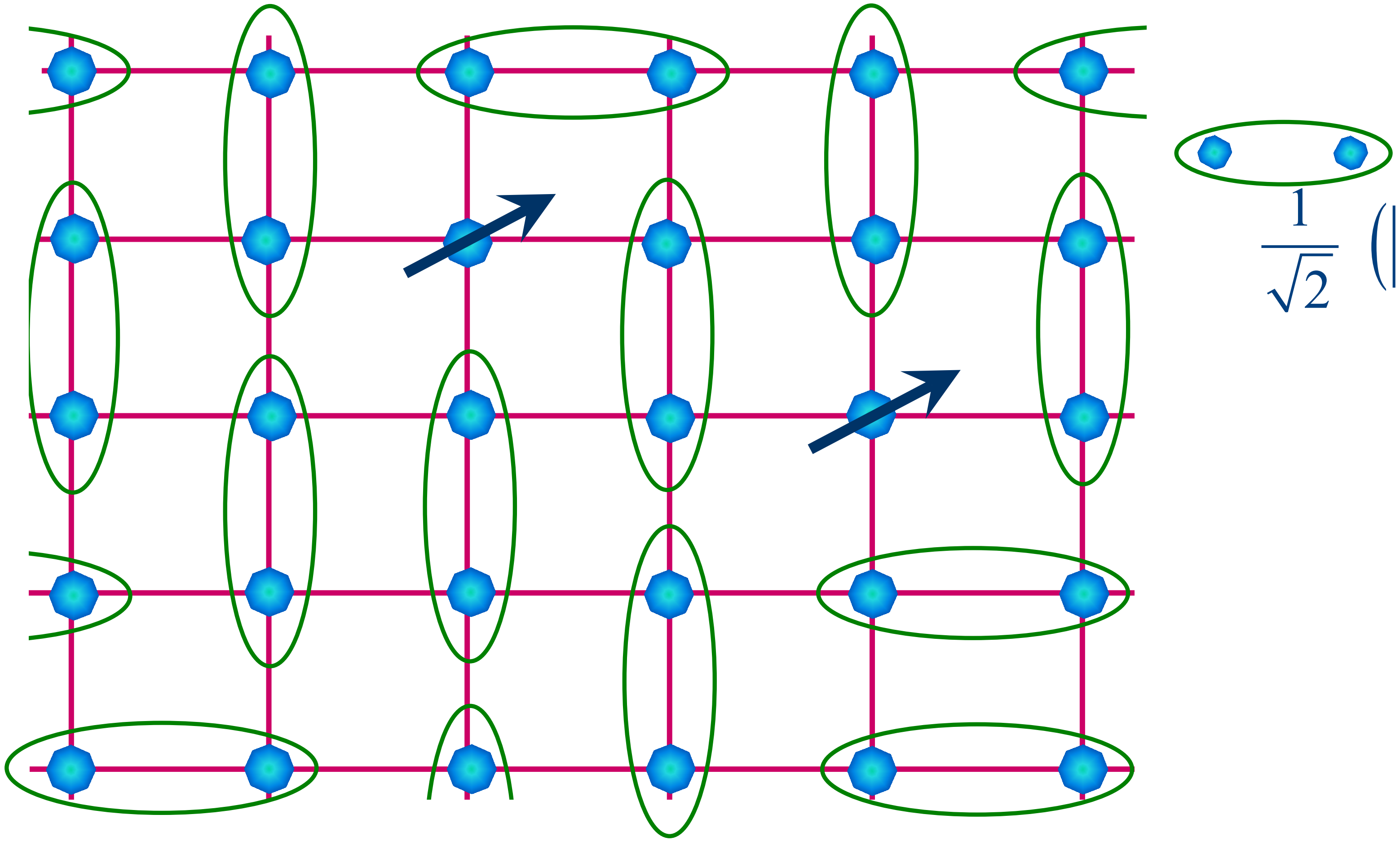
Excitations of RVB liquid



 $=$

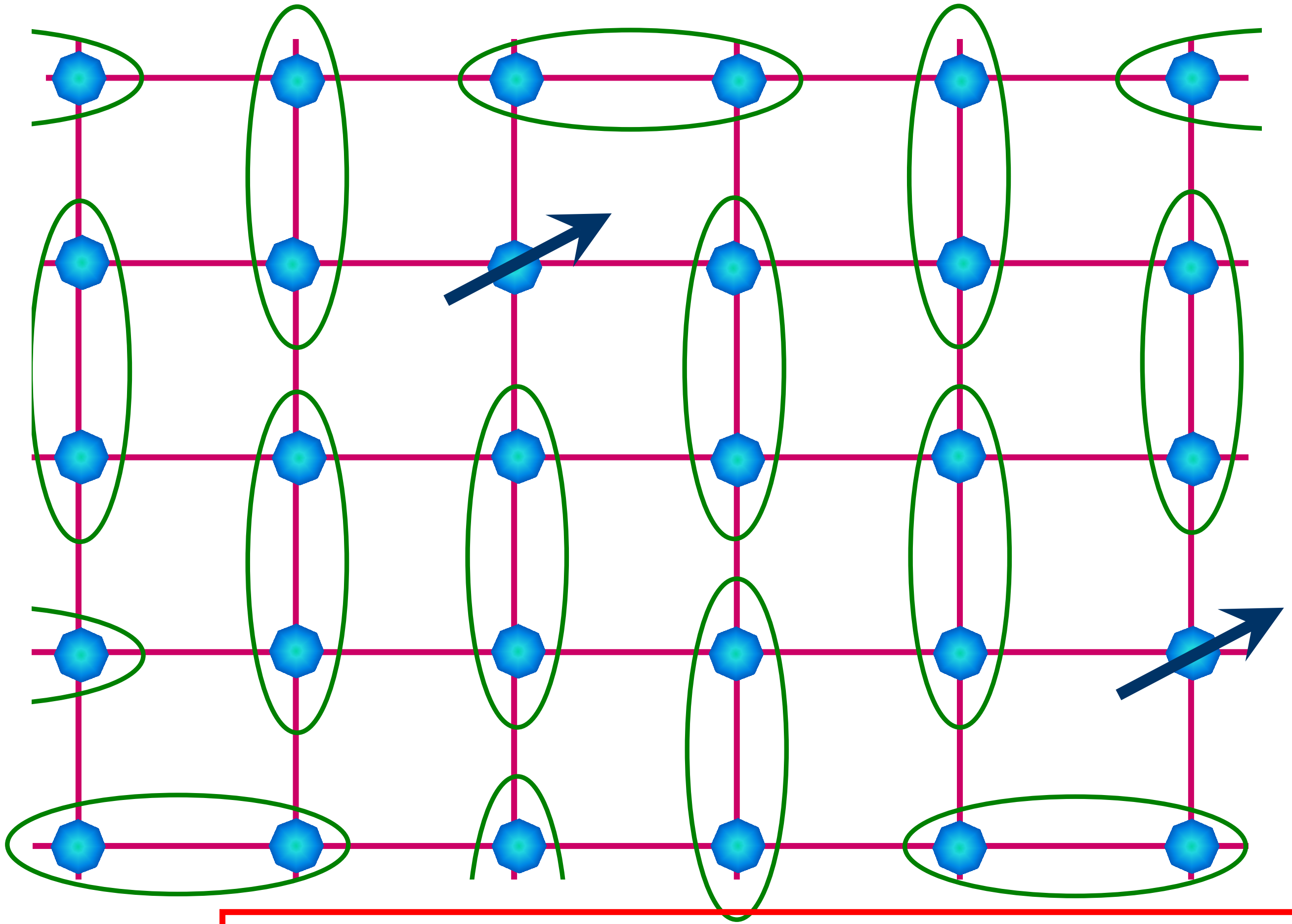
$$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

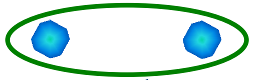
Excitations of RVB liquid



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

Excitations of RVB liquid: Deconfined spinons



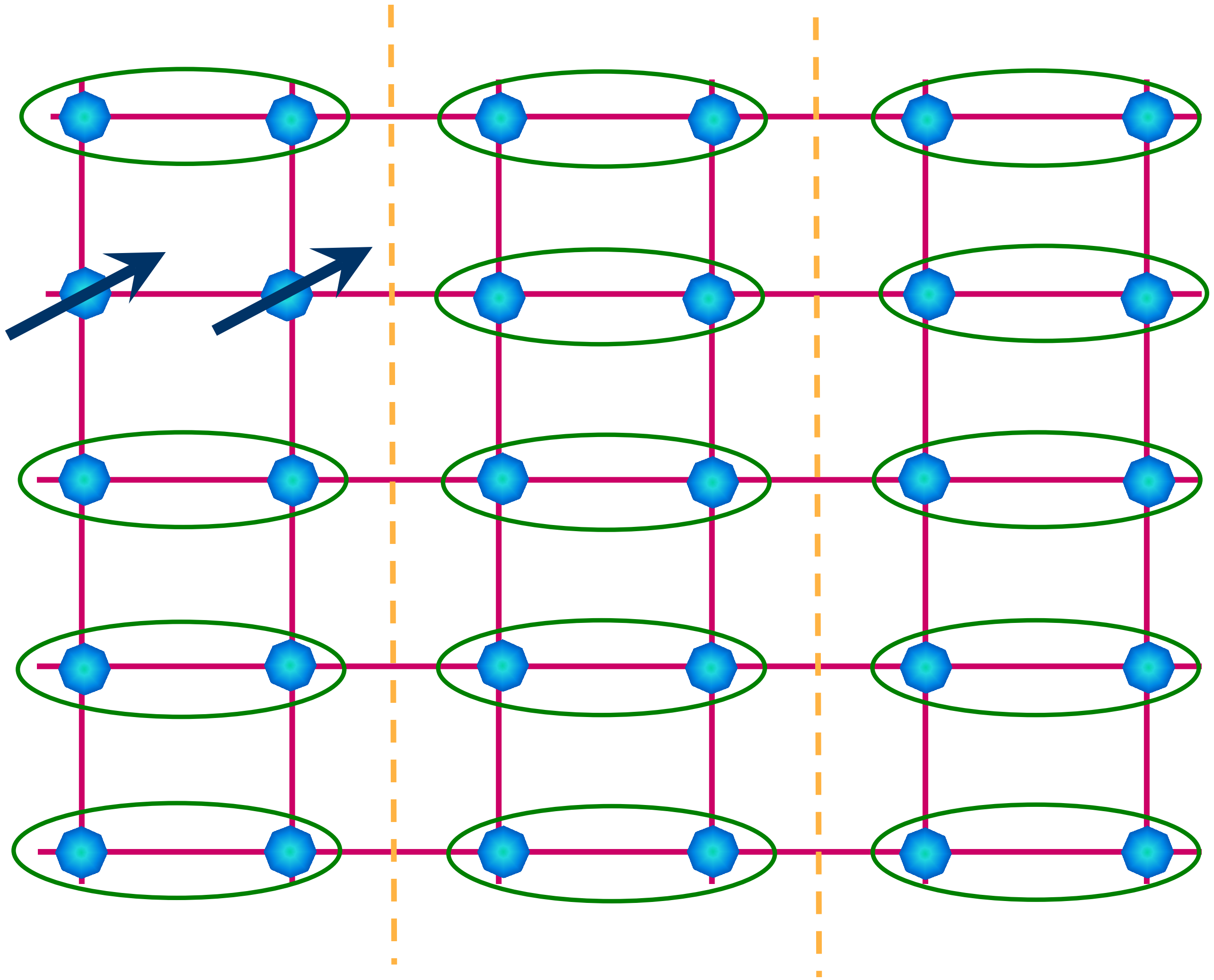
 =

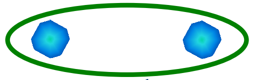
$$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Emergent excitations of RVB state – **Fractionalization**!

- Spinon (spin ½, charge 0, gapped) = „matter“ particle
- Vison (spin 0, charge 0, gapped) = excitation of Z_2 gauge field

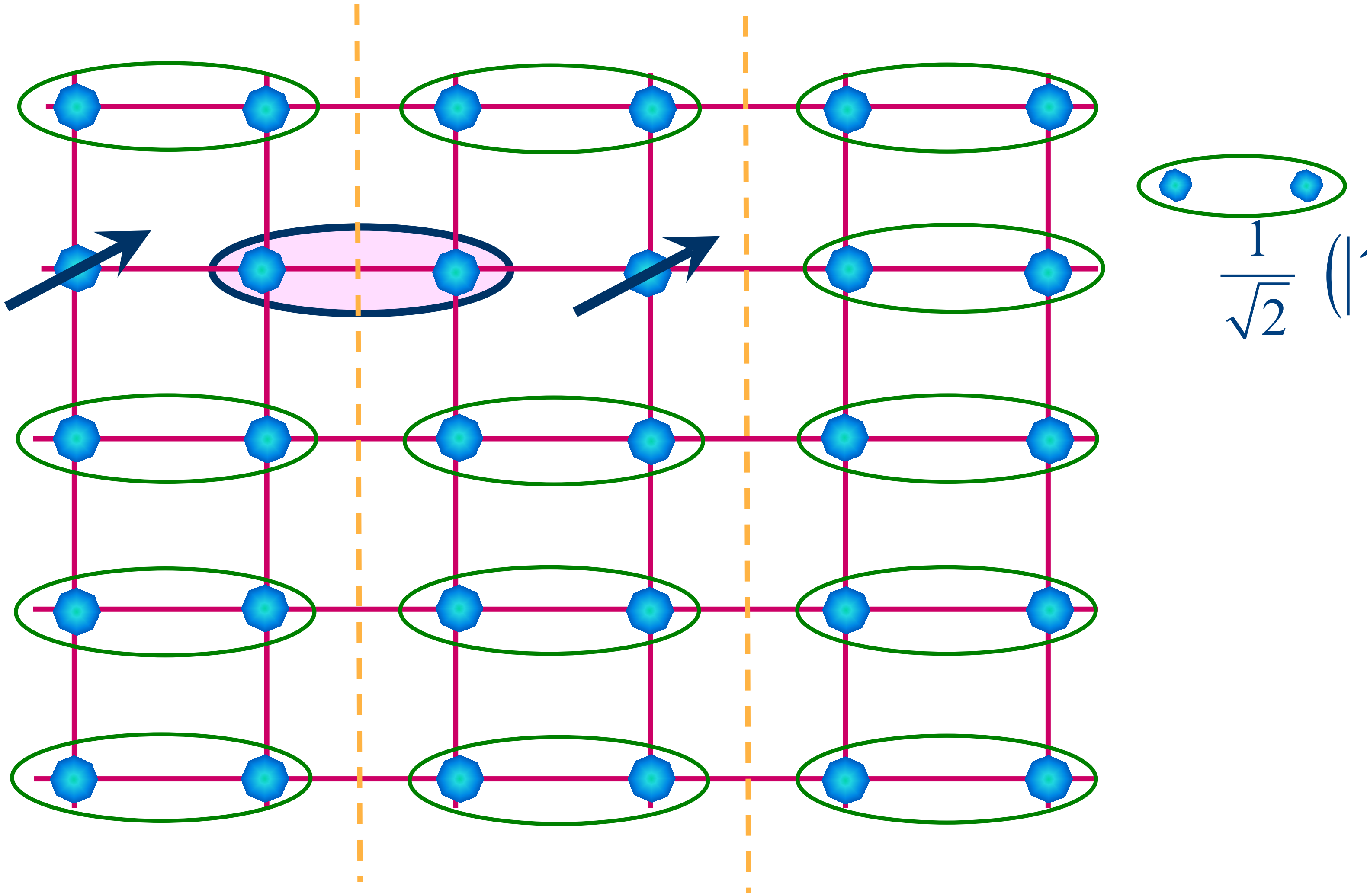
Excitations of the valence-bond solid





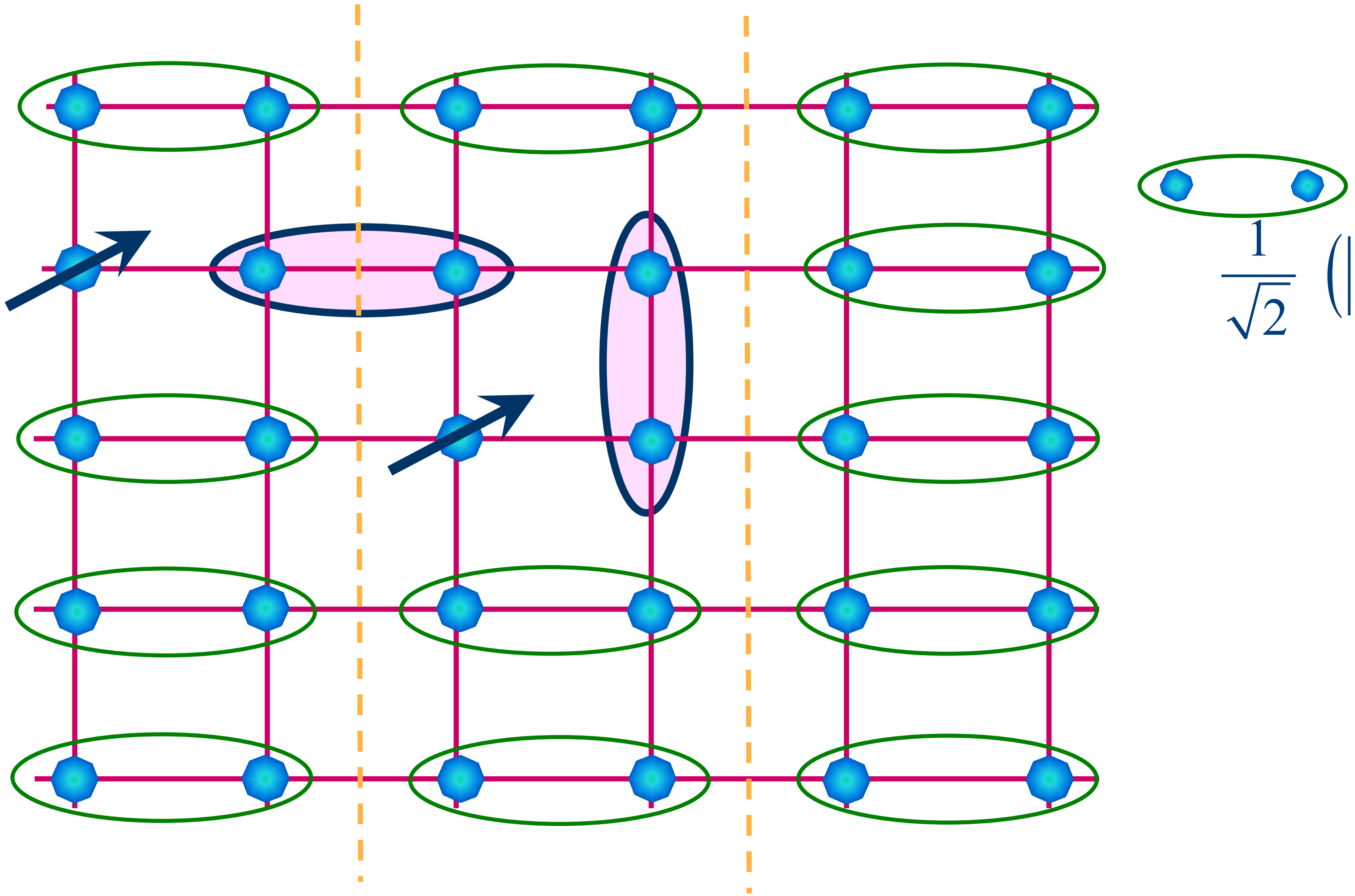
$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Excitations of the valence-bond solid



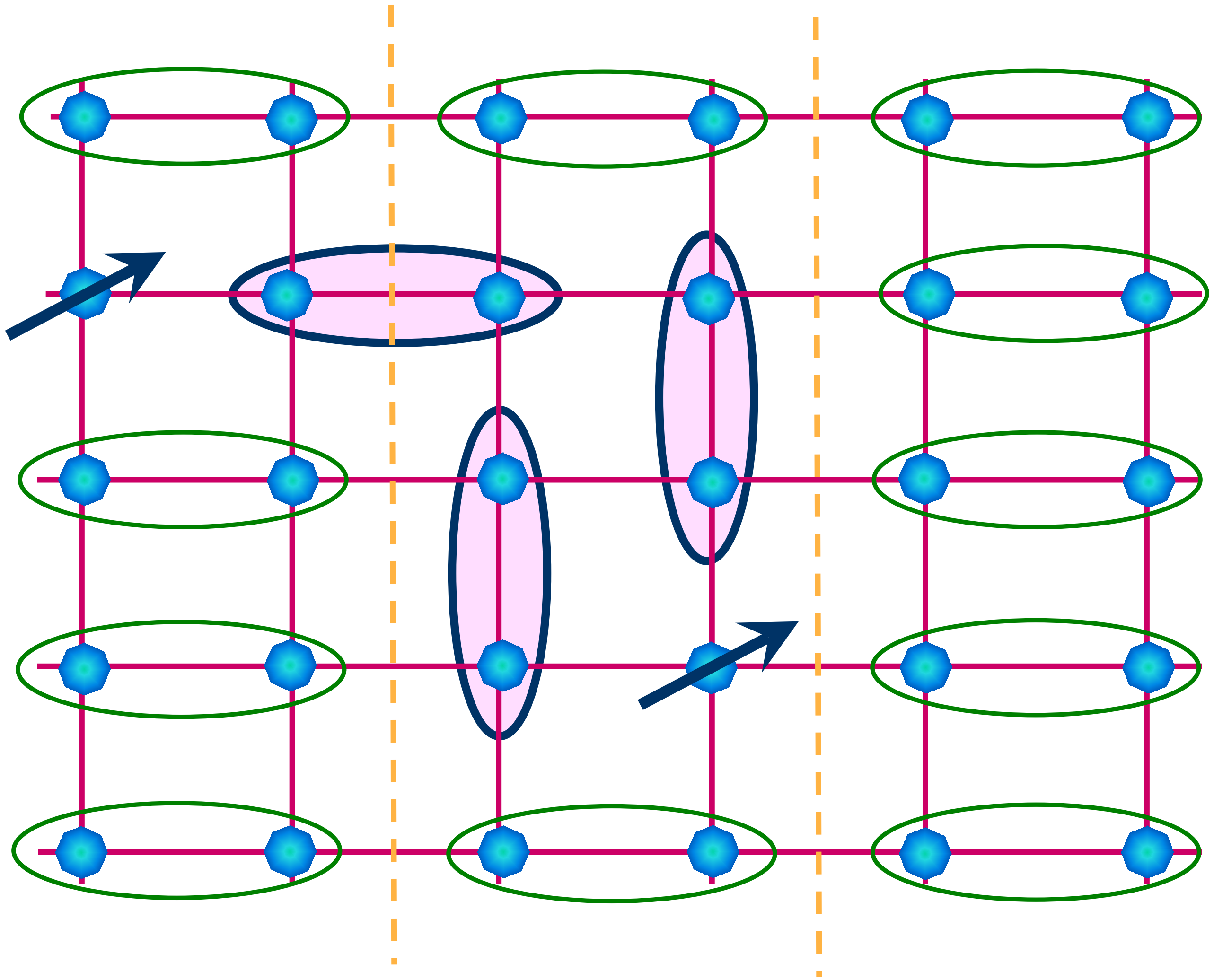
$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

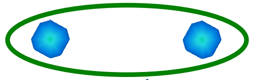
Excitations of the valence-bond solid



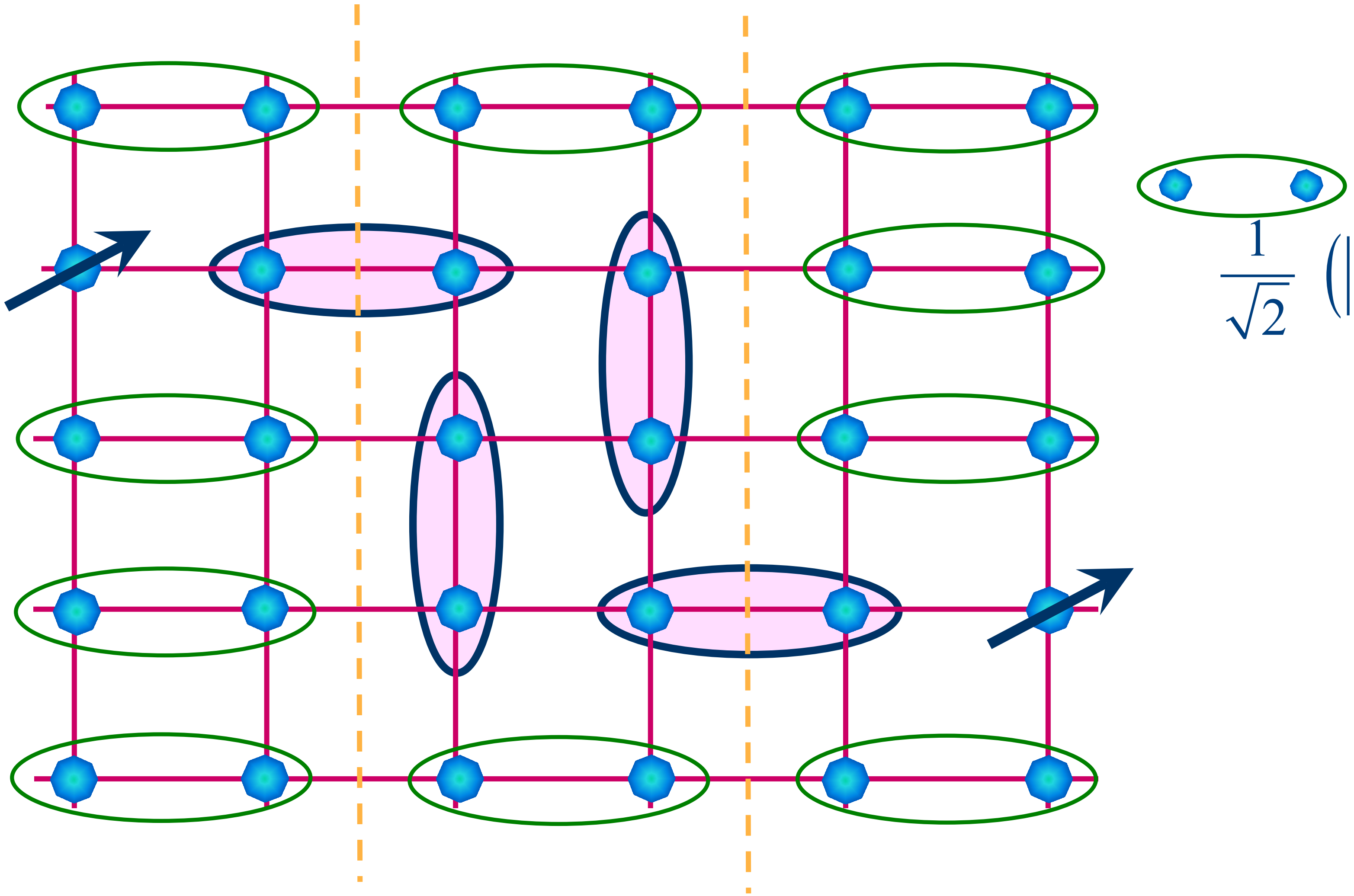
$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Excitations of the valence-bond solid



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

Excitations of the valence-bond solid



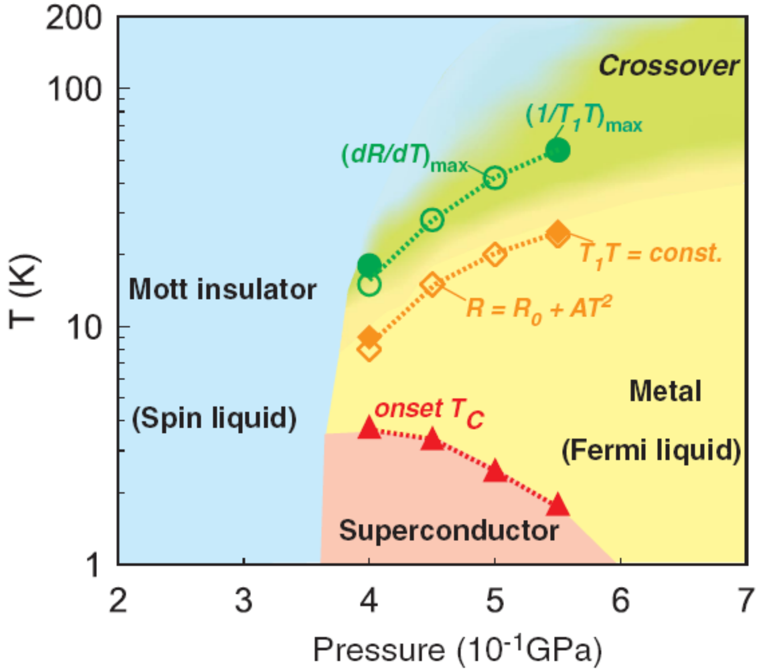
$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Spinons are unable to move apart:
no fractionalization, but **confinement**

Experiment: Spin liquids and valence-bond solids

κ-$(ET)_2Cu_2(CN)_3$

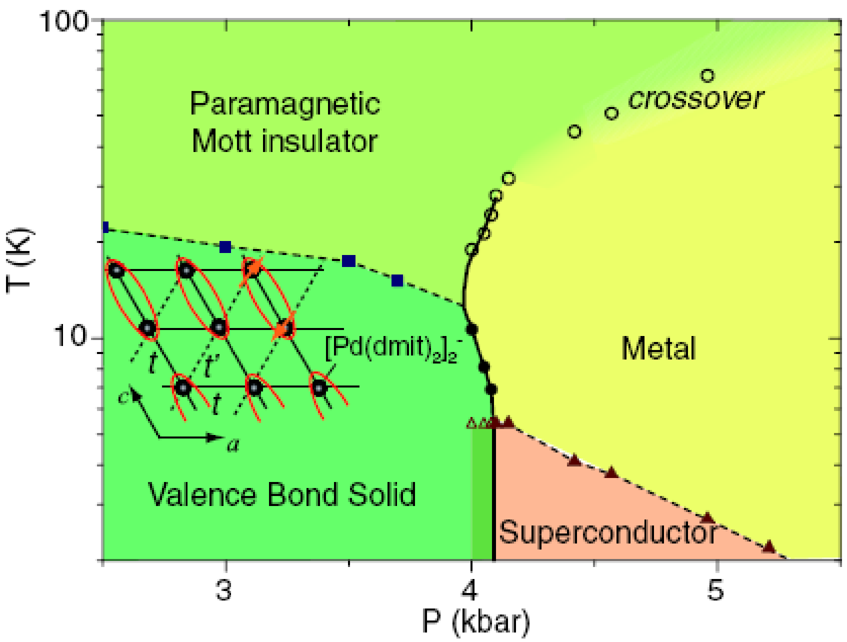
Spin liquid



Kurosaki *et al.*, PRL (2005)

$[Pd(dmit)_2]_2$

Valence-bond solid



Shimizu *et al.*, PRL (2007)

Microscopics: half-filled triangular-lattice Hubbard model

Exotic quantum phase transitions in frustrated magnets

Quantum phase transitions: beyond LGW

Degrees of freedom:
emergent fractionalized particles and gauge fields

QPT through condensation of

- matter particles
- gauge-field defects (e.g. vortices)
- composites thereof

Parton construction: U(1) spin liquid

Consider magnet with collinear magnetic fluctuations

$$\vec{S}_i = \mathfrak{Re}\left(\vec{\phi} e^{i\vec{K}\cdot\vec{x}_i}\right) = \vec{n}_1 \cos(\vec{K}\cdot\vec{x}_i) + \vec{n}_2 \sin(\vec{K}\cdot\vec{x}_i)$$

with $\vec{n_1} \parallel \vec{n_2}$

Parametrization in terms of „spinons“:

$$\boxed{\vec{\phi} = \sum_{\sigma\sigma'} z_\sigma^\dagger \vec{\tau}_{\sigma\sigma'} z_{\sigma'}/2} \qquad \sum_\sigma |z_\sigma|^2 = 1$$

Invariant under local U(1) transformation:

$$z_\sigma \to e^{i\Theta} z_\sigma$$

Arovas/Auerbach, PRB **38**, 316 (1988)
Read/Sachdev, PRL **62**, 1694 (1989)

Effective theory for U(1) spin liquid

Low energy spinon theory for "quantum disordering" the Néel state is the CP^1 model

$$\mathcal{S}_z = \int d^2x d\tau \Big[c^2 \left|(\nabla_x - iA_x)z_\alpha\right|^2 + \left|(\partial_\tau - iA_\tau)z_\alpha\right|^2 + s\left|z_\alpha\right|^2 + u\left(\left|z_\alpha\right|^2\right)^2 + \frac{1}{4e^2}\left(\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda\right)^2 \Big]$$

where A_μ is an emergent U(1) gauge field (the **"photon"**) which describes low-lying spin-singlet excitations.

Phases:

$$\langle z_\alpha \rangle \neq 0 \quad \Rightarrow \quad \text{Néel (Higgs) state}$$
$$\langle z_\alpha \rangle = 0 \quad \Rightarrow \quad \text{Spin liquid (Coulomb) state}$$

Parton construction: Z_2 spin liquid

Consider magnet with non-collinear magnetic fluctuations

$$\vec{S}_i = \mathfrak{Re}\left(\vec{\phi} e^{i\vec{K}\cdot\vec{x}_i}\right) = \vec{n}_1 \cos(\vec{K}\cdot\vec{x}_i) + \vec{n}_2 \sin(\vec{K}\cdot\vec{x}_i)$$

with $\vec{n}_1 \cdot \vec{n}_2 = 0 \quad ; \quad \vec{n}_1^2 = \vec{n}_2^2 = 1$

Parametrization in terms of „spinons“:

$$\boxed{\vec{\phi} = \vec{n}_1 + i\vec{n}_2 = \epsilon_{\sigma\sigma'} z_{\sigma'} \frac{\vec{\sigma}_{\sigma\tau}}{2} z_\tau} \qquad \sum_\sigma |z_\sigma|^2 = 1$$

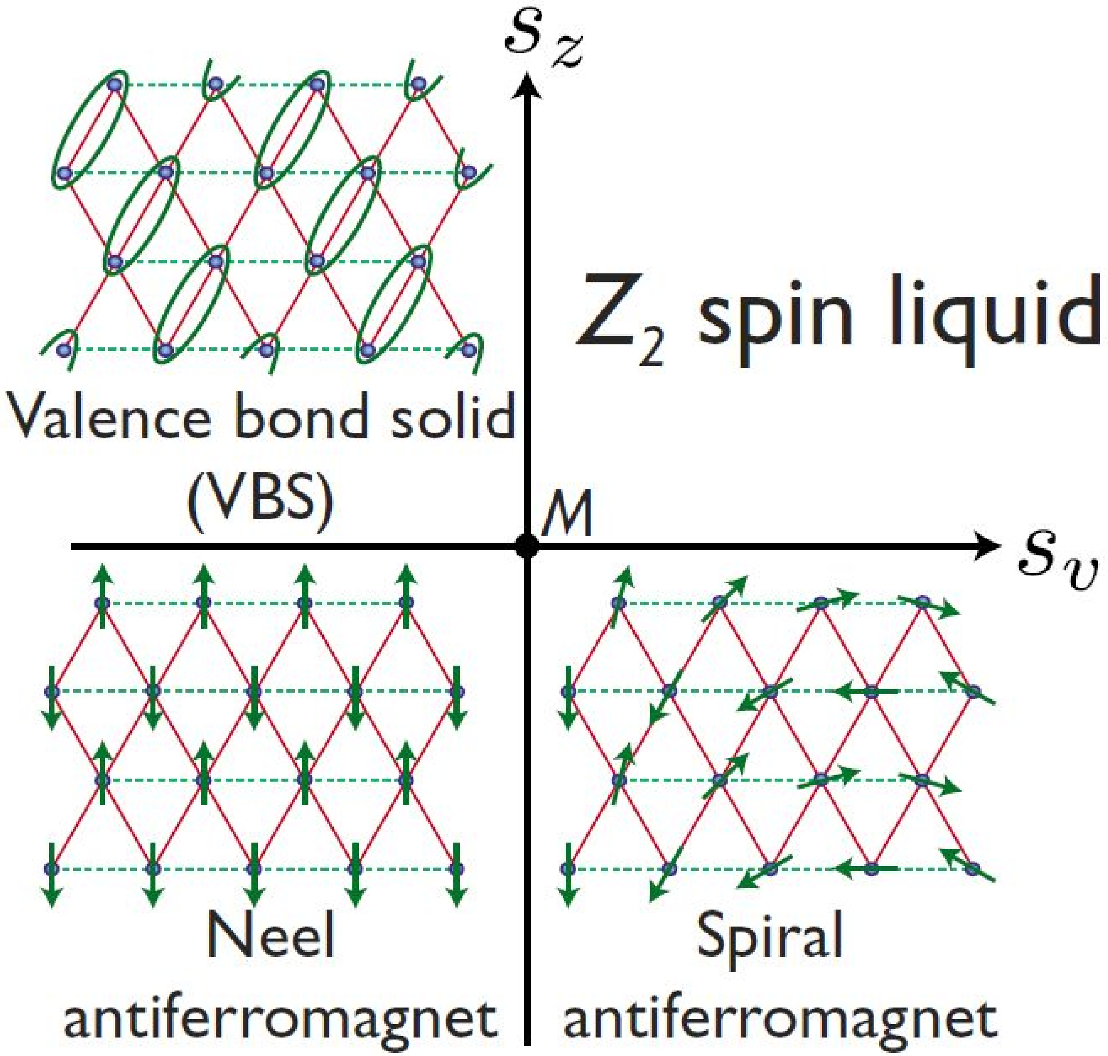
Invariant under local Z_2 transformation:

$$z_\sigma \rightarrow \eta z_\sigma \text{ with } \eta = \pm 1$$

Reduction from U(1) to Z_2 can be understood through (BCS) pairing of spinons

Arovas/Auerbach, PRB **38**, 316 (1988)
Read/Sachdev, PRL **62**, 1694 (1989)

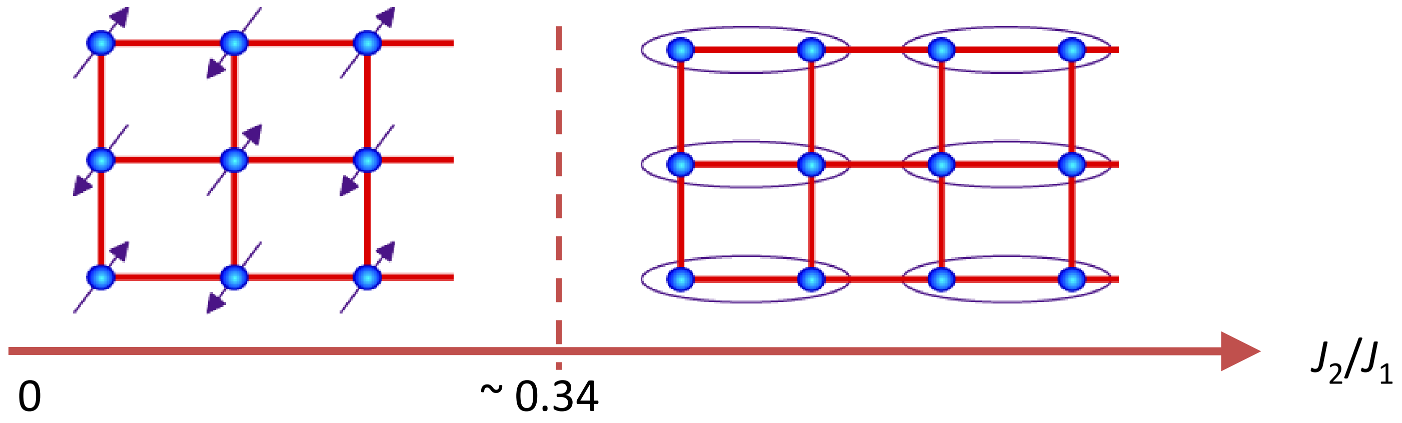
Spin liquids and symmetry-breaking descendants



Xu/Sachdev, PRB **79**, 064405 (2009)

Deconfined criticality in frustrated magnets

Phase diagram of frustrated square-lattice Heisenberg model



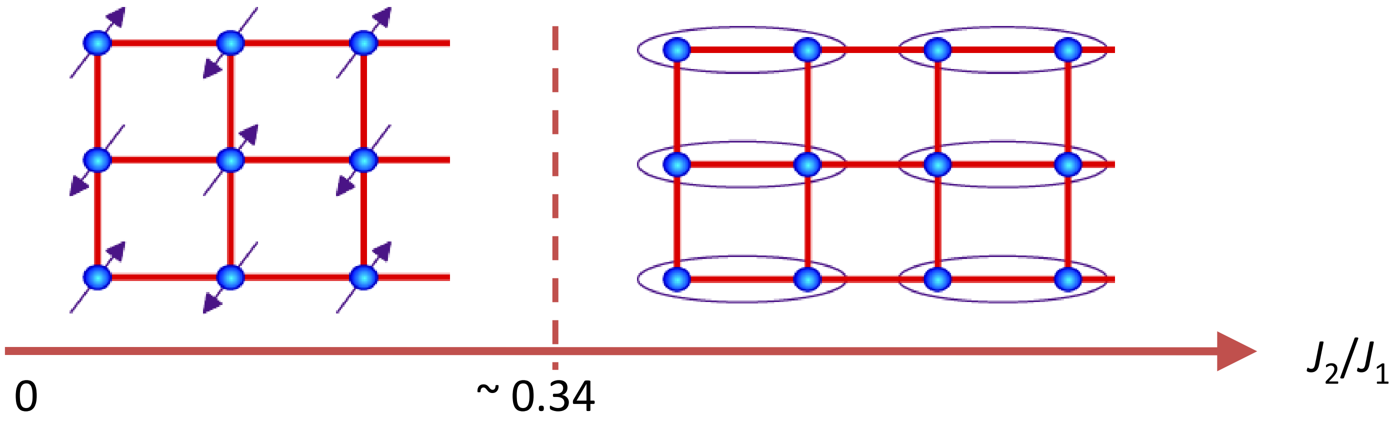
Néel and valence-bond solid states break **different** symmetries!
Landau theory would predict direct first-order transition or intermediate phase.

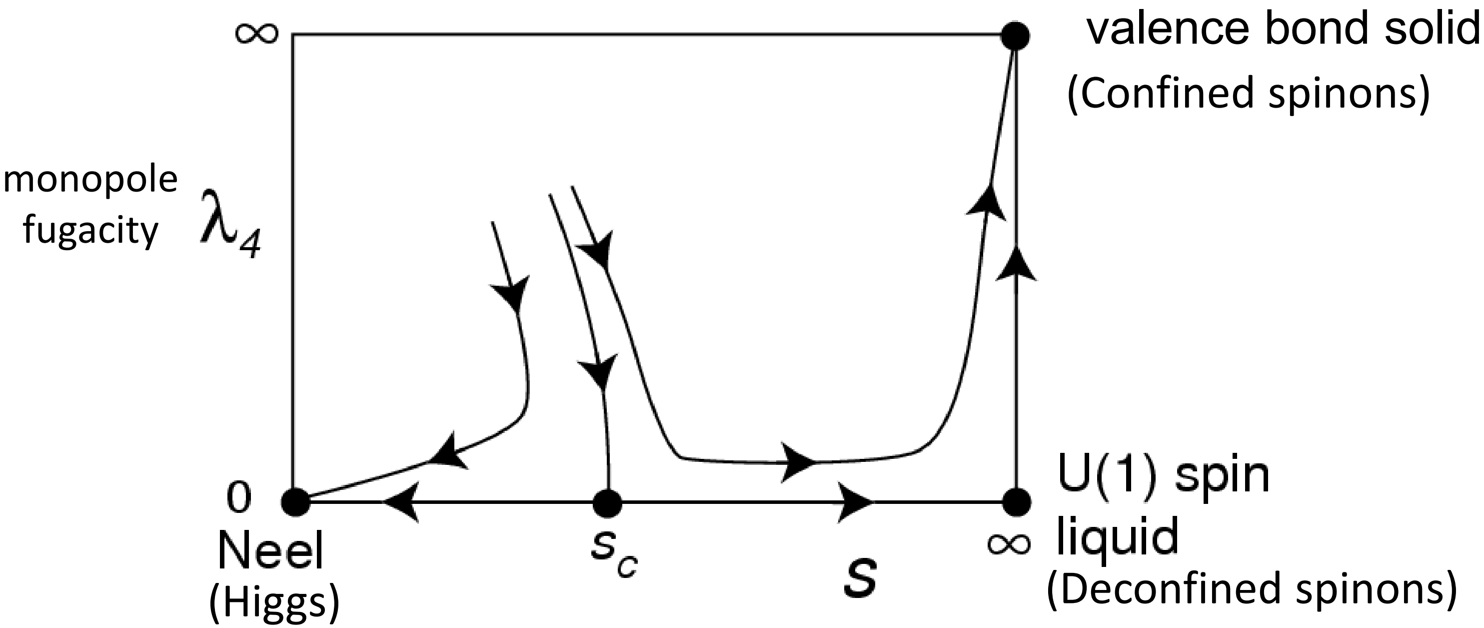
How can direct continuous transition take place?
→**Deconfined quantum criticality**

Primary degrees of freedom are spinons,
but are deconfined only at critical point.

Deconfined criticality in frustrated magnets

Phase diagram of frustrated square-lattice Heisenberg model





T. Senthil et al., Science **303**, 1490 (2004)

More general fractionalization schemes …

PRL **105,** 057201 (2010) PHYSICAL REVIEW LETTERS week ending 30 JULY 2010

Majorana Liquids: The Complete Fractionalization of the Electron

Cenke Xu and Subir Sachdev

Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA
(Received 9 May 2010; revised manuscript received 23 June 2010; published 27 July 2010)

We describe ground states of correlated electron systems in which the electron fractionalizes into separate quasiparticles which carry its spin and its charge, and into real Majorana fermions which carry its Fermi statistics. Such parent states provide a unified theory of previously studied fractionalized states: their descendants include insulating and conducting states with neutral spin $S = 1/2$ fermionic spinons, and states with spinless fermionic charge carriers. We illustrate these ideas on the honeycomb lattice, with field theories of such states and their phase transitions.

Xu/Sachdev, PRL **105**, 057201 (2010)

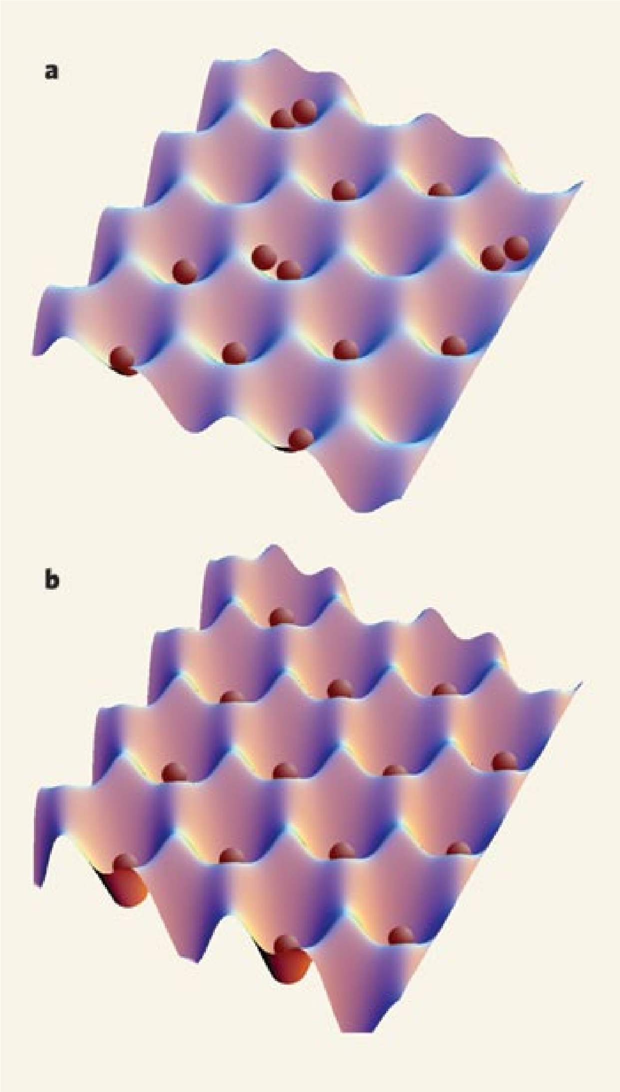
Beyond insulators:
Mott criticality

What is a Mott insulator?

System of interacting fermions
moving in a lattice with kinetic energy *t*,
and subject to local repulsion *U*.

$U \gg t$, half-filling:
(<*n*>=1 particles per site)

Particles localized due to interactions!
Mott insulator



Characteristics:
- Gap to charge excitations
- No Fermi surface
- Residual spin degrees of freedom → magnetism

Bandwidth-controlled Mott transition: Questions

- Conductivity always finite at $T>0$ → transition only well defined at $T=0$?
- What is fate of **Fermi surface** at transition?
  What happens to low-energy quasiparticles?
- Is **magnetism** relevant for transition?

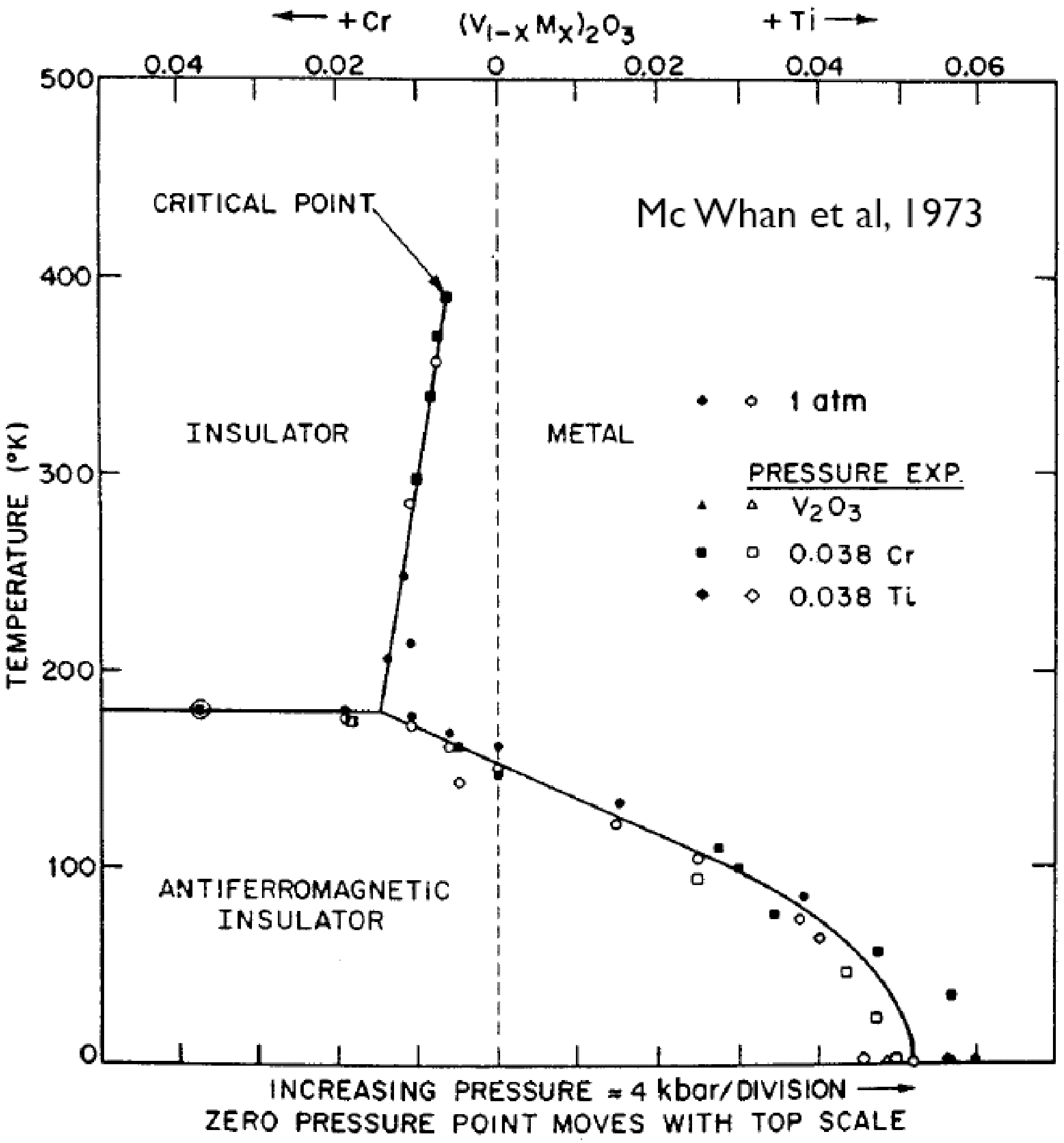
…

- Does genuine **Mott quantum criticality** exist?
  (metal ←→ topological spin liquid)

Senthil, PRB **78**, 045109 (2008)
Qi / Sachdev, PRB **77**, 165112 (2008)
Mishmash *et al*, PRB **91**, 235140 (2015)
+ many others

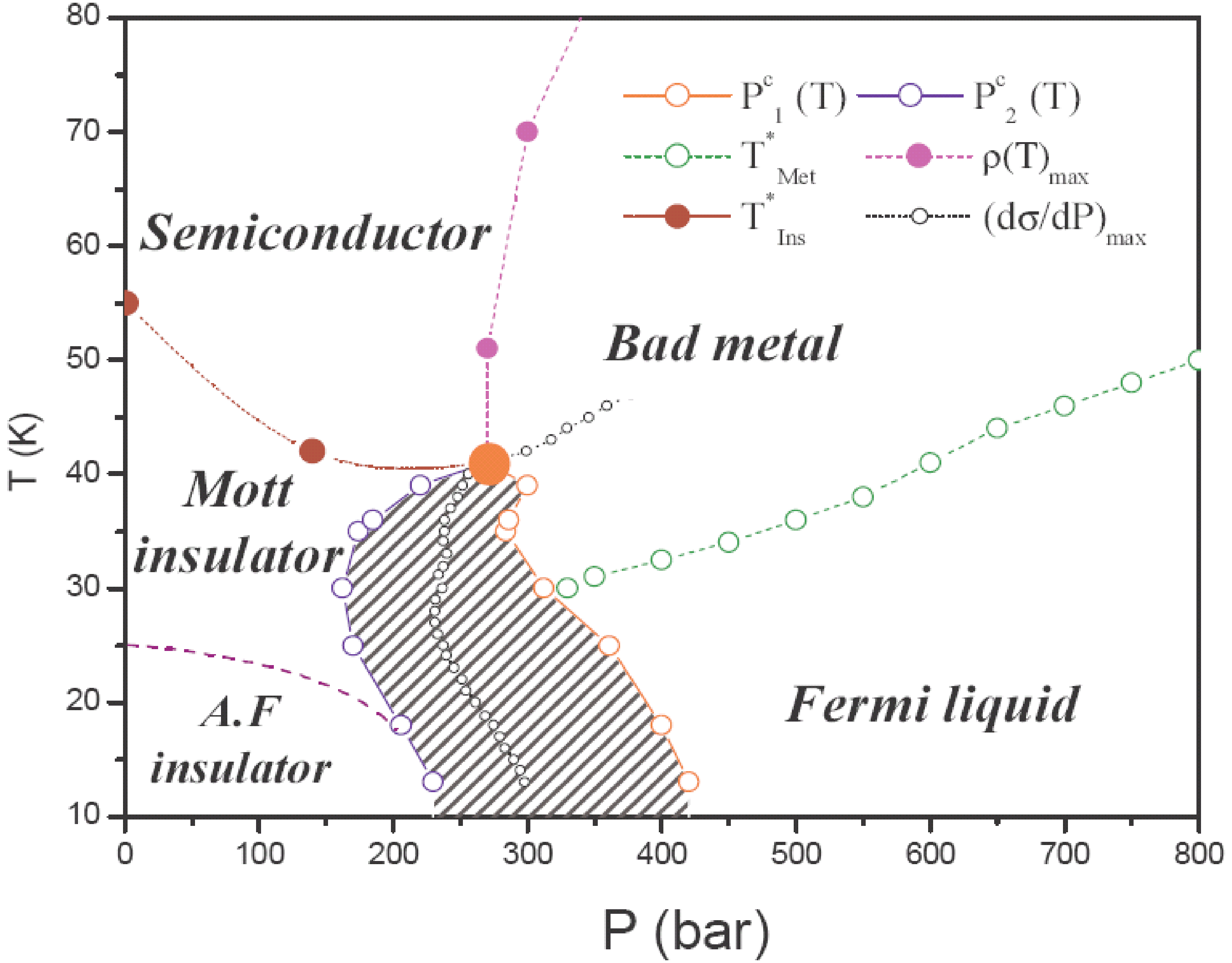
Mott transition: Experiments

V_2O_3



Mott transition: Experiments

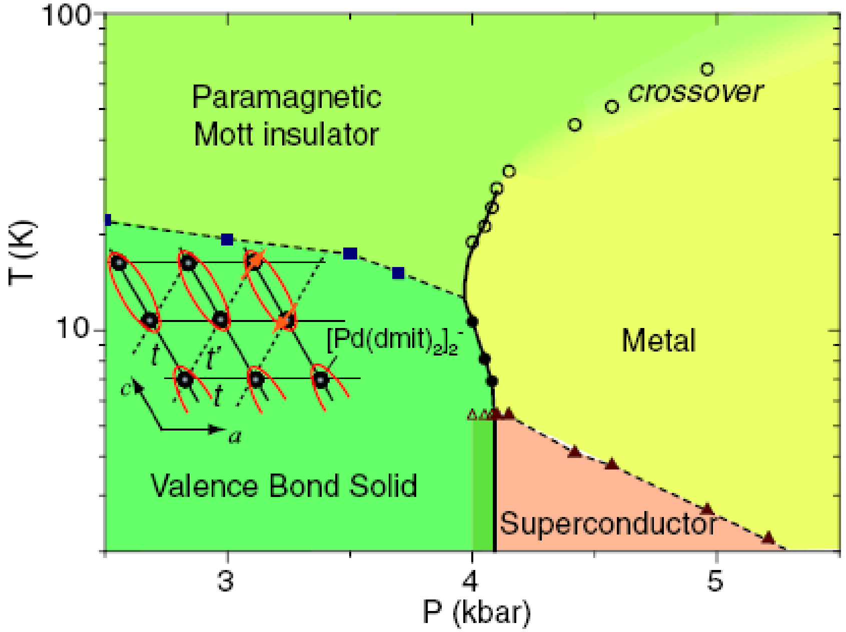
κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl



Limelette *et al*, PRL **91**, 016401 (2003)

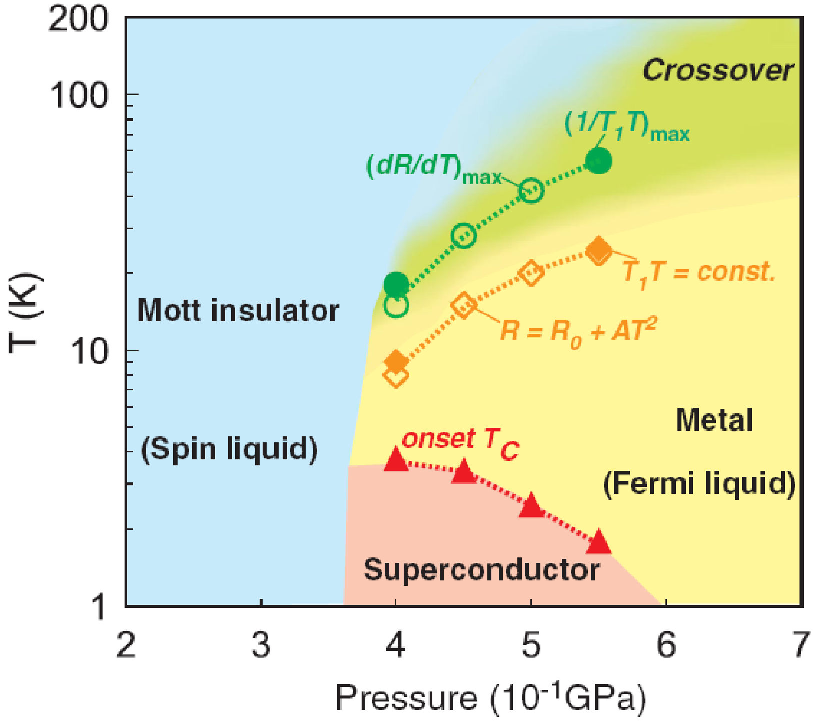
Mott transition: Experiments

$[Pd(dmit)_2]_2$



Shimizu *et al.*, PRL (2007)

κ-$(ET)_2Cu_2(CN)_3$



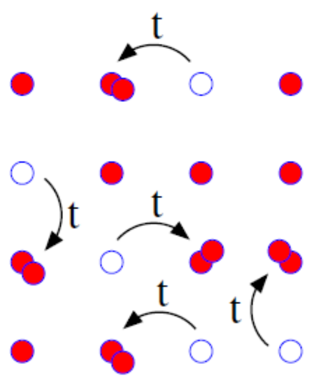
Kurosaki *et al.*, PRL (2005)

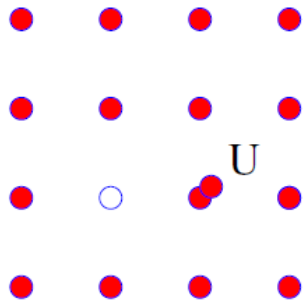
Hubbard model

$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Kinetic energy
(bandwidth $W \sim t$)

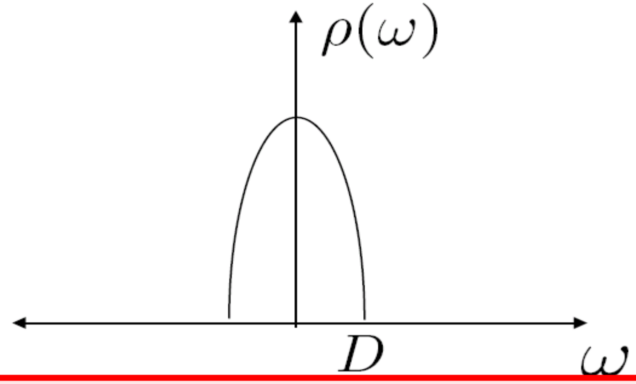
Coulomb repulsion
(local strength U)





Mott transition: Single-particle spectrum @ half-filling

Uncorrelated metal, *U*=0

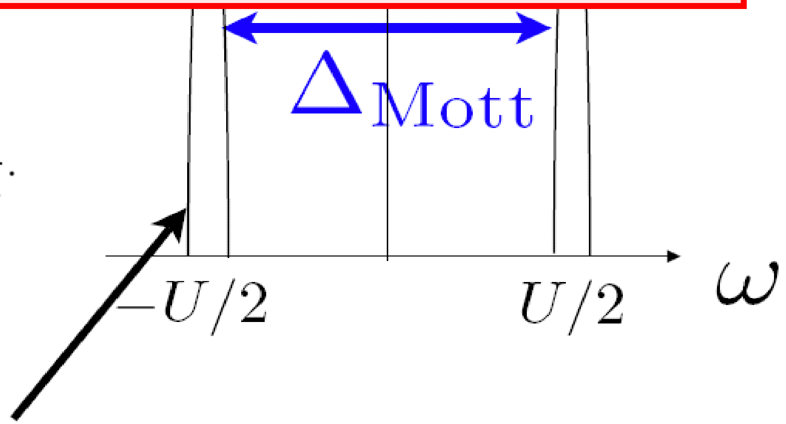


What happens at low energies at $U = U_c$?

- **Quasiparticle weight Z → 0 ?**
- **Effective mass m*→ ∞ ?**
- **Mott gap Δ → 0 ?**

Mott insulator, *U* large
(close to atomic limit!)

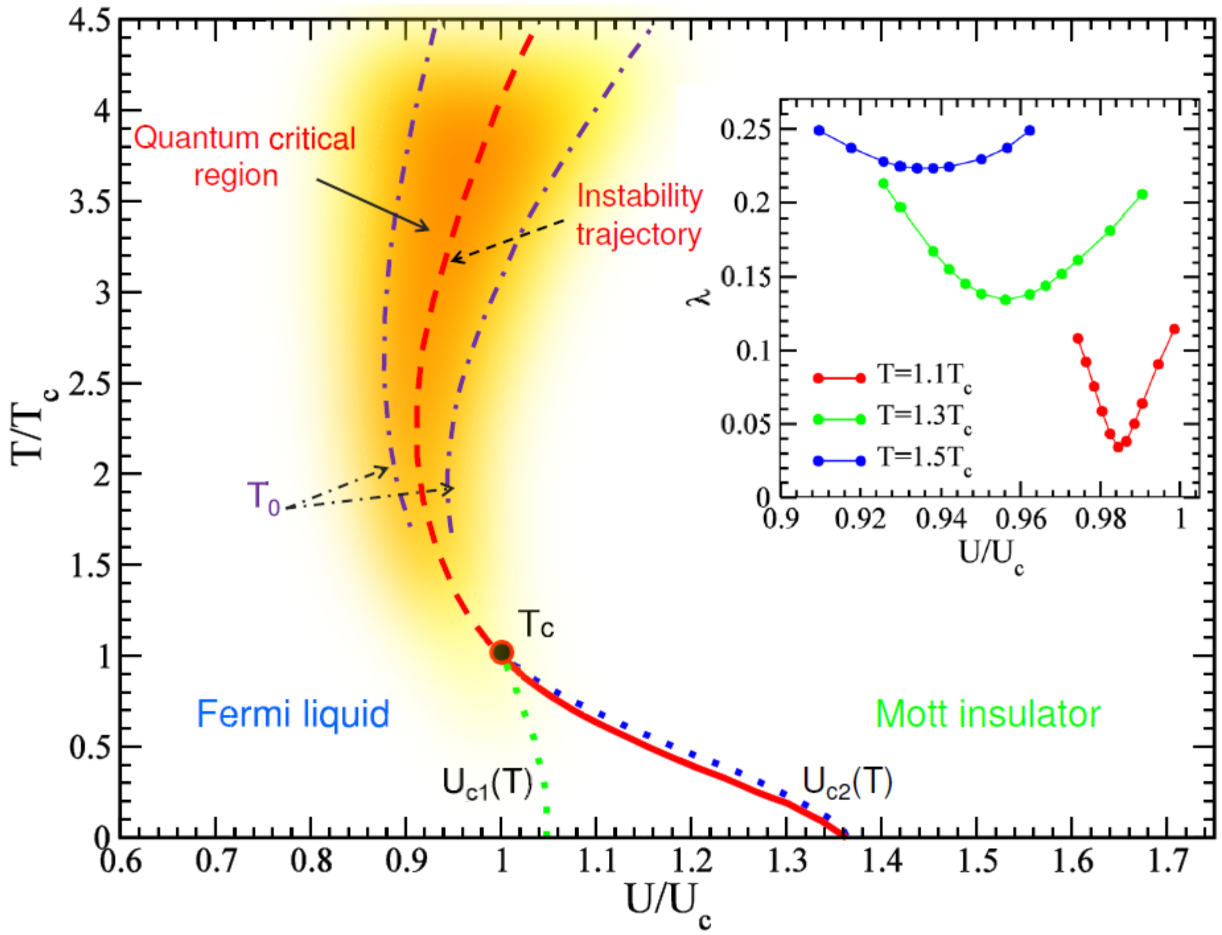
$$G(i\omega_n)_{\rm at} = \frac{1/2}{i\omega_n + U/2} + \frac{1/2}{i\omega_n - U/2}.$$



Hubbard bands
(reflect local moments)

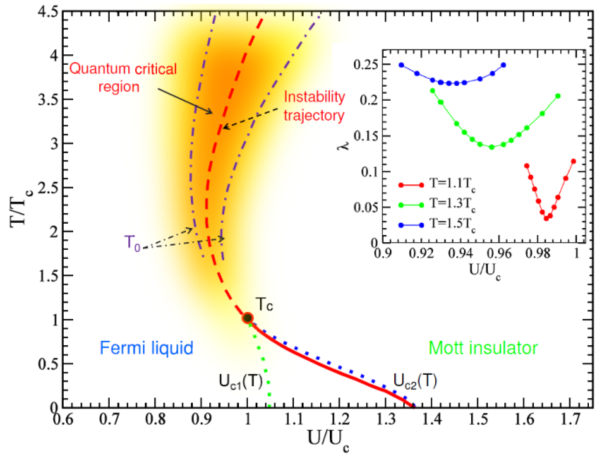
Mott transitions & quantum criticality?

Signs of **quantum** criticality in DMFT for single-band Hubbard model

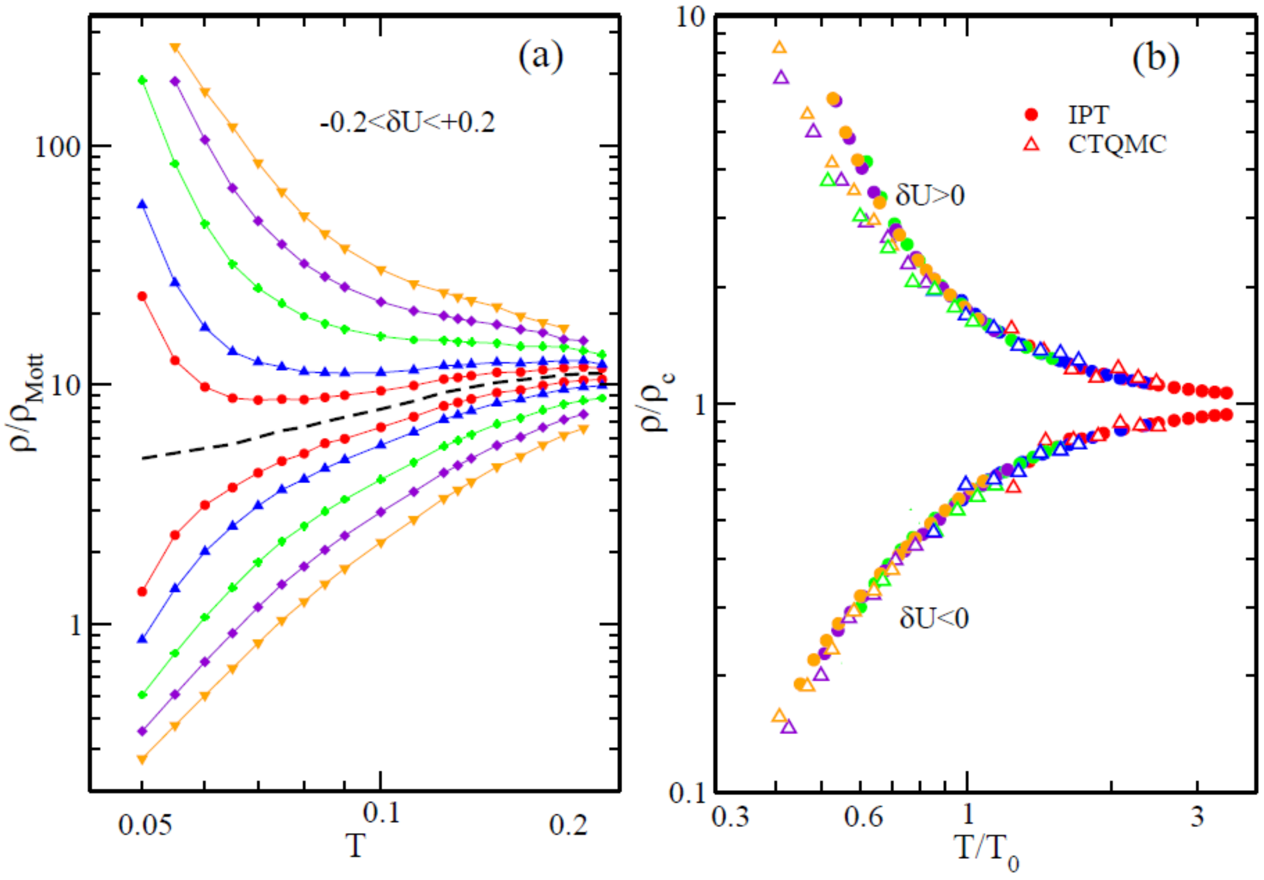


Terletska / Dobrosavljevic *et al*, PRL **107**, 026401 (2011)

Mott transitions & quantum criticality?



Resistivity near Mott endpoint



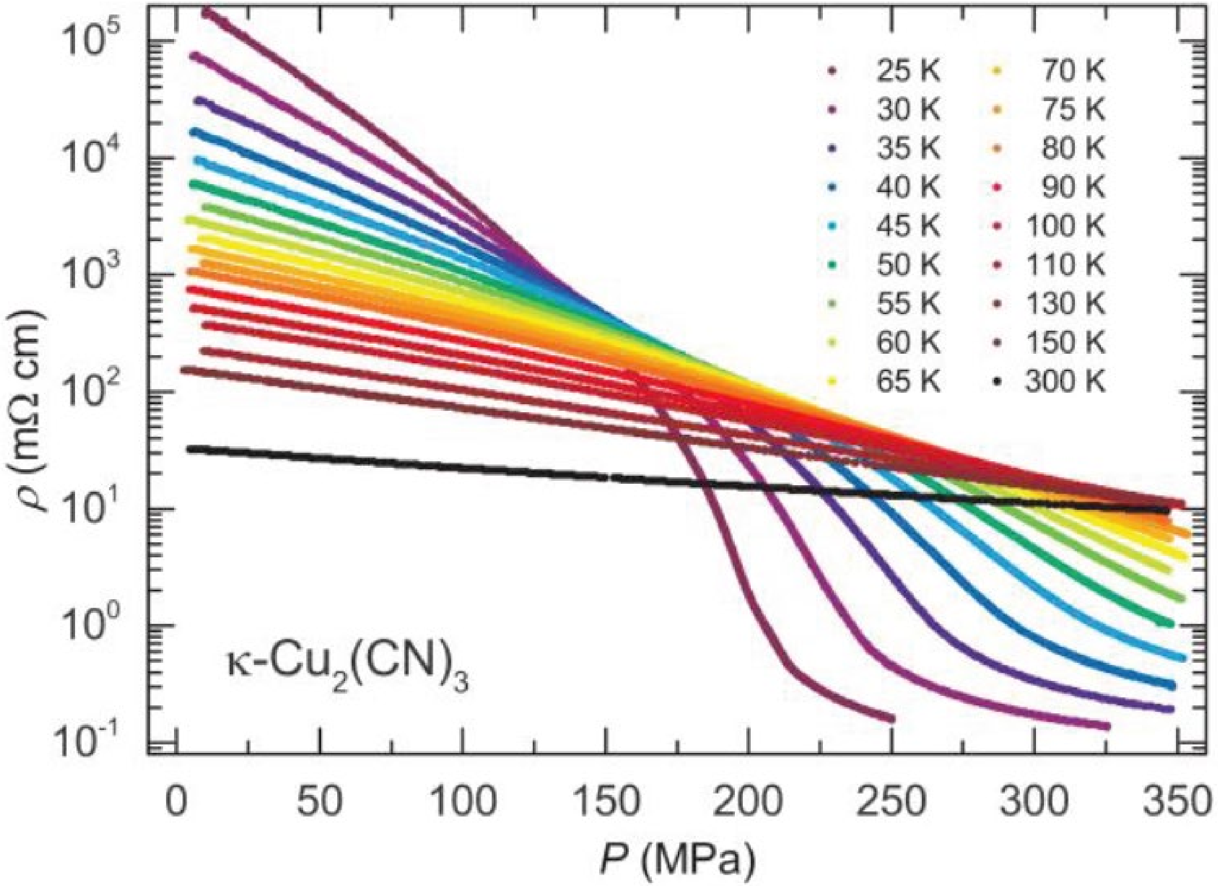
Terletska / Dobrosavljevic *et al*, PRL **107**, 026401 (2011)

Mott transitions & quantum criticality!

κ-$(ET)_2Cu_2(CN)_3$

κ-$(ET)_2Cu[N(CN)_2]Cl$

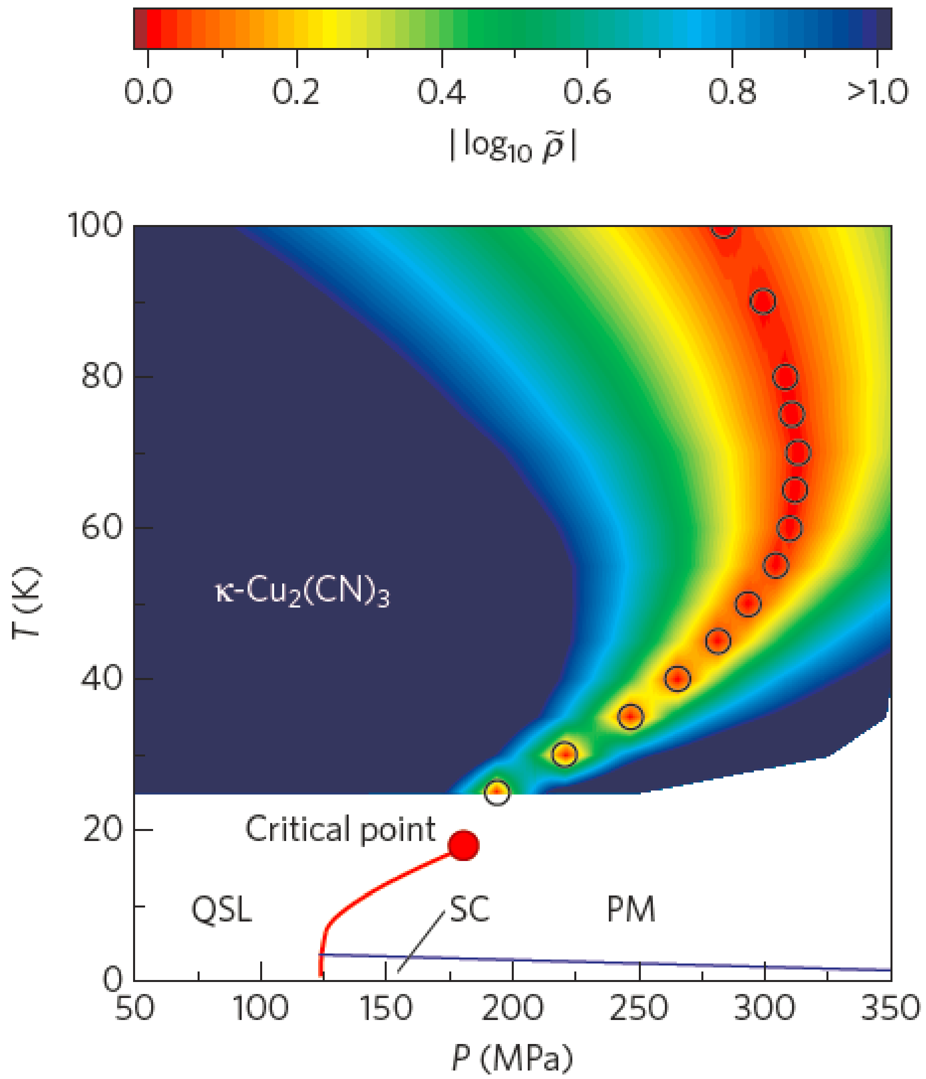
$EtMe_3Sb[Pd(dmit)_2]_2$



Furukawa / Kanoda *et al.,* Nat. Phys. **11**, 221 (2015)

Mott transitions & quantum criticality!

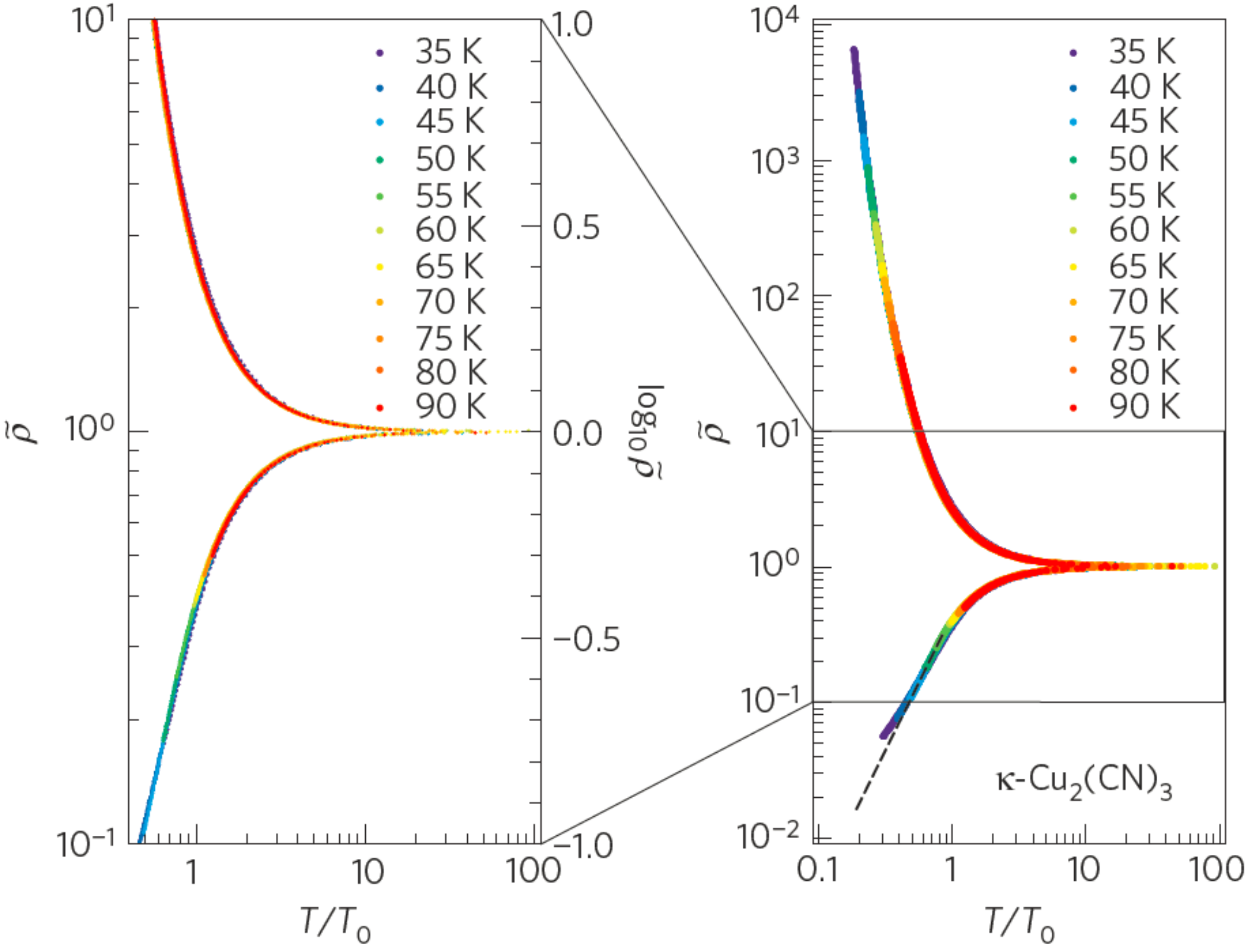
κ-$(ET)_2Cu_2(CN)_3$
κ-$(ET)_2Cu[N(CN)_2]Cl$
$EtMe_3Sb[Pd(dmit)_2]_2$

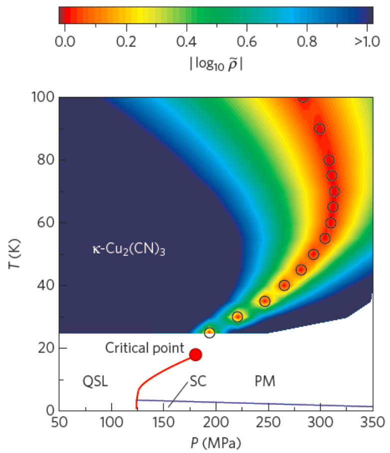


$$\tilde{\rho}(\delta P, T) \equiv \rho(\delta P, T)/\rho_c(T)$$
$$\rho_c(T) \equiv \rho(\delta P = 0,\ T)$$

Furukawa / Kanoda *et al.,* Nat. Phys. **11**, 221 (2015)

Mott transitions & quantum criticality!



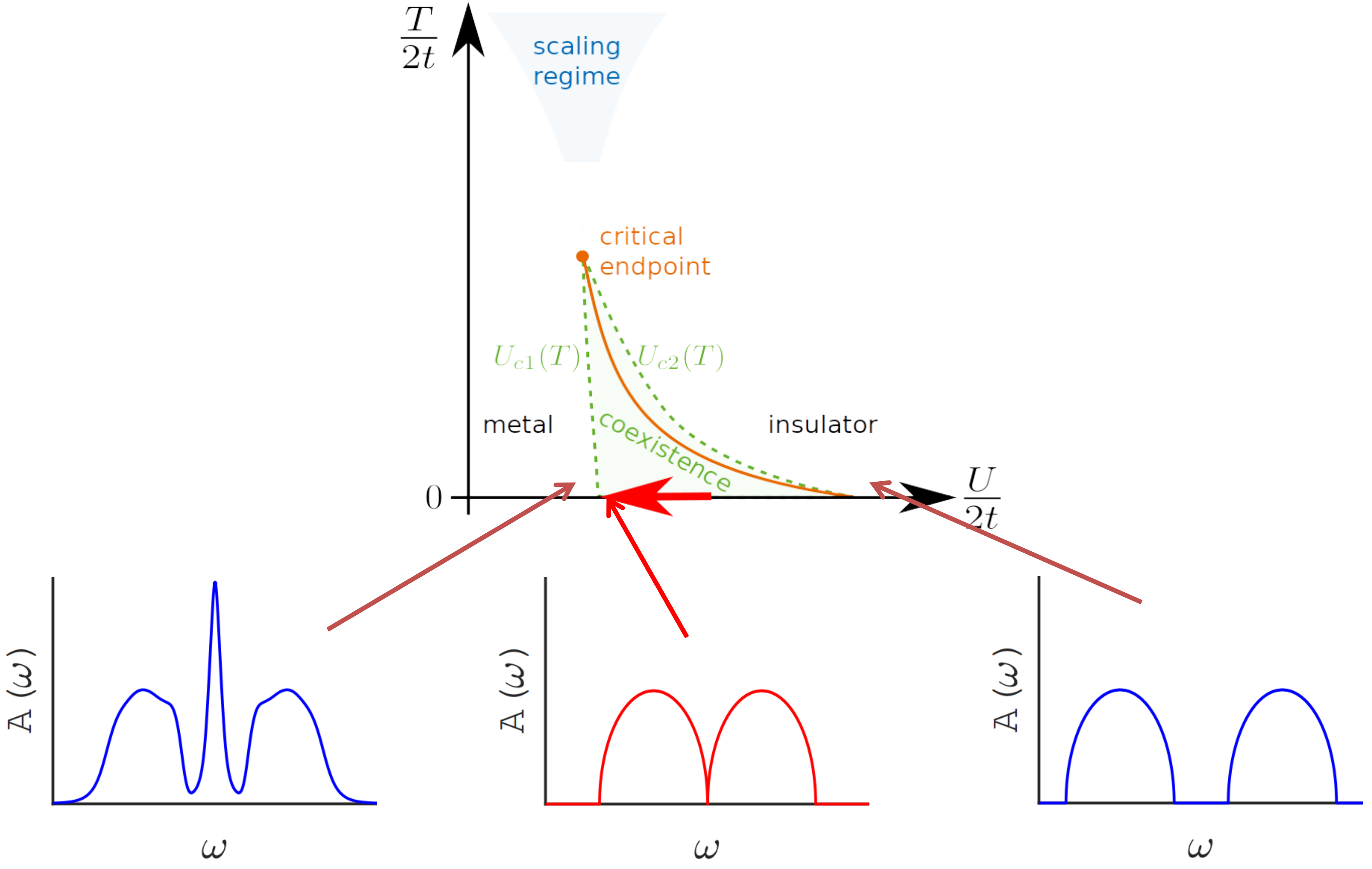


$$\tilde{\rho}(\delta P, T) \equiv \rho(\delta P, T)/\rho_c(T)$$
$$\rho_c(T) \equiv \rho(\delta P = 0,\ T)$$

$$T/T_0 = T/|c\delta P|^{z\nu}$$
$$z\nu = 0.62$$

Furukawa / Kanoda *et al.,* Nat. Phys. **11**, 221 (2015)

Scale-invariant single-particle spectra? (frequency power laws)

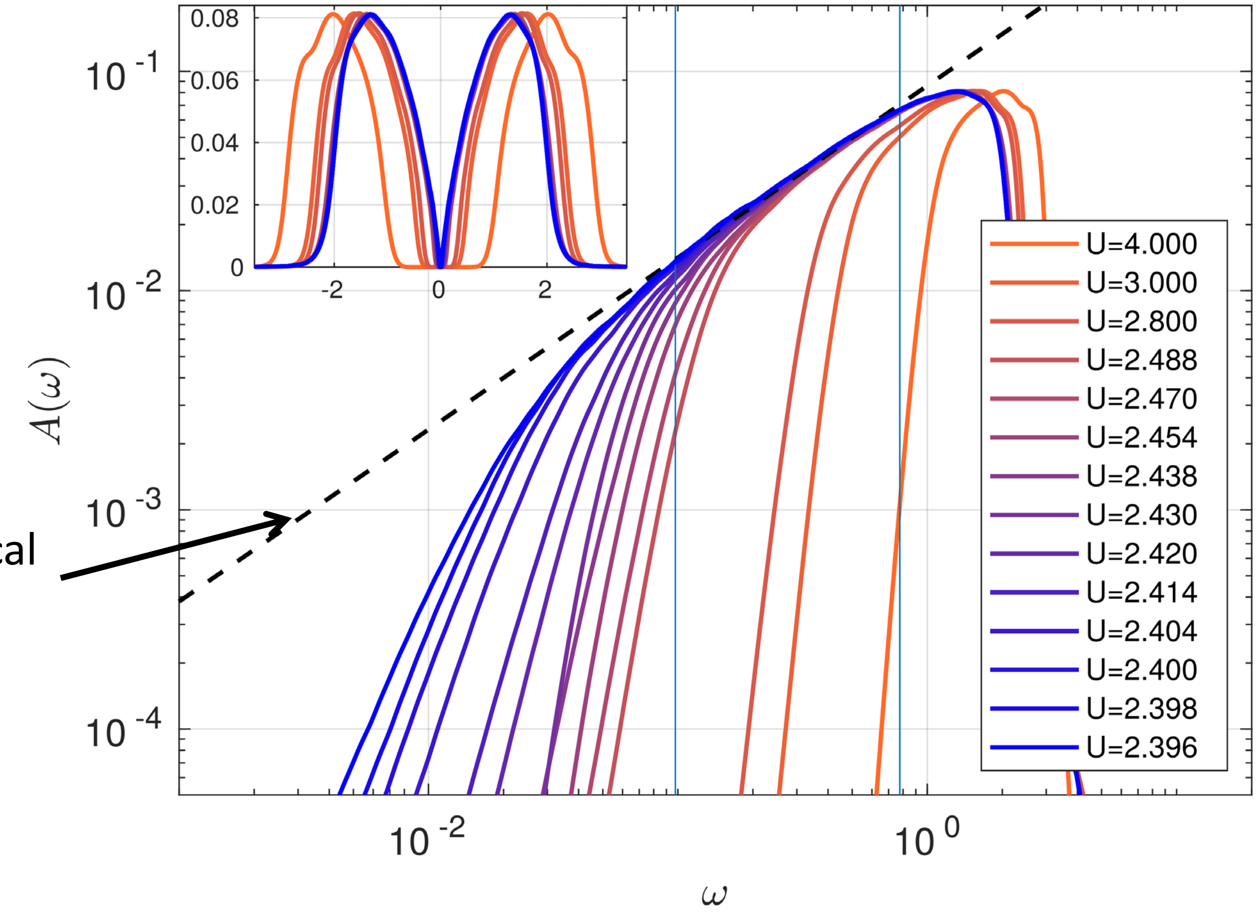


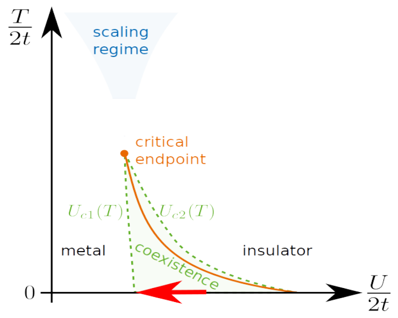
Metastable insulator at $U \rightarrow U_{c1}^{+}$
could develop frequency power laws (!)

Metastable insulator: DMFT results

Single-particle spectrum of insulating solution at T=0 upon approaching U_{c1}

quantum critical power law

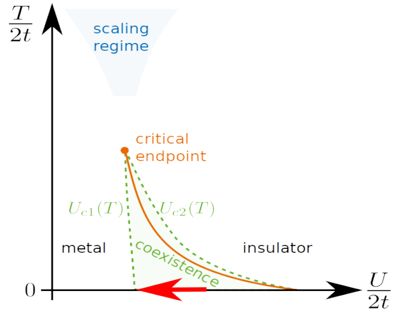


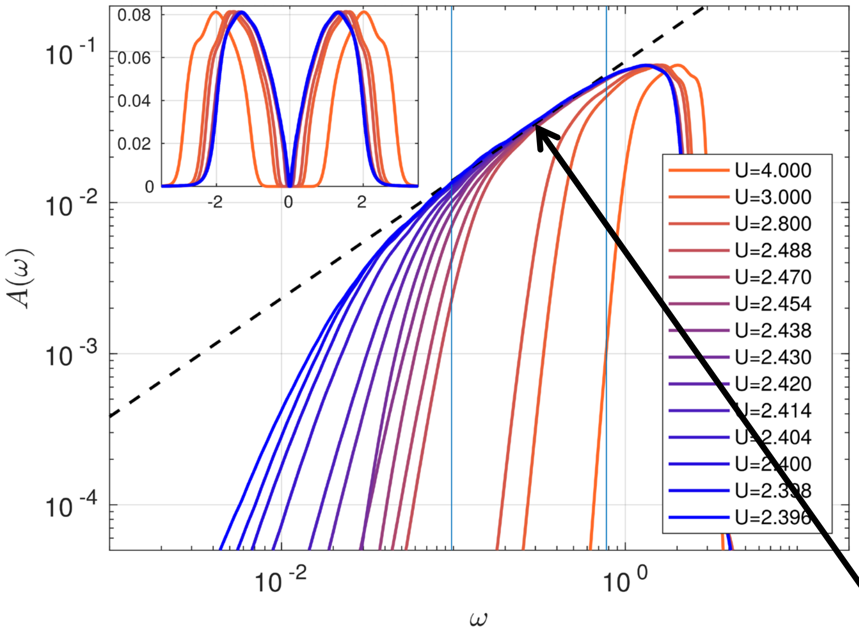


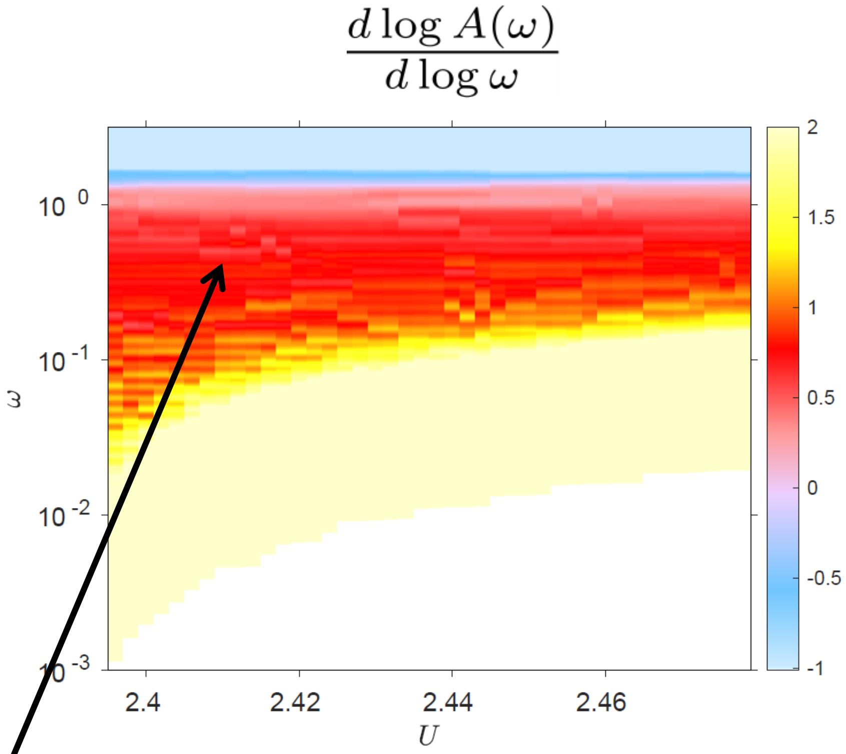
Eisenlohr / Lee / Vojta, PRB **100**, 155152 (2019)

Metastable insulator: DMFT results

Single-particle spectrum of insulating solution at T=0 upon approaching U_{c1}

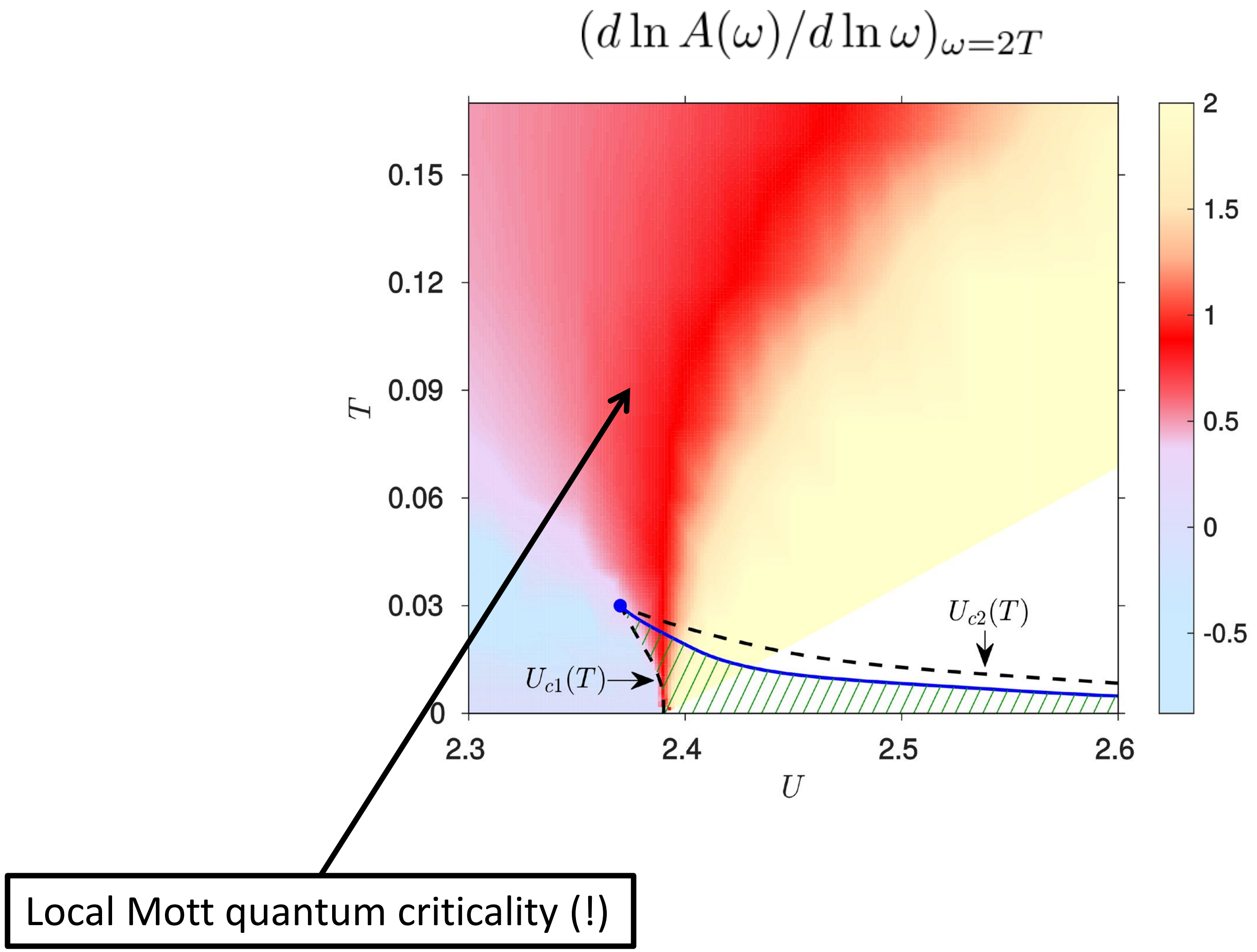






quantum critical power law

Finite-*T* phase diagram from DMFT



Eisenlohr / Lee / Vojta, PRB **100**, 155152 (2019)

Outlook

Conventional quantum criticality in clean insulators well understood (bosonic order parameter, LGW).

More complicated:

- QPT in metals (low-lying particle-hole excitations)
- QPT in the presence of quenched disorder
- QPT of emergent fractionalized degrees of freedom
- Topological QPT

Open:

- Genuinely fermionic QPT (Mott? …?)
- QPT without underlying quasiparticles (Mott? …?)