Quantum Magnetism: In- and Out-of-Equilibrium

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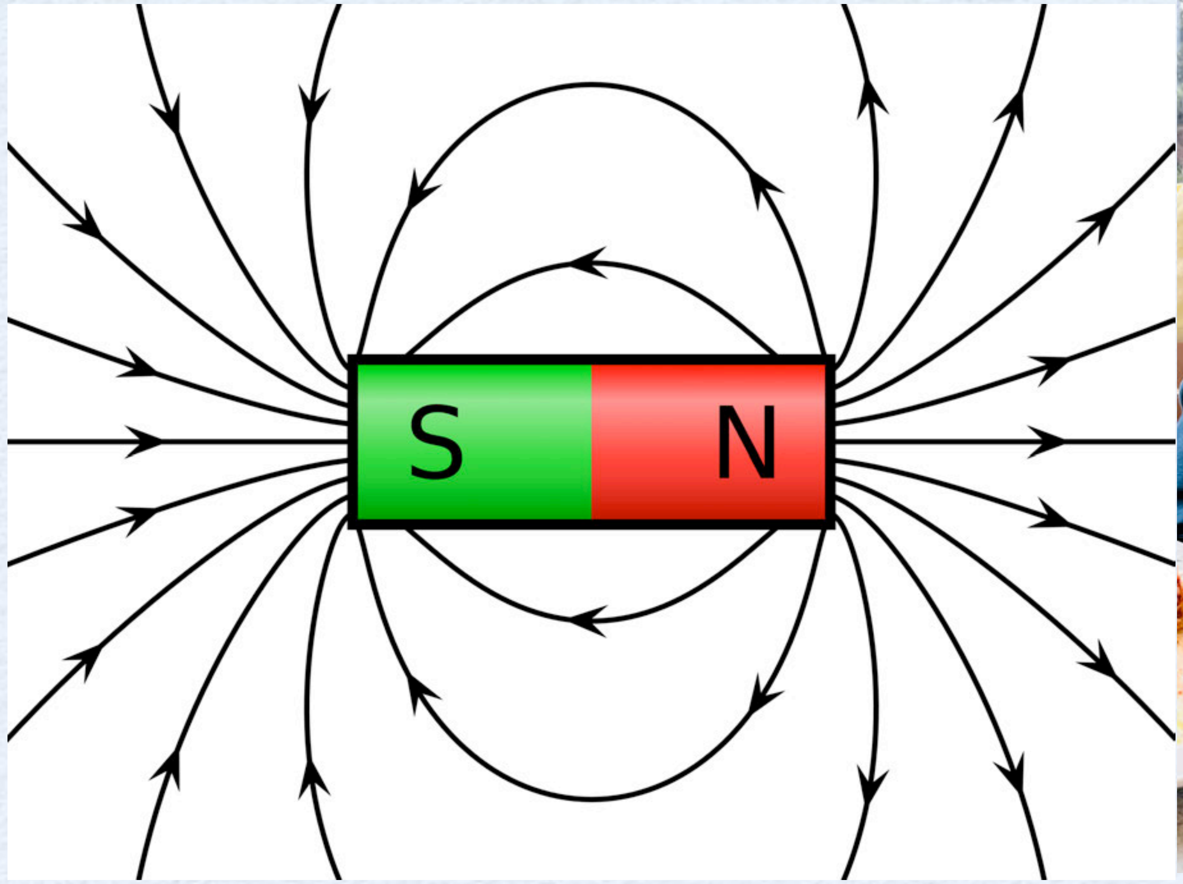
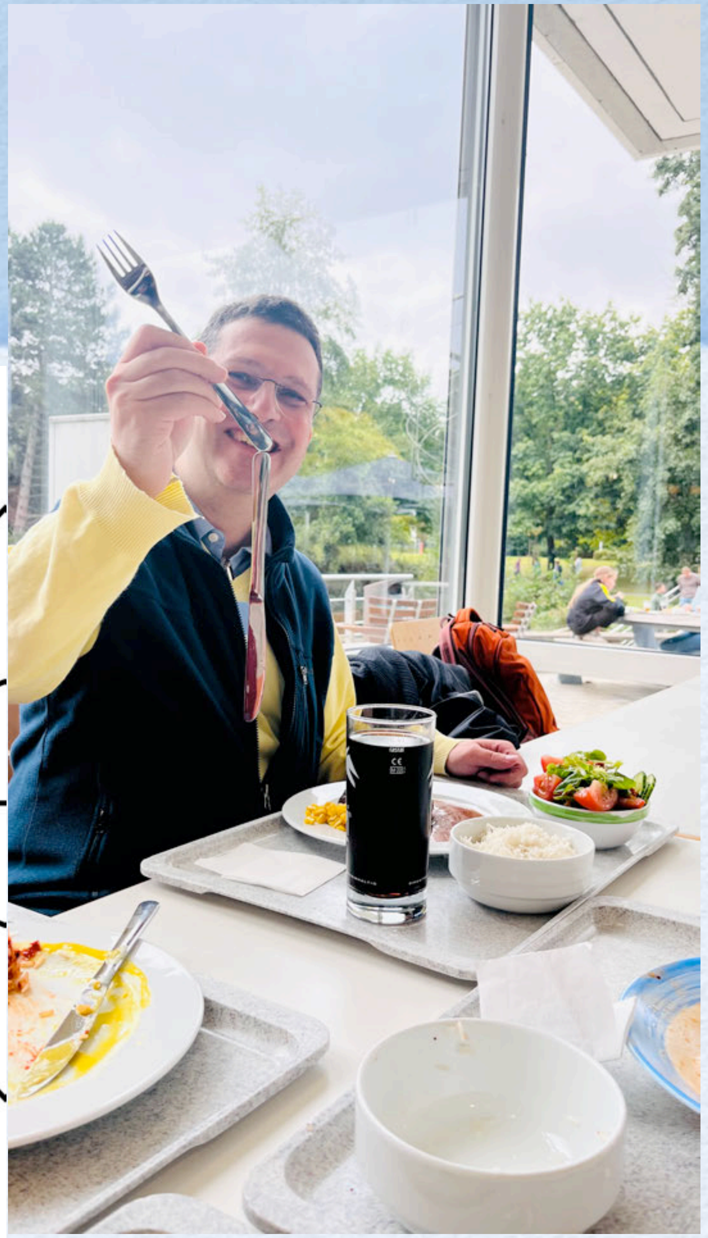
$[q,p]=i\hbar$

Autumn School on Correlated Electrons: Correlations and Phase Transitions

FZ Jülich, September 16th – 20th 2024

Magnetism





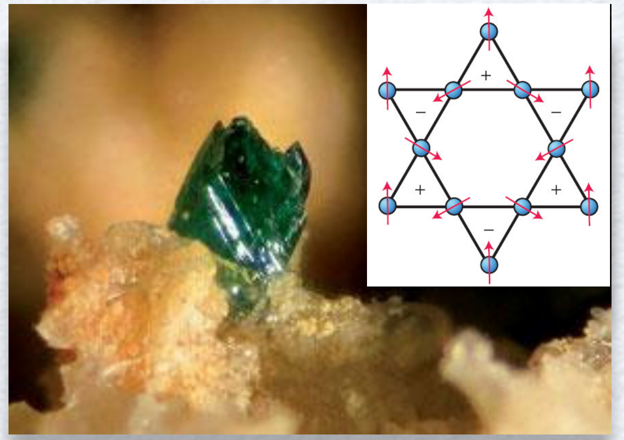
- Magnetism occurs in natural minerals like magnetite — already discovered in ancient times, used, e.g., in China
- Classically, magnetism is not possible — Bohr-van Leeuwen theorem!

$$Z \propto \int d^{3N}p \int d^{3N}r\, e^{-\beta H\left(\mathbf{p}_i - \frac{q_i}{c}\mathbf{A}(\mathbf{r_i}), \mathbf{r}_i\right)} \longrightarrow \int d^{3N}p' \int d^{3N}r\, e^{-\beta H(\mathbf{p}_i', \mathbf{r}_i)}$$

$\Longrightarrow$ Partition function independent of B, hence also all thermodynamic observables do not respond to B:
No magnetization possible!

⇒ Magnetization in materials must be due to quantum effects. Quantum magnetism? Cooperative effect!

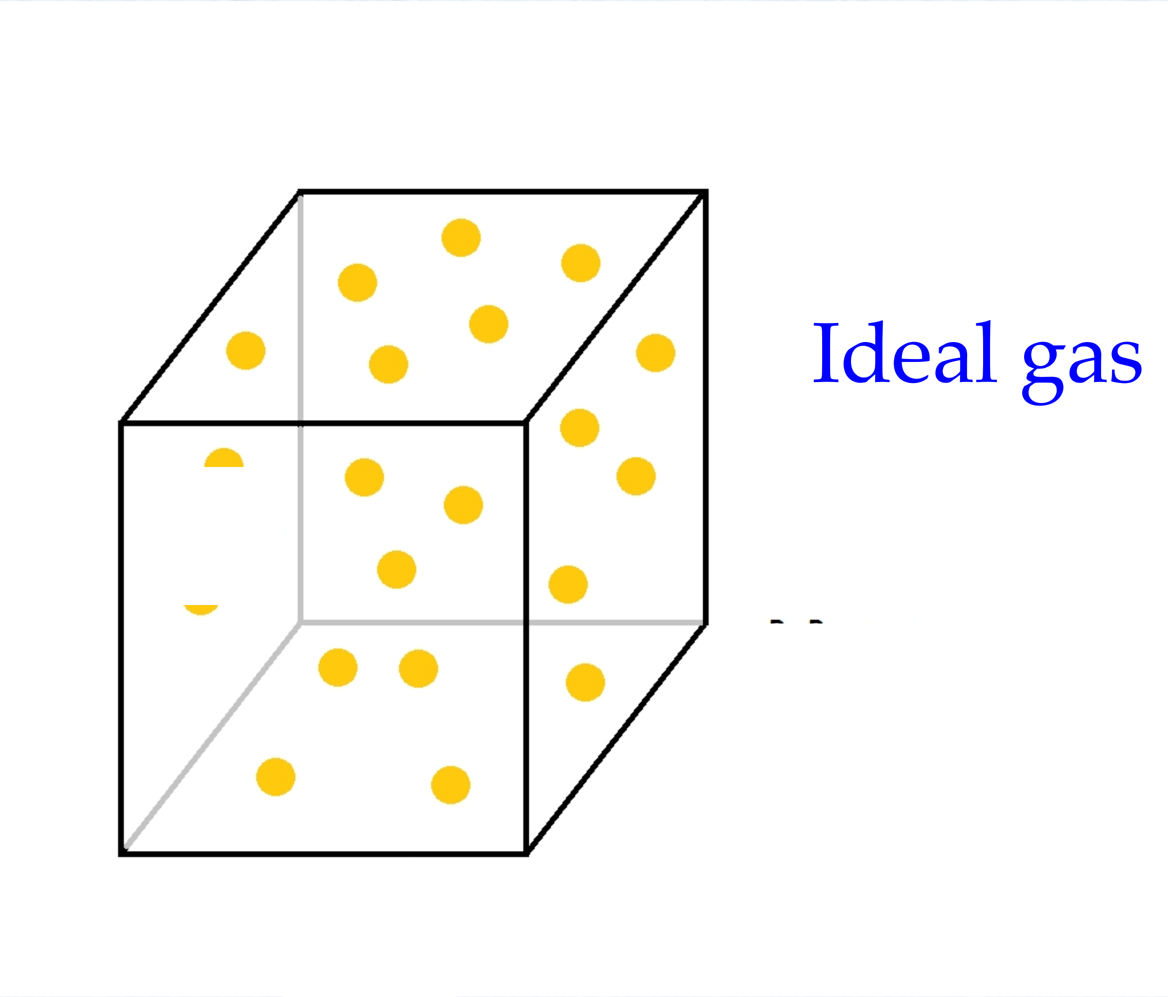
Part I: General Overview



Many-Body Systems?

➟ Interactions

No interactions:



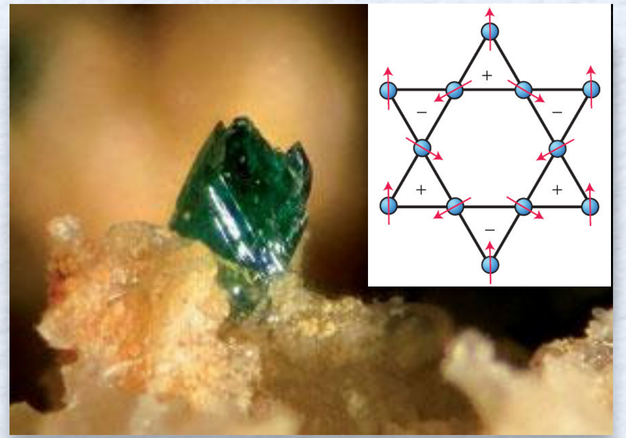
With interactions:

➟ Interactions lead to interesting physics.

Quantum Many-Body Systems: in Nature and in the Lab

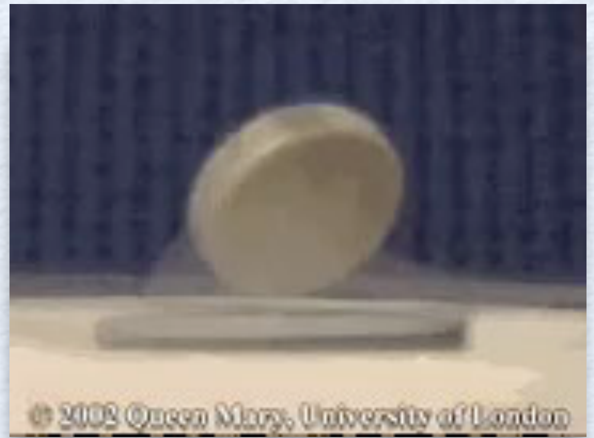
Quantum Magnetism in Natural Minerals

Synthesized Materials: Cuprates



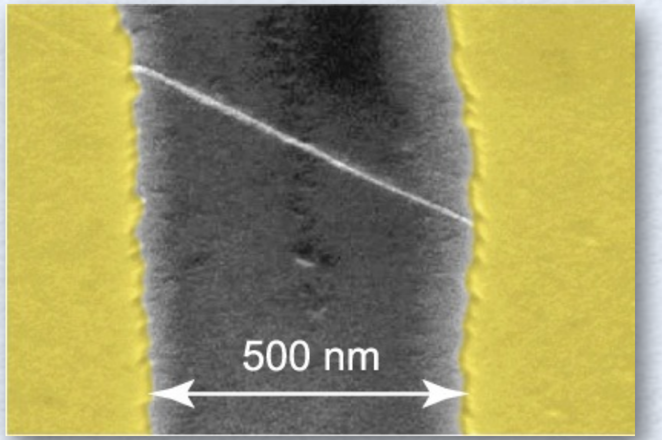
Introduction to Frustrated Magnetism
C. Lacroix, P. Mendels, F. Mila, Springer (2011)

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m_i}\vec{\nabla}_i^2 + \sum_{i\neq j} \hat{V}\left(\vec{x}_i, \vec{x}_j\right)$$



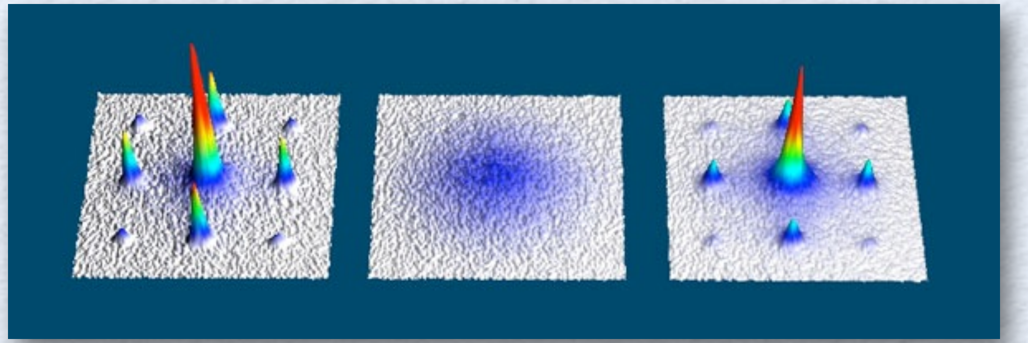
Correlated Electrons in high-temperature superconductors
E. Dagotto, Rev. Mod. Phys. (1994)

Goal: Identify new states of matter



Quantum Physics in One Dimension,
T. Giamarchi, Clarendon Press (2004)

Quantum Wires, Low Dimensions



Many-body physics with ultracold gases
I. Bloch, J. Dalibard & W. Zwerger, Rev. Mod. Phys. (2008)

Ultracold Gases (Optical Lattices)

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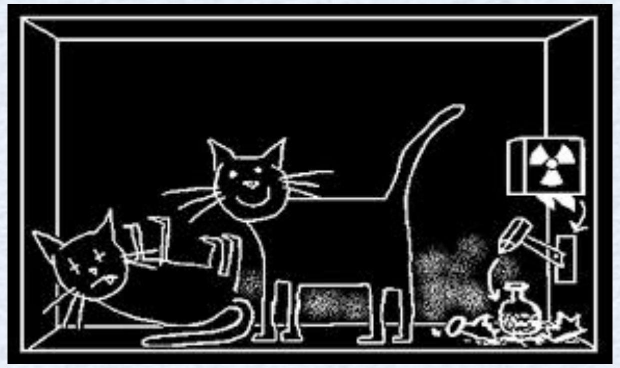
Quantum Many-Body Systems:

Superposition & Entanglement

I) Superposition of states is *also* a possible state

$$|\psi\rangle = |\text{dead}\rangle + |\text{alive}\rangle$$



II) Entanglement: spin-1/2 particles (e.g., electrons)

2 particles: 4 possible states

$$|\psi\rangle = \begin{cases} |\uparrow\rangle \otimes |\uparrow\rangle \\ |\uparrow\rangle \otimes |\downarrow\rangle \\ |\downarrow\rangle \otimes |\uparrow\rangle \\ |\downarrow\rangle \otimes |\downarrow\rangle \end{cases}$$

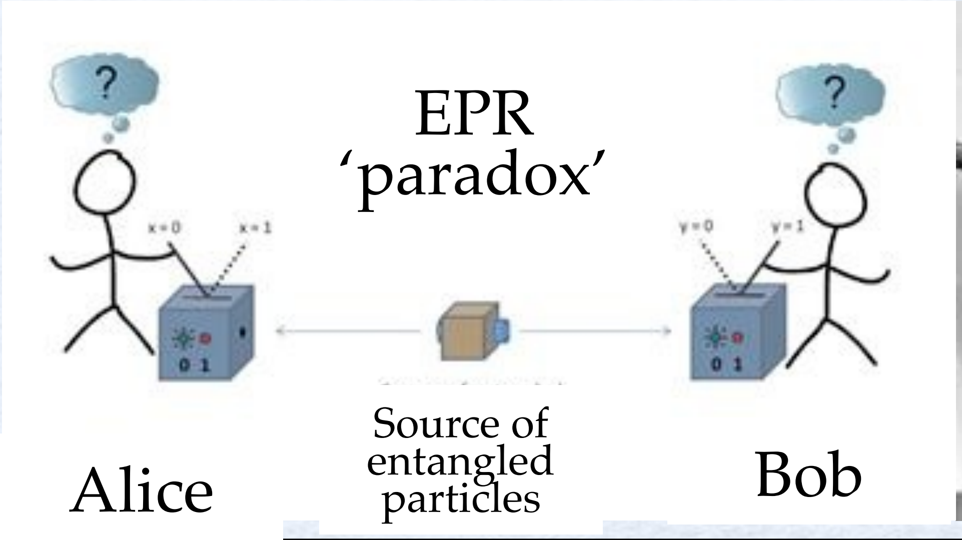
“classical”, “product state”

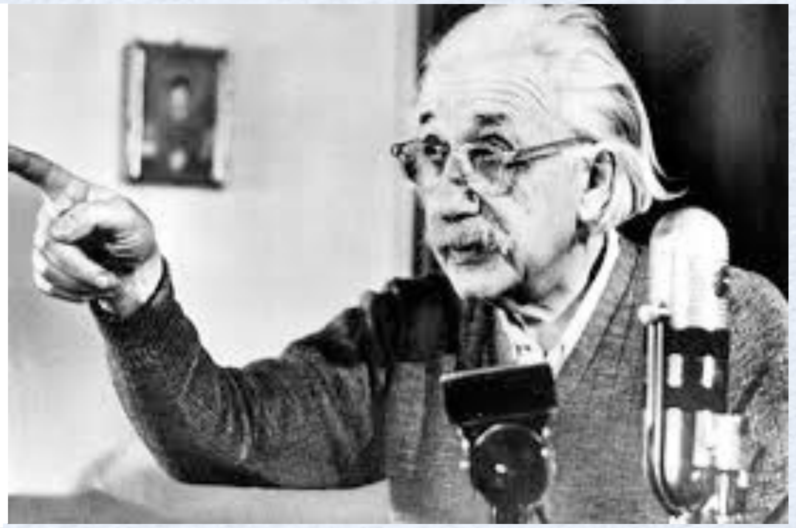
$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \otimes |\uparrow\rangle + |\downarrow\rangle \otimes |\downarrow\rangle\right)$$

“entangled”: not a product state

Einstein:

«spooky action at a distance»





Quantum Many-Body Systems:

Correlations

Correlated states:

"mean-field" picture of independent particles breaks down

$$\langle S_1^z S_2^z \rangle \neq \langle S_1^z \rangle \langle S_2^z \rangle + \langle (S_1^z - \langle S_1^z \rangle)(S_2^z - \langle S_2^z \rangle) \rangle$$

➠ Expectation values of observables for particles 1 and 2 *correlate with each other*

a) because of entanglement

b) because of mutual interactions.

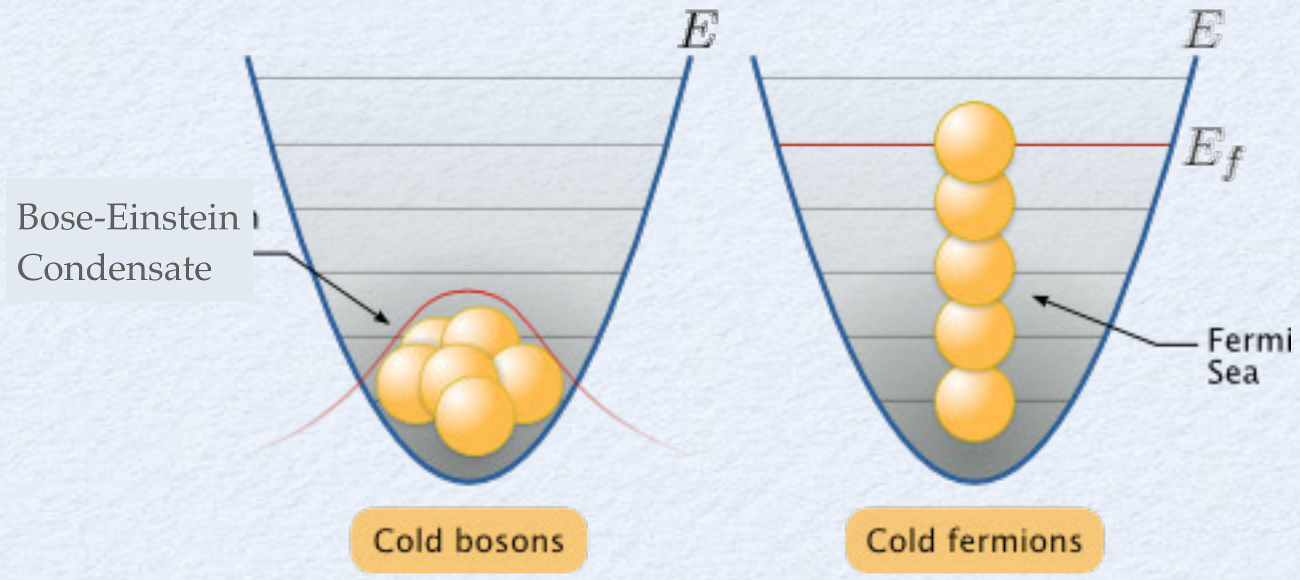
Small numerical values: need *accurate* methods

Quantum Many-Body Systems:

Quantum Statistics

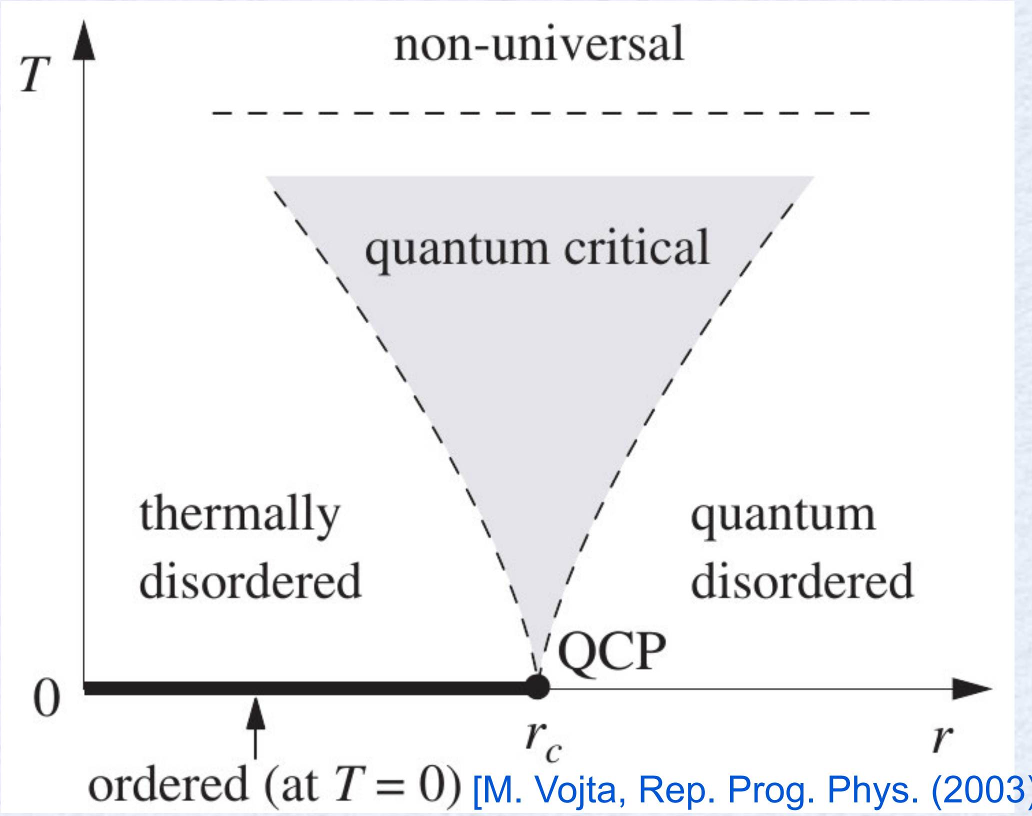
Exchange statistics:

Behavior at low temperatures:



At T=0:

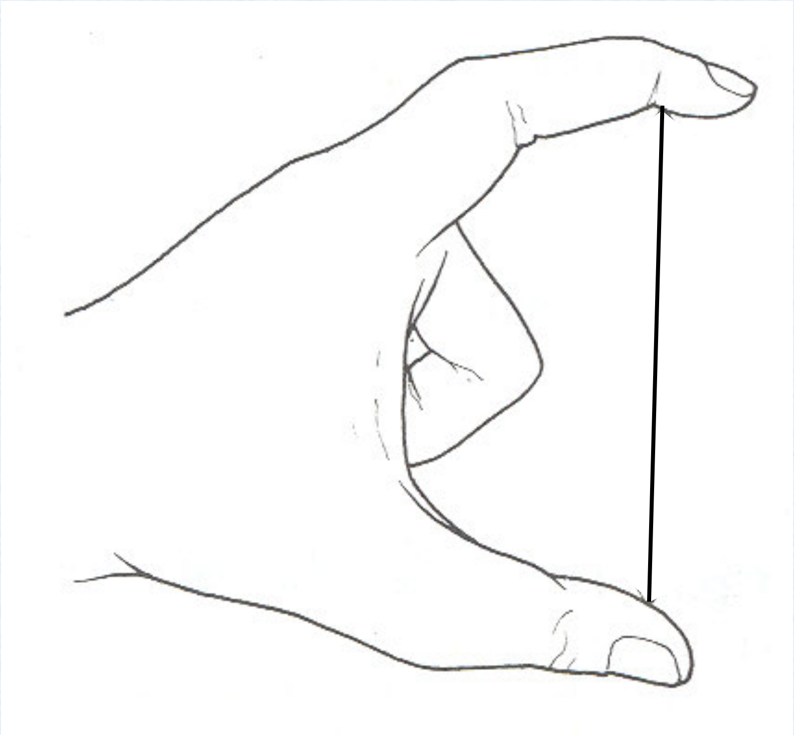
Quantum fluctuations drive "quantum phase transitions".



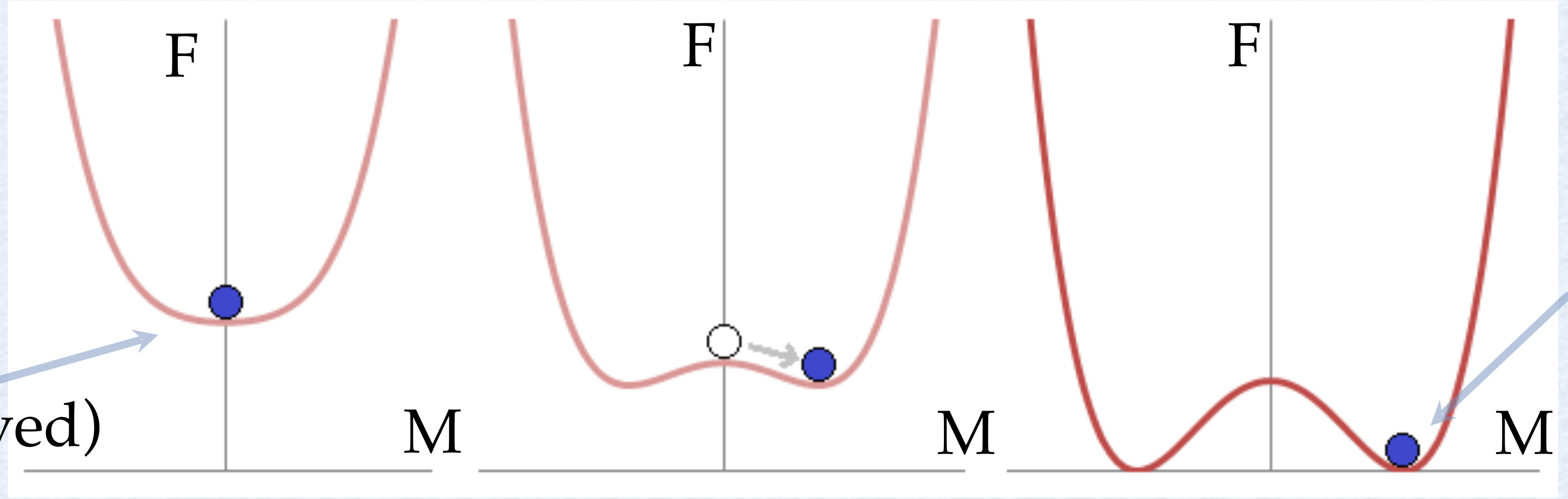
[M. Vojta, Rep. Prog. Phys. (2003)]

Quantum States of Matter:
Spontaneous Breaking of Symmetries

Continuous phase transitions:



$$F[M] = aM^2 + bM^4 \text{ (Landau)}$$



no “order”
(symmetry preserved)

finite
“order parameter”:
broken symmetry

How to investigate this?
Which quantities to compute?

expectation values:
local order parameters,
correlation functions, …

Unconventional States:
Topological Phases

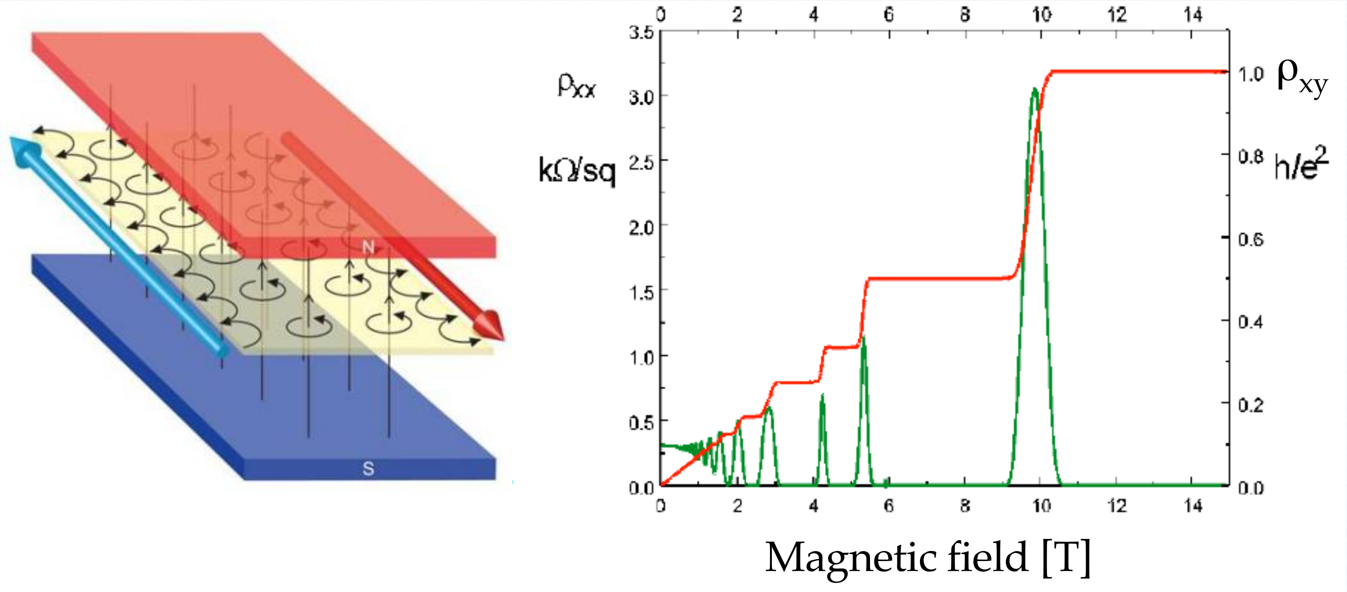
Nobel Prize
2016

"Topological order": <u>beyond</u> Landau paradigm

No local order parameter, instead:

- *topological invariants* (integer numbers)
  ↪ protection against local noise: quantum computing
- metallic surface states
  ↪ dissipationless transport

Examples: integer and fractional quantum Hall effect 

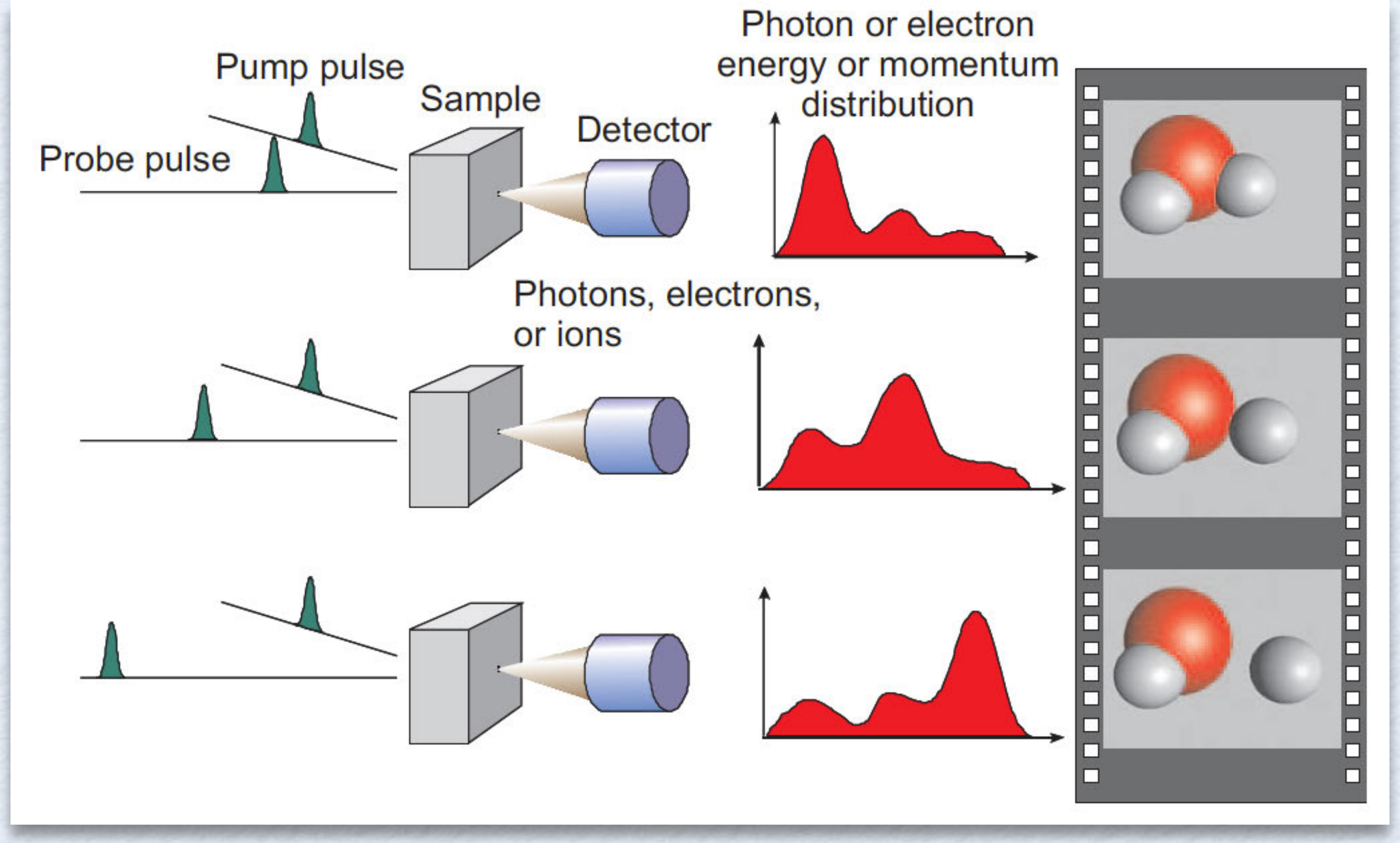


Phase transitions:
jumps in transverse conductivity

How to investigate this?
Which quantities to compute?

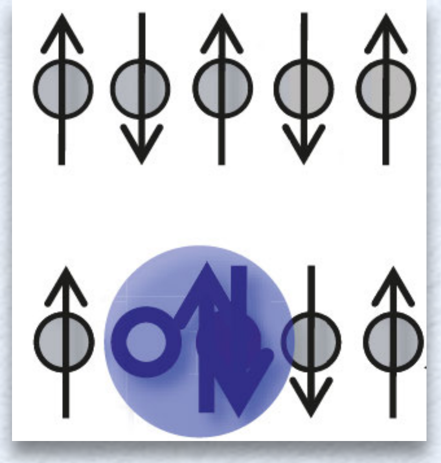
⇒ topological invariants,
energy gaps,
entanglement properties,
…

Many-Body Systems Out-Of-Equilibrium:
Highly Excited Materials



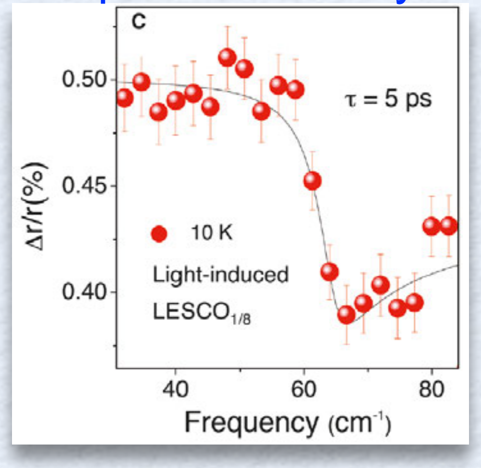
F. Krausz & M. Ivanov, RMP (2009)

Photo-excitation of Mott insulators



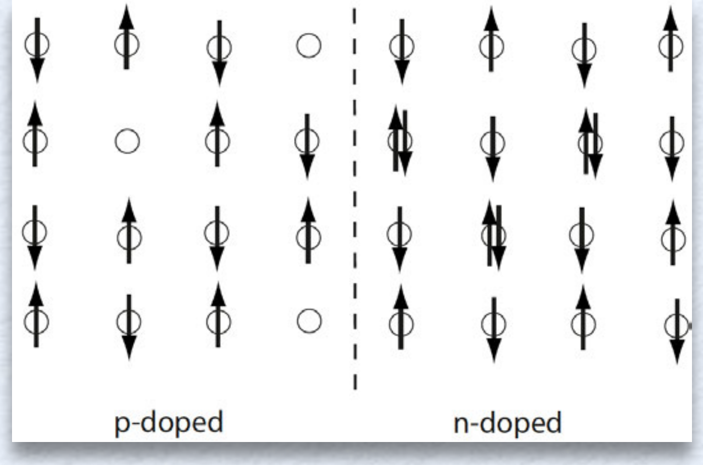
S. Wall et al., Nature Physics (2010)

"Light-induced superconductivity"



D. Fausti et al., Science (2011)

Photovoltaic effects

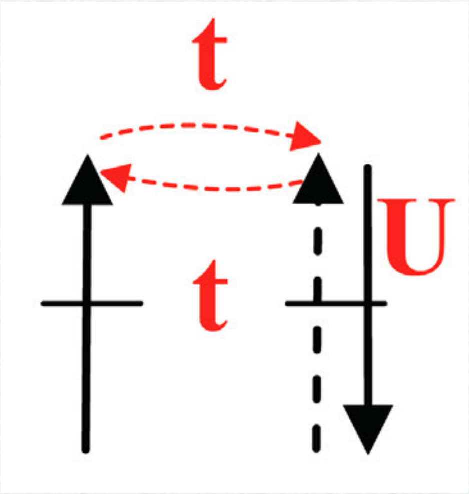


E. Manousakis PRB (2010)

How to investigate this?
Which quantities to compute?

→ Formation of transient order?
Creation of quasiparticles?

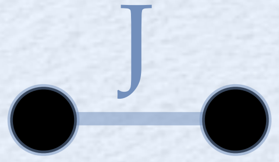
Part II: Basic Properties of Quantum Magnets



1, 2, 3:

Adding spins

one single spin-1/2 object: two states, ↑ or ↓, and superpositions $\left|\psi\right\rangle = \alpha \left| \uparrow \right\rangle + \beta \left| \downarrow \right\rangle, \alpha^2 + \beta^2 = 1$ — Qubits!



$J\,\mathbf{S}_1 \cdot \mathbf{S}_2$

J>0:  antiferromagnetic

J<0:  ferromagnetic

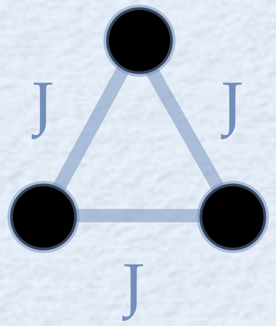
Four eigenstates:

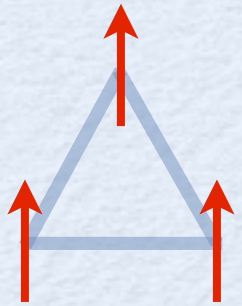
no classical analog!

$$
\begin{aligned}
|s\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \\
|t_1\rangle &= |\uparrow\uparrow\rangle \\
|t_0\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\
|t_{-1}\rangle &= |\downarrow\downarrow\rangle
\end{aligned}
$$

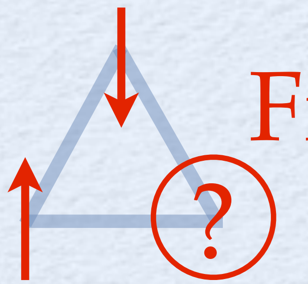
singlet state, energy $E_S = -\frac{3}{4}J$

triplet states, energy $E_T = \frac{1}{4}J$ (3x degenerate)





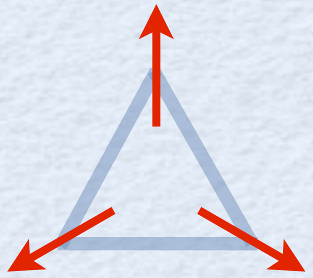
ferromagnetic



antiferromagnetic

Frustration!

Highly degenerate Ground state

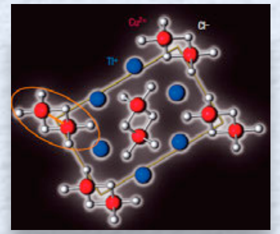


New configurations!

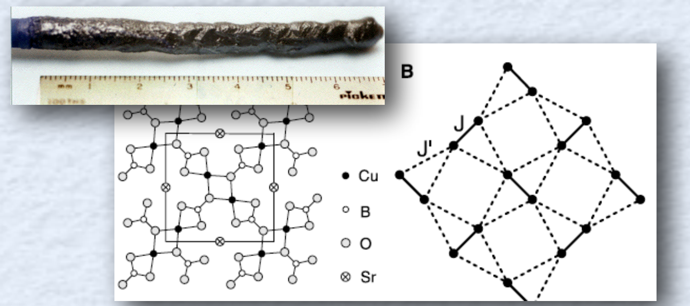
Quantum Magnets as realization of strongly correlated systems: Examples

Quantum magnetic materials: networks of many spins, realize collective quantum phenomena, e.g.

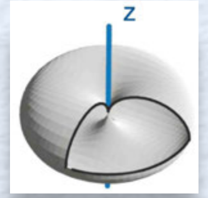
- $TlCuCl_3$ (S = ½ ladder):
  Bose-Einstein-Condensation of Magnons



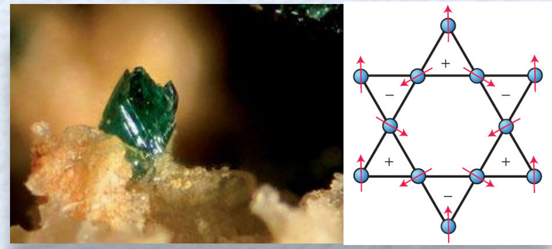
- $SrCu_2(BO_3)_2$ (S = ½ Shastry-Sutherland lattice):
  Fractional magnetization plateaux, magnetic superstructures (supersolid?)



- Sr_2IrO_4 (square lattice iridate material):
  Spin-nematic state?



- Herbertsmithite $ZnCu_3(OH)_6Cl_2$ (S = ½ kagome lattice):
  Algebraic spin liquid? More exotic state?



'Standard model': Heisenberg exchange on different geometries

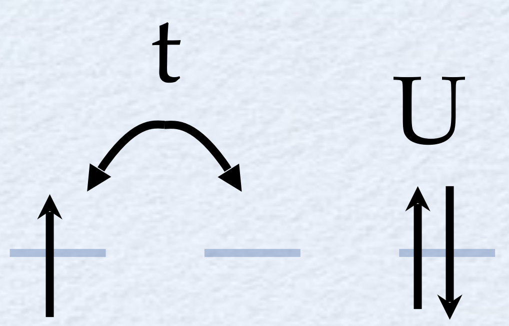
$$H = \mathbf{J} \sum_{\langle j,m \rangle} \mathbf{S}_j \cdot \mathbf{S}_m$$

Real materials: further effects, like spin-orbit coupling

Quantum Many-Body Systems: Typical Lattice Models

Hubbard model (1D):

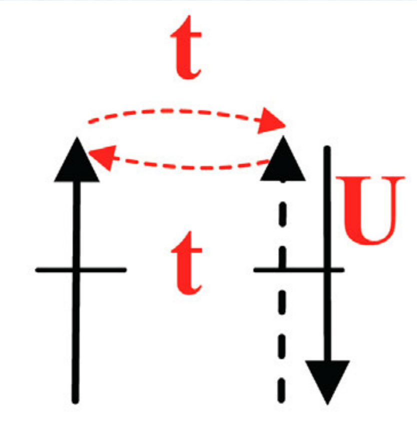
$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} \left[c^{\dagger}_{i+1,\sigma} c_{i,\sigma} + h.c. \right] + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$



Heisenberg exchange: 2nd order perturbation theory for $U \gg t$

$$J \, \vec{S}_1 \cdot \vec{S}_2$$

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



Often anisotropy in one direction, XXZ model:

$$\mathcal{H} = J_{\perp} \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right) + \Delta \sum_{\langle i,j \rangle} S_i^z S_j^z$$

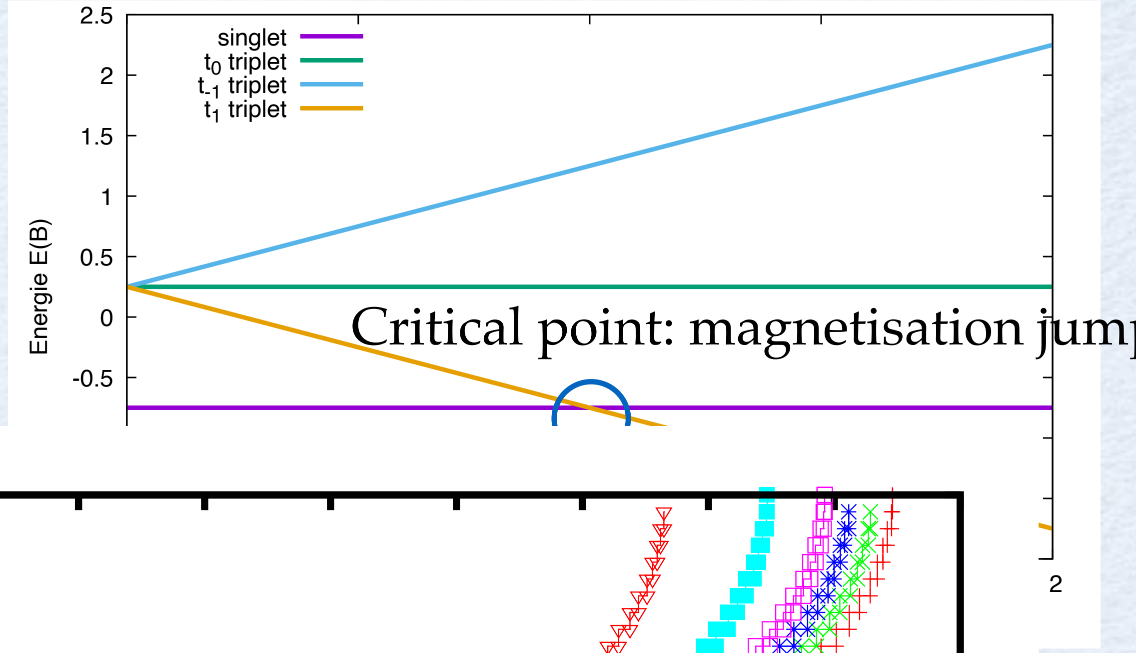
Basic properties:

Magnetisation Curves

Dimer in magnetic field: $\mathscr{H} = J\mathbf{S}_1 \cdot \mathbf{S}_2 - B(S_1^z + S_2^z)$

Energies of the singlet: $E_S(B) = -\frac{3}{4}J$

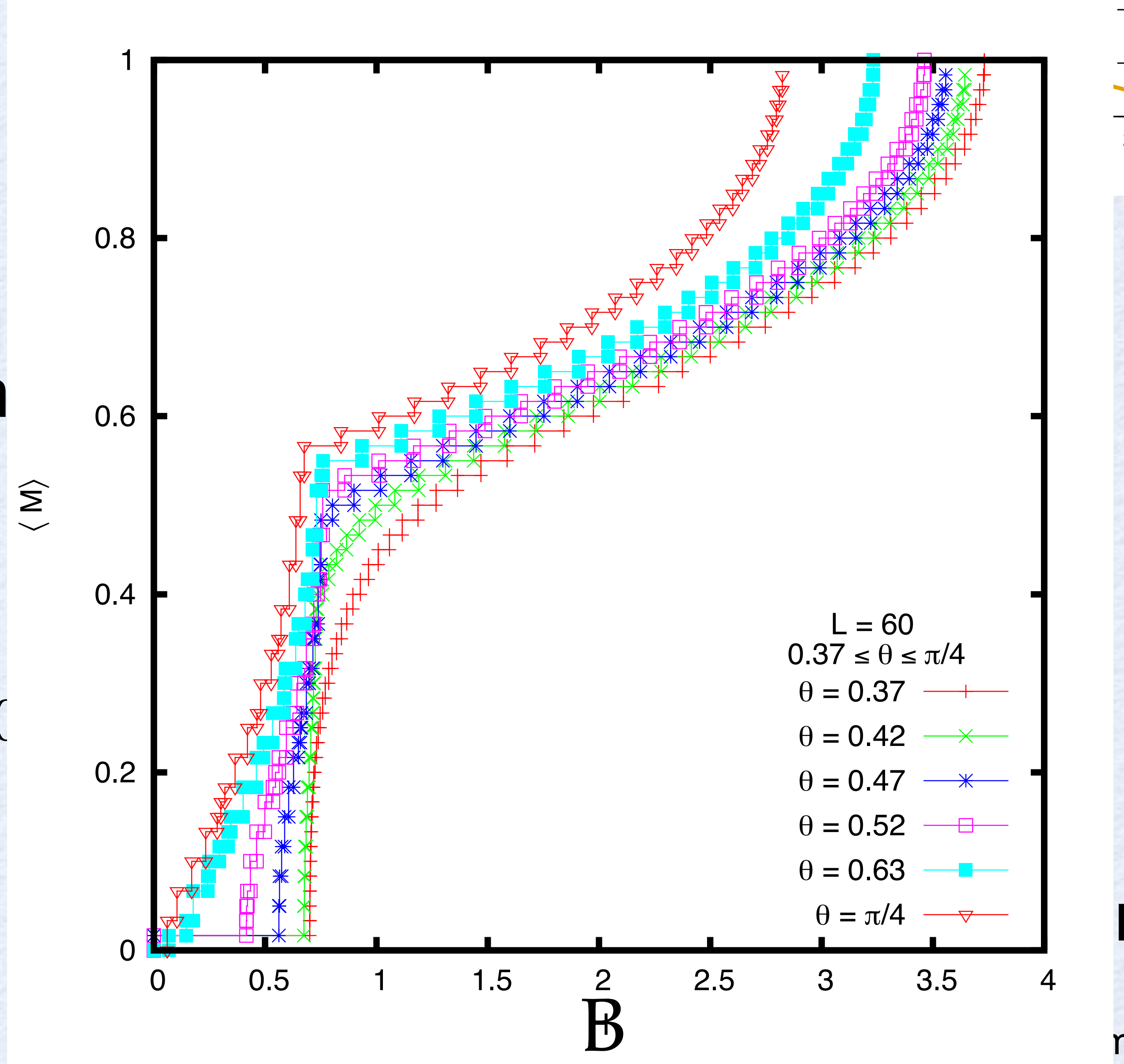
Energies of the triplets: $E_{t_1}(B) = \frac{1}{4}J - B\,,$



In general, obtain $M(B)$ via:

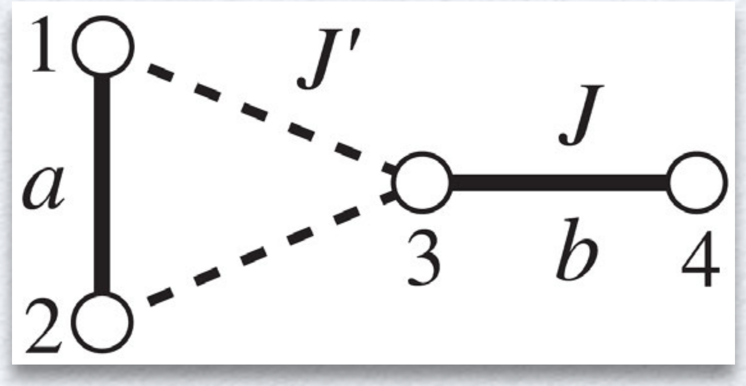
Legendre transform (if $S^z_{\text{total}} = \sum_j S_j^z$ is a good quantum

$$M(B) = \langle S^z_{total}\rangle \Big|_{[E_0(S^z_{total},B=0}$$



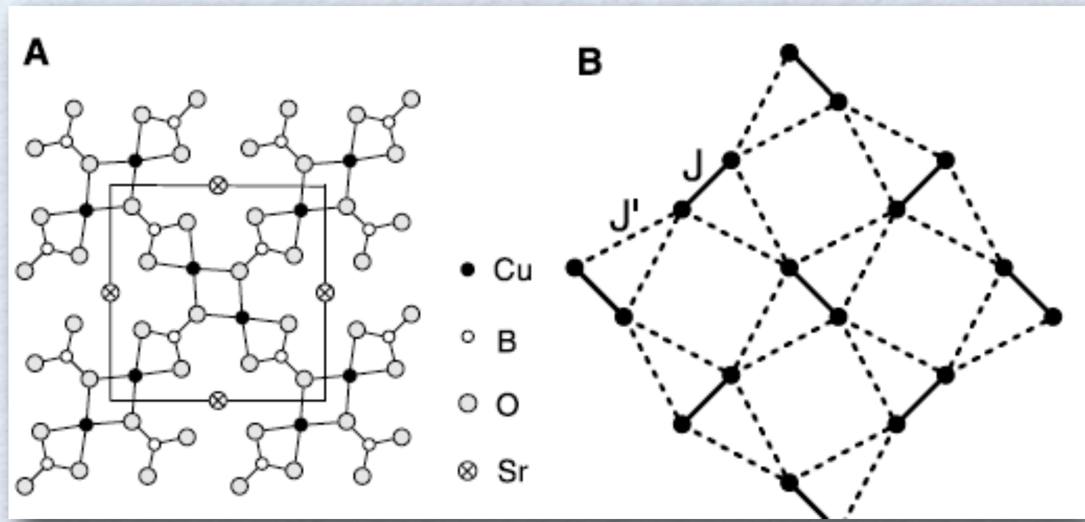
(Or directly as expectation value $M(B) = \sum_j \langle S_j^z\rangle(B)$ if … r)

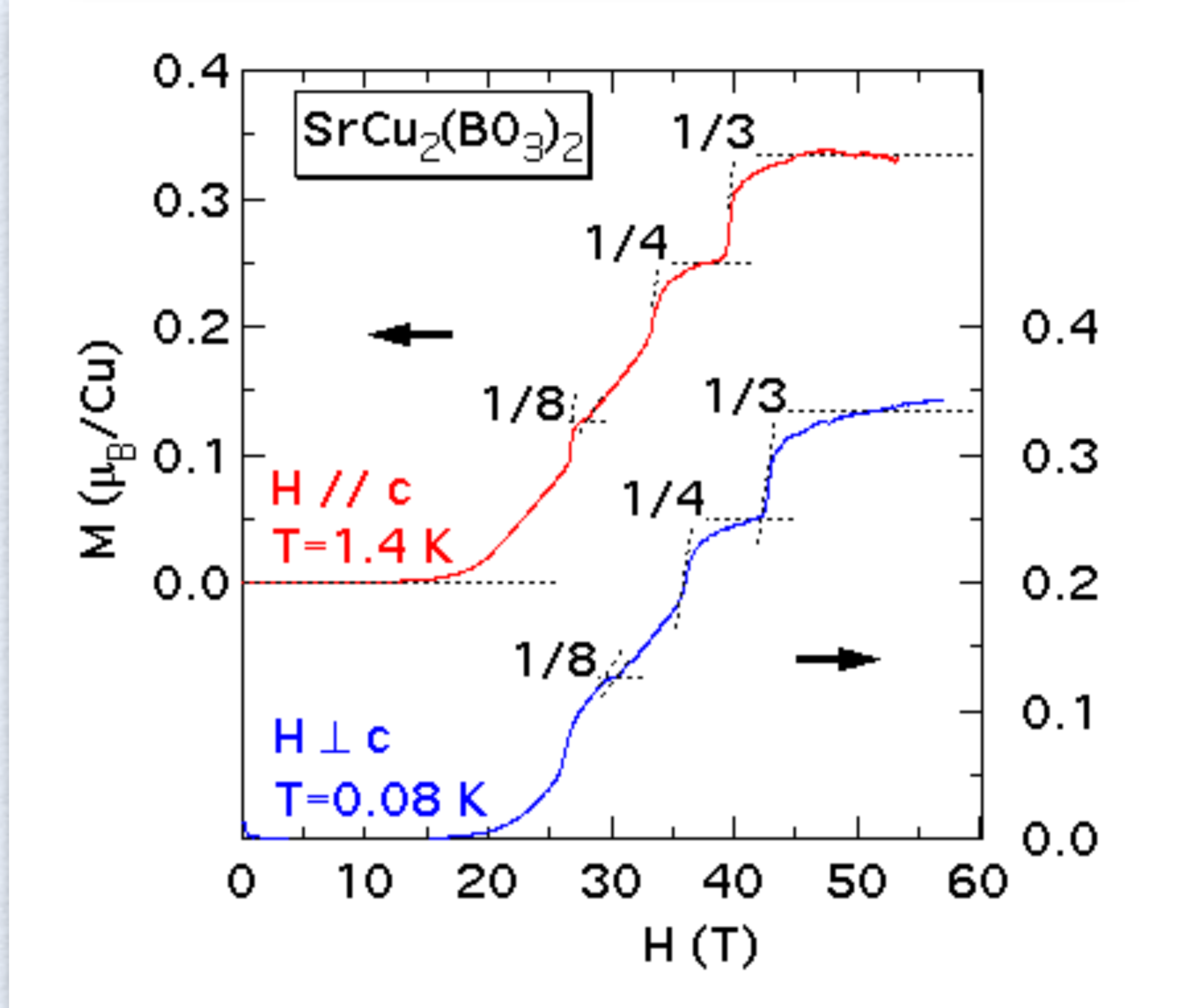
Part III: First example — dimer system in a magnetic field



A highly frustrated quantum magnet: $SrCu_2(BO_3)_2$

[H. Kageyama *et al.*, PRL **82**, 3168 (1999), K. Kodama et al., Science **298**, 395 (2002)]

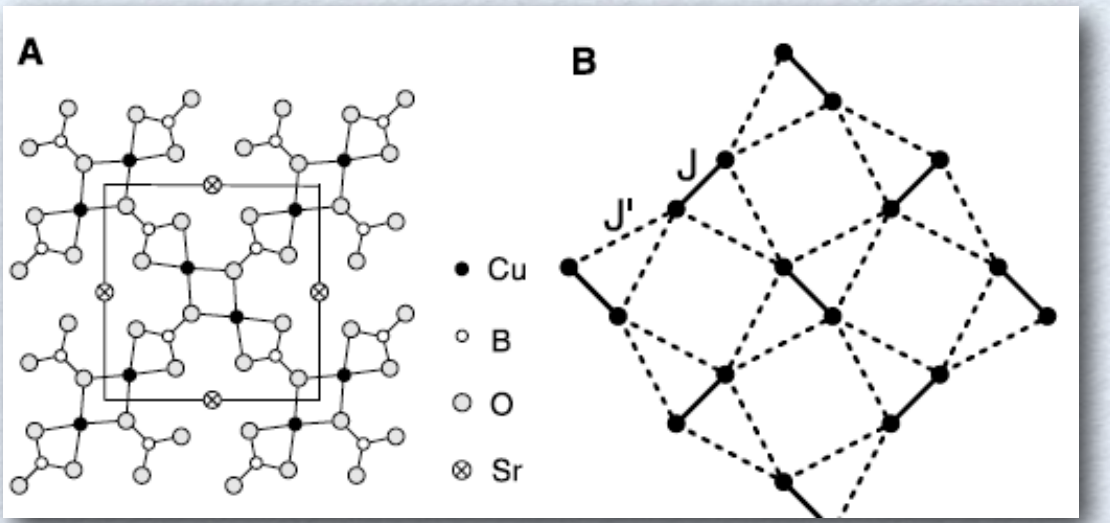




- Network of orthogonal dimers in a plane:
  2D Shastry-Sutherland lattice
- Series of fractional magnetization plateaux, e.g., at 1/8, 1/4, and 1/3 (+ further)
- Exotic states (e.g. spin-supersolid) in the vicinity or on the plateaux?
- Theoretical treatment of the full 2D system very challenging

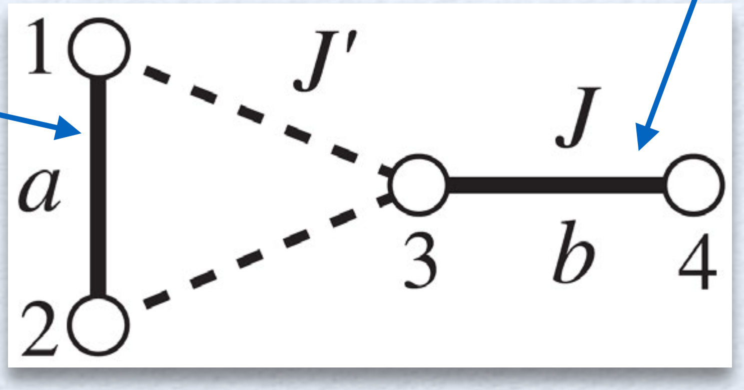
A highly frustrated quantum magnet: $SrCu_2(BO_3)_2$

[H. Kageyama *et al.*, PRL **82**, 3168 (1999),
K. Kodama et al., Science **298**, 395 (2002)]



$J > 0$: singlet

$J > 0$: singlet



Fluctuations between dimers a and b:

$$\mathcal{H}_{ab} = J'(\boldsymbol{S}_1 + \boldsymbol{S}_2) \cdot \boldsymbol{S}_3$$

$$S_1 = S_2 = 1/2 \Rightarrow \mathbf{S}_1 + \mathbf{S}_2 = \begin{cases} 0 \\ 1 \end{cases}$$

$$\mathcal{H}_{ab} |s\rangle_a |\psi\rangle_b = 0$$

singlet dimer is always an eigenstate

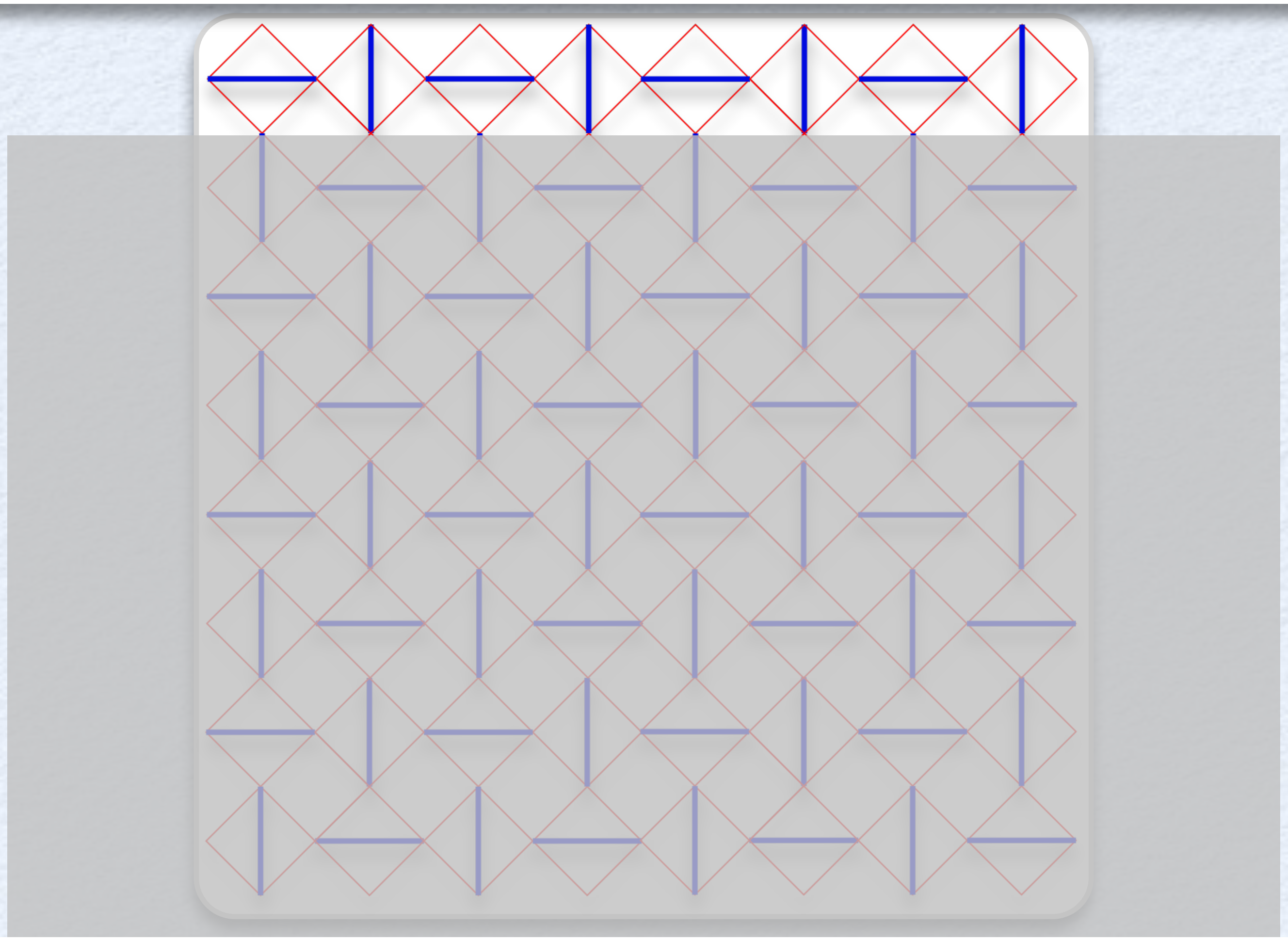
$J' \ll J$ → Ground state is a product state of singlets on the dimers
➟ this remains true as long as no phase transition is happening (no closing of a gap)

Shastry-Sutherland Lattice:

From 1D to 2D

Heisenberg model on orthogonal dimer network:

$$\mathcal{H} = J \sum_{\ll i,j \gg} \vec{S}_i \cdot \vec{S}_j + J' \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j - H \sum_i S_i^z$$



- Full 2D system too difficult ➙ take a stripe
- simplest stripe: ‘orthogonal dimer chain’ [Schulenburg & Richter, PRB 65, 054420 (2002)]

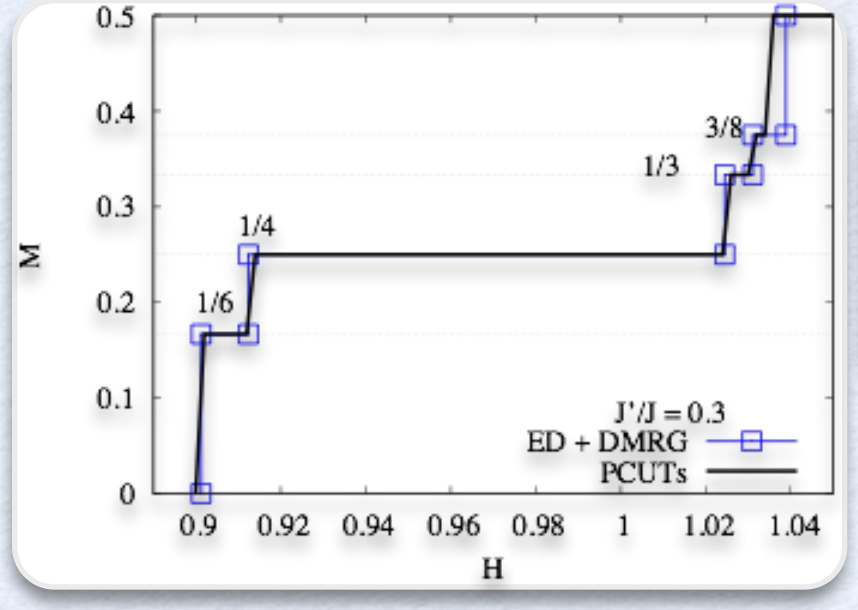
  infinite series of plateaux between M = 1/4 and 1/2
- 2 orthogonal dimer chains with transverse PBC: peculiar system, ‘Shastry-Sutherland tube’
- crossover to 2D system: increase number of orthogonal dimer chains

Quasi-1D version of the Shastry-Sutherland lattice: "2-leg Shastry-tubes"

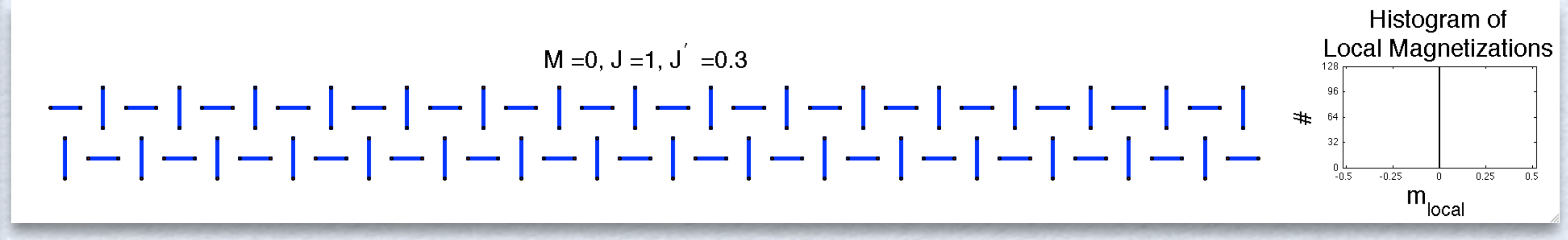
Magnetization curve: Compute ground state energies at different values of S^z_{total}

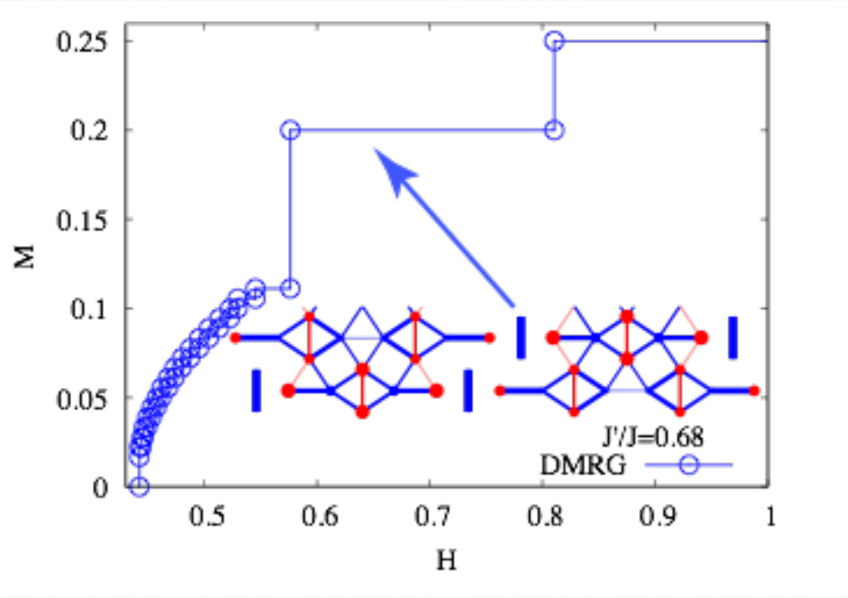
Do a Legendre-transform

[S.R. Manmana, J.-D. Picon, K.P. Schmidt, and F. Mila, EPL **94**, 67004 (2011)]

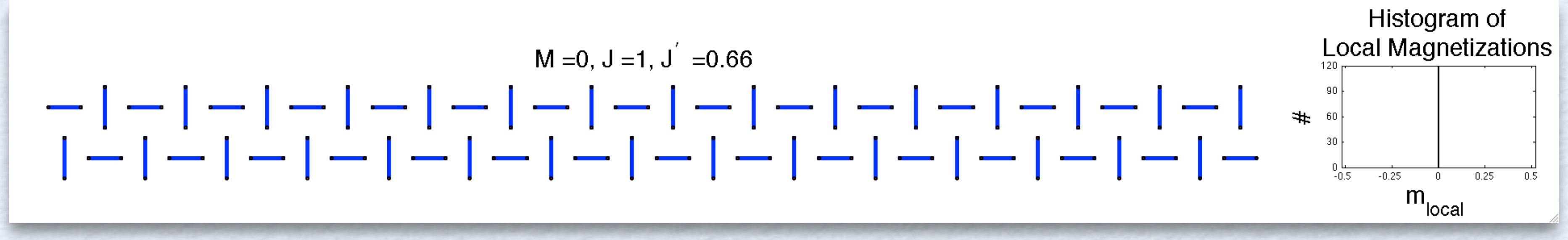


J'/J = 0.3 ("perturbative regime")





J'/J = 0.66 ("intermediate regime")

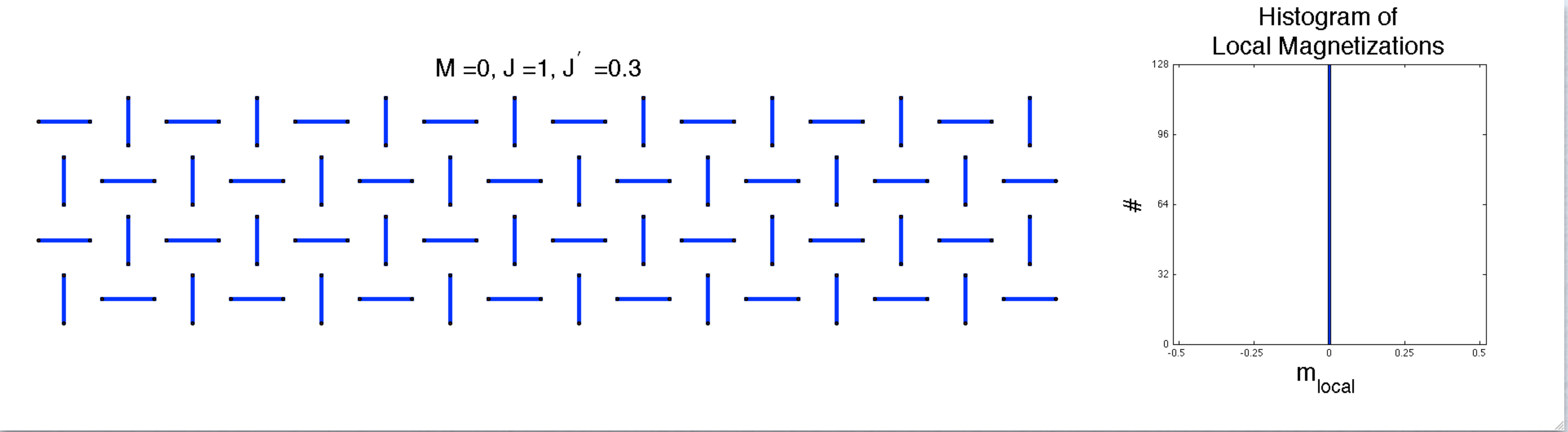


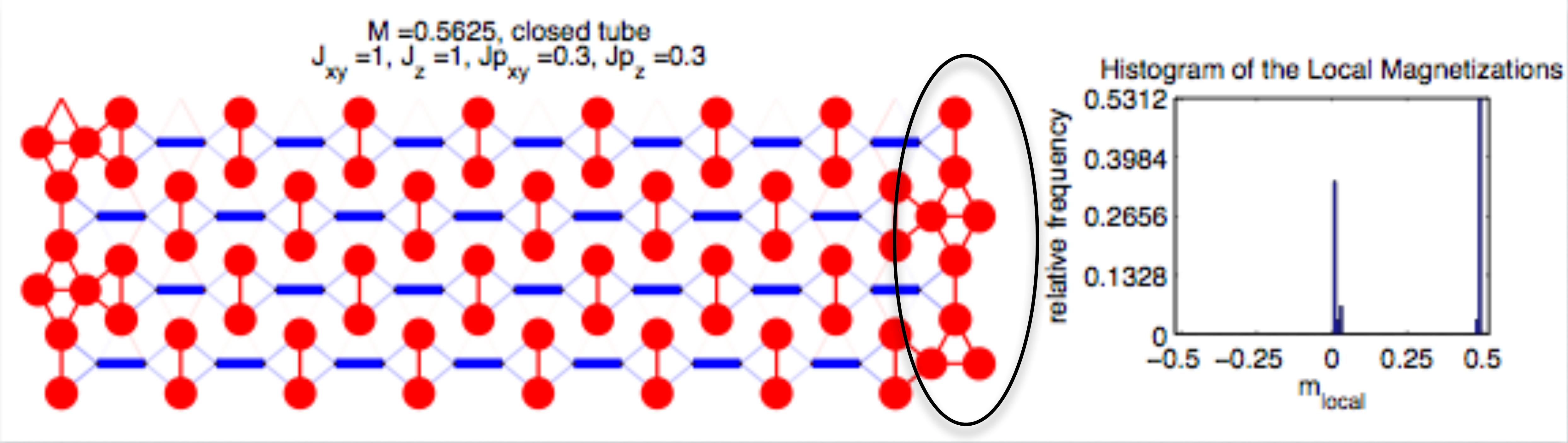
➥ Magnetization plateau of *bound states* of triplons

➟ *Qualitative* change of elementary building blocks: single triplons → multi-triplon bound states

Salvatore R. Manmana

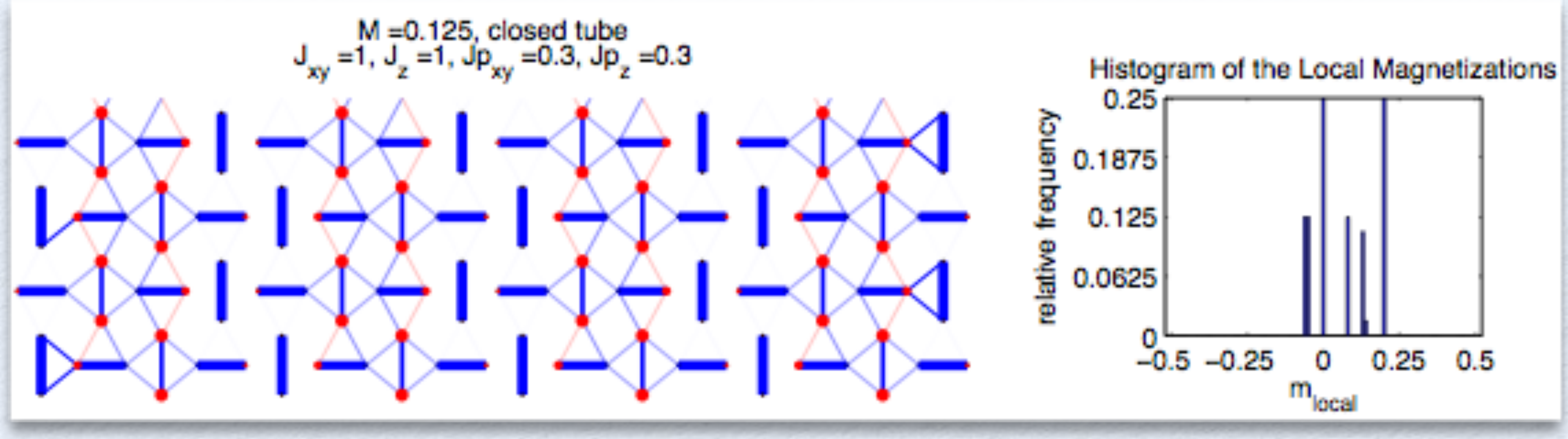
Quasi-2D version of the Shastry-Sutherland lattice:
"4-leg Shastry-tubes"



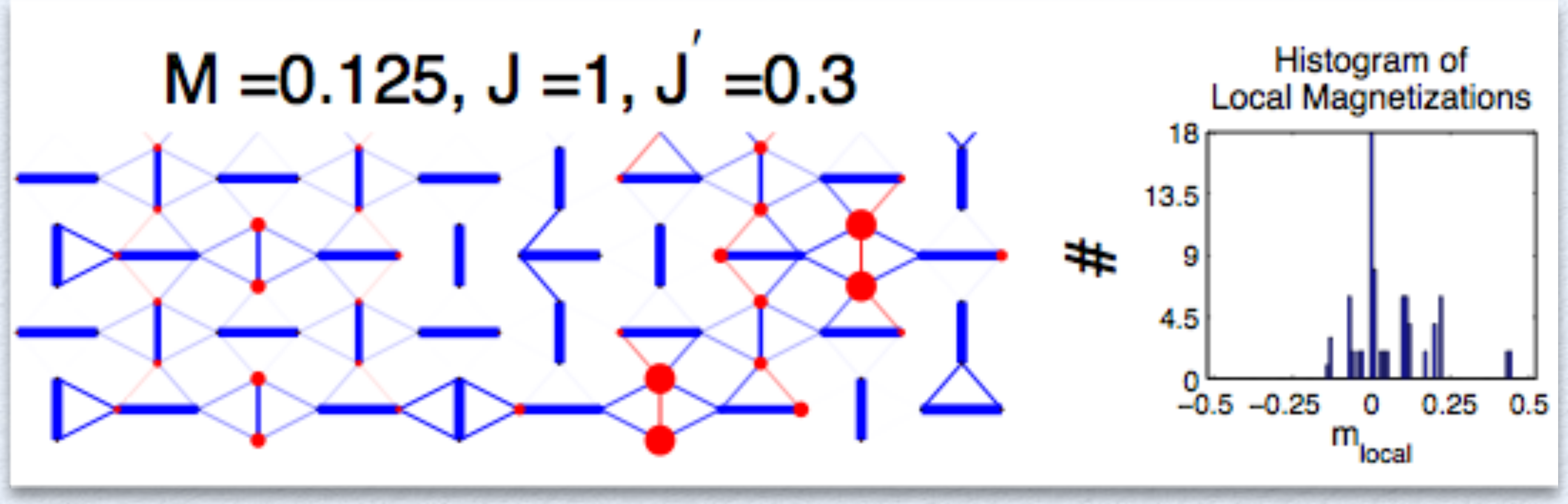


- Excited states by injecting triplons, but fluctuations much more pronounced
- Periodic patterns of triplons: magnetization plateaux?
- At boundaries: emerging 1D structures?

Quasi-2D Shastry-Sutherland lattice:
DMRG on the 1/8 plateau



E/N = -0.319238530384945



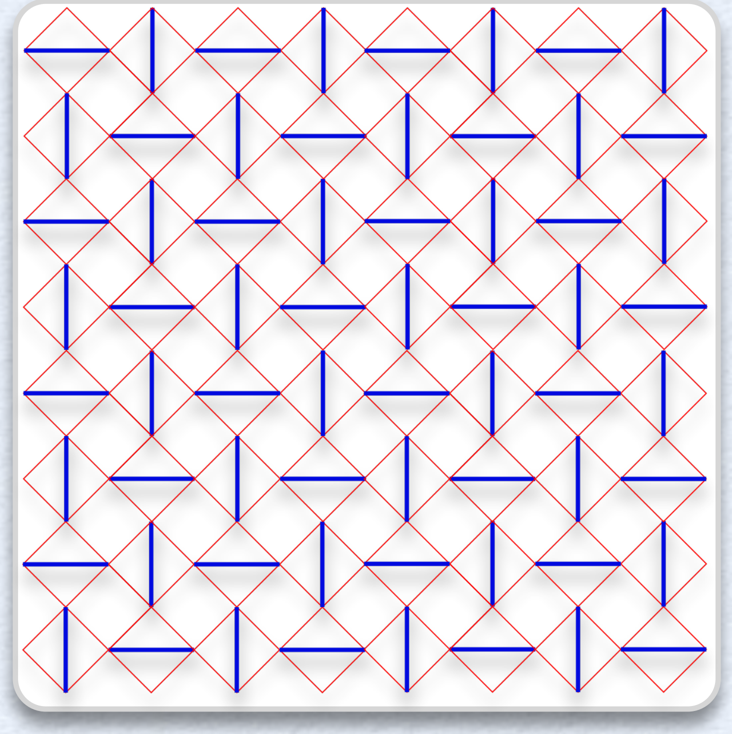
E/N = -0.319179928025625

Difference in E/N: only 6e-5 !!!
[S. White on Kagome: difference between VBC and spin-liquid ≈ 1e-3]

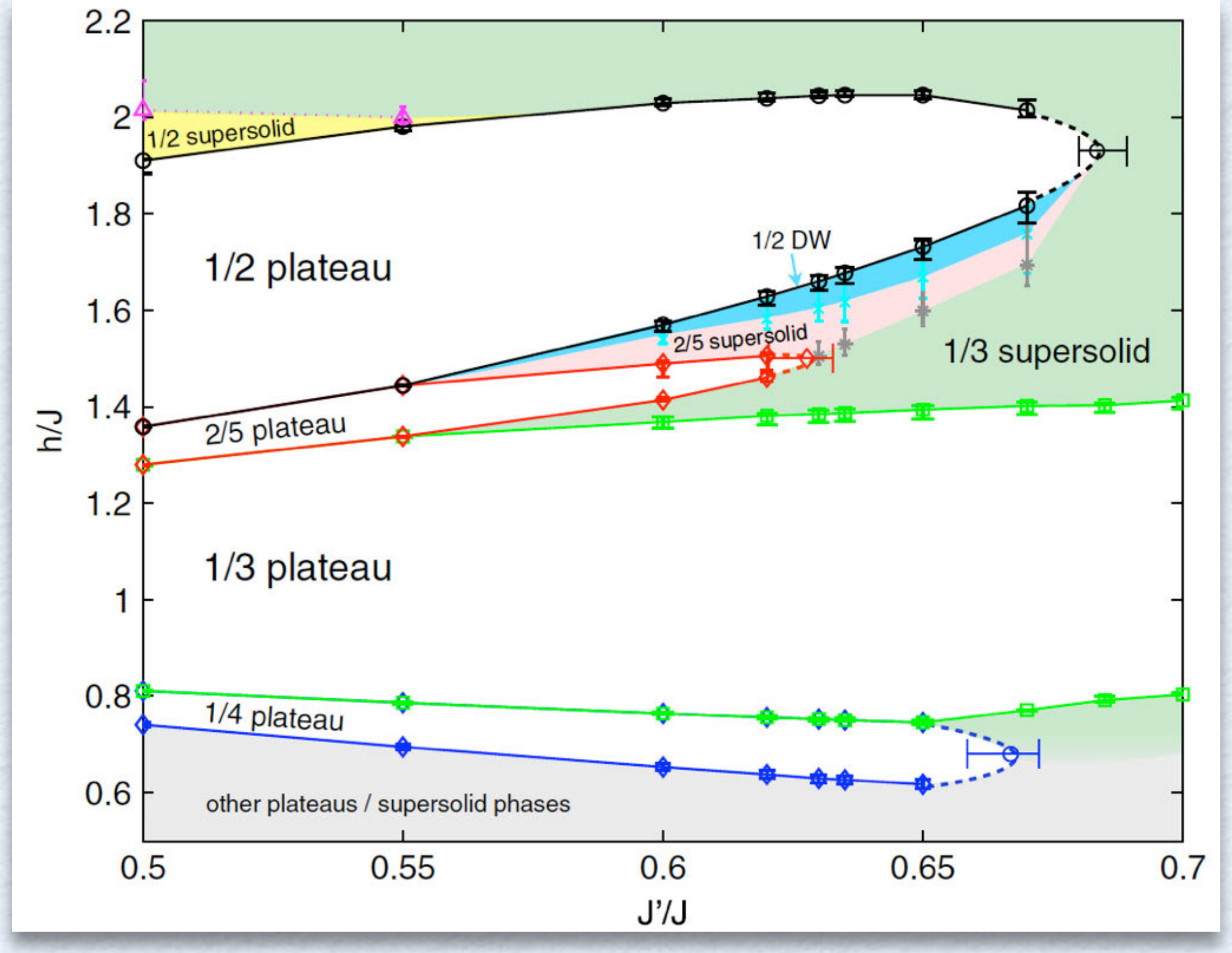
Approaching the 2D Shastry-Sutherland lattice: magnetization curve & comparison to experiments

[Y.H. Matsuda, N. Abe, S. Takeyama, H. Kageyama, P. Corboz, A. Honecker, S.R. Manmana, G.R. Foltin, K.P. Schmidt, and F. Mila, PRL **111**, 137204 (2013)]

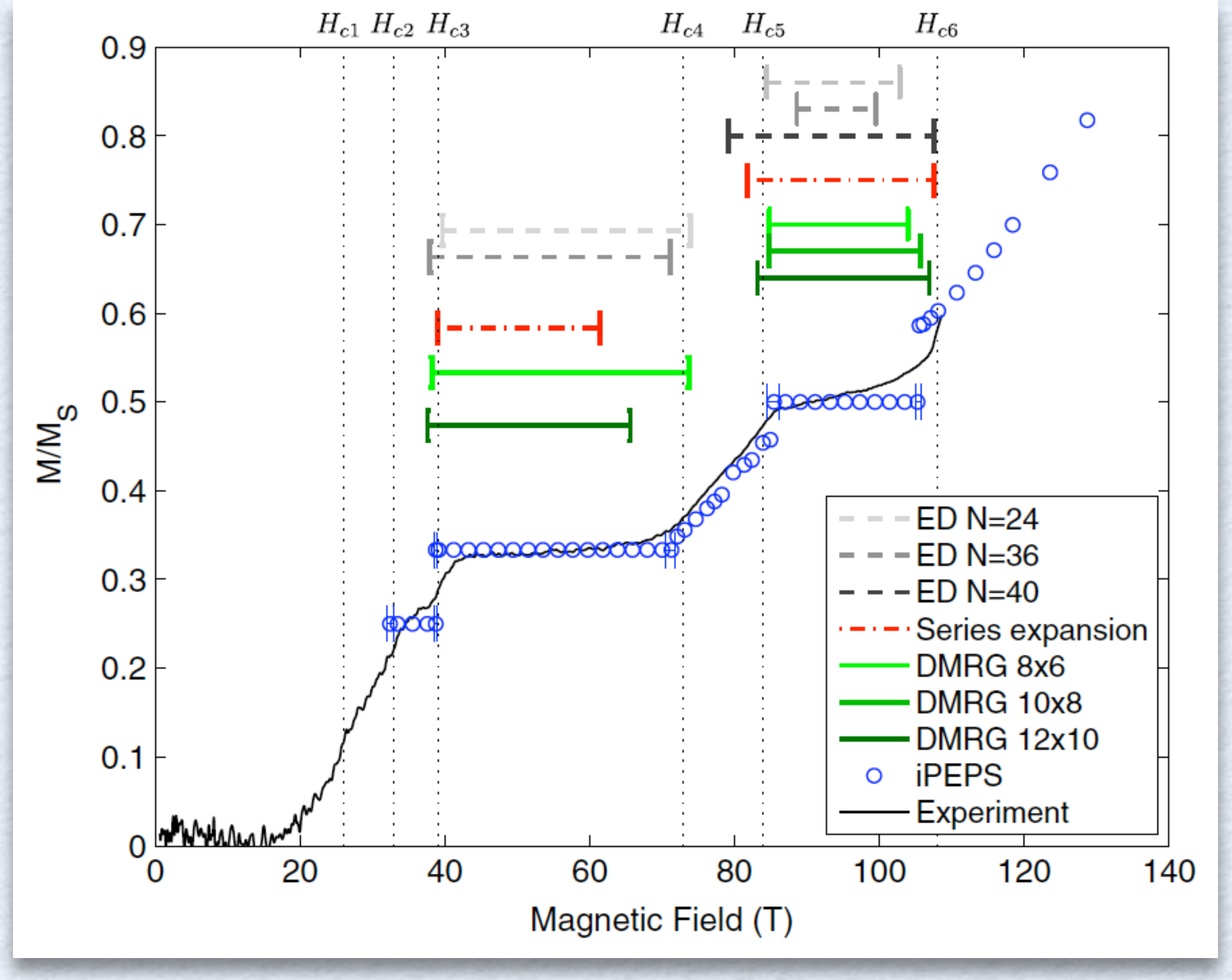
2D system:



iPEPS (2D, thermod. limit)



J'/J = 0.63:



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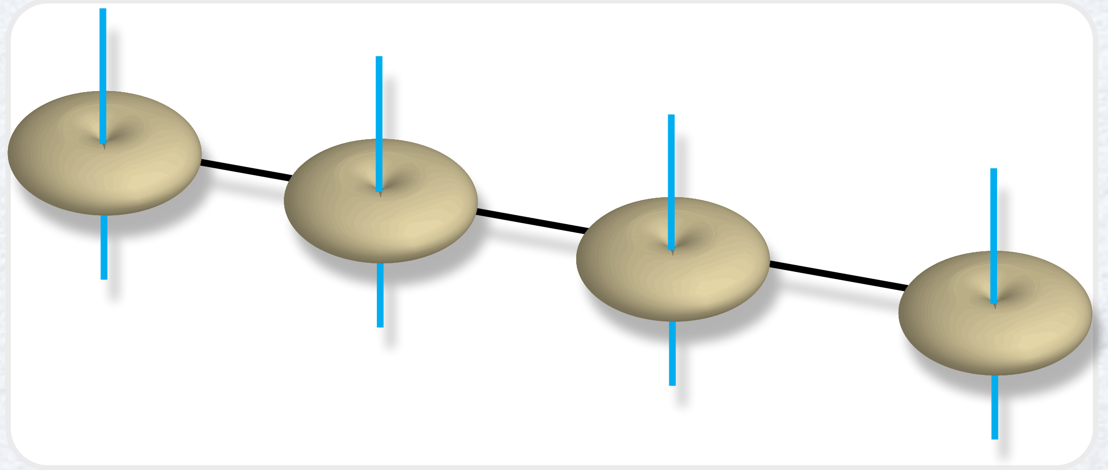
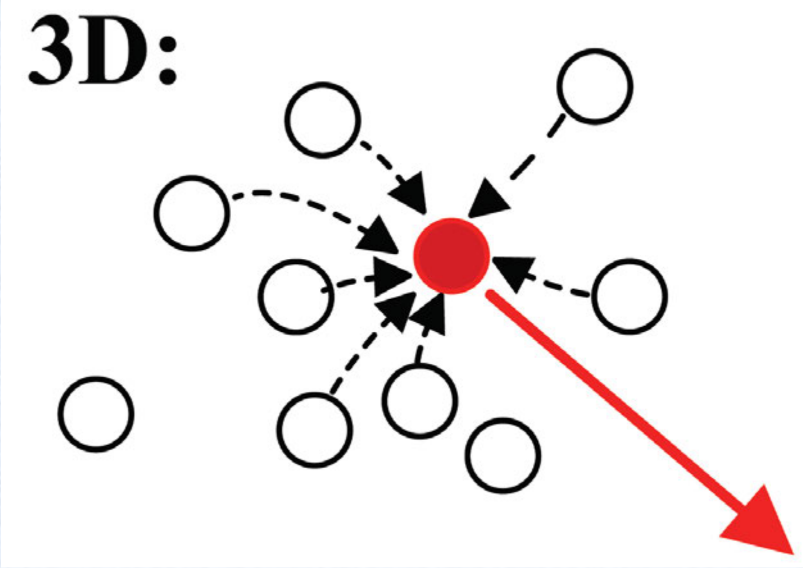
Part IV: Even more unconventional States of Matter



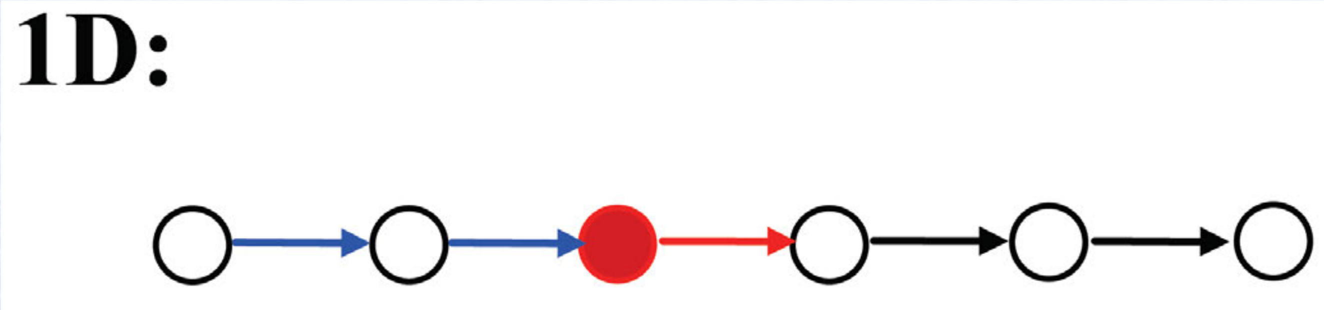
One-Dimensional Systems:

Luttinger Liquids

[T. Giamarchi, *Quantum Physics in one dimension*]

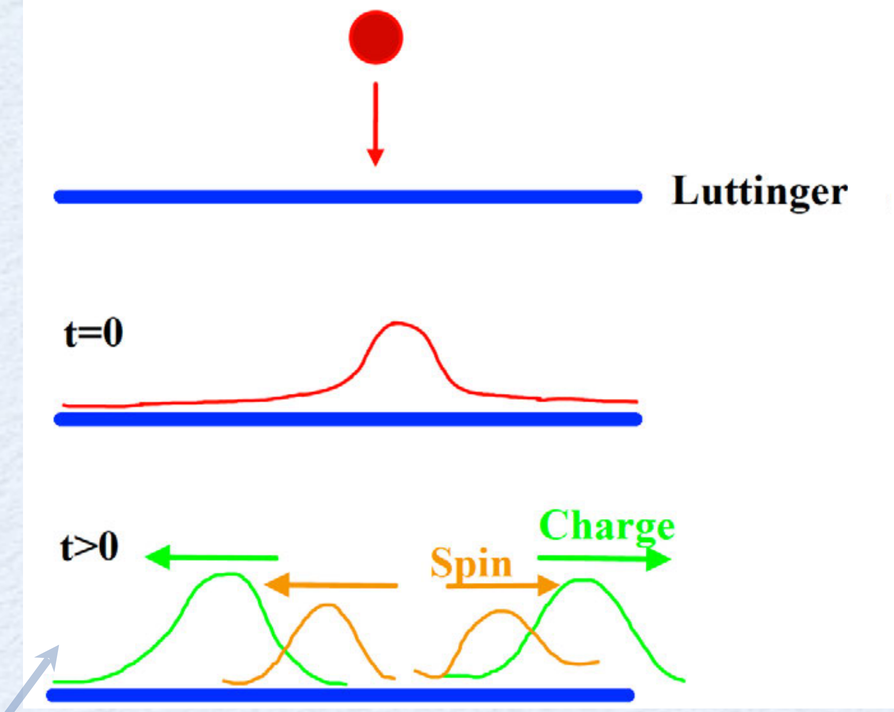


Fermi liquid:
quasi-free quasiparticles

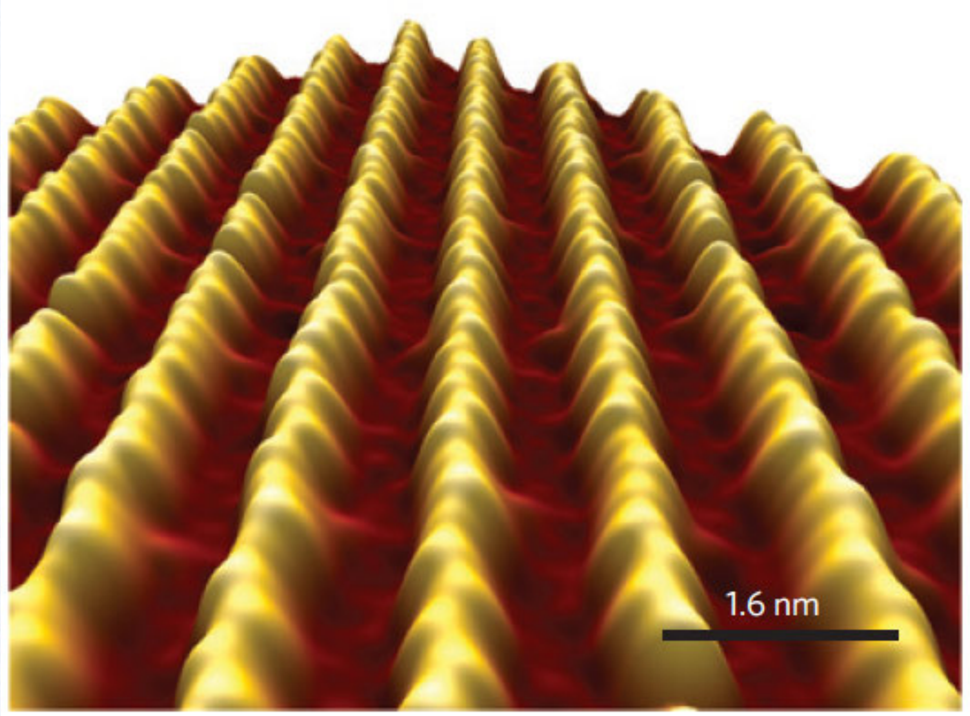


Interaction & geometry don't allow for 'quasi-free' motion:
collective excitations!

Spin- and charge degrees of freedom feel different influence:
Spin-Charge-Separation!



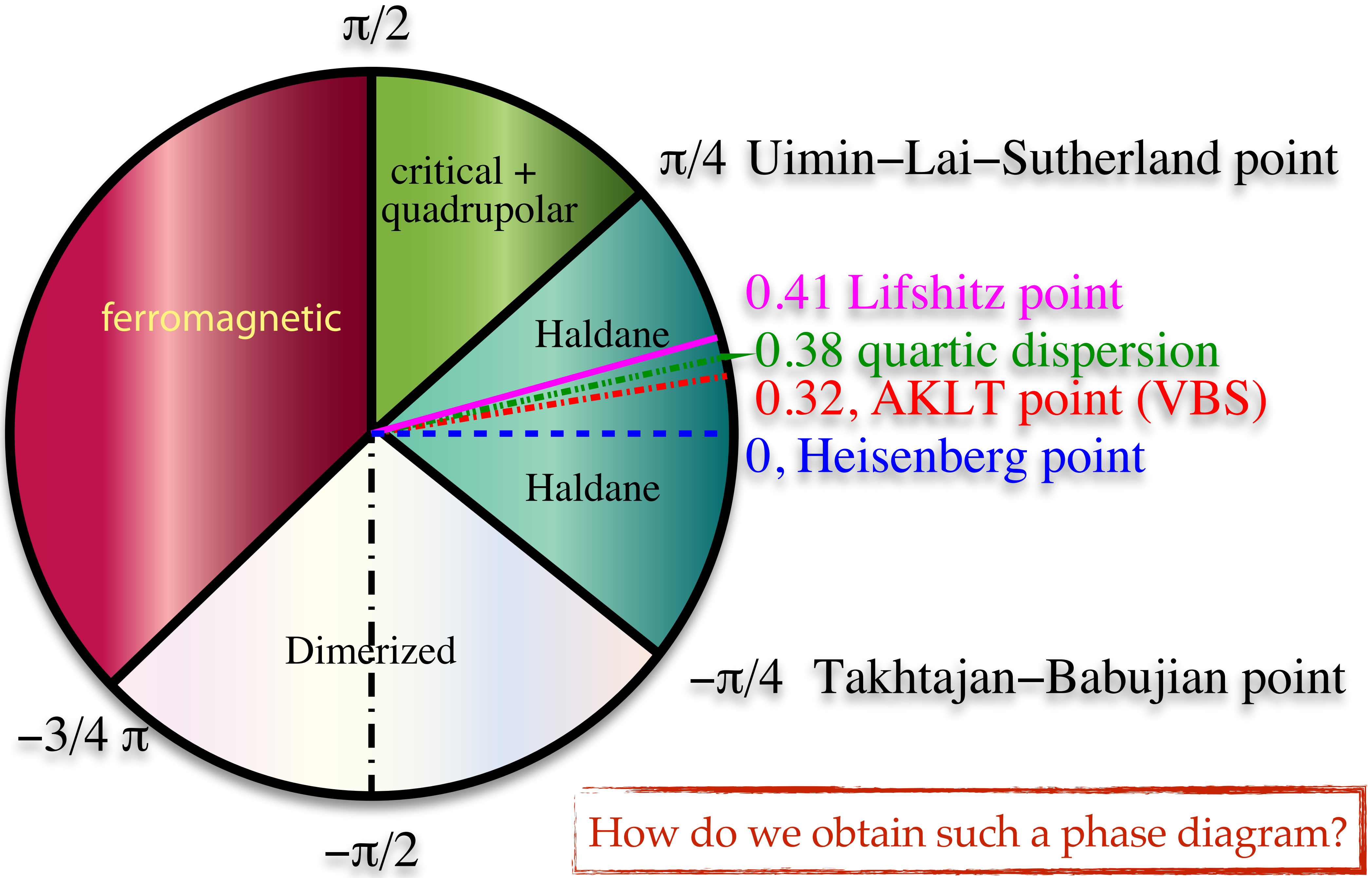
Experiments:



[C. Blumenstein et al., Nat. Phys. (2011)]

The bilinear-biquadratic S=1 Heisenberg chain: Ground state phase diagram at B=0

$$\hat{H} = J \sum_{i,j} \left[\cos(\theta) \mathbf{S}_{j,i} \mathbf{S}_{j+1,i} + \sin(\theta) \left(\mathbf{S}_{j,i} \mathbf{S}_{j+1,i} \right)^2 \right]$$



How do we obtain such a phase diagram?

(Quasi-)Long-Range-Order in Spin Systems

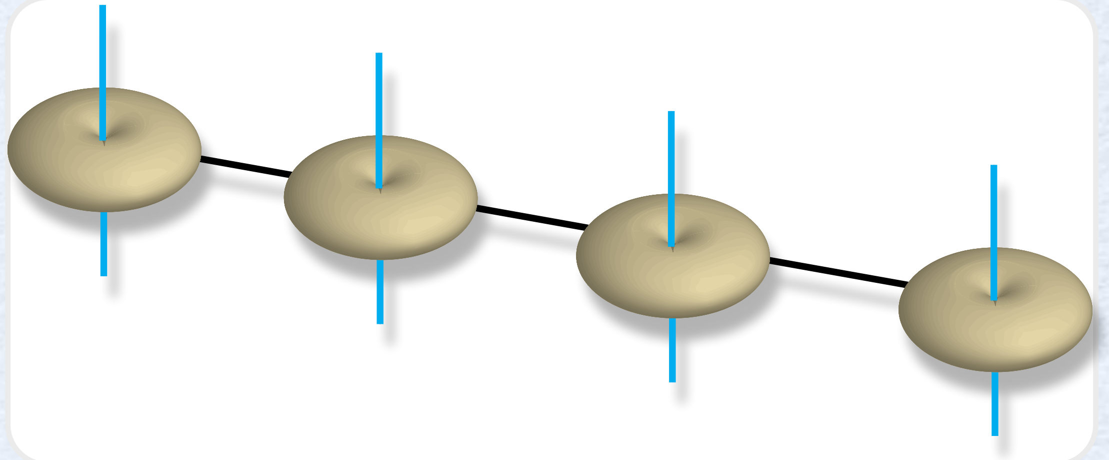
‚Magnetic' long range order in spin systems: spontaneous breaking of the SU(2) symmetry

- S=1/2: breaking of SU(2) signifies finite magnetization
- S>1/2: alternative mechanism to break SU(2) without finite magnetizations
  - ➡ Note that, e.g., $\langle (S_i^+)^2 \rangle \neq 0$ while $\langle S_i^z \rangle = 0$ at the same time

Consider the full operator space (S=1): products of local spin operators ➙ 9 possible elements
- 1 element: length of the spin, $1/3S(S+1)\delta_{\alpha\beta}$
- 3 elements: antisymmetric terms: $1/2\,(S_\alpha S_\beta - S_\beta S_\alpha) = S_\gamma$
- 5 elements: symmetric traceless tensor operator $Q_{\alpha\beta} = 1/2\,(S_\alpha S_\beta + S_\beta S_\alpha) - 1/3S(S+1)\delta_{\alpha,\beta}$

➟ Quadrupolar order parameter:

$$\vec{Q}_i = \begin{pmatrix} \frac{2}{\sqrt{3}}\left[(S_i^z)^2 - \frac{1}{4}\left(S_i^+S_i^- + S_i^-S_i^+\right)\right] \\ \frac{1}{2}\left(S_i^+S_i^z + S_i^zS_i^+ + S_i^-S_i^z + S_i^zS_i^-\right) \\ -\frac{i}{2}\left(S_i^+S_i^z + S_i^zS_i^+ - S_i^-S_i^z - S_i^zS_i^-\right) \\ -\frac{i}{2}\left[(S_i^+)^2 - (S_i^-)^2\right] \\ \frac{1}{2}\left[(S_i^+)^2 + (S_i^-)^2\right] \end{pmatrix}$$



"fluctuations around specific direction" - looks like donuts...

Not "pointing" in specific direction: spin nematic state
(see, e.g., K. Penc, lecture notes ICTP Trieste)

R. Manmana

Spin chains:

How to characterise the phases?

One spatial dimension: no "true" long-range order, but algebraic decay of correlation functions possible

➡ Phases characterized by "dominant" (slowest decaying) correlation functions.

➡ Here we compare:

spin correlations

$$C_S^{long}(i,j) = \langle S_i^z S_j^z \rangle - \langle S_i^z \rangle \langle S_j^z \rangle$$
$$C_S^{trans}(i,j) = \langle S_i^- S_j^+ \rangle$$

longitudinal: magnetic qlro
transverse: quasi-condens. of magnons

quadrupolar correlations:

$$C_Q(i,j) = \langle \vec{Q}_i \cdot \vec{Q}_j \rangle - \langle \vec{Q}_i \rangle \cdot \langle \vec{Q}_j \rangle$$

3 components:
longitudinal: $\Delta S^z = 0$
transverse: $\Delta S^z = 1$
pairing: $\Delta S^z = 2$
→ quasi-condens. of *pairs* of magnons

parity breaking, vector chiral order:

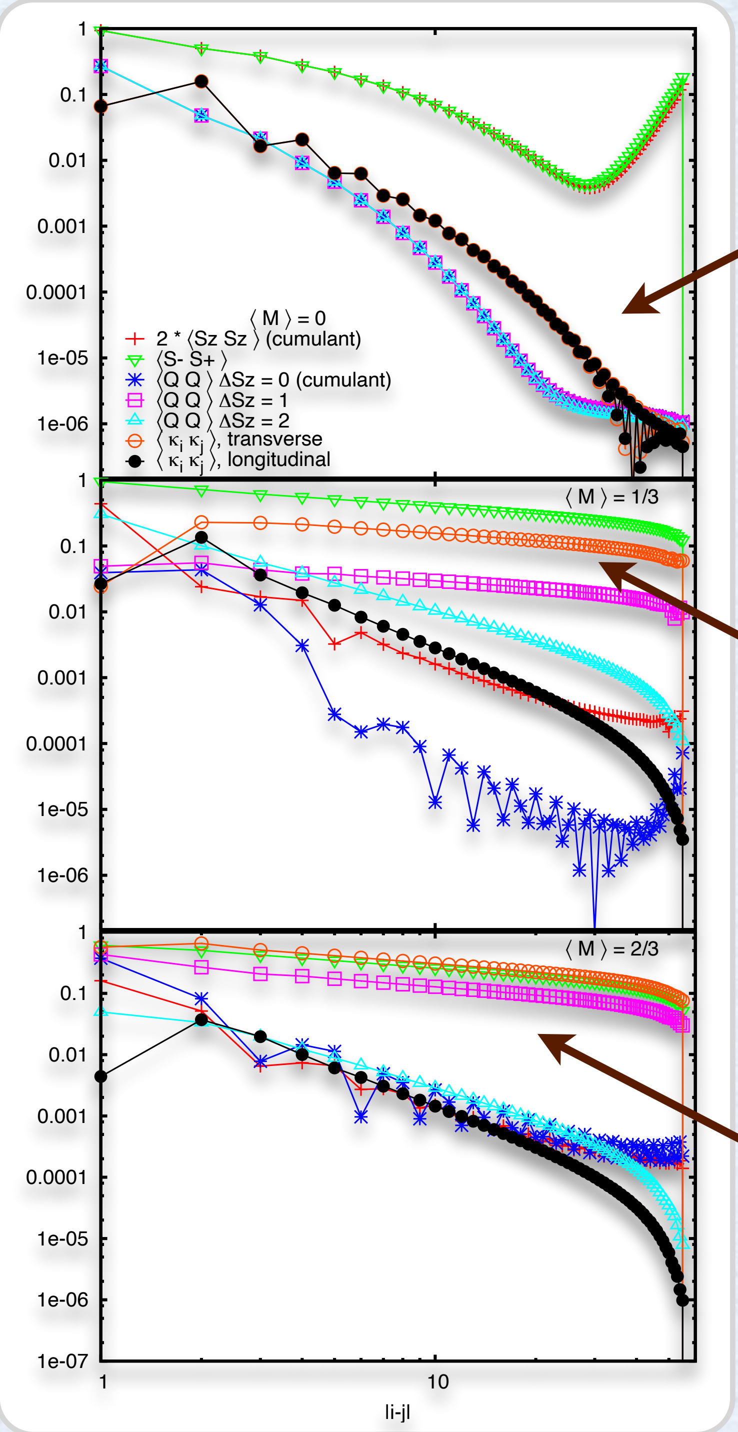
vector chirality $\vec{\kappa}_j = \langle \mathbf{S}_j \times \mathbf{S}_{j+1} \rangle$ $C_\kappa(i,j) = \langle \vec{\kappa}_i \cdot \vec{\kappa}_j \rangle$

2 components:
longitudinal: parity breaking
transverse: ~ transv. spin

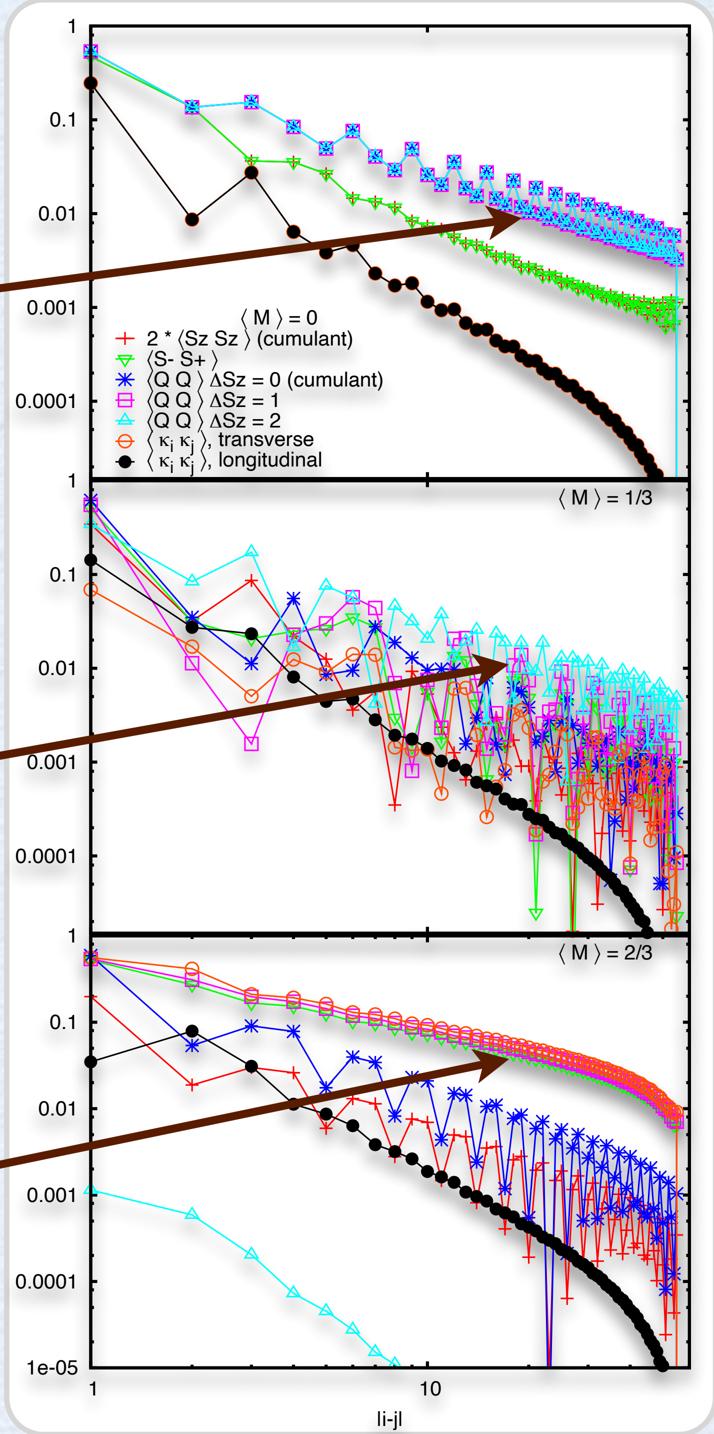
S=1 Bilinear-Biquadratic Heisenberg Chain in Magnetic Fields: Correlation Functions

[S.R. Manmana, A.M. Läuchli, F.H.L. Essler, and F. Mila, PRB **83**, 184433 (2011)]

Θ = 0:



Θ=π/3:



M=0:
exponential decay

quadrupolar correlations dominant

M=1/3:
transverse spin, quadrupolar and chiral correlations, same exponent

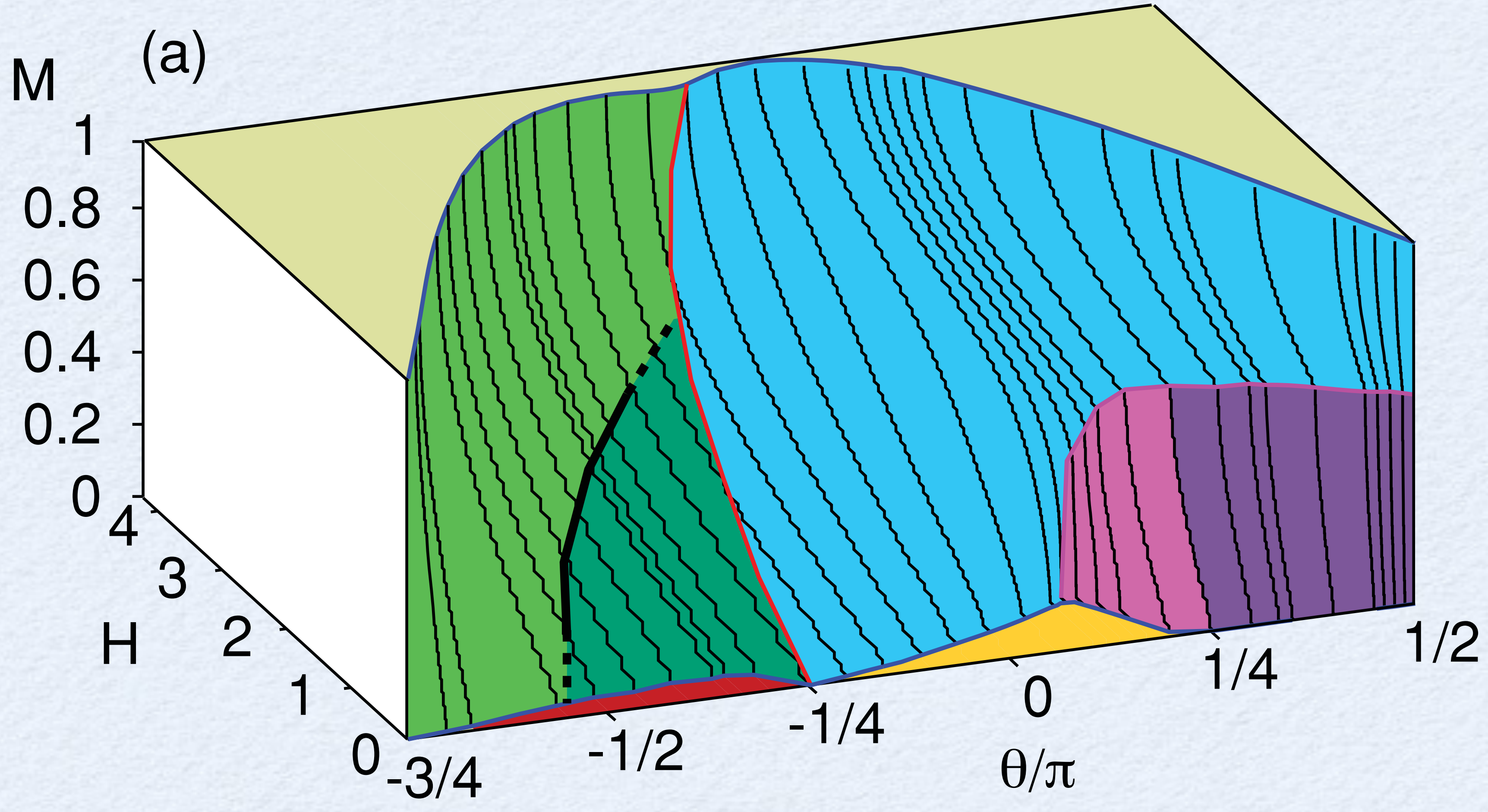
quadrupolar correlations (weakly), no vector chiral order

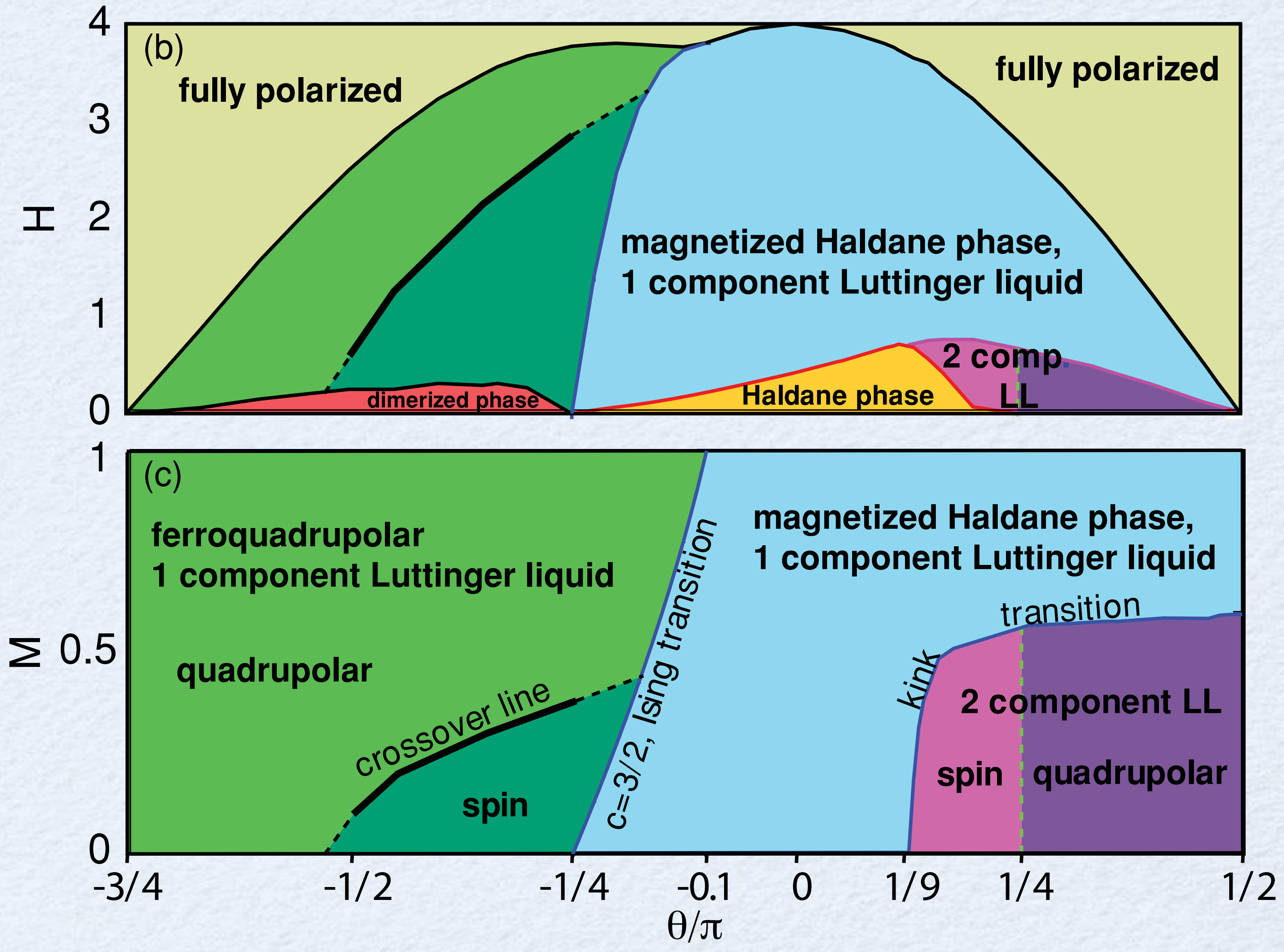
M=2/3:
transverse spin, quadrupolar and chiral correlations, same exponent

- No vector chiral order
- below the kink: Luttinger-liquid phase with spin-nematic quasi-long-range order

The bilinear-biquadratic S=1 Heisenberg chain: Phase Diagram at Finite Magnetic Fields

[S.R. Manmana, A.M. Läuchli, F.H.L. Essler, and F. Mila, PRB **83**, 184433 (2011)]

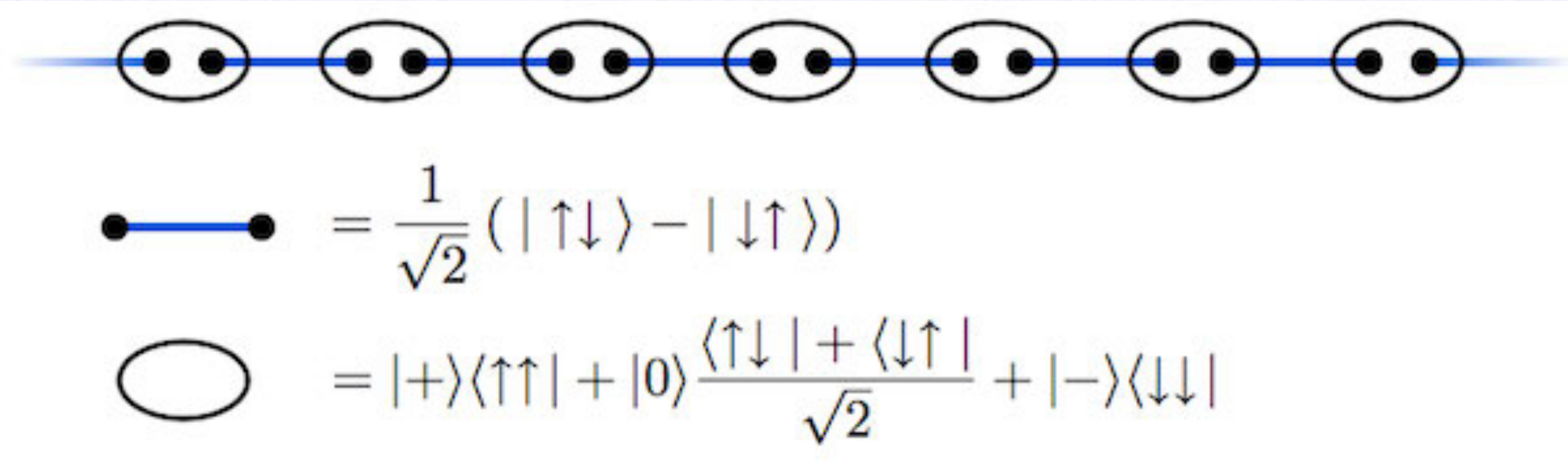




Salvatore R. Manmana

S=1 Bilinear-Biquadratic Heisenberg Chains: The AKLT State

Sketch of the AKLT state:



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

$$\bigcirc = |+\rangle\langle\uparrow\uparrow| + |0\rangle\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$$

- „Topological“ phase (*symmetry protected topological state*, SPT)
- Exact ground state of $\mathscr{H} = \sum_j \left[\mathbf{S}_j \cdot \mathbf{S}_{j+1} + \frac{1}{3}\left(\mathbf{S}_j \cdot \mathbf{S}_{j+1}\right)^2\right]$
- No local order parameter, but string order parameter
- Fractional excitations: effective S=1/2 at the edges

Nobel Prize 2016 for Topol. Phases

More unconventional states:

Symmetry Protected Topological Phases

Possible characterization (X.-G. Wen):

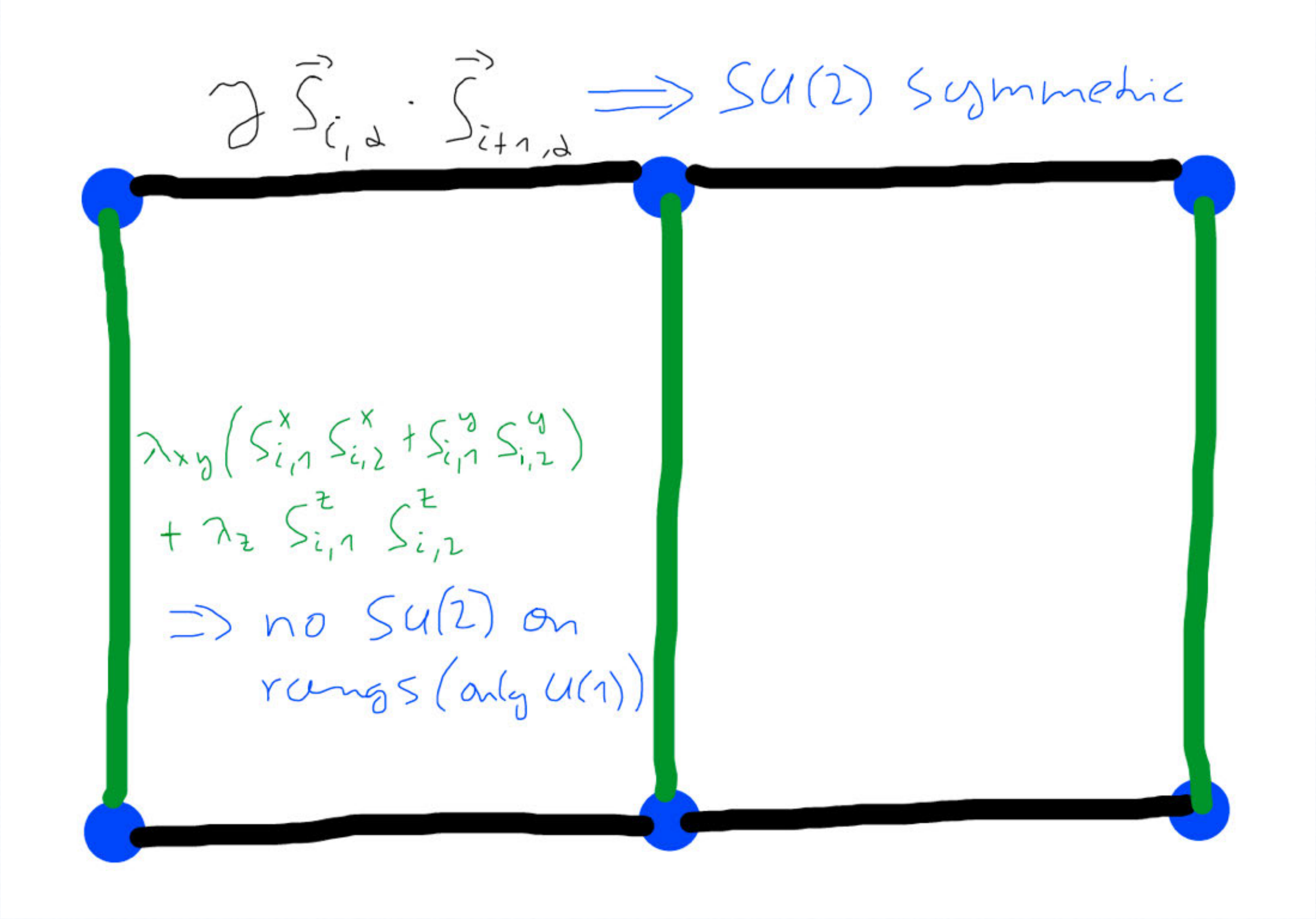
- ➠ new kind of order at T=0
- ➠ SPT phases possess a symmetry and a finite energy gap.
- ➠ SPT states are short-range entangled states with a symmetry.
- ➠ defining properties:

(a) distinct SPT states with a given symmetry cannot smoothly deform into each other without phase transition, if the deformation preserves the symmetry.

(b) however, they all can smoothly deform into the same trivial product state without phase transition, if we break the symmetry during deformation.

Note: “Real” Topological Phases ➠ “long-range entanglement” (Wen)

Simple System with two SPT Phases:
2-leg ladder with anisotropic interactions



Simple System with two SPT Phases:
2-leg ladder with anisotropic interactions

Characterize topological phases via “entanglement spectrum”:

F. Pollmann, A. Turner, E. Berg, and M. Oshikawa, PRB **81**, 064439 (2010)

$$|\psi\rangle = \sum_{j=1}^{\dim\mathcal{H}} \sqrt{\lambda_j}\, |\alpha\rangle_j\, |\beta\rangle_j$$

λ_j: eigenvalues reduced density matrix, give entanglement spectrum

“Entanglement Splitting” test for 2-fold degeneracy:

$$ES = \sum_{j\,\mathrm{odd}} (\lambda_j - \lambda_{j+1})$$

test topological properties!

- staggered magnetization along the legs:

$$\langle m \rangle = \langle S^z_{L/2,\,1} \rangle - \langle S^z_{L/2+1,\,1} \rangle$$

- Spin gaps:

singlet gap: $\Delta^0_S = E_1(S^z_{\mathrm{total}} = 0) - E_0(S^z_{\mathrm{total}} = 0)$

triplet gap: $\Delta^1_S = E_0(S^z_{\mathrm{total}} = 1) - E_0(S^z_{\mathrm{total}} = 0)$

2nd triplet gap: $\Delta^{1,2}_S = E_0(S^z_{\mathrm{total}} = 2) - E_0(S^z_{\mathrm{total}} = 1)$

Simple System with two SPT Phases:
2-leg ladder with anisotropic interactions

[Z.-X. Liu, Z.-B. Yang, Y.-J. Han, W. Yi, and X.-G. Wen, PRB (2012)]

Symmetry of the ladder: $D_2 \times \sigma$ ($D_2 = \{E, R_x, R_y, R_z\}$; σ: rung exchange)

➠ 8 distinct SPT phases: from projective representations, characterized via 'active operators'

	R_z	R_x	σ	Active operators	SPT phases
E_0	1	1	1		Rung-singlet[a], $t_x \times t_x, \ldots$
E_1	I	$i\sigma_z$	σ_y	(S^z_-, S^z_+, SS_-)	$t_x \times t_y$
E_2	σ_z	I	$i\sigma_y$	(S^x_-, S^x_+, SS_-)	$t_y \times t_z$
E_3	$i\sigma_z$	σ_x	I	(S^x_+, S^y_+, S^z_+)	$t_0, t_x \times t_y \times t_z$
E_4	σ_z	$i\sigma_z$	$i\sigma_x$	(S^y_+, S^y_-, SS_-)	$t_x \times t_z$
E_5	$i\sigma_z$	σ_x	$i\sigma_x$	(S^x_+, S^y_-, S^z_-)	t_x
E_6	$i\sigma_z$	$i\sigma_x$	σ_z	(S^x_-, S^y_-, S^z_+)	t_z
E_7	$i\sigma_z$	$i\sigma_x$	$i\sigma_y$	(S^x_-, S^y_+, S^z_-)	t_y

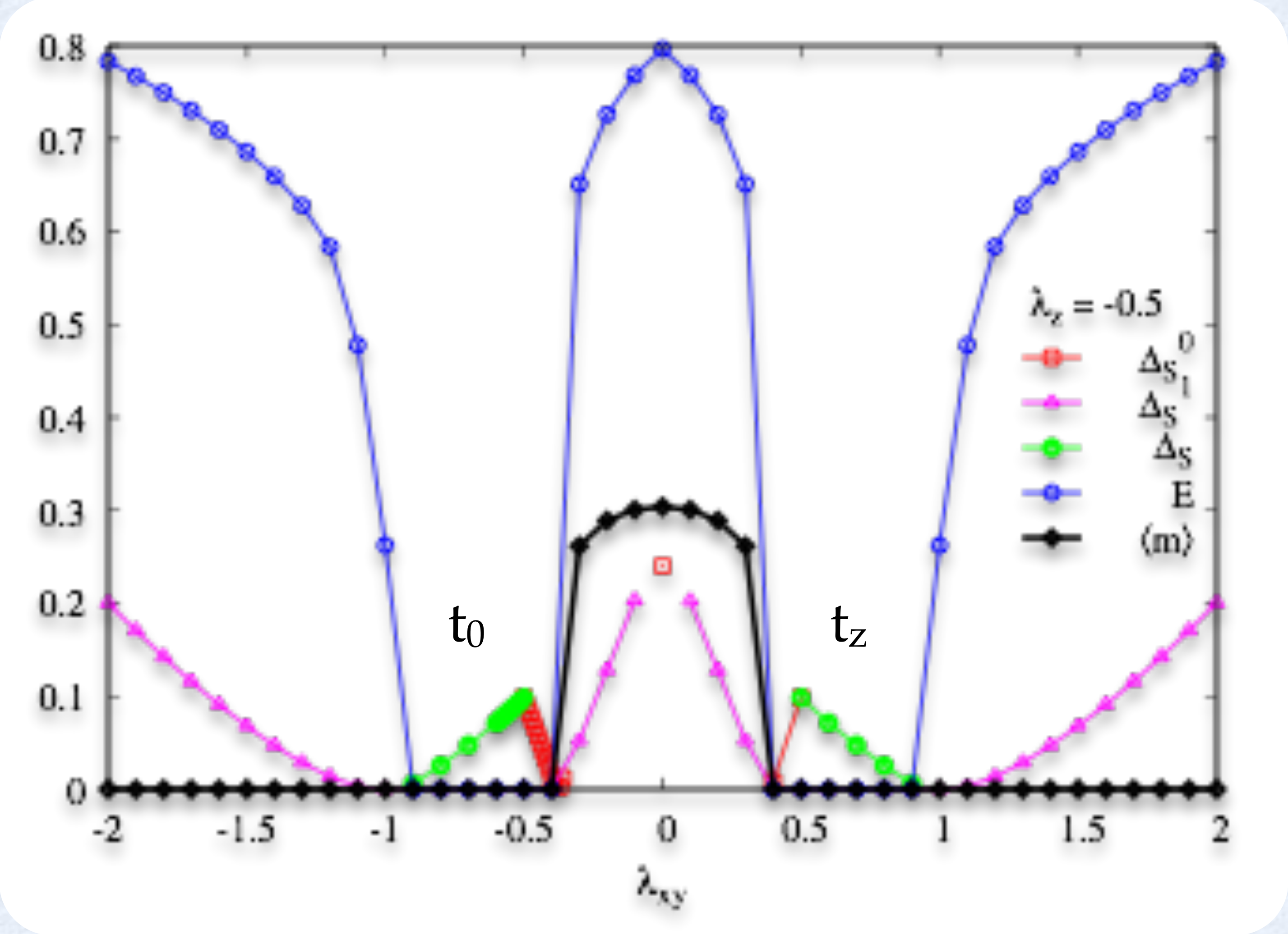
With $O_\pm = O_1 \pm O_2$

$$SS_- = \vec{S}_{i,1} \cdot \vec{S}_{i+1,1} - \vec{S}_{i,2} \cdot \vec{S}_{i+1,2}$$

Simple System with two SPT Phases: 2-leg ladder with anisotropic interactions

[S.R. Manmana *et al.*, PRB (rapid comm.) **87,** 081106(R) (2013)]

Nearest neighbor interactions:
(DMRG with up to 400 rungs)



Ground-state degeneracy:

t_0 phase:

$S_1^x+S_2^x$:
E_0 = -188.25372468551
E_1 = -188.24741526006

$S_1^x-S_2^x$:
E_0 = -188.24728807477
E_1 = -188.2472878754

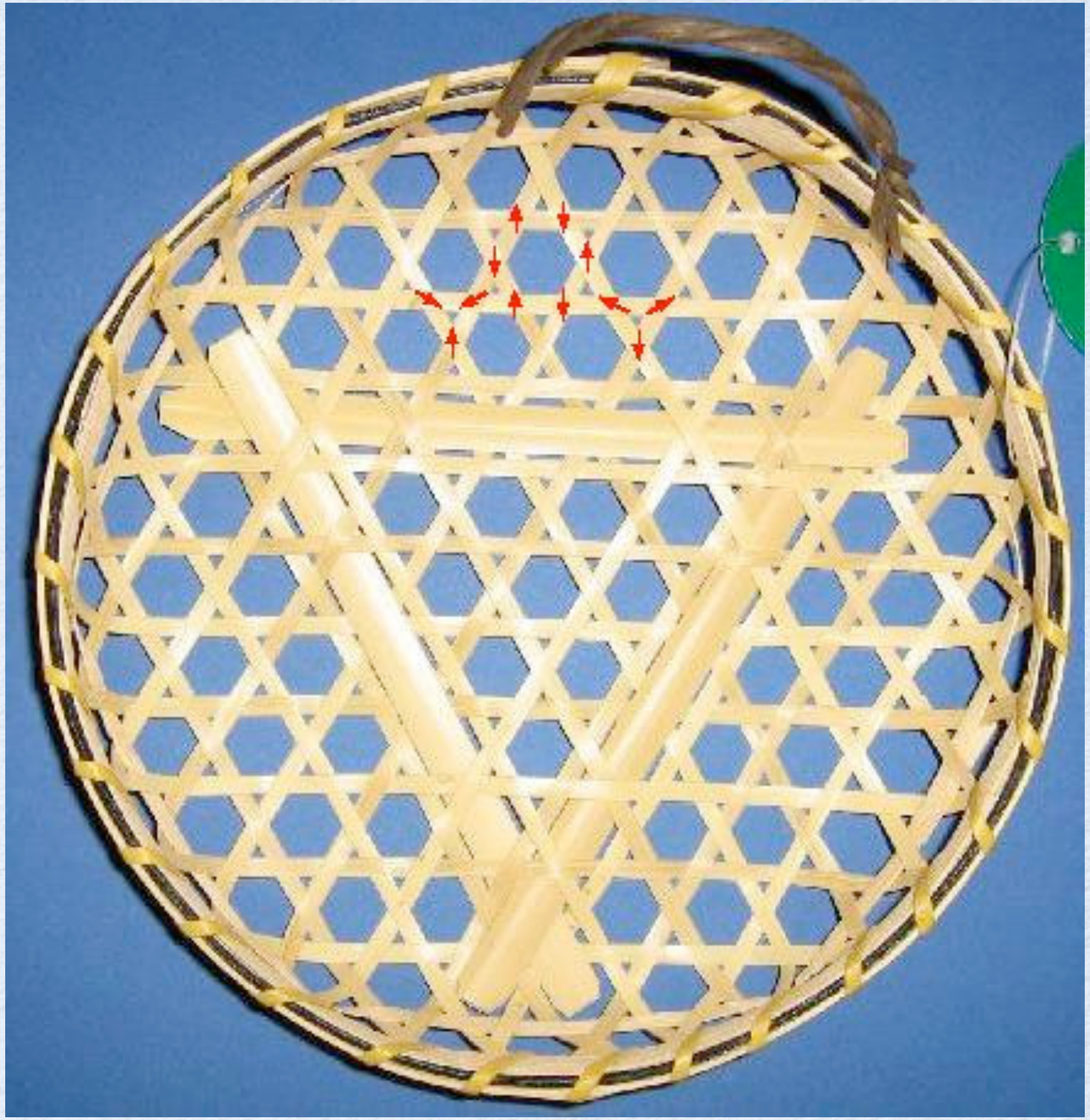
t_z phase:

$S_1^x+S_2^x$:
E_0 = -188.24727291579
E_1 = -188.24727272182

$S_1^x-S_2^x$:
E_0 = -188.25372545779
E_1 = -188.24741603227

The kagome antiferromagnet

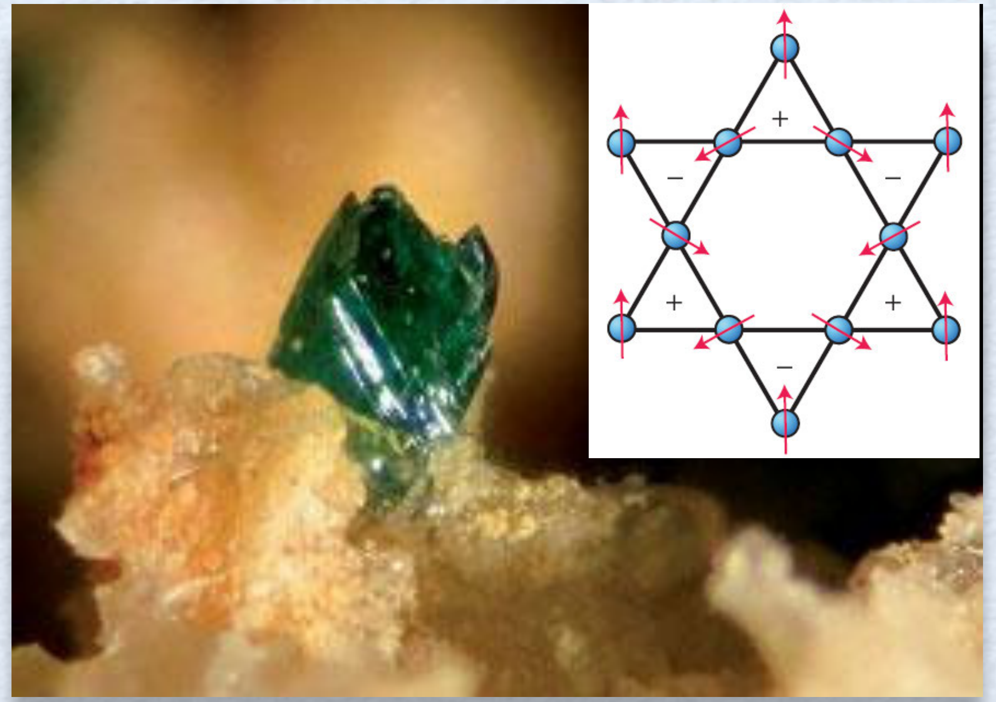
Wikipedia:
kago: bamboo basket
me: “eyes” (holes)
[I. Syôzi, Prog. Theor. Phys. 6, 306 (1951).]



- Highly frustrated system: only corner sharing triangles!
  [see, e.g., G. Misguich & C. Lhuillier, cond-mat/0310405]
- Unconventional properties:
  - Exponential number of singlet excitations above the ground state
  - Candidate for algebraic spin liquid state
- Realization in nature?

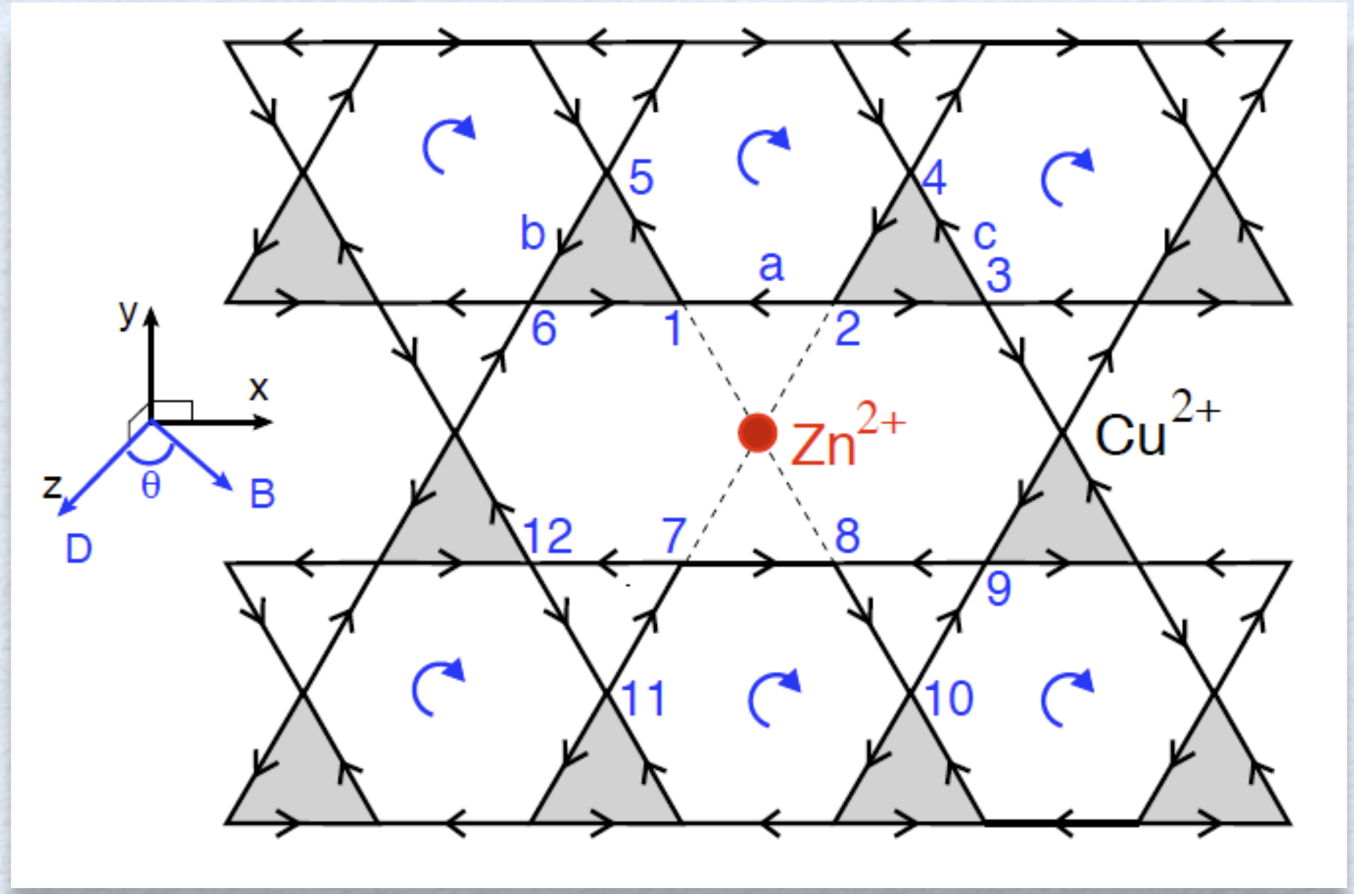
s=1/2 kagome material:

Herbertsmithite $ZnCu_3(OH)_6Cl_2$



Good realization of the s=1/2 Heisenberg system on the kagome geometry, but:

- 5-10% non-magnetic impurities
- significant Dzyaloshinskii-Moriya interactions



Model:

$$\mathcal{H} = J\sum_{\langle ij\rangle} \mathbf{s}_i \cdot \mathbf{s}_j + \sum_{\langle ij\rangle} \mathbf{D}_{ij} \cdot (\mathbf{s}_i \times \mathbf{s}_j) - \mathbf{B} \cdot \mathbf{S}$$

Real materials:

Dzyaloshinsky-Moriya interactions

Heisenberg exchange interaction: $J\,\vec{S}_1 \cdot \vec{S}_2$

Origin due to the "hopping" of the electrons, obtained in 2nd order perturbation theory

Spin-Orbit Coupling: $\sim \lambda\,\vec{L} \cdot \vec{S}$ $\qquad \lambda \ll 1$

Effective magnetic Hamiltonian from 2nd order perturbation theory when including this interaction:

$$\hat{H}_{\text{eff}} = J'\,\vec{S}_1 \cdot \vec{S}_2 + \vec{D} \cdot \left(\vec{S}_1 \times \vec{S}_2\right) + \vec{S}_1 \cdot \mathbf{\Gamma} \cdot \vec{S}_2 + \ldots$$

$$J' \sim \lambda^0 \qquad |\vec{D}| \sim \lambda \qquad |\mathbf{\Gamma}| \sim \lambda^2$$

- DM term antisymmetric under exchange of spins, while Heisenberg term symmetric
- Typically: D ~ 1 - 10% of J
- Standard references:

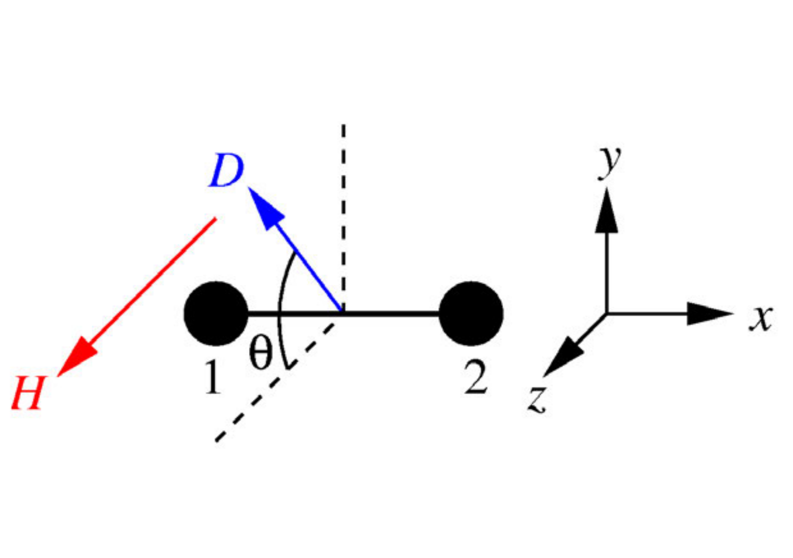
I. Dzyaloshinsky, J. Phys. Chem. Solids **4**, 241-255 (1958).

T. Moriya, Phys. Rev. Lett. **4**, 228 (1960); Phys. Rev. **120**, 91 (1960).

The simplest system:

S=1/2 dimer with DM interaction

[S. Miyahara et al., PRB **75**, 184402 (2007)]



$$\hat{H}_{12} = J\,\vec{S}_1 \cdot \vec{S}_2 + \vec{D} \cdot \left(\vec{S}_1 \times \vec{S}_2\right) - \vec{H} \cdot \left(\vec{S}_1 + \vec{S}_2\right)$$

Moriya's rules: D orthogonal to the dimer.

Symmetries of the Dimer with DM in a magnetic field:
Permutation 1 <-> 2 + Sx -> -Sx. Consequence:

$$\begin{aligned} \langle S_1^x \rangle &= -\langle S_2^x \rangle \\ \langle S_1^y \rangle &= \langle S_2^y \rangle \\ \langle S_1^z \rangle &= \langle S_2^z \rangle \end{aligned}$$

- Staggered magnetization: $$m_s := \frac{1}{2}\langle \vec{S}_1 - \vec{S}_2 \rangle \sim \vec{D} \times \vec{H}$$
- Uniform magnetization:
  Not parallel to H! $$m_u := \frac{1}{2}\langle \vec{S}_1 + \vec{S}_2 \rangle \sim \left(\vec{D} \times \vec{H}\right) \times \vec{D}$$

Characterise the phases?

Correlation Matrix

A. J. Beekman, L. Rademaker, and J. van Wezel, SciPost Phys. Lect. Notes 11 (2019).

Order parameter: only in the thermodynamic limit! $\langle \mathcal{O} \rangle = \lim_{h\to 0} \lim_{N\to\infty} \langle \psi_0(h,N) | \mathcal{O} | \psi_0(h,N) \rangle$,

Finite systems? Correlation matrix $C(x,x') = \langle \psi | \mathcal{O}^\dagger(x) \mathcal{O}(x') | \psi \rangle$

Main properties:

$$\lim_{|x-x'|\to\infty} C(x,x') \propto \begin{cases} \langle \mathcal{O}^\dagger(x) \rangle \langle \mathcal{O}(x') \rangle = const. & \text{long-range ordered} \\ e^{-|x-x'|/l} & \text{disordered}, \end{cases}$$

Example: $\langle \psi | S_j^+ | \psi \rangle = 0$ (for finite systems), but $C_{ij} = \langle \psi | S_i^+ S_j^- | \psi \rangle$ can be finite!

Eigenvalues, eigenvectors:

$$C_{ij} = \sum_\nu \mathbf{v}_\nu \underbrace{\left\langle \psi \left| \left(\sum_i v_{\nu,i}^* S_i^+ \right) \left(\sum_i v_{\nu,j} S_j^- \right) \right| \psi \right\rangle}_{\lambda_\nu} \mathbf{v}_\nu^\dagger$$

If one eigenvalue much larger than the others: $\lim_{|i-j|\to\infty} C_{ij} \approx \lambda_L v_{L,i} v_{L,j}^*$

$$\Rightarrow \lim_{|i-j|\to\infty} C_{ij} = \lim_{|i-j|\to\infty} \sum_\nu v_{\nu,i} \underbrace{\left\langle \psi \left| \sum_k v_{\nu,k}^* S_k^+ \right| \psi \right\rangle}_{\sqrt{\lambda_\nu}^*} \underbrace{\left\langle \psi \left| \sum_l v_{\nu,l} S_l^- \right| \psi \right\rangle}_{\sqrt{\lambda_\nu}} v_{\nu,j}^\dagger = \lim_{|i-j|\to\infty} \langle S_i^+ \rangle \langle S_j^- \rangle$$

Characterise the phases?

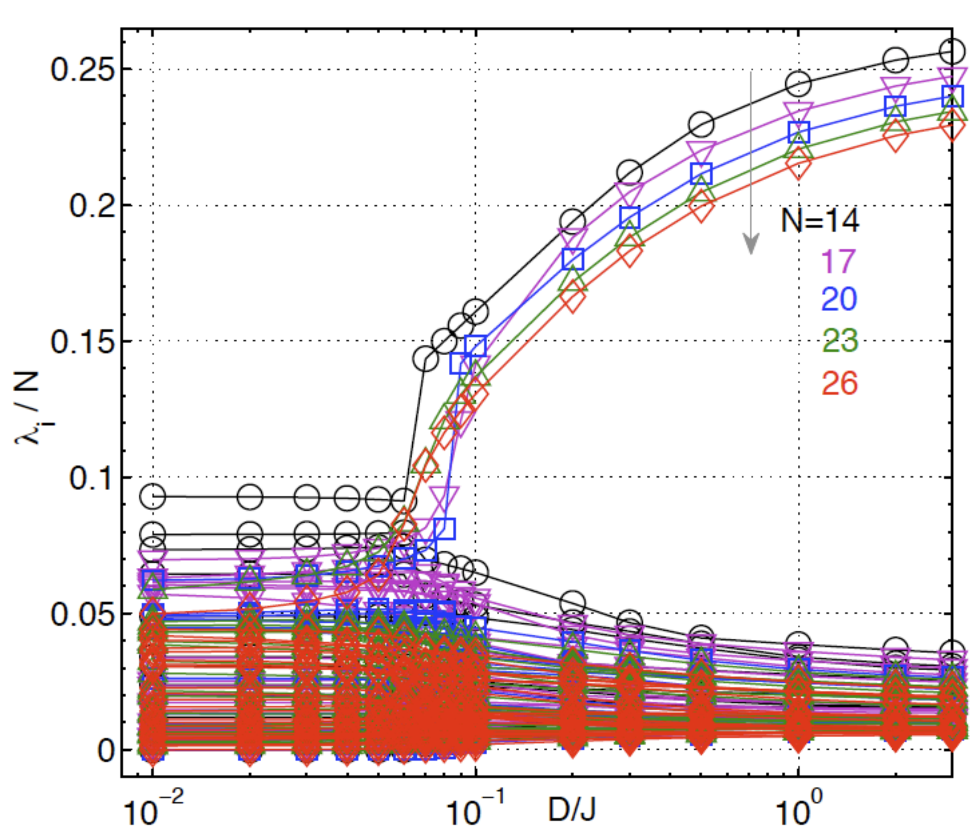
Correlation Matrix

Correlation matrix:

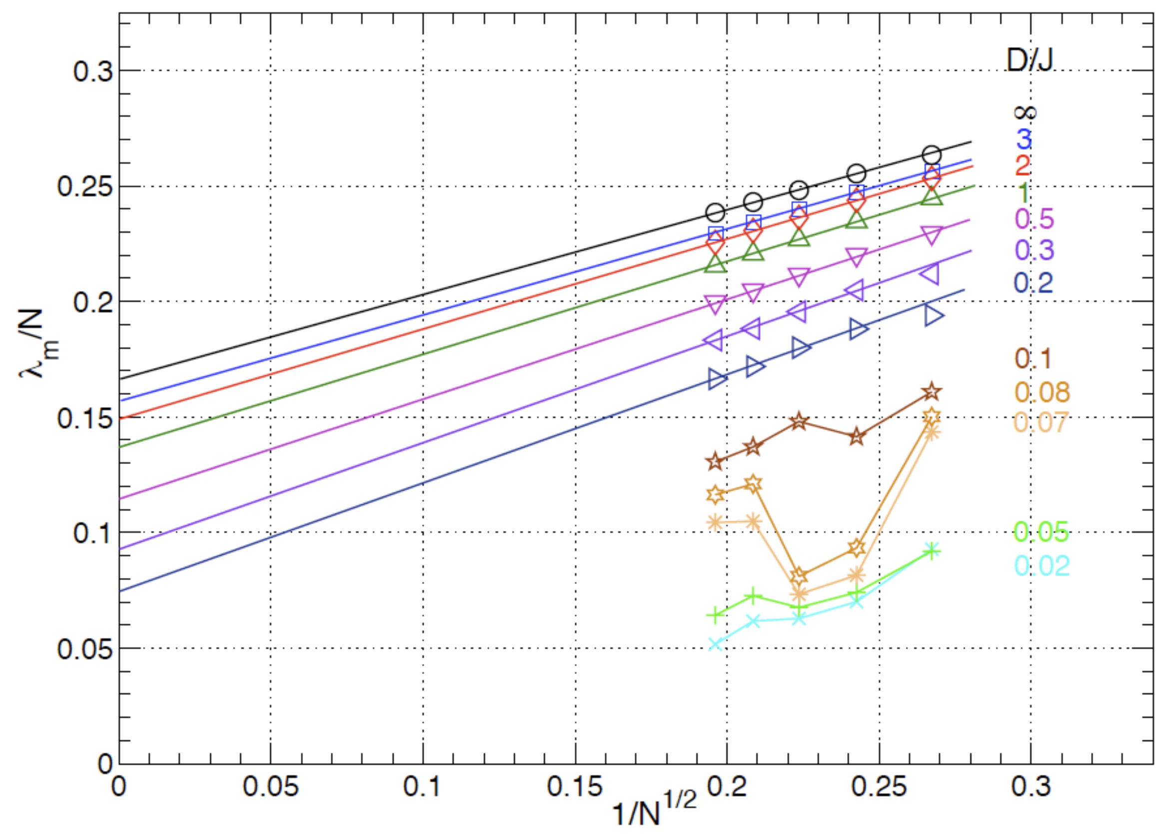
$$C_{i,j} := \langle\Psi_0|s_i^+ s_j^-|\Psi_0\rangle$$

- Dominant eigenstate analogous to condensate wave function in superfluids - natural orbital
- Value of local magnetizations given by $\langle s_j^+\rangle = \langle s_j^x\rangle + i\langle s_j^y\rangle = \sqrt{\lambda_m} v_m(j)$

Eigenvalues in dependence of D:

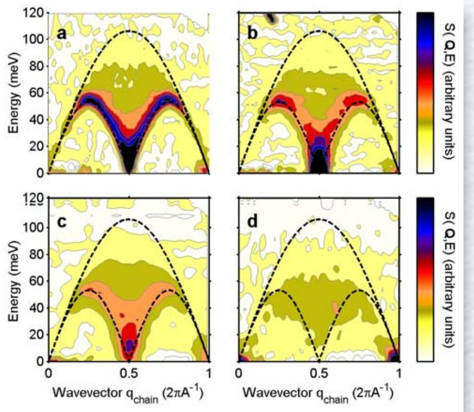


Finite size extrapolation of λ_m:



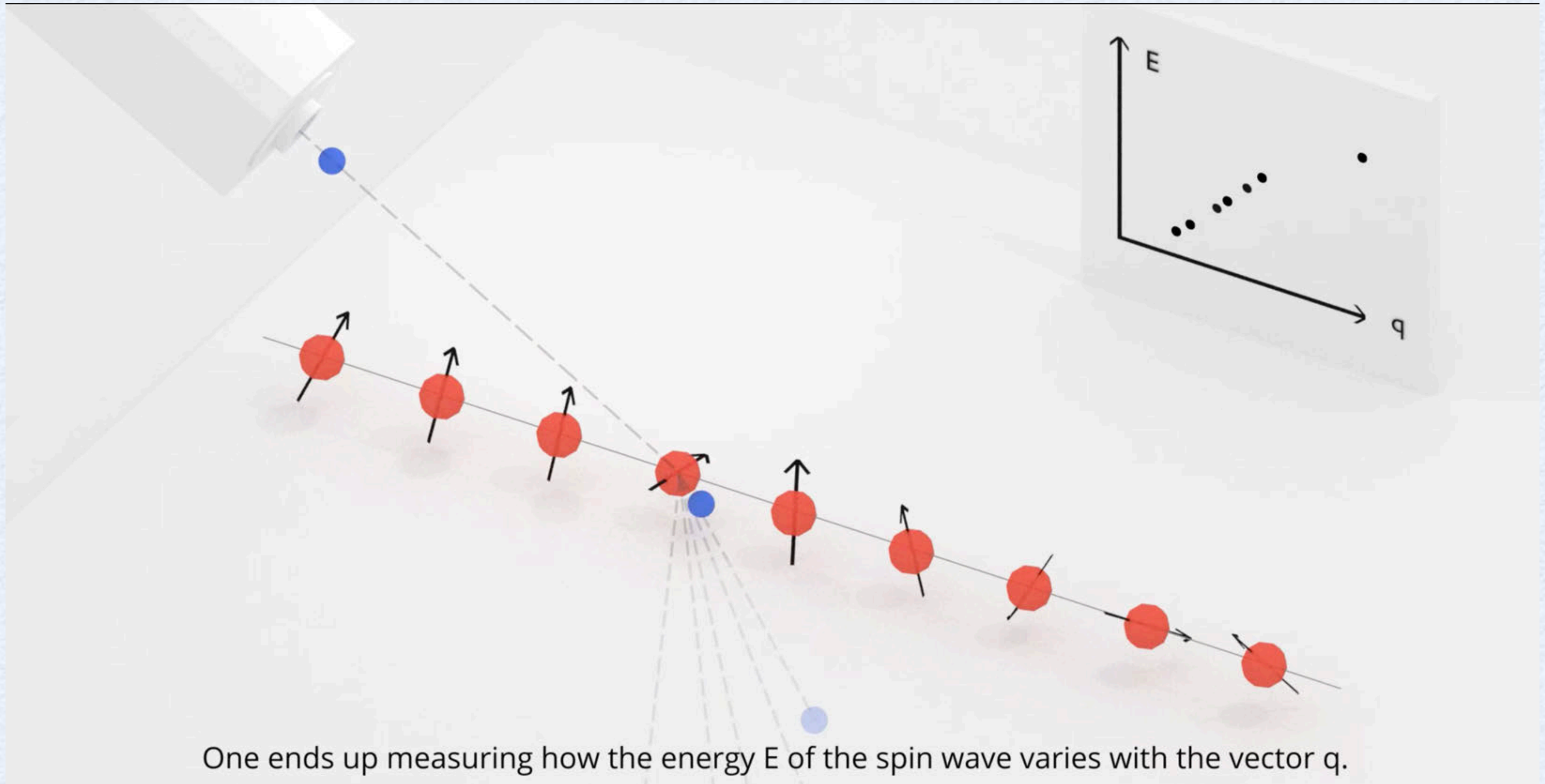
▹ Ordered phase for D/J > 0.1, non-ordered phase for D/J < 0.1

Part V: Dynamics
Structure Factors and Nonequilibrium Behaviour

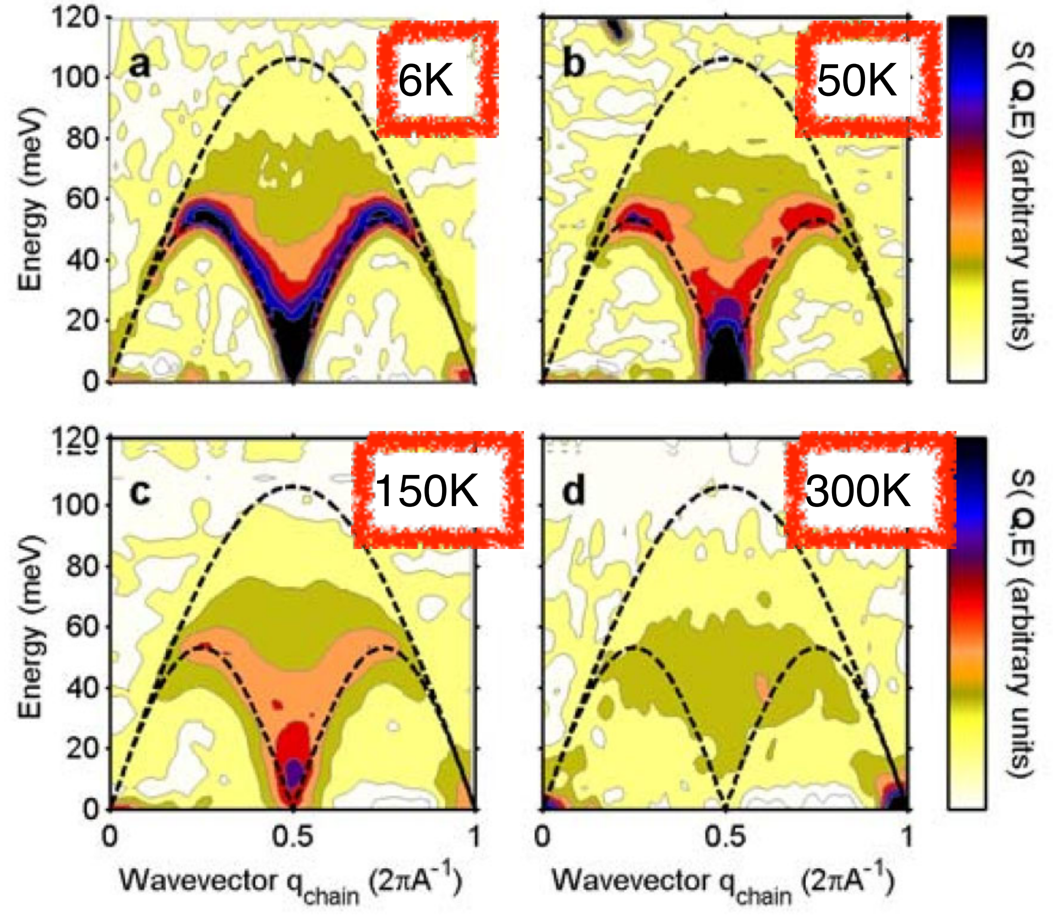


[B. Lake *et al.*, Nat. Mat. 4 (2005) 329]

Inelastic Neutron Scattering:
Dynamical Structure Factors



[Movie on Wikipedia: https://w.wiki/BCgs]



[B. Lake *et al.*, Nat. Mat. 4 (2005) 329]

⟶ Explore elementary excitations of the system

Salvatore R. Manmana

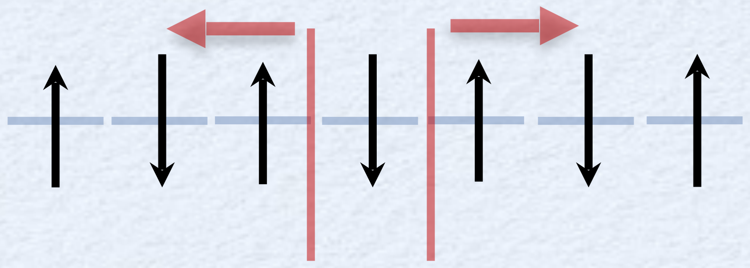
Linear Response:

Spectral Functions at Finite Field

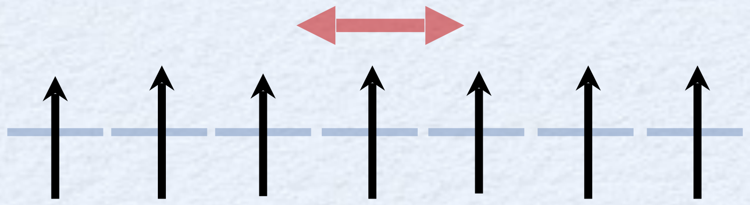
Dynamical structure factor $S^z(k,\omega)$ of a S-1/2 Heisenberg chain when changing an external magnetic field:

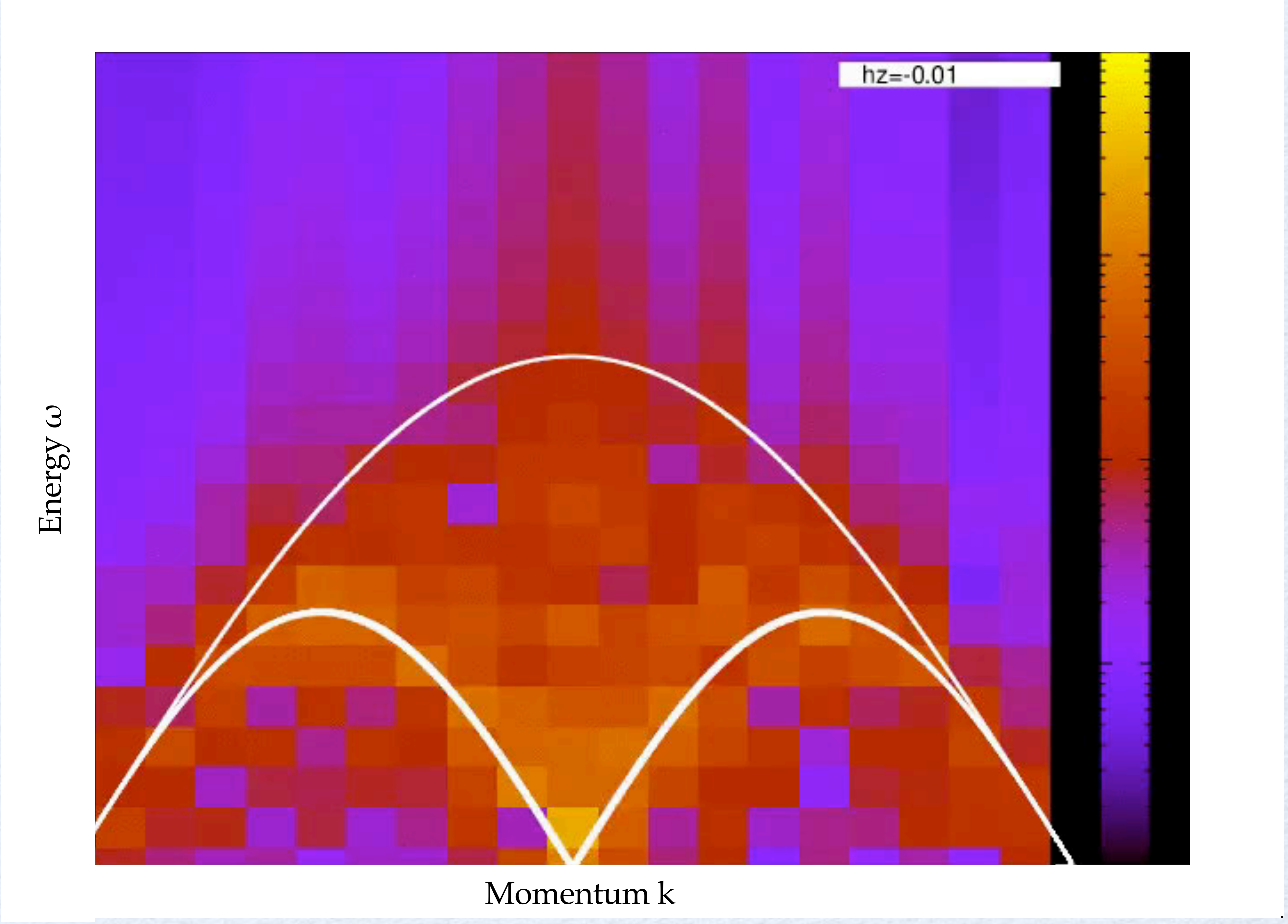
$$\mathcal{H} = J\sum_i \vec{S}_i \cdot \vec{S}_{i+1} - B\sum_i S_i^z$$

small B: spinons



large B: magnons



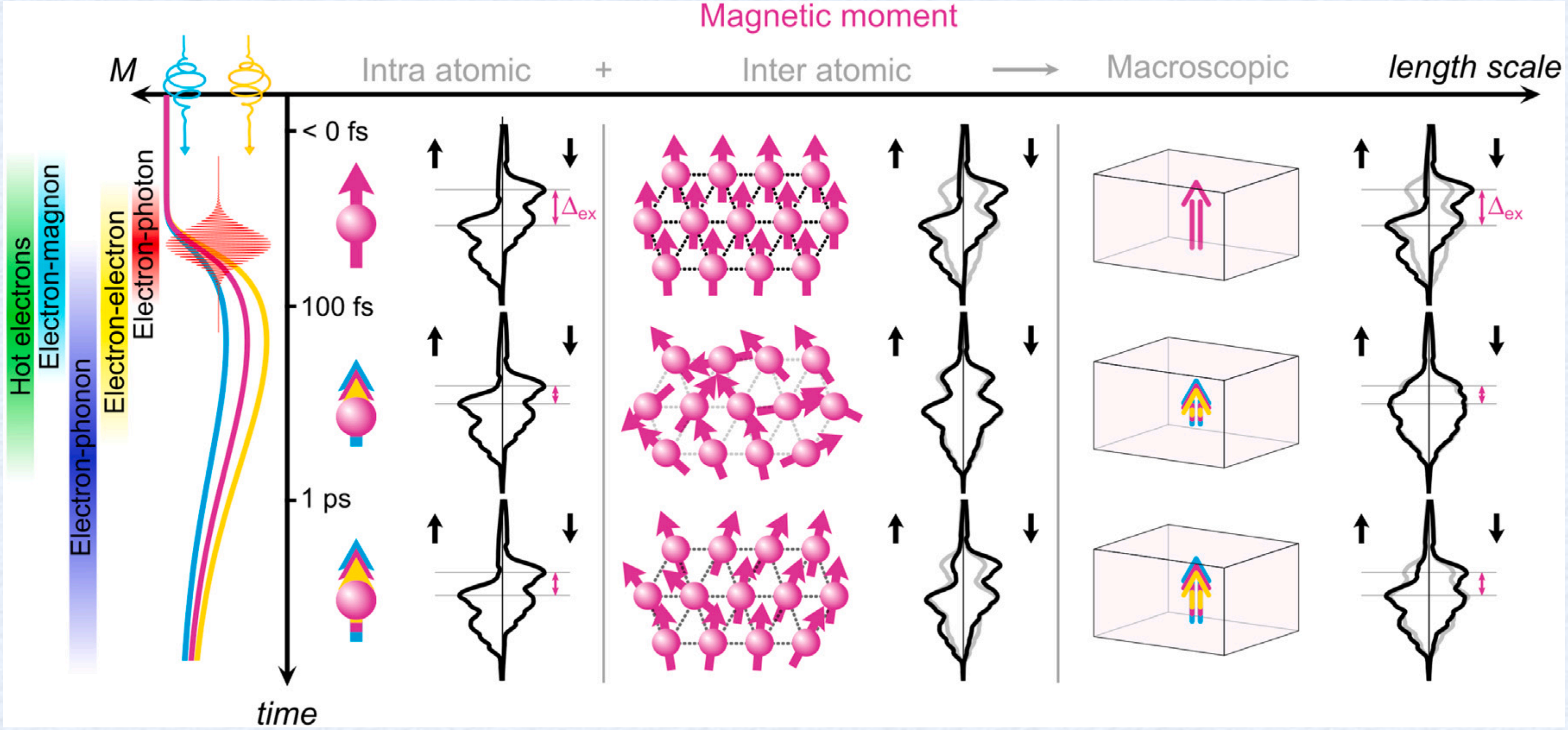


[T. Köhler, Master thesis, U. Göttingen 2013]

Transient states out-of-equilibrium:
Can we change the magnetisation by photo excitation?

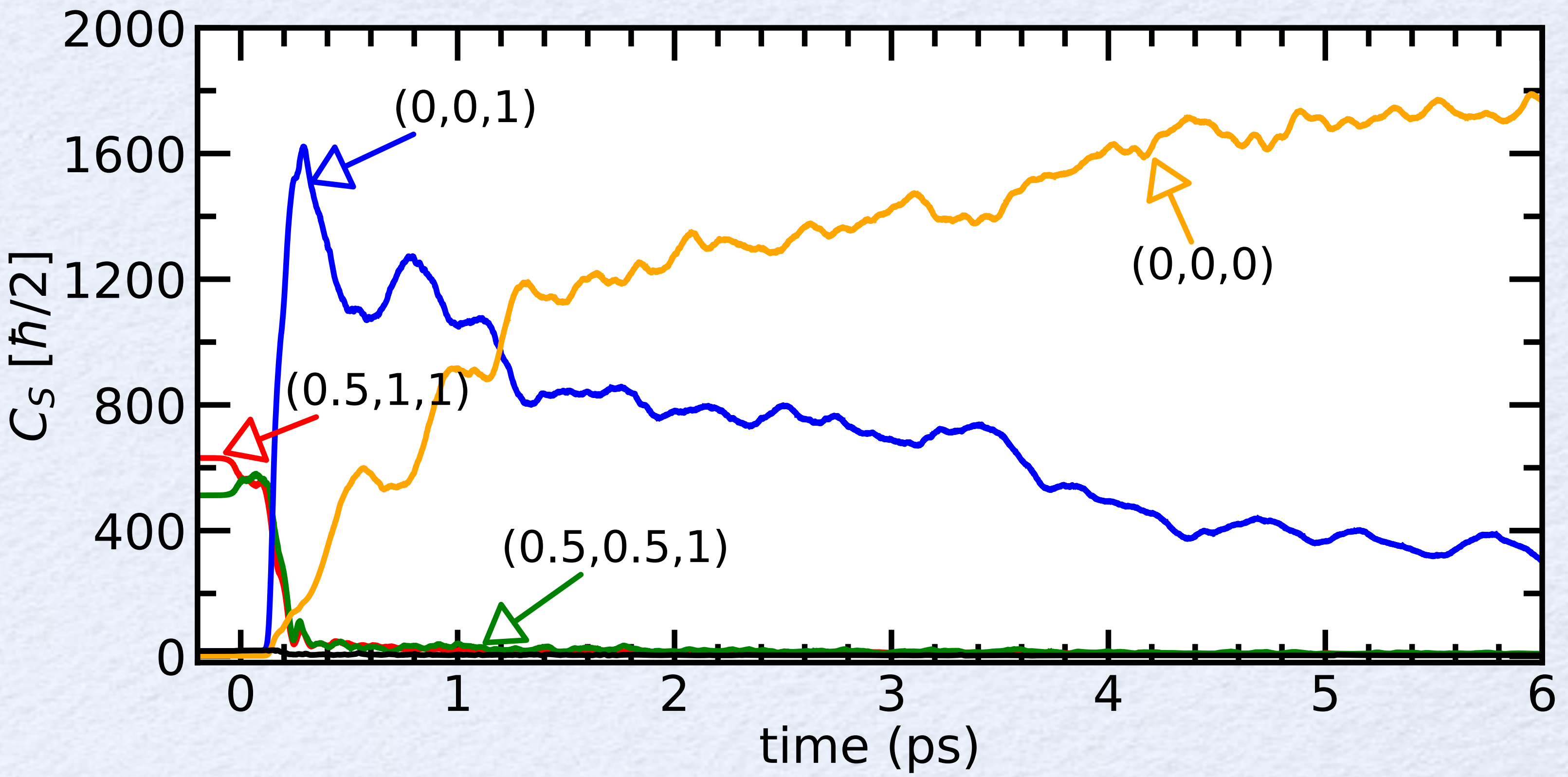
Typical setup: pump-probe experiments (on fs/ps/ns time scales)

Demagnetisation dynamics



[P. Scheid, Q. Remy, S. Lebègue, G. Malinowski, and S. Mangin, J. of Magn. and Magn. Mat. **560**, 169596 (2022)]

Transient ferromagnetic order in manganites



[S. Rajpurohit, C. Jooss, and P.E. Blöchl, Phys. Rev. B **102**, 014302 (2020)]

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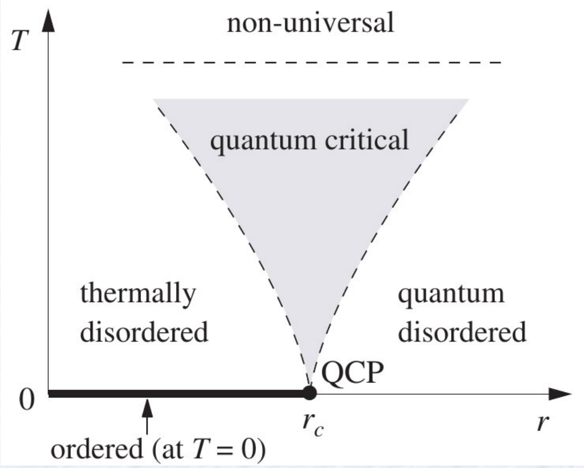
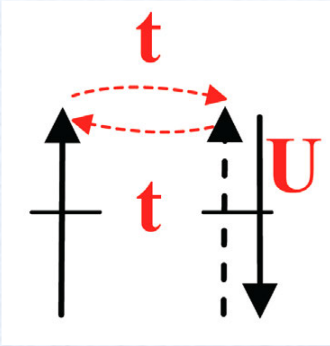
Conclusions & Outlook

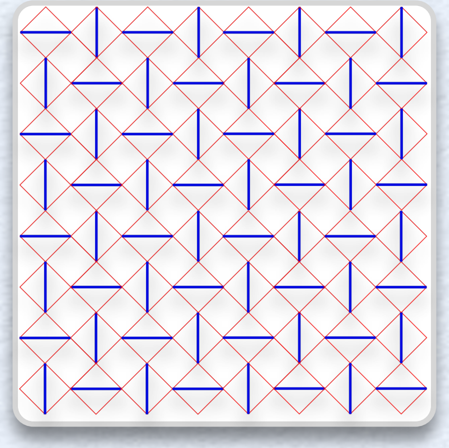
1. Basic properties of Quantum Many-Body Systems



2.Basic properties of Quantum Magnets

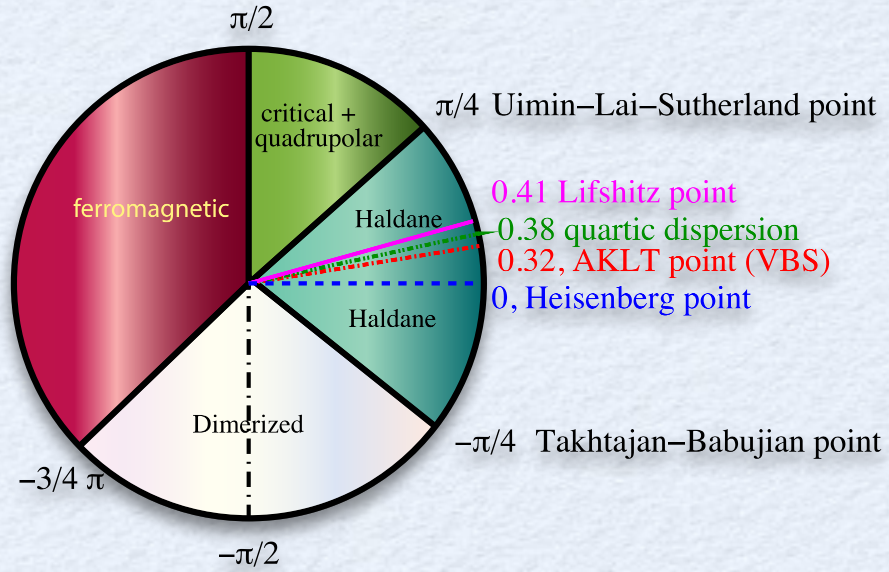


3. Dimer systems in a magnetic field

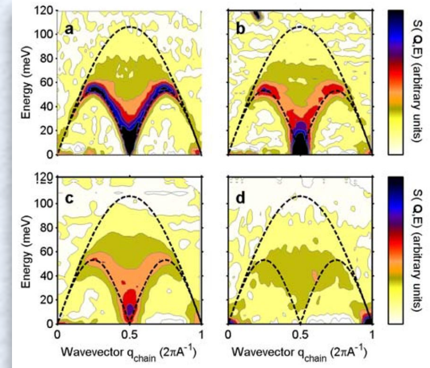


4. Unconventional states of matter: Luttinger liquids, spin nematic states, topological phases

Thank you for your attention!



5. Dynamical sturcture factors and nonequilibrium behavior



[B. Lake *et al.*, Nat. Mat. 4 (2005) 329]

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