Macroscopic entanglement, spin liquids & Kitaev models

Entanglement in Strongly Correlated Systems
Benasque, February 2020

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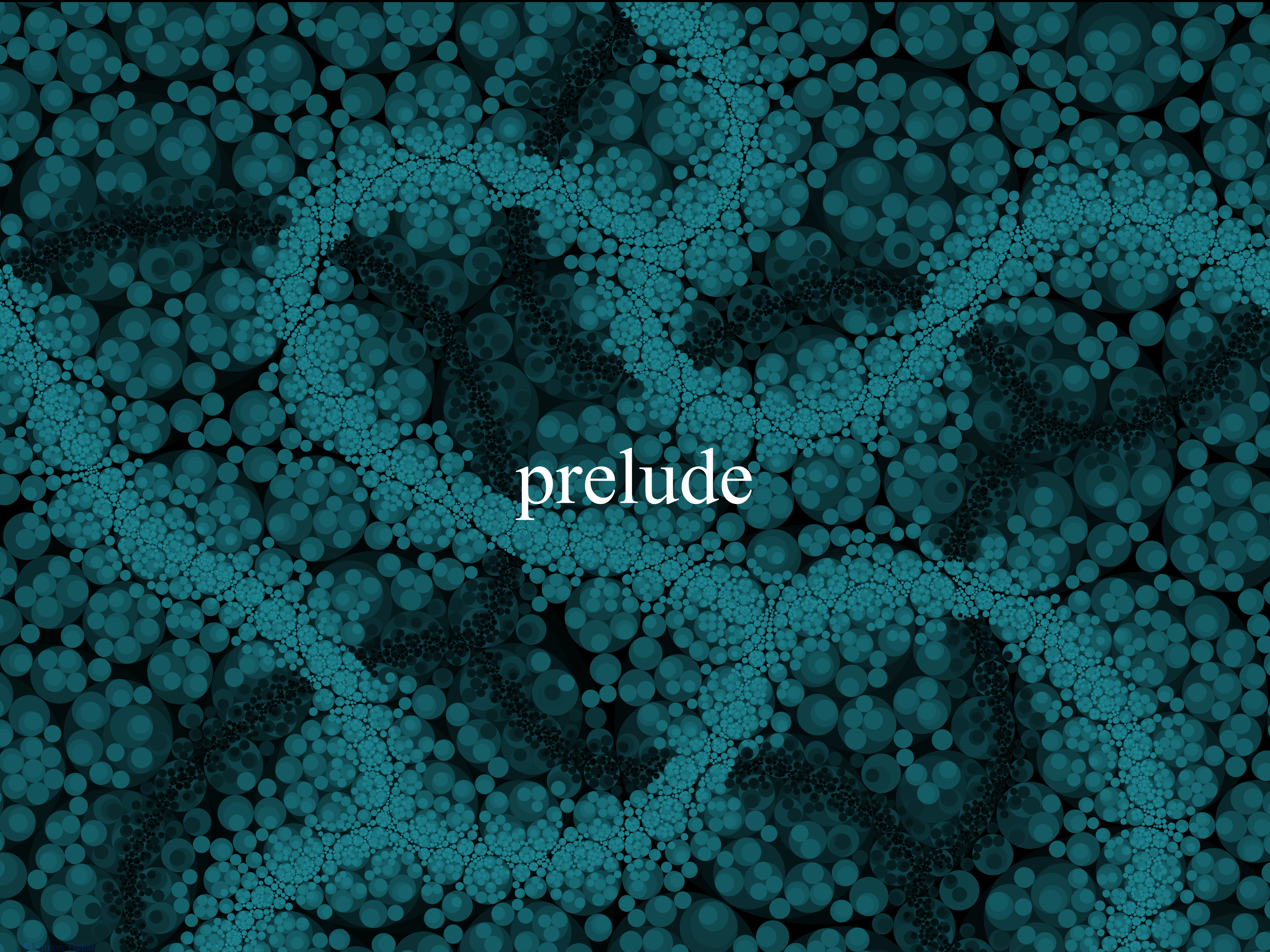
CRC183
ENTANGLED STATES OF MATTER

This week's menu

classical spin liquids

quantum spin liquids

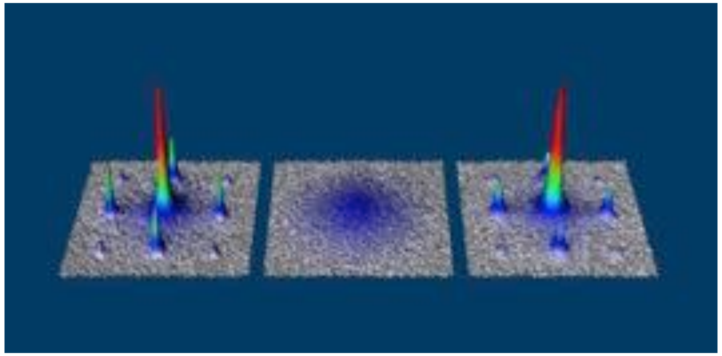
Kitaev materials


prelude

Matter – a collective phenomenon

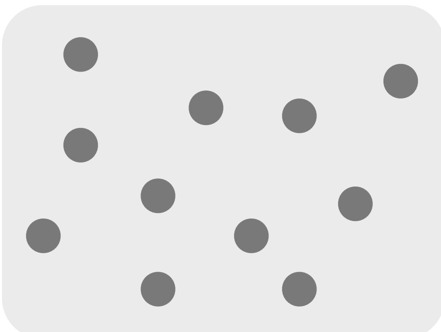
water ice

superconductor



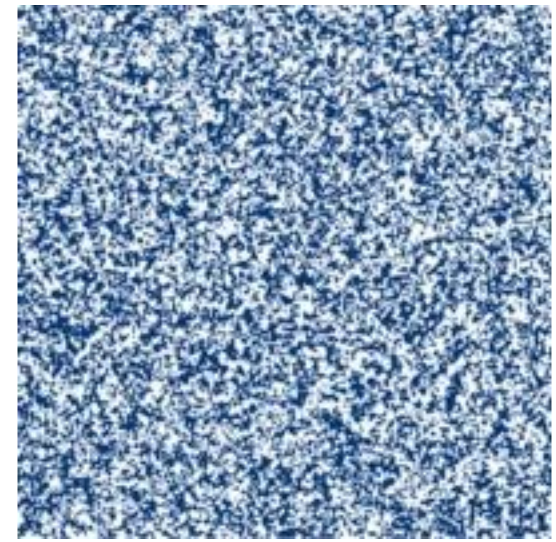
Bose-Einstein condensate

Motivation – a paradigm

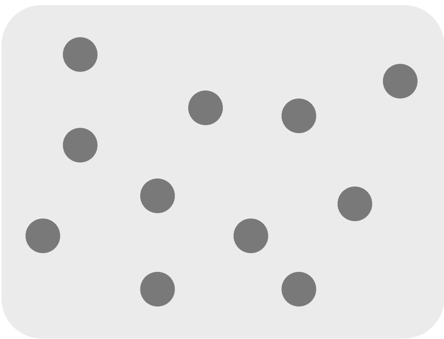


interacting
many-body system

$$\mathcal{H} = -\sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z$$



Motivation – a paradigm



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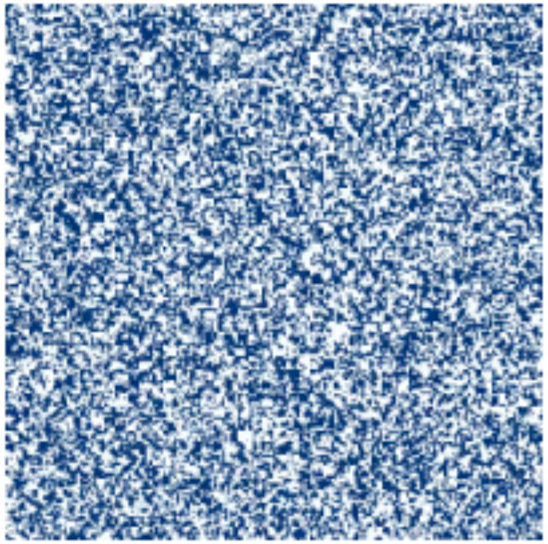
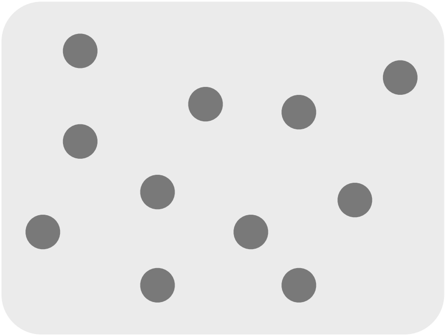


Motivation – a paradigm



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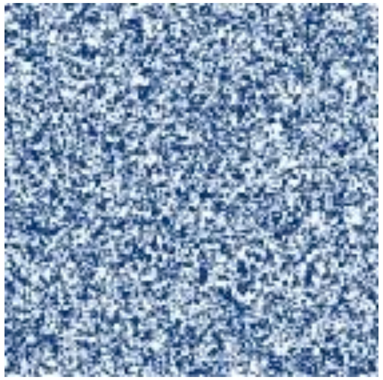
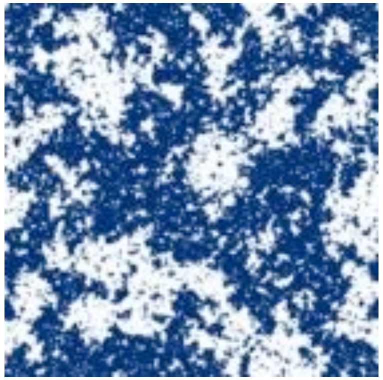
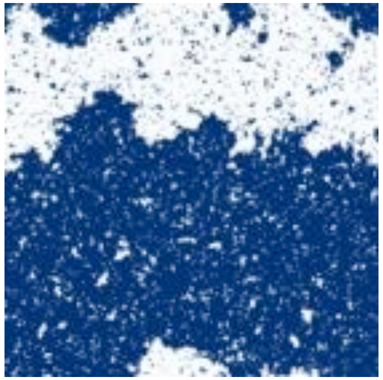




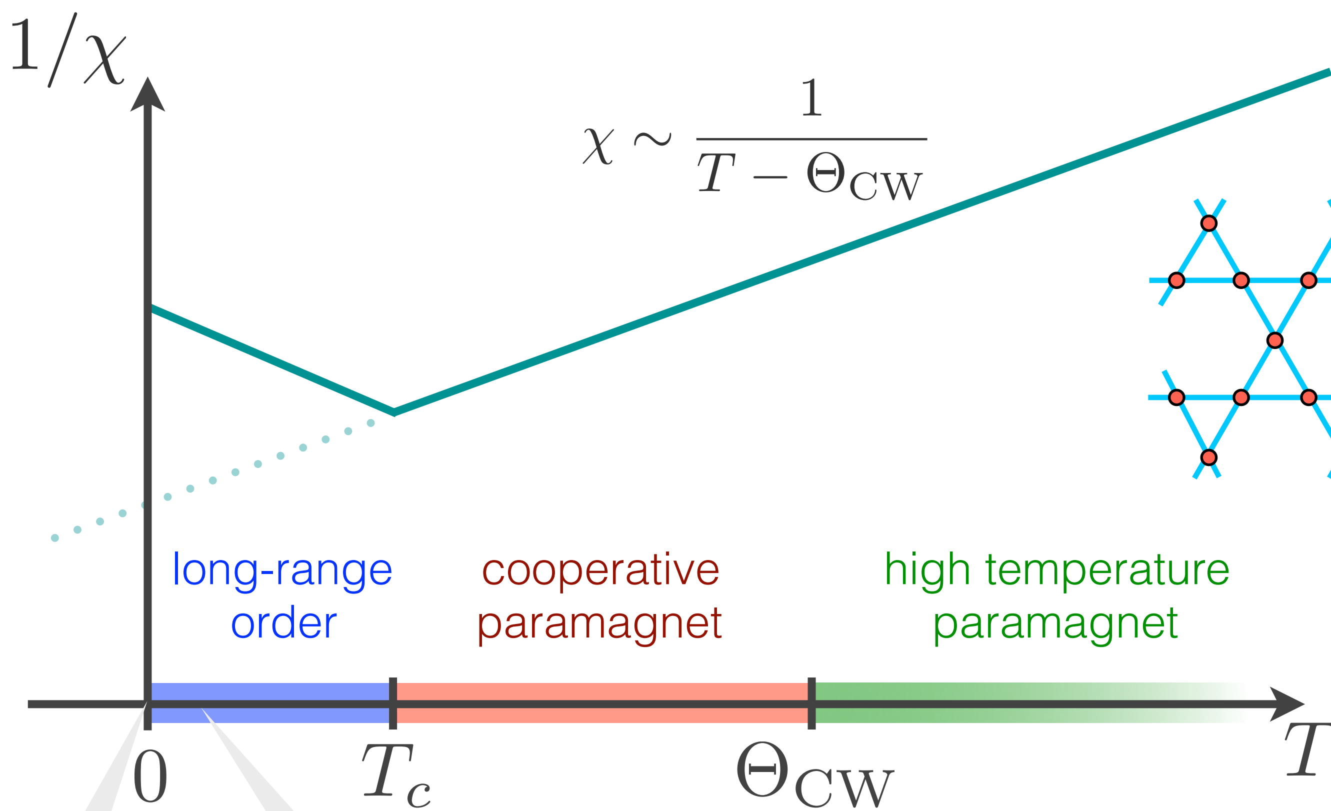


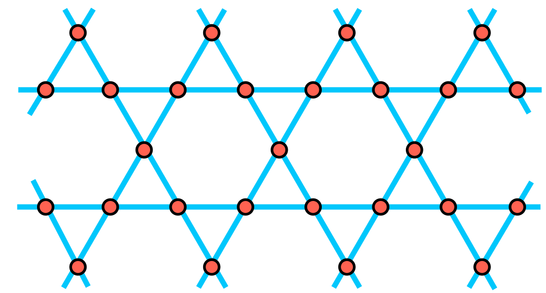
Spontaneous symmetry breaking

- ground state has **less symmetry** than Hamiltonian
- **local** order parameter
- phase transition / **Landau-Ginzburg-Wilson** theory

Beyond the paradigm – frustrated magnets

Insulating magnets with competing interactions.





T=0 residual entropy

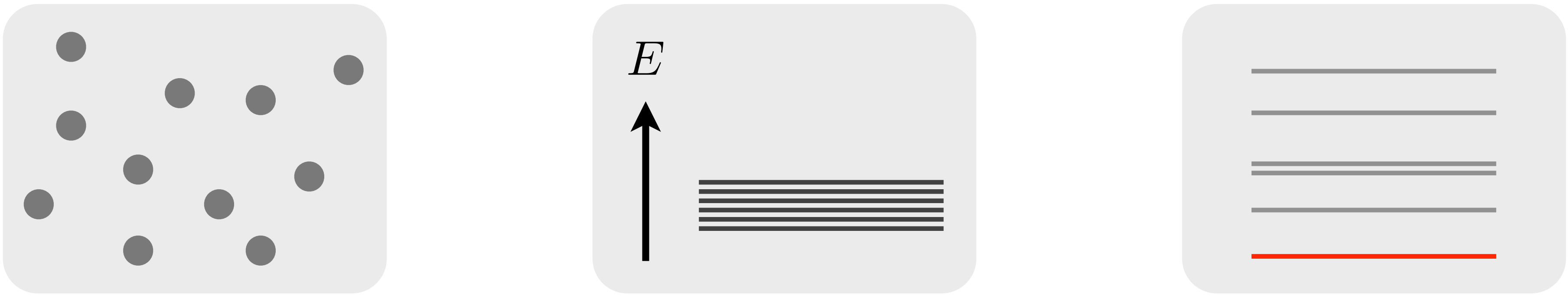
long-range order

How can we quantify ‘frustration’ ?

$$f = \frac{\Theta_{CW}}{T_c}$$

Why we should look for the misfits

Some of the most intriguing phenomena in condensed matter physics arise from the splitting of ‘accidental’ degeneracies.

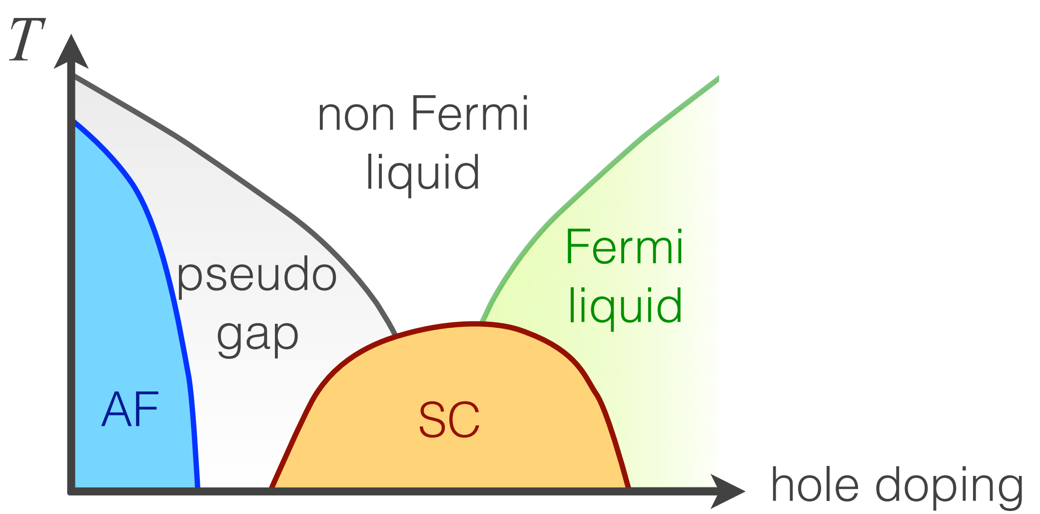


interacting **many-body system**

‘accidental’ **degeneracy**

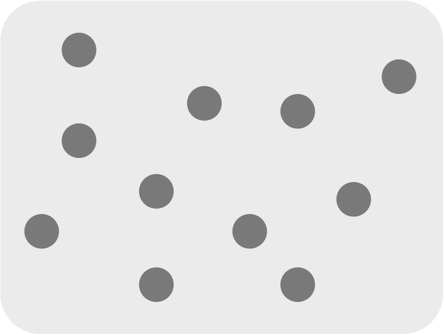
residual effects select ground state

phase diagram of cuprate superconductors

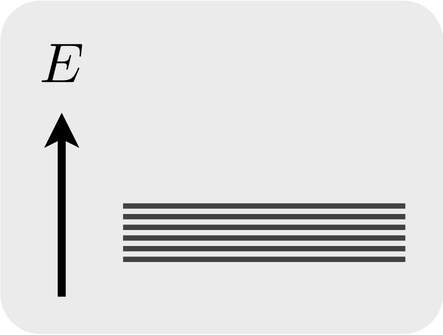


When do interesting things happen?

Some of the most intriguing phenomena in condensed matter physics arise from the splitting of ‘accidental’ degeneracies.



interacting
many-body system



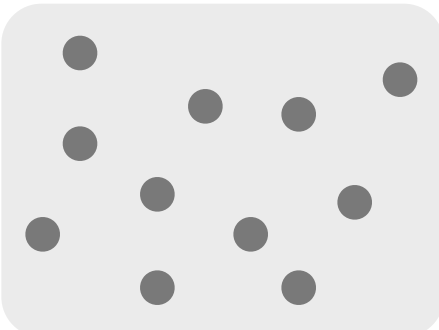
‘accidental’
degeneracy

residual effects
select ground state

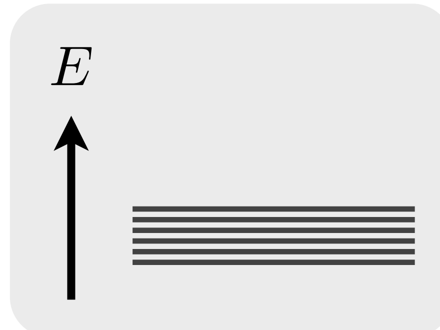
But they are also notoriously difficult to handle, due to

- multiple energy scales
- complex energy landscapes / slow equilibration
- macroscopic entanglement
- strong coupling

Examples in this talk



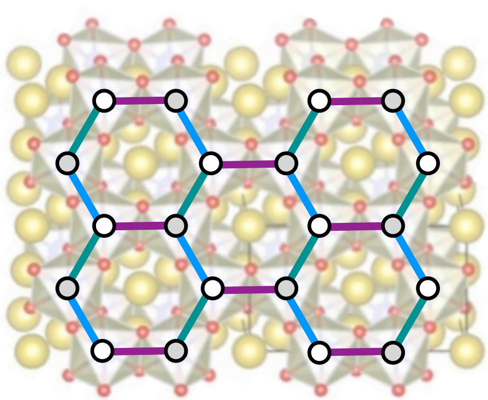
interacting
many-body system



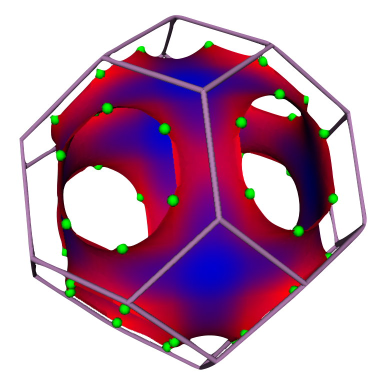
‘accidental’
degeneracy

residual effects
select ground state

classical spin liquids
in layered Iridates



spiral spin liquids
in spinel compounds

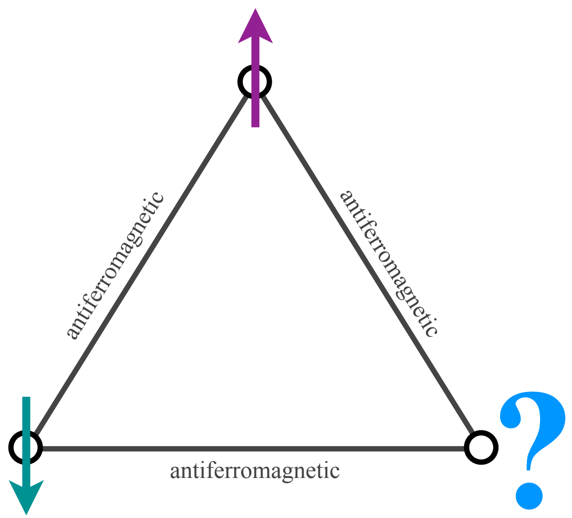


classical spin liquids

– Kitaev model –

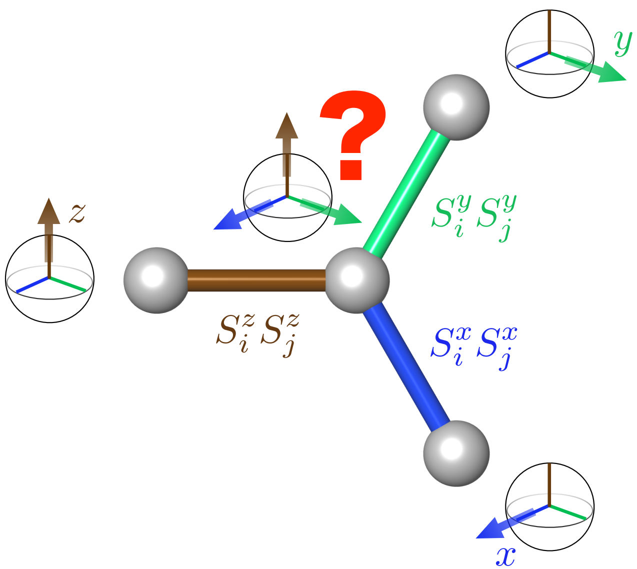
Frustration

Competing interactions lead to frustration.
We will see that frustration can originate interesting spin liquid behavior.



geometric frustration

triangular lattice antiferromagnet
diamond lattice antiferromagnet

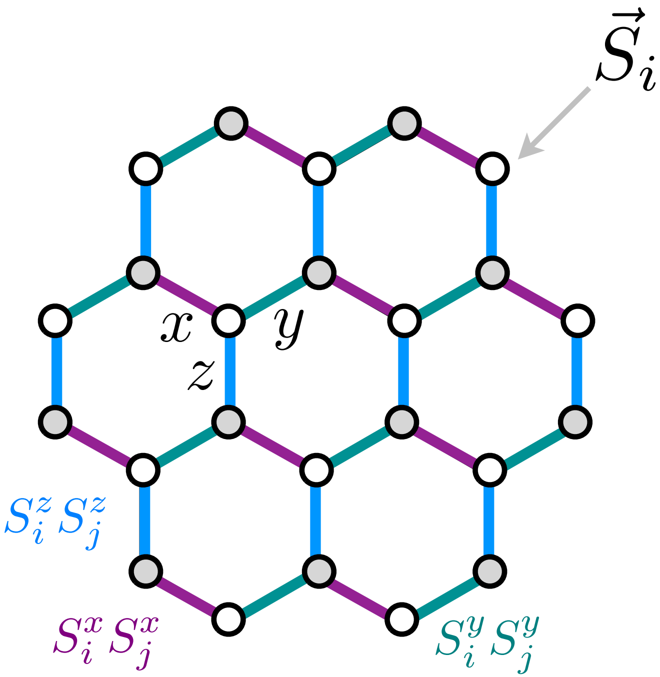


exchange frustration

classical Kitaev model

The Kitaev model

A. Kitaev, Ann. Phys. **321**, 2 (2006)



O(3) Heisenberg spins

$$H_{\text{Kitaev}} = \sum_{\gamma-\text{links}} J_\gamma S_i^\gamma S_j^\gamma$$

Ising-like* interaction

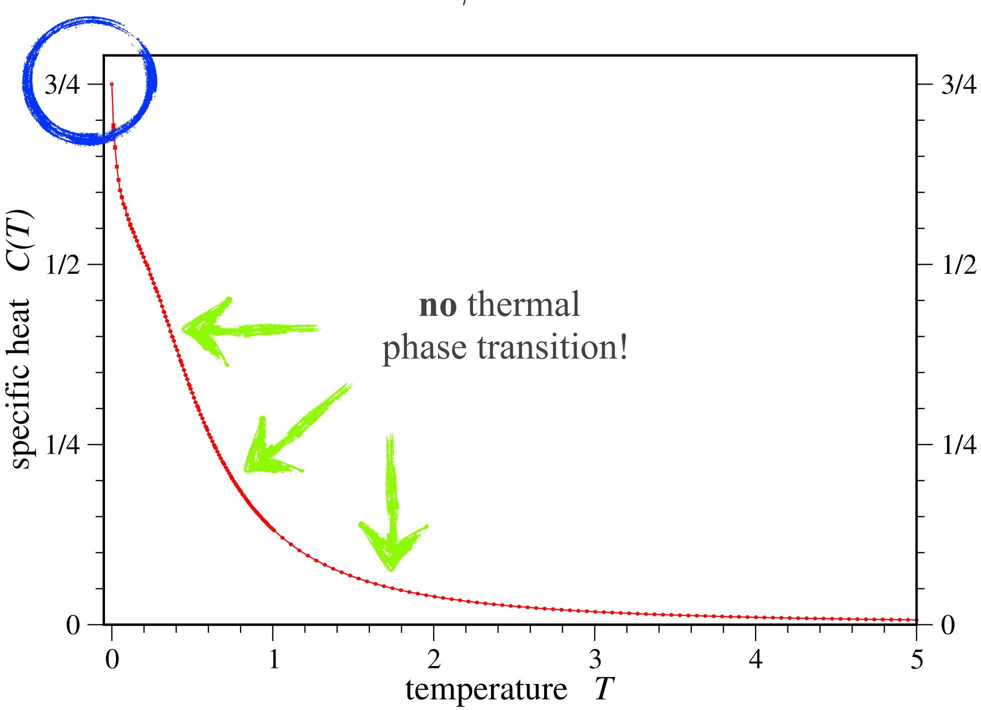
* preferred direction of spin alignment depends on spatial direction of bond

Its quantum mechanical cousin (see also next lecture) is well known for its rare combination of a model of fundamental conceptual importance and an exact analytical solution.

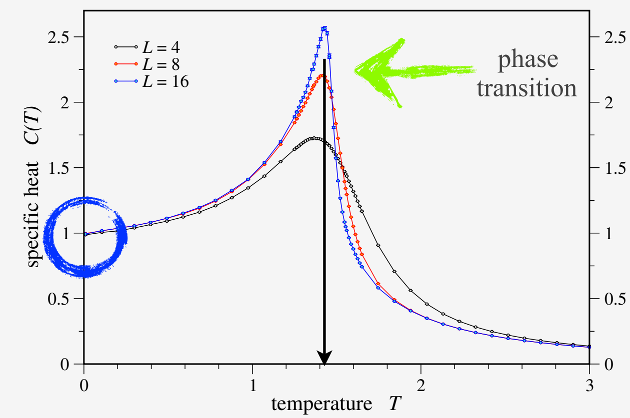
But to a good extent this is also true for the classical model (though much less known).

A first step – numerical simulation

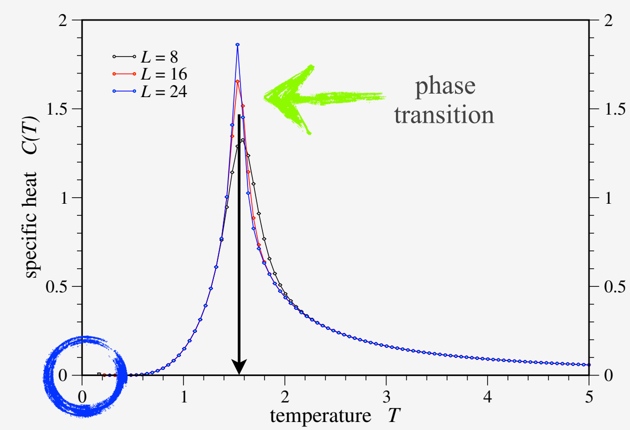
$$H_{\text{Kitaev}} = \sum_{\gamma-\text{links}} J_\gamma S_i^\gamma S_j^\gamma$$



$$H_{\text{Heisenberg}} = \sum_{\gamma-\text{links}} J_\gamma \vec{S}_i \vec{S}_j$$

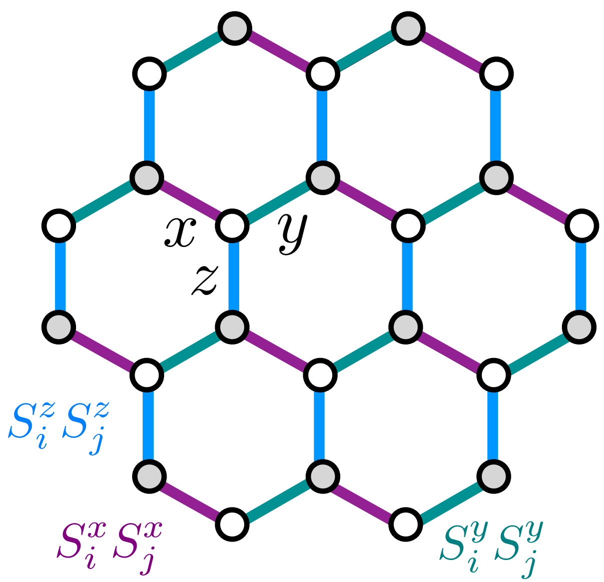


$$H_{\text{Ising}} = \sum_{\gamma-\text{links}} J_\gamma S_i^z S_j^z$$

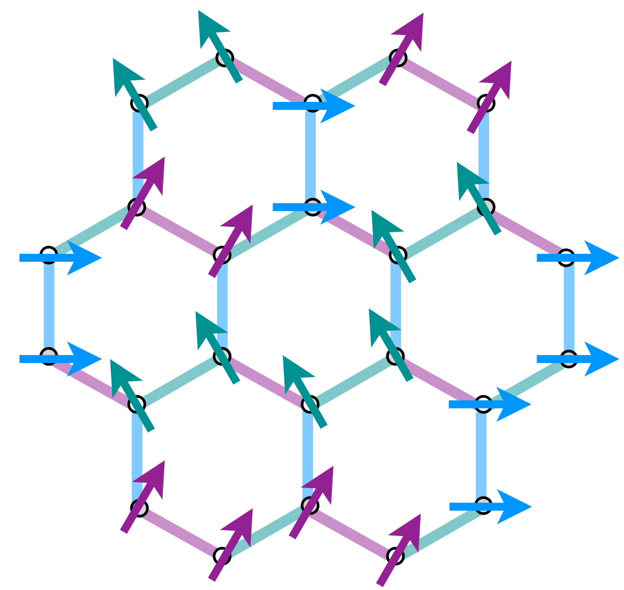


Frustration in the Kitaev model

Observation: no spin configuration can simultaneously satisfy all exchange terms.



T=0 **spin configuration**



$$H_{\text{Kitaev}} = \sum_{\gamma-\text{links}} J_\gamma S_i^\gamma S_j^\gamma$$

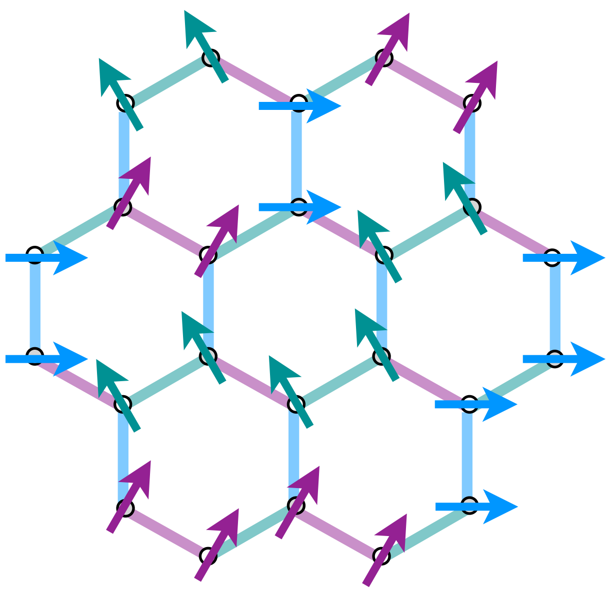
Ising-like* interaction

* preferred direction of spin alignment depends on spatial direction of bond

Every spin can minimize its energy by pointing parallel to precisely one neighbor.

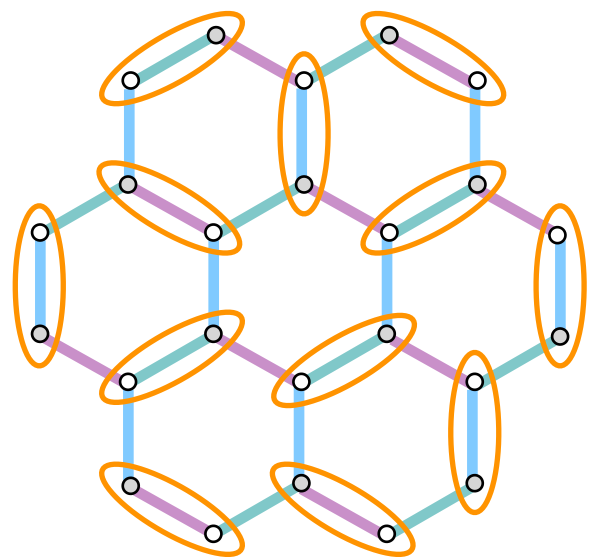
Emergent magnetostatics

T=0 **spin configuration**



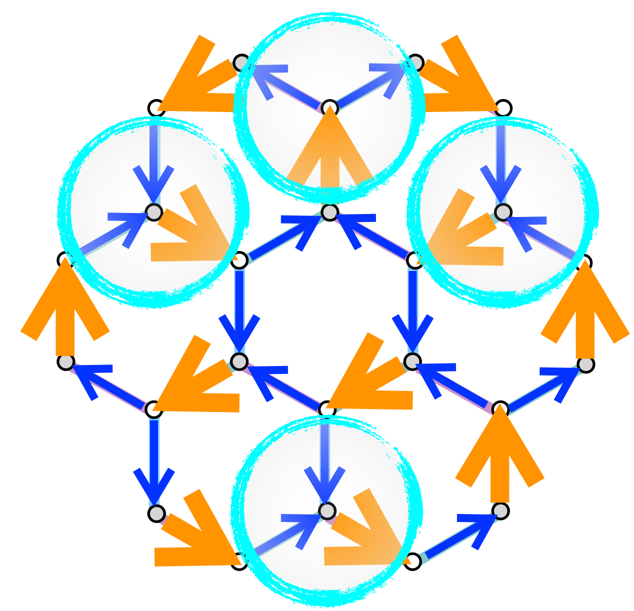
every spin is parallel to *precisely* one neighbor

dimer covering



every site is part of *precisely* one dimer

divergence-free field



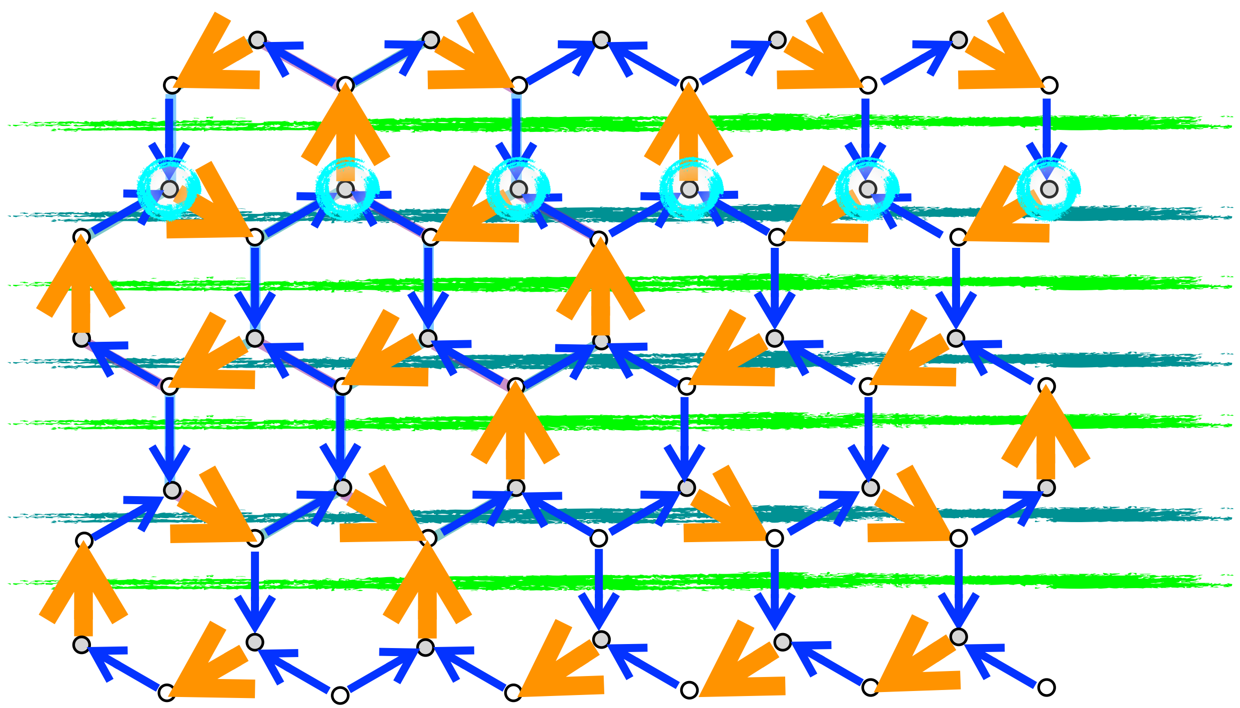
$$\mathrm{div}\ \vec{B} = 0$$

$= \hat{e}_{ij}$

$= -\hat{e}_{ij}/2$

Long-range correlations

divergence-free field



$$\sum_i \vec{b}_i = \vec{M}$$

$$\sum_i \vec{b}_i = -\vec{M}$$

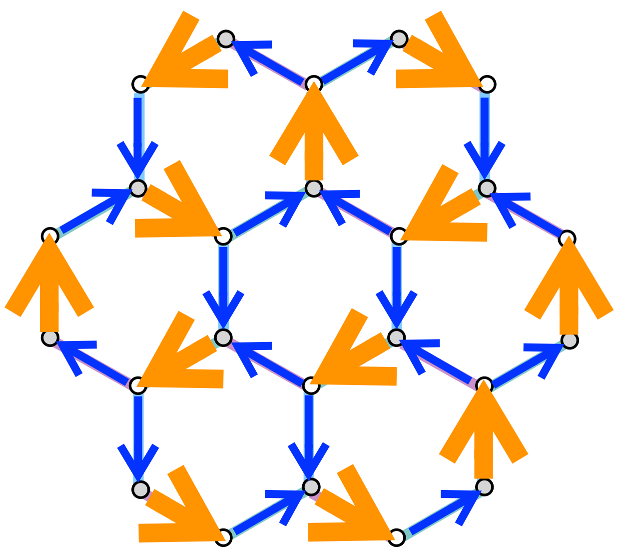
$$\text{div } \vec{B} = 0$$

An immediate consequence from the strictly enforced **local constraint** of a divergence-free field is the emergence of **long-range correlations**.

Emergent magnetostatics – Coulomb phase

look also at D.A. Huse et al., Phys. Rev. Lett. 91, 167004 (2003)

divergence-free field



$$\text{div } \vec{B} = 0$$

orange arrow $= \hat{e}_{ij}$

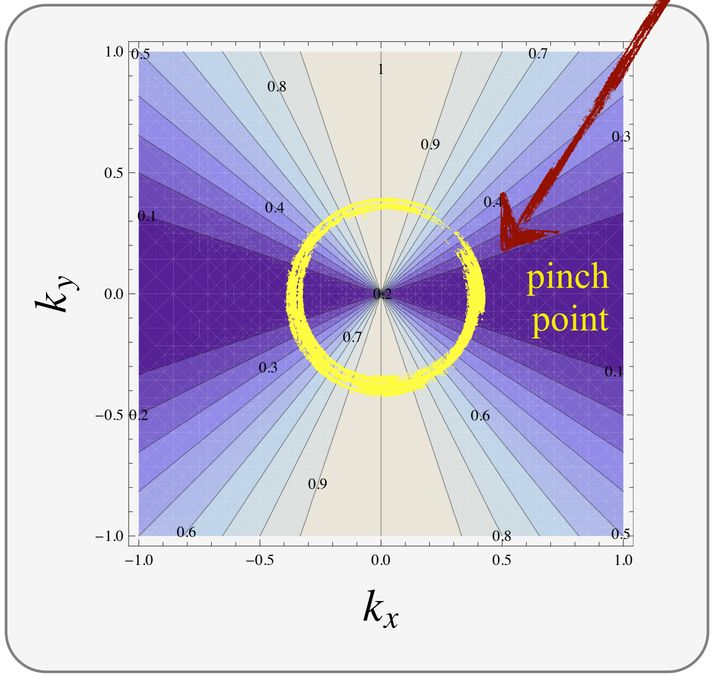
blue arrow $= -\hat{e}_{ij}/2$

dimer-dimer correlations

$$\langle n(\vec{r}) n(0) \rangle \propto \frac{1}{r^2}$$

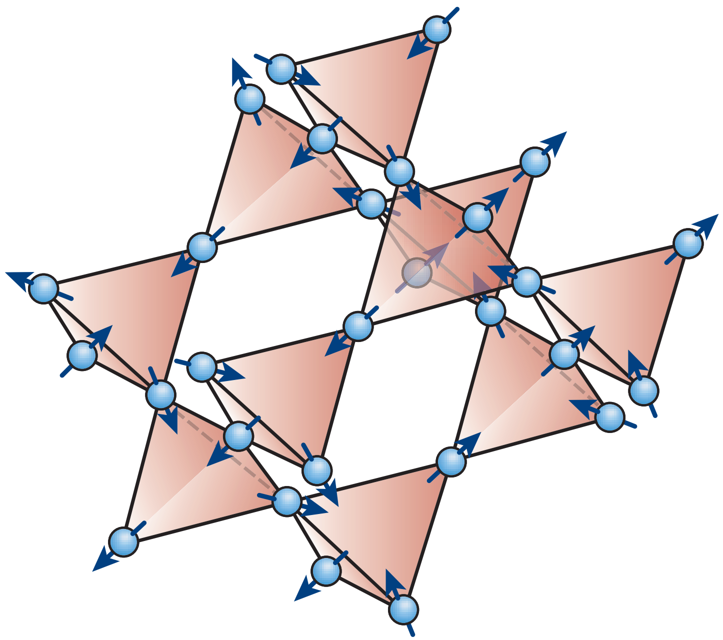
Coulomb phase

... and in Fourier space



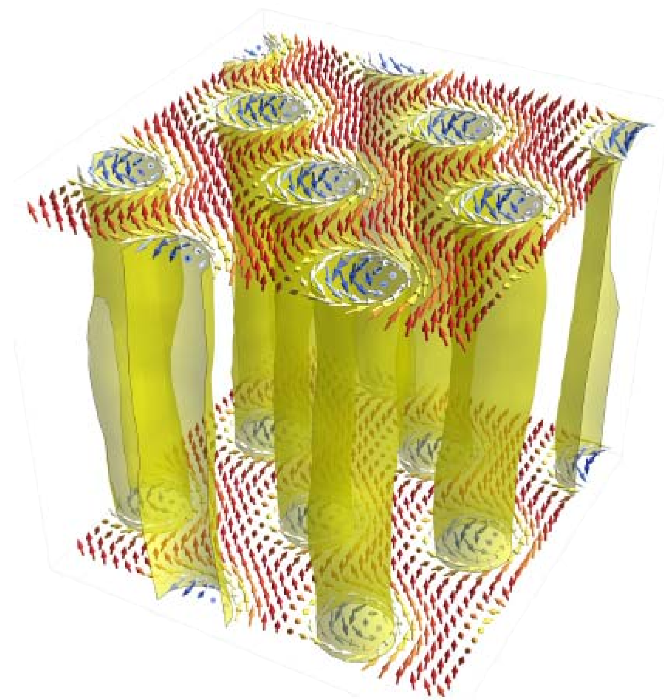
Emergent magnetostatics – Coulomb phase

Such analogies to electromagnetism have also been exploited to discuss the frustrated magnetism in **spin ice** materials and the physics of **skyrmion lattices** in chiral magnets.



spin ice on the pyrochlore lattice

Moessner group
MPI-PKS Dresden

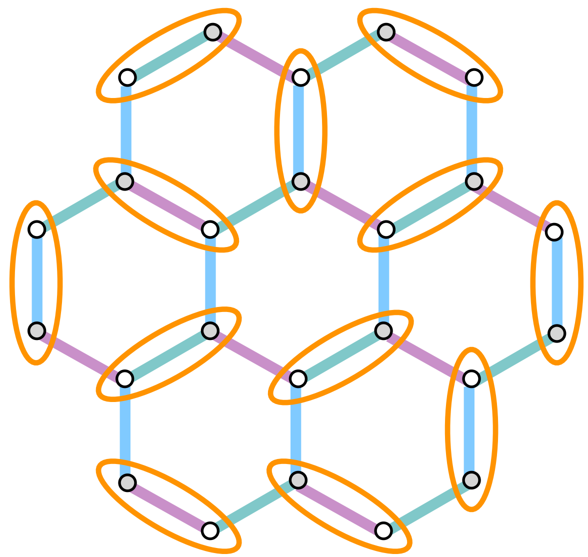


skyrmion lattice in MnSi

Rosch group
University of Cologne

degeneracy – the imprint of frustration

dimer covering



every site is part of *precisely* one dimer

The number of dimer coverings for the hexagonal lattice grows as

$$Z \propto 1.402581^N$$

degeneracy @ $T = 0$

(for periodic boundary conditions)

G.H. Wannier, Phys. Rev. 79, 357 (1950)
P.W. Kasteleyn, J. Math. Phys. 4, 287 (1963)
V. Elser, J. Phys. A: Math. Gen 17, 1509 (1984)

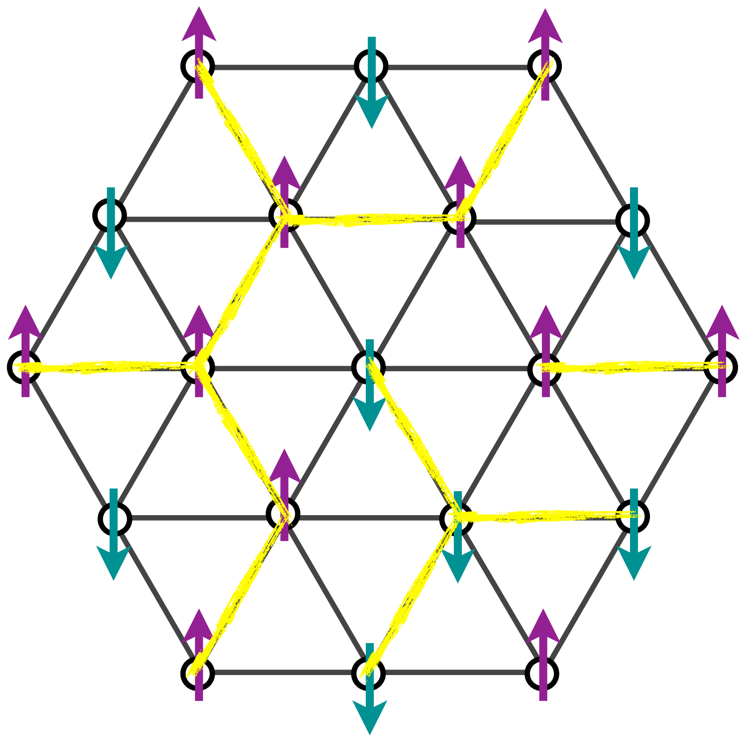
At **finite temperature** this degeneracy will be immediately lifted. Monomer defects are introduced (and screened).

→ screened Coulomb phase

= high-temperature paramagnet

Triangular lattice Ising model

G.H. Wannier, Phys. Rev. 79, 357 (1950)



$$H_{\text{Ising}} = \sum_{\gamma-\text{links}} J_\gamma S_i^z S_j^z$$

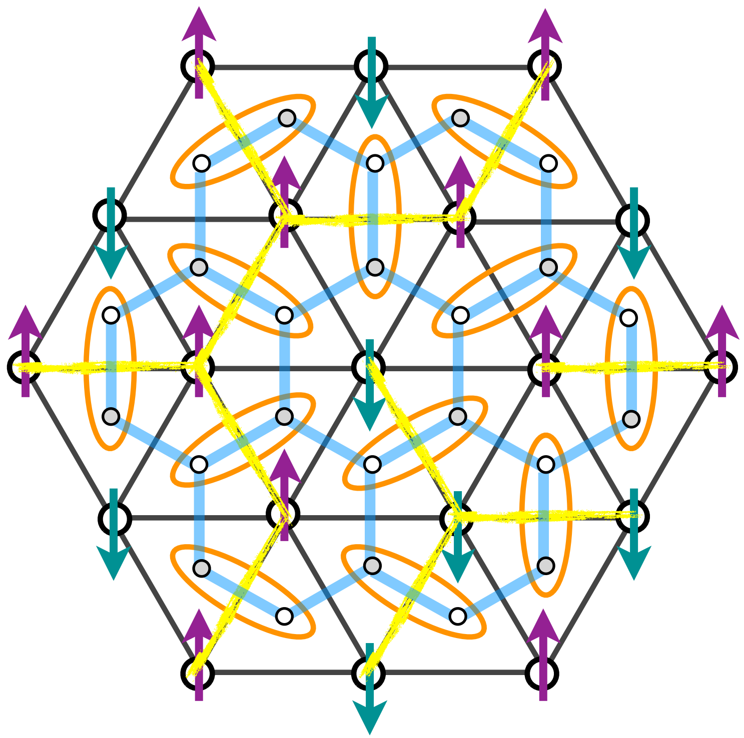
antiferromagnetic

T=0 **spin configuration**

precisely one frustrated bond per triangle

Triangular lattice Ising model

G.H. Wannier, Phys. Rev. 79, 357 (1950)



$$H_{\text{Ising}} = \sum_{\gamma-\text{links}} J_\gamma S_i^z S_j^z$$

antiferromagnetic

T=0 **spin configuration**

precisely one frustrated bond per triangle

T=0 **dual dimer configuration**

precisely one dimer per site on dual honeycomb lattice

→ $Z \propto 1.402581^N$ degenerate spin configurations

→ Coulomb correlations $\langle S^z(\vec{r}) S^z(0) \rangle \propto \frac{1}{r^2}$

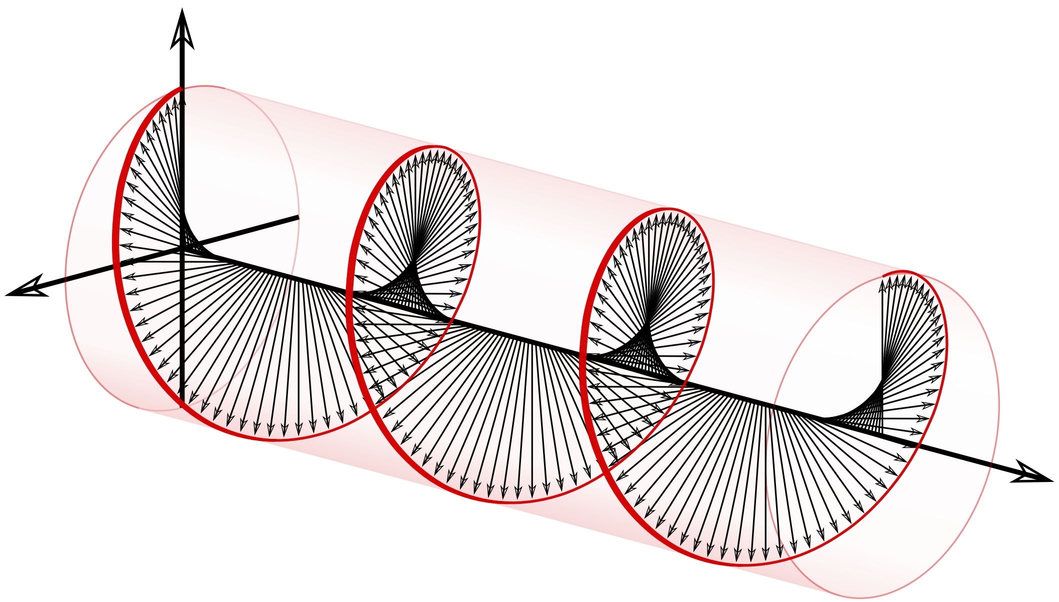
spiral spin liquids

Spin spirals

Coplanar spirals typically arise in the presence of **competing interactions**

Elementary ingredient for

- multiferroics
- spin textures/multi-q states
  - skyrmion lattices
  - Z_2 vortex lattices
- spiral spin liquids



Description in terms of a single wavevector

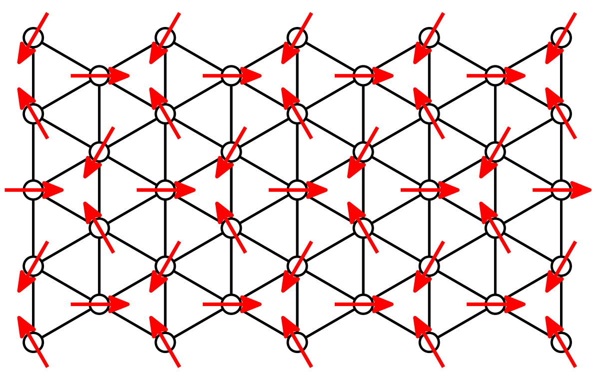
$$\vec{S}(\vec{r}) = \mathrm{Re}\left(\left(\vec{S}_1 + i\vec{S}_2\right) e^{i\vec{q}\vec{r}}\right)$$

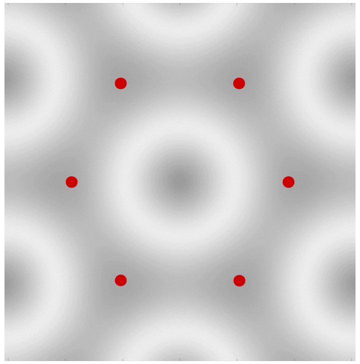
Spin spirals

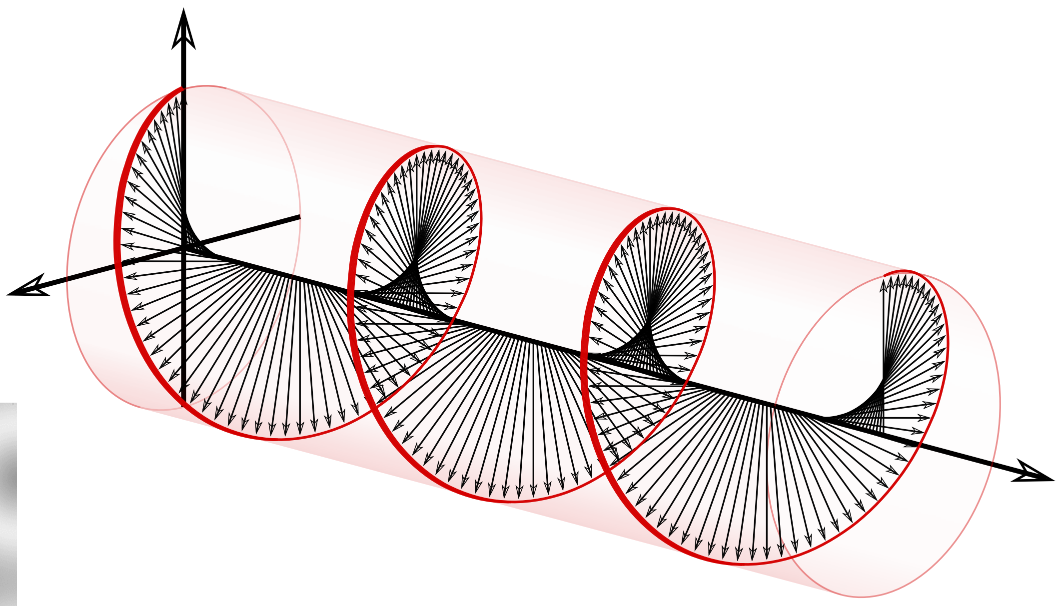
Coplanar spirals typically arise in the presence of **competing interactions**

Familiar example

- **120º order** of Heisenberg AFM on triangular lattice





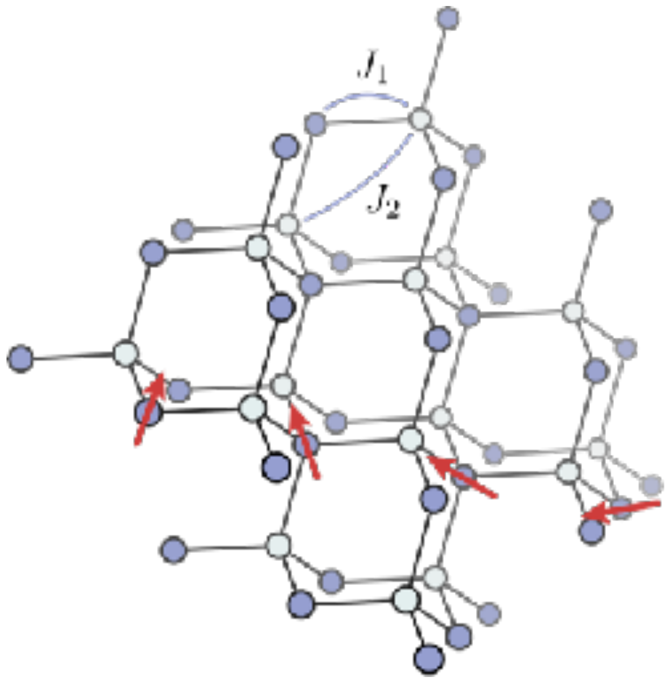


$$\vec{q} = \left(\pm \frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}} \right)$$

$$\vec{S}(\vec{r}) = \mathrm{Re} \left(\left(\vec{S}_1 + i\vec{S}_2 \right) e^{i\vec{q}\vec{r}} \right)$$

Spin spirals

Frustrated diamond lattice antiferromagnets

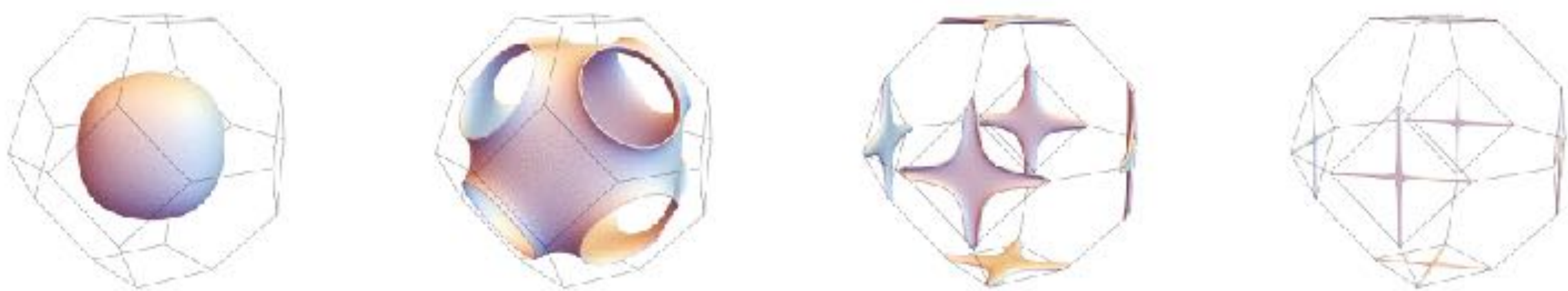


A-site spinels

$MnSc_2S_4$	S=5/2
$FeSc_2S_4$	S=2
$CoAl_2O_4$	S=3/2
$NiRh_2O_4$	S=1

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \vec{S}_j$$

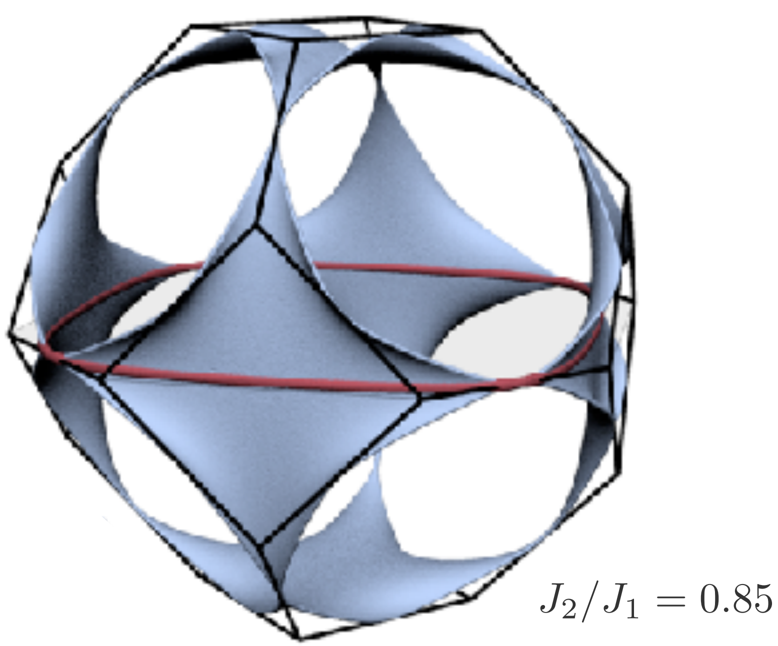
degenerate coplanar spirals form
spin spiral surfaces in *k*-space



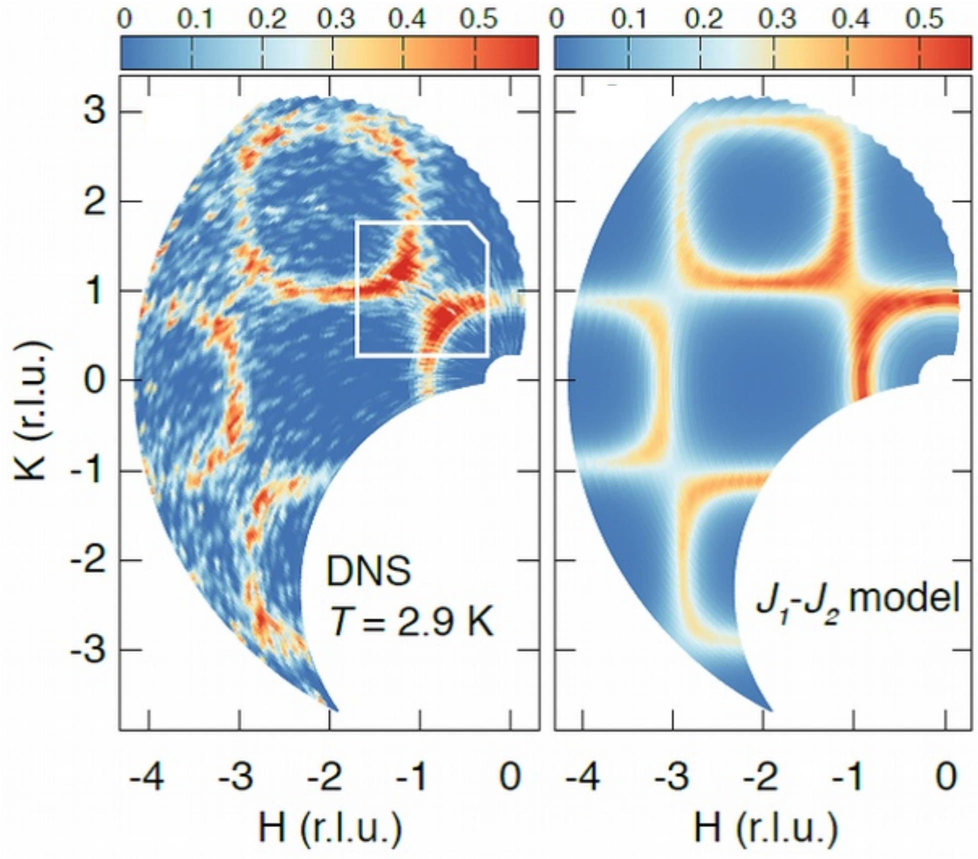
$J_2/J_1 = 0.2$ $J_2/J_1 = 0.4$ $J_2/J_1 = 3$ $J_2/J_1 = 100$

Spin spirals

Experimental observation of spin spiral surface in inelastic neutron scattering of $MnSc_2S_4$.



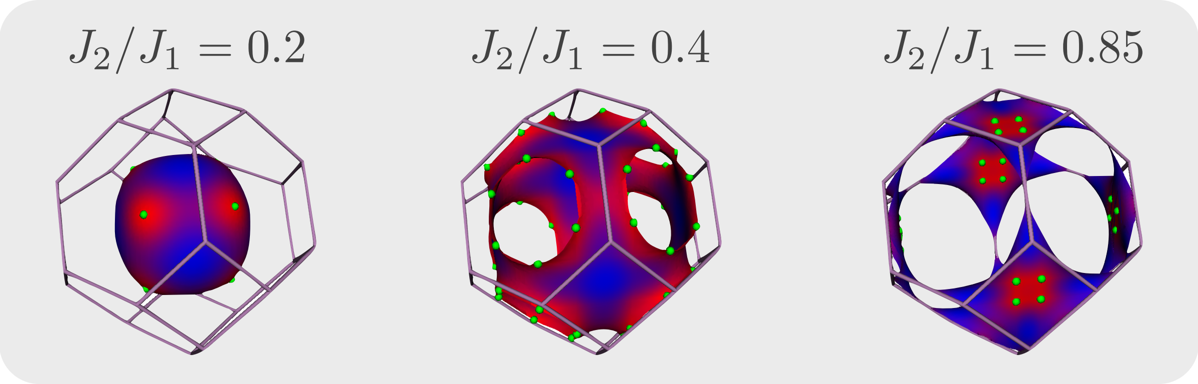
Nature Phys. **3**, 487 (2007)

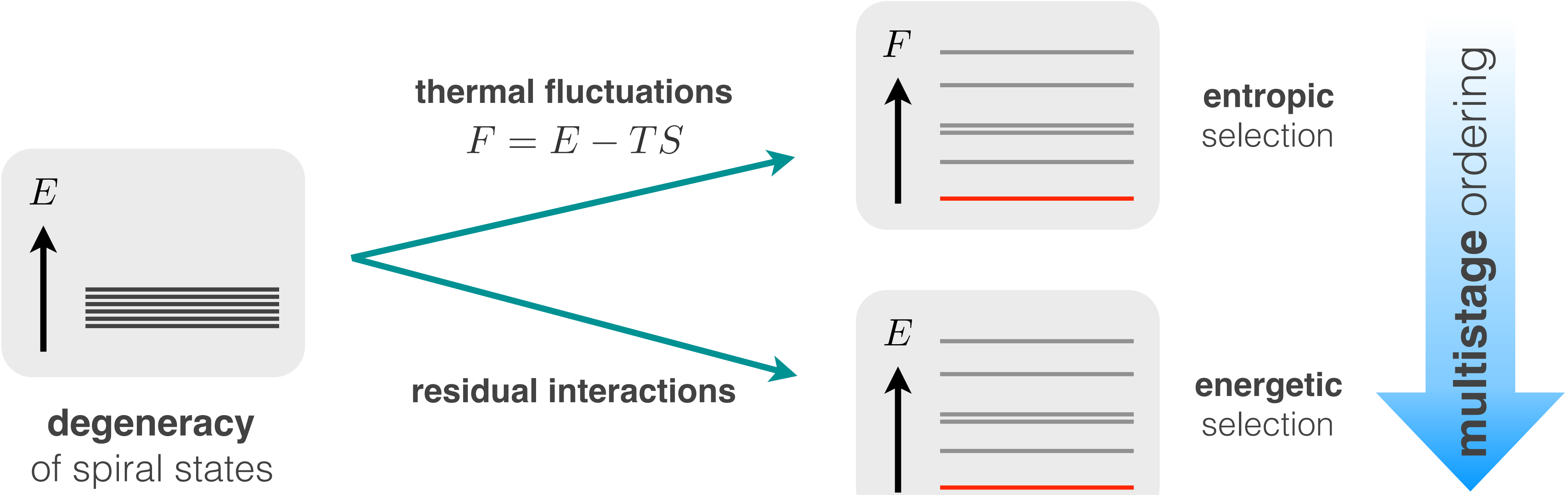


Nature Phys. **13**, 157 (2017)

Order by disorder

Nature Physics 3, 487 (2007).



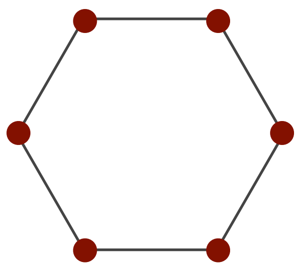


supersymmetry

Spin spiral manifolds

Spiral manifolds are extremely reminiscent of **Fermi surfaces**

triangular lattice

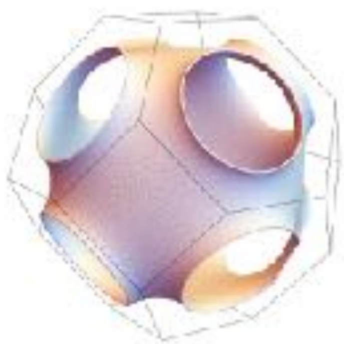


Dirac points

FCC lattice

nodal lines

diamond lattice



Fermi surface

But:
Spiral manifolds describe ground state of classical spin system, while Fermi surfaces are features in the middle of the energy spectrum of an electronic quantum system.

Spin spiral manifolds

Luttinger-Tisza

spin spirals in a nutshell

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{ij} \, \vec{S}_i \vec{S}_j$$

Fourier transform of spin model

$$= \sum_{\vec{k}} \sum_{A,B} S^A_{\vec{k}} \, \mathbf{M}_{A,B}(\vec{k}) \, S^B_{-\vec{k}}$$

diagonalize matrix

$$\mathbf{M}_{A,B}(\vec{k}) = \sum_{\vec{r}^A_{B,j}} J_{\vec{r}_j} \, e^{-i\vec{k}\cdot\vec{r}_j}$$

find **minimal** eigenvalues

$$\lambda_j(\vec{k})$$

free fermions in a nutshell

$$\mathcal{H} = \sum_{\langle i,j \rangle} t_{ij} \, c_i^\dagger c_j$$

Fourier transform of spin model

$$= \sum_{\vec{k}} \sum_{A,B} {c^\dagger}_{A,\vec{k}} \, \mathbf{H}_{A,B}(\vec{k}) \, c_{B,\vec{k}}$$

diagonalize matrix

$$\mathbf{H}_{A,B}(\vec{k}) = \sum_{\vec{r}^A_{B,j}} t_{\vec{r}_j} \, e^{-i\vec{k}\cdot\vec{r}_j}$$

find **zero** eigenvalues

$$\epsilon_j(\vec{k})$$

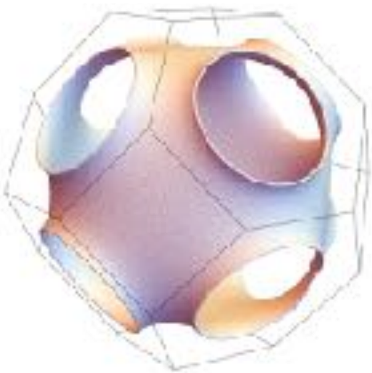
Spin spiral manifolds

spin spirals in a nutshell

$\mathbf{M}_{A,B}(\vec{k})$

with **minimal** eigenvalues

$\lambda_j(\vec{k})$



make ansatz

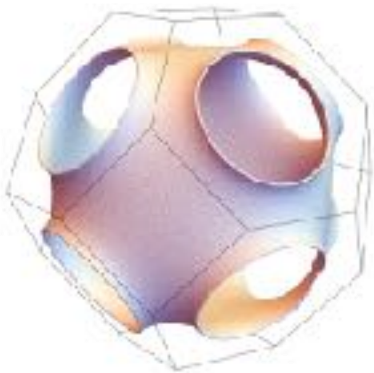
$$\mathbf{M}(\vec{k}) = \mathbf{H}(\vec{k})^2 - E_0 \cdot \mathbf{1}$$

free fermions in a nutshell

$\mathbf{H}_{A,B}(\vec{k})$

with **zero** eigenvalues

$\epsilon_j(\vec{k})$



$\mathbf{H}(\vec{k})^2$ has eigenvalues $\epsilon_j(\vec{k})^2$

zero eigenvalues of $\mathbf{H}(\vec{k})$ are minimal eigenvalues of $\mathbf{H}(\vec{k})^2$

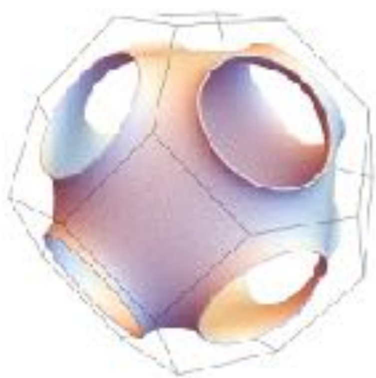
Mapping classical to quantum

spin spirals in a nutshell

$\mathbf{M}_{A,B}(\vec{k})$

with **minimal** eigenvalues

$\lambda_j(\vec{k})$



$\mathbf{H}(\vec{k})^2$

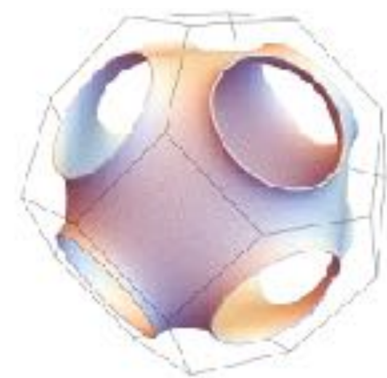
$\sqrt{\mathbf{M}(\vec{k})}$

free fermions in a nutshell

$\mathbf{H}_{A,B}(\vec{k})$

with **zero** eigenvalues

$\epsilon_j(\vec{k})$



$$\mathbf{M}(\vec{k}) = \mathbf{H}(\vec{k})^2 - E_0 \cdot \mathbf{1}$$

mapping of a classical to quantum system
(of same spatial dimensionality)
via a 1:1 matrix correspondence

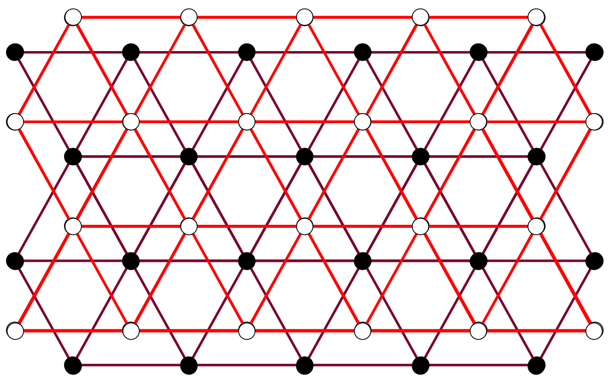
→ reminiscent of “topological mechanics”

Mapping classical to quantum

$$\mathbf{M}(\vec{k}) = \mathbf{H}(\vec{k})^2 - E_0 \cdot \mathbf{1}$$

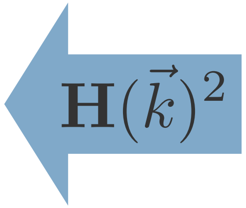
What does **"squaring"** of quantum system mean?

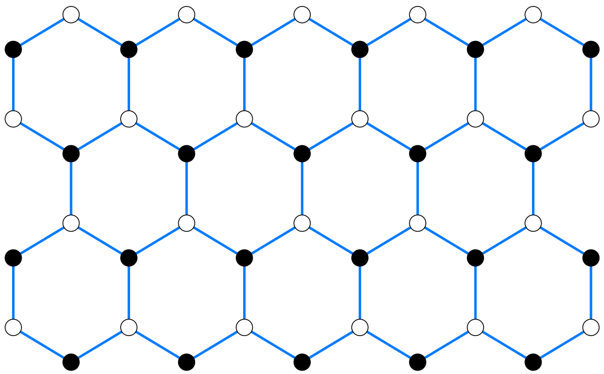
Explicit **lattice construction**.



coplanar spirals on triangular lattice

$$\vec{q} = \left(\pm\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}}\right)$$





free fermions on honeycomb lattice

$$\vec{q} = \left(\pm\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}}\right)$$

Mapping classical to quantum

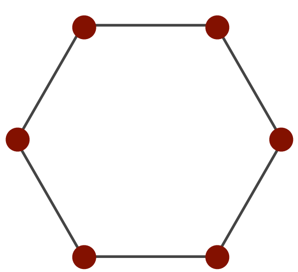
$$\mathbf{M}(\vec{k}) = \mathbf{H}(\vec{k})^2 - E_0 \cdot \mathbf{1}$$

What does **"squaring"** of quantum system mean?

Explicit **lattice construction**.

spin spirals
triangular lattice

120^o order



Dirac points

free fermions
honeycomb lattice

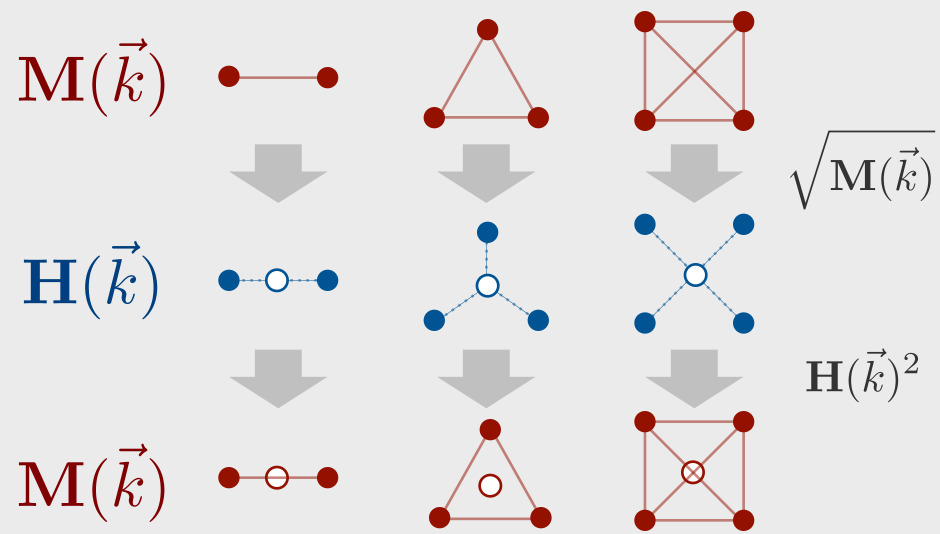
spin spirals
FCC lattice

degenerate spirals

nodal lines

free fermions
diamond lattice

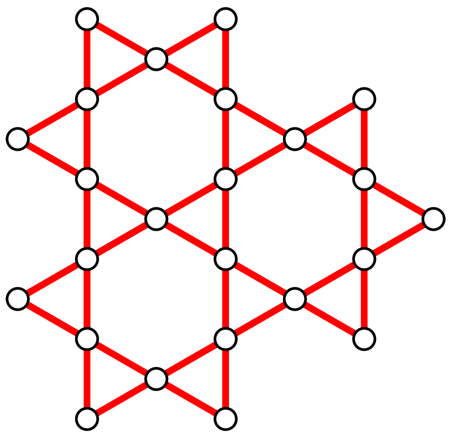
general lattice construction

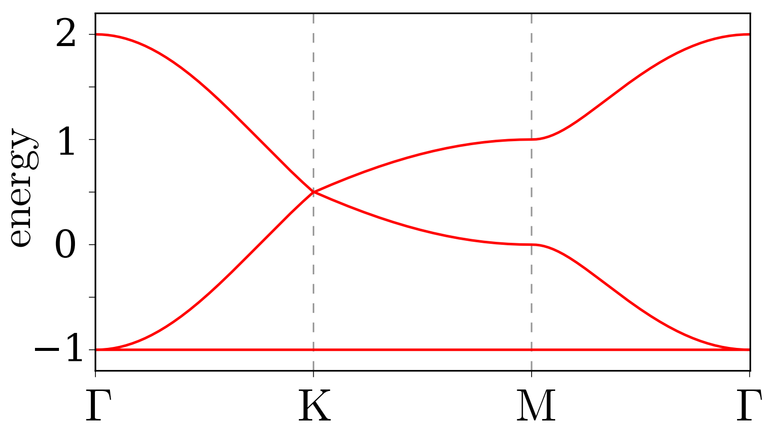


Examples

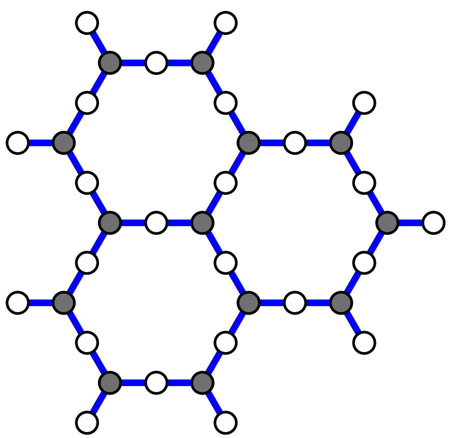
Spectra of the **kagome** and **extended honeycomb** lattice.

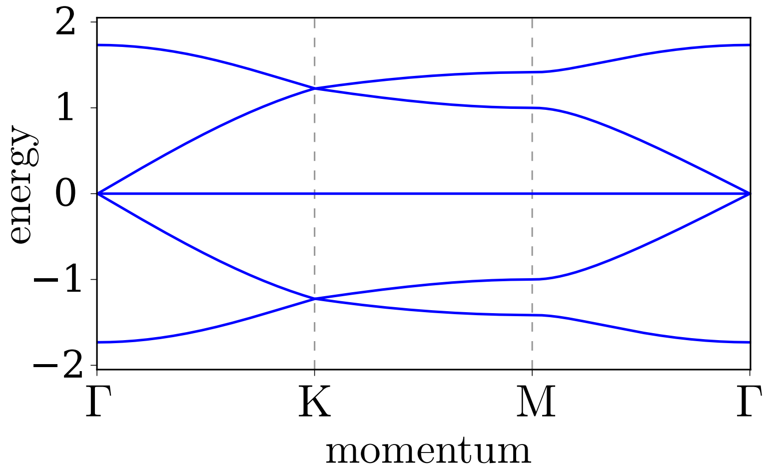
spins





fermions

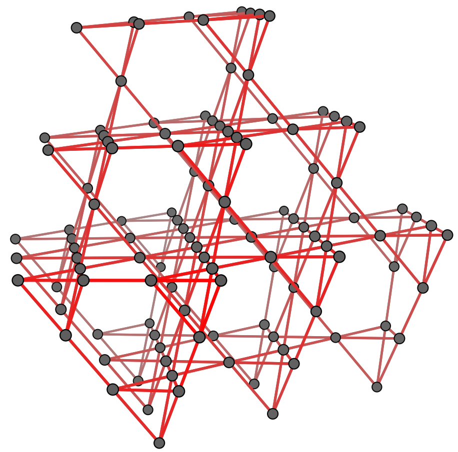


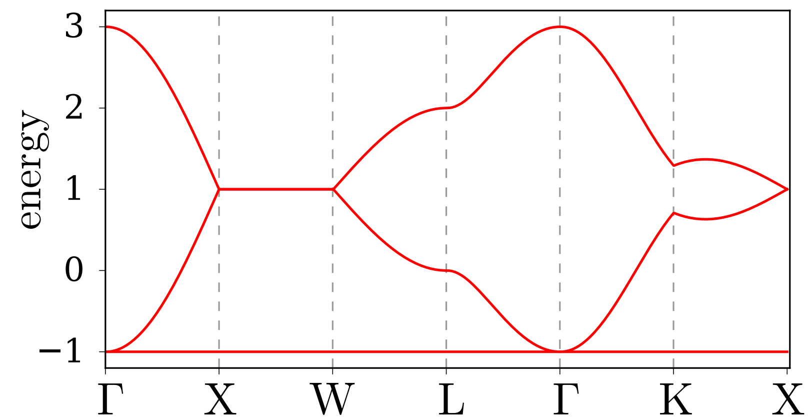


Examples

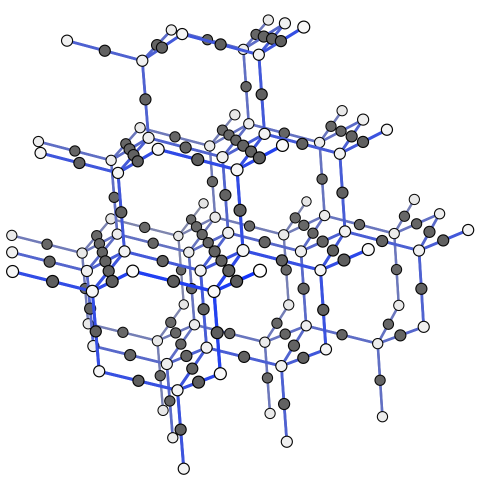
Spectra of the **pyrochlore** and **extended diamond** lattice.

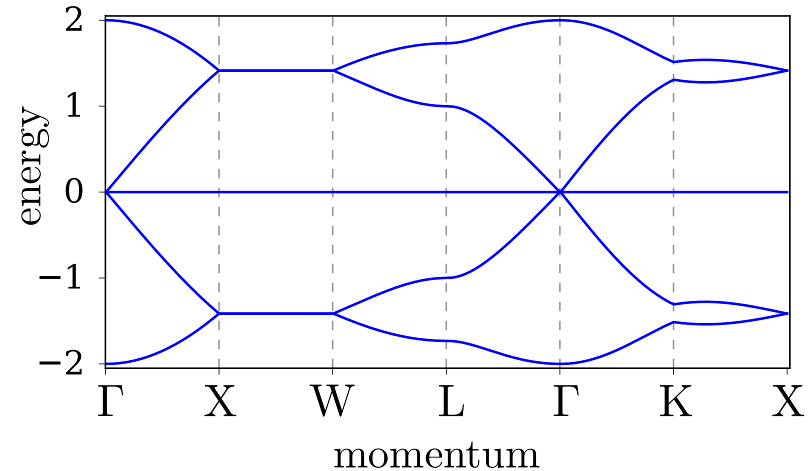
spins



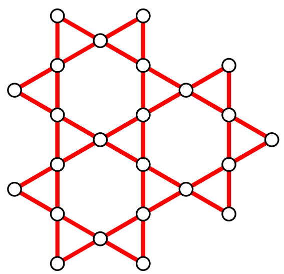


fermions

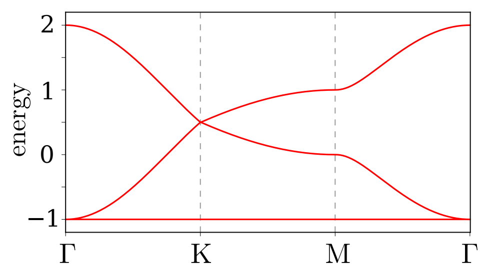


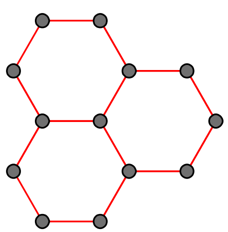


SUSY formulation

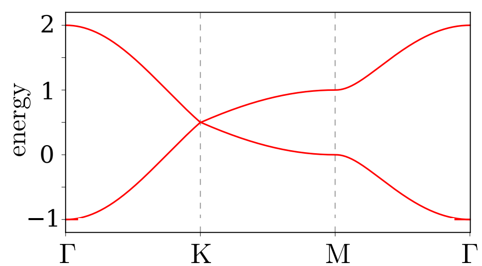


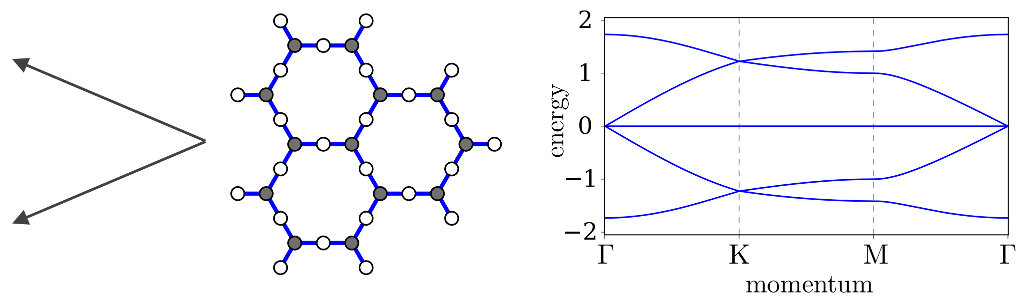
"boson"





"fermion"





SUSY charge

$$\mathcal{H}^2 = \begin{pmatrix} \mathbf{Q}^\dagger \mathbf{Q} & 0 \\ 0 & \mathbf{Q}\mathbf{Q}^\dagger \end{pmatrix}$$

square root →

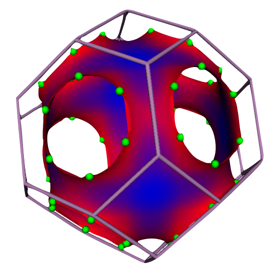
$$\mathcal{H} = \begin{pmatrix} 0 & \mathbf{Q}^\dagger \\ \mathbf{Q} & 0 \end{pmatrix}$$

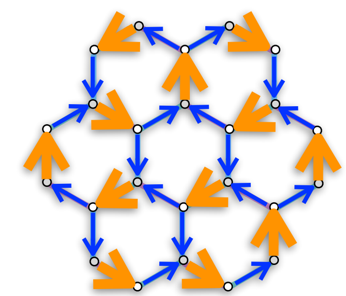
We are done with part I.

So what did we learn?

Summary

- Frustrated magnets are a source of **remarkably diverse behavior**
  - complex collective phenomena
  - exotic ordered phases
  - spin liquids





- Frustration brings along an enhanced **sensitivity to otherwise residual effects**, which will split degenerate states and reorganize the collective state of a system.

All slides of this presentation will become available on our group webpage at **www.thp.uni-koeln.de/trebst**

Thanks!

@SimonTrebst