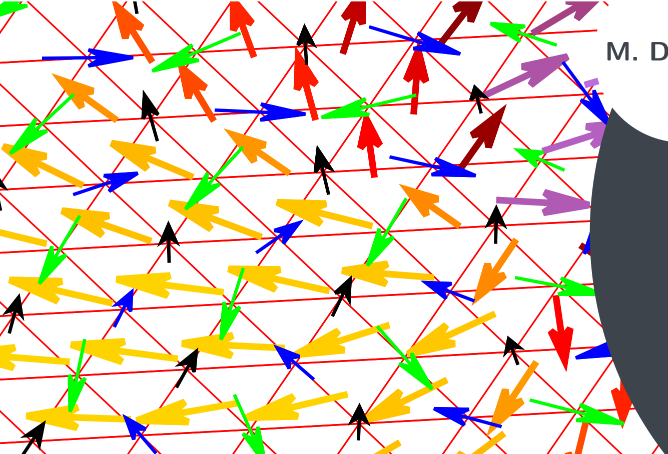
Universität Stuttgart



M. Daghofer

# Frustrated Magnets

# Topics to be Covered

- What are 'frustrated' magnets?
  - Criteria for frustration
  - Susceptibility vs. long-range ordering
  - realizations and examples
- Why do we care about them?
  - boring states suppressed
  - $\Rightarrow$ unconventional statistics, patterns ...
- What do we do about them?
  - first try 'standard' approaches
  - numerics often especially hard
  - compare numerics and effective theory

# Starting point: localized spins

- localized spins = correlated system
- Can't be band insulator: $\uparrow$ and $\downarrow$ would cancel
- Can't be partially filled non-interacting band: would be itinerant metal
  - $\epsilon_{\uparrow/\downarrow}(\vec{k}) = \epsilon(\vec{k}) \mp \frac{g\mu_B}{2}|B|$, fill both bands up to $\mu$
  - temperature hardly enters susceptibility: $\chi = \frac{\partial M}{\partial B} \approx \mu_B \rho(E_F) + \mathcal{O}(T^2)$
- discuss non-interacting spins $H = -\frac{g\mu_B}{2} B \sum_i \sigma_i^z$ and $M = \frac{g\mu_B}{2N} \sum_i \langle \sigma_i^z \rangle$
- $\Rightarrow \quad \chi = \frac{g\mu_B}{2N} \sum_i \frac{\partial \langle \sigma_i^z \rangle}{\partial B}$
- sums go over only two states:

$$\langle \sigma_i^z \rangle = \frac{\sum_j \langle \sigma_i^z \rangle_j e^{-\beta E_j}}{\sum_j e^{-\beta E_j}} = \frac{e^{-\beta(-\frac{g\mu_B}{2}B)} - e^{-\beta(\frac{g\mu_B}{2}B)}}{e^{-\beta(-\frac{g\mu_B}{2}B)} + e^{-\beta(\frac{g\mu_B}{2}B)}} = \tanh \frac{g\mu_B B}{2k_b T} \tag{1}$$

- linear in $B$ for $\mu_B B \ll k_B T$

$$\Rightarrow \quad \chi \approx \frac{\partial}{\partial B} g^2 \mu_B^2 \frac{B}{4k_b T} = \frac{g^2 \mu_B^2}{4k_b T} = \frac{C}{T}\,. \tag{2}$$

- Curie: $\chi \propto 1/T$ indicates localized spins

# Interacting spins: Heisenberg and Ising Models

$$H = \sum_{i,j} J_{i,j} \vec{S}_i \vec{S}_j \qquad \text{resp.} \qquad H = \sum_{i,j} J_{i,j} S_i^z S_j^z \ . \tag{3}$$

- arises in 2nd order perturbation theory for half-filled band at $t_{i,j} \ll U$
- Heisenberg preserves rotational spin invariance: starting point of ignorance
- less symmetric corrections may arise (spin-orbit coupling)

Mean-field approach:

- decoupling $\vec{S}_i \vec{S}_j \to \langle \vec{S}_i \rangle \vec{S}_j + \vec{S}_i \langle \vec{S}_j \rangle - \langle \vec{S}_i \rangle \langle \vec{S}_j \rangle$
- for one bond:

$$H_{a,b} = \sum_{i=a,b} \left( -\mu \vec{B} + J_{i,\bar{i}} \langle \vec{S}_{\bar{i}} \rangle \right) \vec{S}_i - \text{const.} \tag{4}$$

  each spin sees effective field from the other
- Ising a bit easier for now
- ferromanget even more so: because it is not frustrated!

# Mean-Field approach

- effective field for each spin given by all others:

$$H_i = -\mu \vec{B}_{i,\text{eff}} \vec{S}_i = \left( -\mu \vec{B} + \sum_j J_{i,j} \langle \vec{S}_j \rangle \right) \vec{S}_i \tag{5}$$

- assume translationally invariant (ferromagnetic) solution along $z$, i.e., $\langle \vec{S}_i \rangle \to \langle \vec{S} \rangle = \langle S \rangle \vec{e^z}$ (reasonable for $J < 0$)
- consider nearest-neighbor coupling to $z$ neighbors:

$$\mu B_{\text{eff}} = \mu B - zJ \langle S \rangle \tag{6}$$

- apply independent-spin formula (mean-field!)

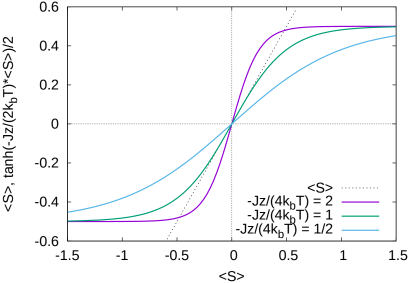
$$\langle S \rangle = \frac{1}{2} \langle \sigma^z \rangle = \frac{1}{2} \tanh \frac{g\mu_B B_{\text{eff}}}{2k_b T} = \frac{1}{2} \tanh \frac{g\mu_B B - zJ \langle S \rangle}{2k_b T} \ . \tag{7}$$

# Curie Temperature $T_C$

important parameter at $B = 0$: critical temperature $T_C = \frac{z(-J)}{4k_B}$

- implicit equation for $\langle S \rangle$:

$$\langle S \rangle = \frac{1}{2} \tanh \frac{z(-J)\langle S \rangle}{2k_b T} \quad \rightarrow \quad \langle S \rangle = \frac{1}{2} \tanh \frac{2T_C \langle S \rangle}{T} \qquad (8)$$




- solve implicit equation for $\langle S \rangle$ numerically
- graphic solution:
  - slope of tanh $< 1 \Rightarrow$ only 1 solution $\langle S \rangle = 0$
  - slope of tanh $> 1 \Rightarrow$ solutions with $\langle S \rangle \neq 0$
- for $T < T_C$: solutions with $\langle S \rangle \neq 0$ have lower free energy $\Rightarrow$ equilibrium state
- relevant criterion: $T$ vs. critical temperature $T_C = \frac{z(-J)}{k_B 4}$

# High-temperature susceptibility

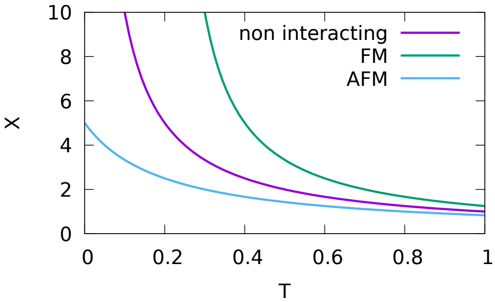
- susceptibility for large $k_B T \gg k_B T_C$:

$$\chi = \frac{g\mu_B}{2}\frac{\partial}{\partial B}\tanh\frac{g\mu_B B - zJ\langle S\rangle}{2k_b T} \approx \frac{g\mu_B}{2}\frac{\partial}{\partial B}\left(\frac{g\mu_B B}{2k_b T} + \frac{2T_C\langle S\rangle}{T}\right) = \frac{g^2\mu_B^2}{4k_b T} + \frac{T_C}{T}\underbrace{g\mu_B\frac{\partial\langle S\rangle}{\partial B}}_{=\chi}$$

- $\Rightarrow$ Curie's law: $\chi = \frac{C}{T-T_C}$
- approximation not valid for $T \lesssim T_C$
- 'expected' $T_C$ can be inferred from fit to high-$T$ susceptibility

# Antiferromagnetism

- non-interacting spins: $\chi = \frac{C}{T}$
- ferromagnetic: $\chi = \frac{C}{T - T_C}$
  - for $T \to T_C$, spins form giant magnetic moment that reacts a lot to (small) $B$




- (unfrustrated) nearest-neighbor antiferromagnetism:
- physics: spins orient opposite ⇒ cancel each other rather than reacting to $B$
- math: same calculation as above, but with one sign change ⇒ $\chi = \frac{C}{T + T_N}$
- $T_N$: Néel temperature, where mean-field theory gives AFM order
- (approximation still only valid for large $T$)

# Frustrated Magnetism

- high-temperature susceptibility:
  - $\chi_{T\gg} \propto \frac{1}{T+T_N}$ with substantial $T_N$
  - $\Rightarrow$ localized spins
  - $\Rightarrow$ spin-spin interactions that suppress $\chi$
- low-temperatures:
  - either no ordering
  - or only at much lower temperatures: actual $T_N$ much smaller than that derived from fitting $\chi_{T\gg}$
- interactions are there and active at short distance, but 'frustrated' at longer distance
- various origins possible:
  - nearest- vs. next-nearest neighbors
  - triangular lattice
  - directionality, e.g. via spin-orbit coupling
  - ...

# Classic Example: triangular lattice

PHYSICAL REVIEW VOLUME 79, NUMBER 2 JULY 15, 1950

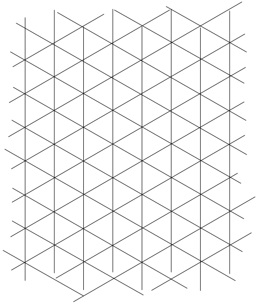
## Antiferromagnetism. The Triangular Ising Net

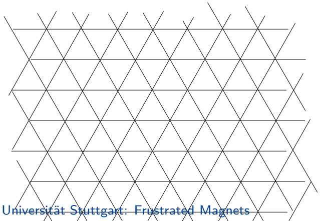
G. H. Wannier
*Bell Telephone Laboratories, Murray Hill, New Jersey*
(Received February 11, 1950)

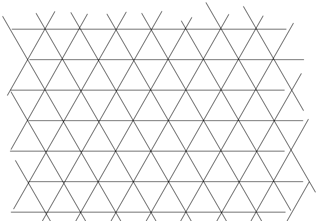
In this paper the statistical mechanics of a two-dimensionally infinite set of Ising spins is worked out for the case in which they form either a triangular or a honeycomb arrangement. Results for the honeycomb and the ferromagnetic triangular net differ little from the published ones for the square net (Curie point with logarithmically infinite specific heat). The triangular net with antiferromagnetic interaction is a sample case of antiferromagnetism in a non-fitting lattice. The binding energy comes out to be only one-third of what it is in the ferromagnetic case. The entropy at absolute zero is finite; it equals

$$S(0)=R\frac{2}{\pi}\int_0^{\pi/3}\ln(2\cos\omega)d\omega=0.3383R.$$

The system is disordered at all temperatures and possesses no Curie point.







# Beyond the triangular lattice

What we can take from here:

- 'obvious' state suppressed: here, the 'normal' AFM state that optimizes all interactions
- some 'local' rule is obeyed by low-energy states: here, for each triangle
- globally, many states fulfill local rules ($\rightarrow$ spin ice)

Other observations:

- extensive ground-state degeneracy unlikely
- usually, something else happens
  - other interactions select ground state
  - quantum/thermal fluctuations select ground state ('order by disorder')
  - completely different state, e.g., spin liquid
  - that state possibly interesting
- but sometimes, it survives well

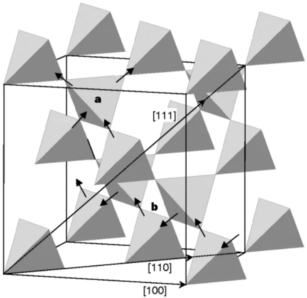
# Ice rules

- originally for water ice:
  - each oxygen has two hydrogens, coupled by 'short' bonds
  - is coupled to other $H_2O$ by 'long' hydrogen bridges
  - which two of the four bonds are long/short, is arbitrary
- $\Rightarrow$ a lot of entropy remains (Pauling):
  - look at tetrahedron of H, $N/2$ tetrahedra
  - total number of configurations: $4^2 = 16$
  - of which 6 agree with ice rules
  - $\Rightarrow$ fraction of states available at $T \to 0$: $Z = 2^N \left(\frac{6}{16}\right)^{N/2} = \left(\frac{6}{4}\right)^{N/2}$
  - $\frac{\log Z}{N} = \frac{1}{2} \log \frac{3}{2} \approx 0.20273$
  - agrees well with numerics
- analogous ideas for Ising spins on pyrochlore/checkerboard lattices

# Spin ice

$Dy_2Ti_2O_7$

- uniaxial spin: along direction to center
- spin can point 'in' or 'out'
- ferromagnetic interactions: two-in–two-out
- Ising-like degree of freedom
- 2D version: checkerboard: large degeneracy seen




A. P. Ramirez, A. Hayashi, R. J. Cava, R. Siddharthan, B. S. Shastry, Nature **399**, 333 (1999)

- states per site at $T \gg 0$: 2
- $\Rightarrow \log 2 = S_0 + \int_0^\infty \frac{C_V(T)}{T} \mathrm{d}T$

# Interesting properties of Spin ice

- defects, e.g. 3-in–1-out
- relevant in a magnetic field
- Coulomb-like effective interaction (from long-range dipole-dipole interactions)
- become "magnetic monopoles"
- $\Rightarrow$ transition in magnetic field becomes crystallization of monopoles

Current topics:

- quantum spin ice
- artificial spin ice

# Heisenberg spins

- can point in arbitrary direction (also an idealization)
- defined by commutators between components:

$$[\hat{S}_k, \hat{S}_l] = i\hbar\epsilon_{klm}\hat{S}_m \tag{9}$$

- unfrustrated square lattice: ordered moment reduced from classical Néel state
- Starting point: classical spins
  - you have to start somewhere
  - often quite good
  - solution will at least be plausible competitor for quantum model as well
- example: triangular lattice with $120^\circ$ order

# Luttinger-Tisza Method

basic ingredients:

- formally relax length of spin
  - find solutions for $x/y/z$ components
  - have to fulfill $(S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 = 1$ ('strong' condition)
  - relax this to 'weak' condition:

$$\sum_i (S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 = N \tag{10}$$

  - afterwards worry about individual spins
- Fourier transform:

$$\sum_{i,j} J_{ij} \vec{S}_i \vec{S}_j \quad \rightarrow \quad \sum_q J_q \vec{S}_q \vec{S}_{-q} \tag{11}$$

J. M. Luttinger and L. Tisza, Phys. Rev. **70**, 954 (1946)

# Luttinger-Tisza Method: example I

- Bravais lattice: all sites equivalent, crystal momentum $k$ good quantum number
- minimize with weak constraint:

$$\sum_{ij} J_{ij}\vec{S}_i\vec{S}_j - \lambda\left(\sum_i |\vec{S}_i|^2 - N\right) \tag{12}$$

- Derivative:

$$\sum_\delta J_\delta \vec{S}_{i+\delta} - 2\lambda\vec{S}_i = 0 \tag{13}$$

- Ansatz: $\vec{S}_i = \vec{u}\mathrm{e}^{i\vec{q}\vec{r}_i}$

$$\sum_\delta J_\delta \vec{u}\mathrm{e}^{i\vec{q}(\vec{r}_i+\vec{\delta})} = 2\lambda\vec{u}\mathrm{e}^{i\vec{q}\vec{r}_i} \quad \Rightarrow \quad \underbrace{\sum_\delta J_\delta \mathrm{e}^{i\vec{q}\vec{\delta}}}_{=J_{\vec{q}}} = \tilde{\lambda} \tag{14}$$

# Luttinger-Tisza Method: example II

- find $\vec{q}$ that minimizes $J_{\vec{q}}$
- Examples:
  - NN AFM Heisenberg: $\vec{q} = (\pi, \pi)$)
  - NN FM Heisenberg: $\vec{q} = (0, 0)$)
  - dominant AFM NNN coupling: $\vec{q}_1 = (\pi, 0)$ and $\vec{q}_2 = (0, \pi)$
- set up solution that obeys strong constraint:

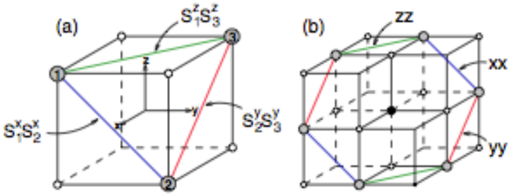
$$\vec{S}_i = \vec{u} \cos \vec{q}\vec{r}_i + \vec{v} \sin \vec{q}\vec{r}_i \quad \text{with} \quad \vec{u}\vec{v} = 0 \tag{15}$$

- coplanar spiral in $\vec{u}$-$\vec{v}$ plane (e.g. $\vec{u} = \vec{e}_x$ and $\vec{v} = \vec{e}_y$)
- examples:
  - triangular lattice $120^\circ$ pattern
  - 1D chain: spiral

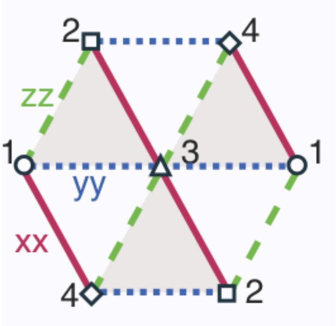
# Conclusions from Luttinger-Tisza

- does not necessarily work for more than one spin per unit cell
- many $\vec{q}$ might optimize $J_{\vec{q}}$
- coplanar spiral may not be unique ground state (kagome!)
- anisotropic interactions: $S^{x/y/z}$ may prefer different $\vec{q}$
- example: skyrmions
  - Dzyaloshinskii-Moriya interaction provide anisotropies
  - one solution: spirals
  - competing solution: superposition of spirals
  - length is then not always one
  - $\Rightarrow$ way out can be skyrmions
- Step beyond Luttinger-Tisza: Classical simulation, e.g. by Markov-chain Monte-Carlo
  - 'straightforward' optimization
  - many parameters!
  - MCMC helps to get out of local minima

# Example: Anisotropic couplings



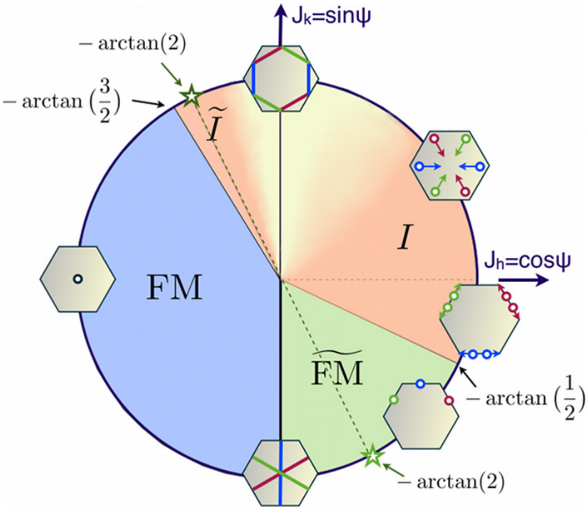

- $90^\circ$ bond angle: Isotropic coupling reduced
- Such bonds in honeycomb $A_2IrO_3$, $RuCl_3$
- Or in triangular lattice ($Ba_3IrTi_2O_9$)




$$\mathcal{H} = J_K \sum_{\gamma} \sum_{\langle i,j \rangle \| \gamma} S_i^\gamma S_j^\gamma + J_H \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j$$

G. Jackeli and G. Khaliullin, PRL **102**, 017205 (2009); J. Chaloupka, G. Jackeli, and G. Khaliullin, PRL **105**, 027204 (2010).

# Kitaev-Heisenberg on a triangular lattice



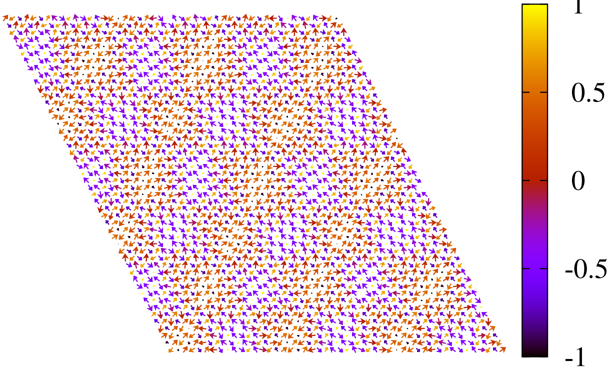

- **Frustration:** Tendency to incommensurate states
- **But:** Each spin component $S^\gamma$ optimized by different momentum $\mathbf{Q}^\gamma$.
- **What about** $I$?

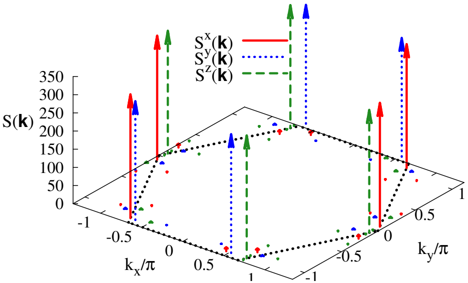
  Incommensurate spiral makes only one $S^\gamma$ happy.
- **Next step:** Markov-chain Monte Carlo

I. Rousochatzakis *et al.*, PRB **93**, 104417 (2016)

# Monte Carlo 'close to' Heisenberg model

$S^\gamma(\mathbf{k}) = |\sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} S_i^\gamma|^2$ for $J_H = 1,\ J_K = -0.3$



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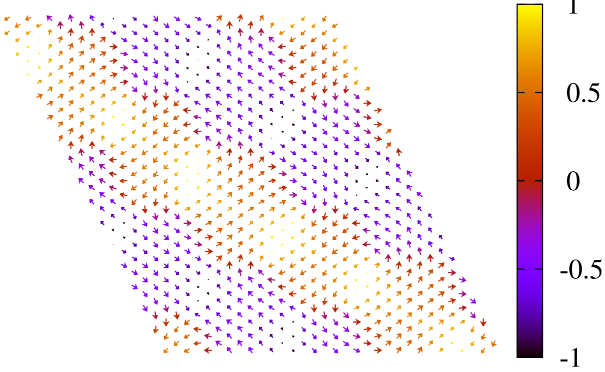
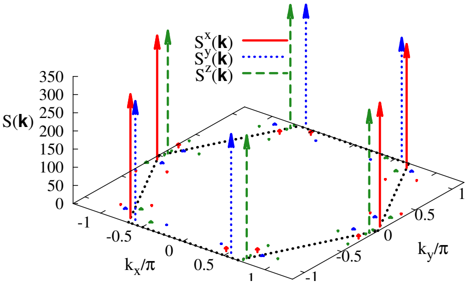
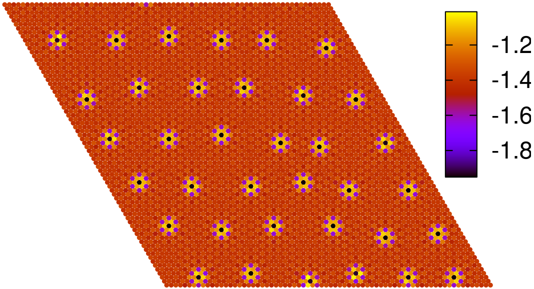
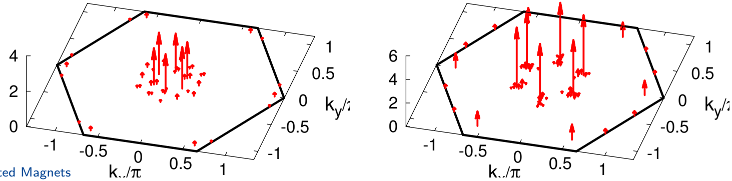


# Local Energy: defects



# Continuum limit

- Vortices form lattice
- Lattice constant depends on $J_K/J_H$
- Lattice constant much larger than that of underlying lattice
- Make original triangular lattice continuum, on which vortices ('particles') arise
- Inhomogeneous solutions of homogeneous problem:
  Particle-like solutions usually unstable

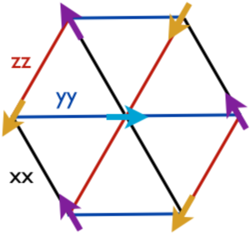
# Lifshitz invariants allow ‘particles’

- Lifshitz invariants $(\mu\partial_\gamma\nu - \nu\partial_\gamma\mu)$ needed for ‘particles’
- Non-centrosymmetric systems
  - Multiferroics

    S. C. Chae *et al.*, PNAS **107**, 21366 (2010)
  - Helimagnets: $DM \times \nabla M \Rightarrow$ skyrmions

    U. K. Rößler, A. N. Bogdanov, and C. Pfleiderer, Nature **442**, 797 (2006)
  - Chiral liquid crystals $\Rightarrow$ blue phases

    D. Wright and N. Mermin, RMP **61**, 385 (1989)
- Here: Hamiltonian inversion symmetric,
  $120°$ order breaks inversion symmetry



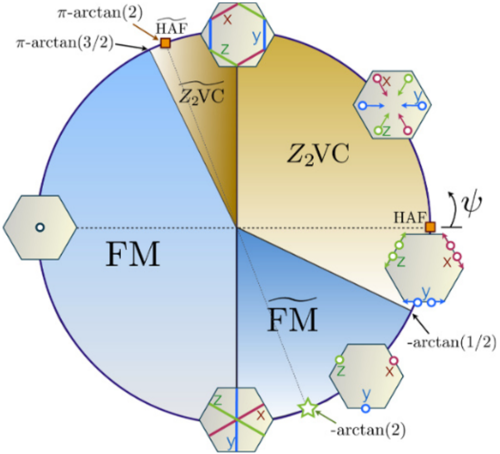
# Lifshitz invariants

- Order parameter $SO(3)$
- Spins on plaquette at origin: To corners of planar triangle
- Spins on plaquette at $\vec{r}$:
  - (non co-planar)
  - plane rotated; triangle rotated within plane

$$\mathbf{R}(\mathbf{r}) = \Big(\boldsymbol{\mu}(\mathbf{r}), \boldsymbol{\nu}(\mathbf{r}), \boldsymbol{\mu}(\mathbf{r}) \times \boldsymbol{\nu}(\mathbf{r})\Big)$$

- Assumption: $\mathbf{R}(\mathbf{r})$ changes slowly with $\mathbf{r}$
  $\Rightarrow$ Taylor expansion
- Heisenberg terms: $(\partial_x \boldsymbol{\mu})^2$
  elastic terms, favor $120^\circ$ state
- Kitaev terms: $\mu_x \partial_c \nu_x - \nu_x \partial_c \mu_x$
  Lifshitz invariants, favor twisting

# Potential classical ground state




- Continuum analysis would put vortices all over incomm. phase
- But:
  - Thermal fluctuations prefer more directional/collinear order
    I. Rousochatzakis *et al.*, PRB **93**, 104417 (2016)
  - Quantum fluctuations prefer more collinear order M. Becker *et al.*, PRB **91**, 155135 (2015); G. Jackeli & A. Avella, PRB **92**, 184416 (2015); T. Shirakawa & S. Yunoki, arXiv:1604.00721
- ⇒ discuss QUANTUM spins

# From classical to Quantum: add spin waves

## Holstein-Primakoff transformation

$$S_i^z = 1 - a_i^\dagger a_i\,, \qquad S_i^+ = \sqrt{2S - a_i^\dagger a_i}\,a_i\,, \qquad S_i^- = a_i^\dagger\sqrt{2S - a_i^\dagger a_i} \tag{16}$$

- in principle exact
- but we plan to drop $a_i^\dagger a_i$ from $\sqrt{\ldots}$: 'linear spin-wave theory'
- $\Rightarrow \langle a_i^\dagger a_i \rangle \ll 2S$
- $\langle S_i^z \rangle$ should be large $\forall i$
- $\Rightarrow$ choose $z$ axis along direction locally preferred by classical order

$\Rightarrow$ bilinear Hamiltonian, but with terms $\propto a_i^\dagger a_j^\dagger$:

$$H_{\mathrm{LSW}} = \sum_{i,j}\left(A_{ij}a_i^\dagger a_j^\dagger + B_{ij}a_i^\dagger a_j\right) + \mathrm{H.c.} + \sum_i C_i a_i^\dagger a_i \tag{17}$$

$A_{ij}$, $B_{ij}$ and $C_i$ depend on classical ground state!

# Bogoliubov and Fourier transforms

solution very similar to BCS theory for superconductors:

$$\alpha_k = u_k a_k + v_k a^\dagger_{-k} \tag{18}$$

with

$$\omega_k = \sqrt{B_k^2 - A_k^2}, \quad u_k = \sqrt{\frac{B_k + \omega_k}{2\omega_k}}, \quad v_k = \mathrm{sgn}(A_k)\sqrt{\frac{B_k - \omega_k}{2\omega_k}} \tag{19}$$

Hamiltonian is then diagonal:

$$H_{\mathrm{LSW}} = \sum_k \omega_k \left( a^\dagger_k a_k + \frac{1}{2} \right) + E_0 \tag{20}$$

ground-state energy

- classical energy $E_0$
- zero-point energy $\frac{1}{2}\sum_k \omega_k$ depending on on classical pattern
- $\Rightarrow$ classical degeneracy may be lifted!

# Conclusions from linear spin-wave theory

- gives excitation spectrum ($\rightarrow$ neutron scattering)
- any $\omega_k < 0$: staring point was not actually a ground state!
- may lift ground-state degeneracy
- $\langle a_i^\dagger a_i \rangle$ gives quantum correction to classical ordered moment:
  - if it is too large $\Rightarrow$ LSWT invalid $\Rightarrow$ different ground state?
  - e.g. triangular lattice: $\langle a^\dagger a \ \rangle \approx 0.26$
  - $\Rightarrow$ ordered moment $M_S = 0.24$ rather than $S = \frac{1}{2}$
  - numerics (ED, DMRG ...): $M_S \approx 0.2$
- LSWT surprisingly good

# What happened so far?

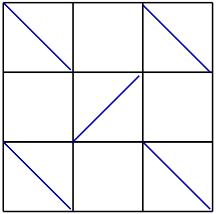
- Ising spins:
  - triangular lattice: ground-state degeneracy
  - pyrochlore: spin ice
  - 'magnetic monopoles' as excitations
- Heisenberg spins:
  - Luttinger-Tisza: frustration can give incommensurate states (e.g. spirals)
  - classical continuum limit: skyrmions, vortices
  - linear spin-wave theory:
    - first step towards quantum spins
    - excitations
    - may select ground state
    - may destabilize ordered moment

# What else can happen?

- look at quantum spins
- beyond Ising (Ising is always classical)
- focus on $S = \frac{1}{2}$: LSWT better for larger spins
- valence bond crystal
- quantum spin liquid a possibility
  - short-range correlations
  - no long-range order
  - but: long-range entanglement
  - topological order
  - exotic excitations with fractional quantum numbers

# Pairing into singlets

e.g. Shastry-Sutherland

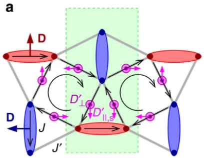


- singlets on diagonals ⇒ magnetism gone in ground state
- ⇒ investigate magnetic field
- gapped excitations: 'triplon'
- triplons can move

$SrCu_2(BO_3)_2$

- quite some additional frustration via Dzyaloshinskii-Moriya

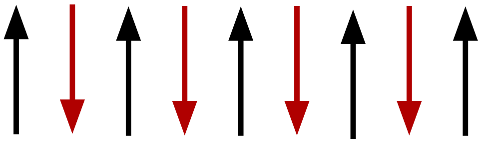
**Figure 1: The $SrCu_2(BO_3)_2$ lattice.**




- magnetic field: triplons topologically non trivial

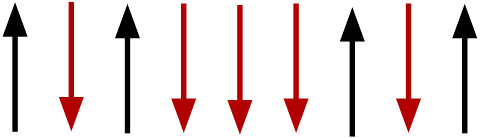
J. Romhányi *et al.*, Nat. Commun. **6**, 6805 (2015); P. McClarty *et al.*, Nat. Phys. **13**, 736 (2017)

# Cartoon for one dimension



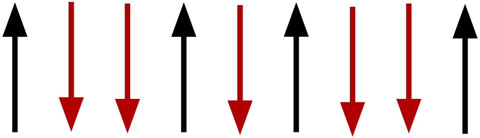
- AFM chain, only NN interactions

# Cartoon for one dimension



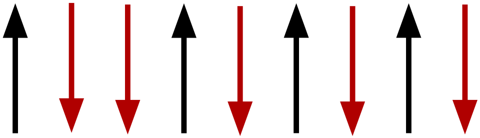
- AFM chain, only NN interactions
- create one excitation (usually 'magnon'):
  $\Delta S = 1$

# Cartoon for one dimension



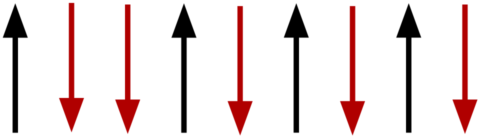
- AFM chain, only NN interactions
- create one excitation (usually 'magnon'): $\Delta S = 1$
- two 'spinons' move apart

# Cartoon for one dimension



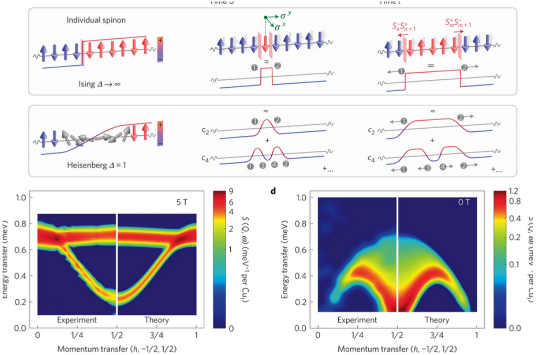
- AFM chain, only NN interactions
- create one excitation (usually 'magnon'): $\Delta S = 1$
- two 'spinons' move apart
- each spinon carries $S = \frac{1}{2}$

# Cartoon for one dimension



- AFM chain, only NN interactions
- create one excitation (usually 'magnon'): $\Delta S = 1$
- two 'spinons' move apart
- each spinon carries $S = \frac{1}{2}$

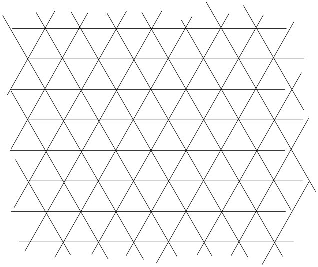
cartoon is extremely well supported by numerics and experiment

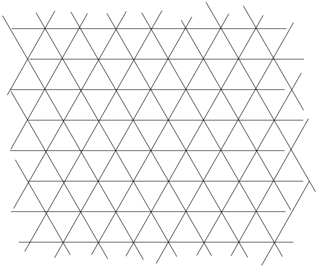



M. Mourigal *et al.*, Nat. Phys. **9**, 435 (2013)

# (Resonating) valence bonds in two dimensions

- valence-bond crystal: spins form (static) NN singlets, magnetism gone
- valence-bond liquid: change partners dynamically ⇒ very entangled

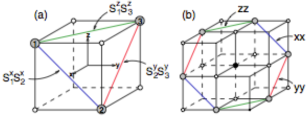




topological sector: odd/even number of dimers cut

# Candidates

- anisotropic triangular-lattice organic compounds
- Herbertsmithite
- volborthite




- different route: 'Kitaev' model
  - $RuCl_3$ with magnetic field
  - $H_3LiIr_2O_6$ ...
  - interactions at first sight very frustrated
  - but can be solved exactly!
  - gapless/gapped spinon excitations
  - experiment: difficult to distinguish interacting spinons from interacting magnons

# How to treat frustrated magnets I

- read the literature
- (find plausible parameter ranges)
- first look at classical model
  - check whether Luttinger-Tisza works
  - if so, check whether coplanar state *only* solution
  - if not: numerics (e.g. Monte Carlo)
- linear spin-wave theory
  - as a check (classical solution stable?)
  - resolve classical degeneracies
  - get excitation spectra

By now, you ideally have an idea what might happen in your system.

# More elaborate treatments of quantum model

- variational approaches
  - your Ansatz needs to contain the right physics!
  - first advantage: energy estimate converges easily
  - disadvantage: energy estimate converges easily, i.e., crappy approximation may still look good!
  - real advantage: better solution always lower energy
- if your system is (quasi–)one-dimensional: DMRG

- exact diagonalization
  - tiny systems
  - but no additional approximations
  - not affected by frustration
- DMRG for higher dimensions
- Quantum Monte Carlo
  - usually sign problem for frustrated systems
  - unless you find the right basis ($\rightarrow$ variational)

# Example: What can you do with exact diagonalization?

- Lanczos method for sparse Hermitian matrices
  - needs to store a few vectors worth of data
  - ground state converges fast
  - Green's functions (excitations) also accessible
- ground state energy to compare approximations with
- ground state to try to understand (Which patterns have large weight?)
- a few excited states
- excitation spectra to compare with experiment
- finite-temperature properties with modified algorithms

If your cluster is too small for the relevant physics, there is not much you can do about it.
(Possibly: use information gained to reduce Hilbert space.)

# Example: What can you do with Monte Carlo?

classical MCMC:

- start from some configuration (random or ordered) $\rightarrow$ extra check on convergence
- good at getting out of local minima
- can be complemented by optimization once one is close to ground state
- gives upper bound for classical energy
- configurations to look at
- correlation functions
- finite-temperature properties

Quantum MCMC:

- an art of its own
- frustration often causes 'sign problem'
- 'language' needs to be adapted to problem at hand
- $\Rightarrow$ you need to have some idea first
- if it works, it can give excellent information
- correlations, order parameters
- finite-size scaling
- excitations (analytic continuation)

# Sources of frustration

- 'pure' geometry (triangular motif)
- longer-range couplings ($J_1$-$J_2$ square lattice)
- directionality
  - Dzyaloshinskii-Moriya from spin-orbit coupling
  - 'Kitaev' Ising-like interactions (from SOC of $t_{2g}$ orbitals)
  - Kanamori-Goodenough rules: connection of spin and orbital without SOC
- other processes:
  - two holes in $t_{2g}$: strong SOC wants $\vec{L} + \vec{S}$ to form singlet $\rightarrow$ triplon as excitation
  - double exchange from electron itineracy wants ferromagnetism
- competition more generally

# Summary

Frustrated magnets can be interesting:

- residual degeneracy
- exotic excitations (monopoles, spinons)
- toological order

Frustrated magnets can be hard:

- the point is that the 'obvious' solution does not work
- sometimes a differnt point of view helps (Kitaev's spin liquid)
- method needs to be adapted to problem

Competing interaction are also simply often present and have to be dealt with.