Tutorial:
Quantum Spin Liquids (Part I)

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Three questions:

1. What *is* a spin liquid?
   Why are they interesting?
2. How to *stabilize* a spin liquid?
3. How to *detect* a spin liquid?

1) Quantum Spin Ice
2) Kitaev's Spin Liquid

What can go wrong?

What is a spin liquid?

- *Broad* sense:

[1]*Doesn't spontaneously break any symmetries*

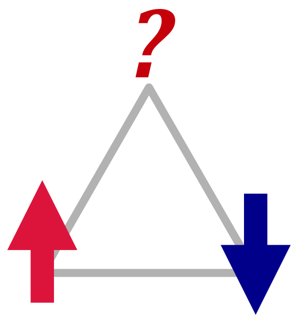
Magnet that *doesn't order*[1] down to zero temperature **and** is *distinct*[2] from a *trivial paramagnet*[3]

[2]*Not "smoothly connected"*

[3]*Has some kind of "topological order"*

Valence bond solid? ***No***
Frozen product state due to disorder? ***No***
One dimension? ***Complicated***

- Typically *highly frustrated*
- Broad *cooperative paramagnet* regime, *well below* characteristic scale



*No choice to satisfy **all** bonds*

What do we mean by *magnet*?

- General (*pseudo-) spin-1/2* model can take the form

Heisenberg – Align or Anti-align

*In **weak** SOC limit $J >> D >> \Gamma$*

Γ is a symmetric 3x3 matrix

$$\sum_{ij}\left[J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j + \mathbf{D}_{ij}\cdot\left(\mathbf{S}_i\times\mathbf{S}_j\right) + \mathbf{S}_i\cdot\left(\boldsymbol{\Gamma}_{ij}\cdot\mathbf{S}_j\right)\right]$$

Dzyaloshinskii-Moriya (DM) interaction

Symmetric anisotropy (pseudo-dipolar, Ising, etc)

If **strong** SOC, *no prescribed form* **–** only constrained by discrete lattice symmetries

Common limits:

Heisenberg $J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j$

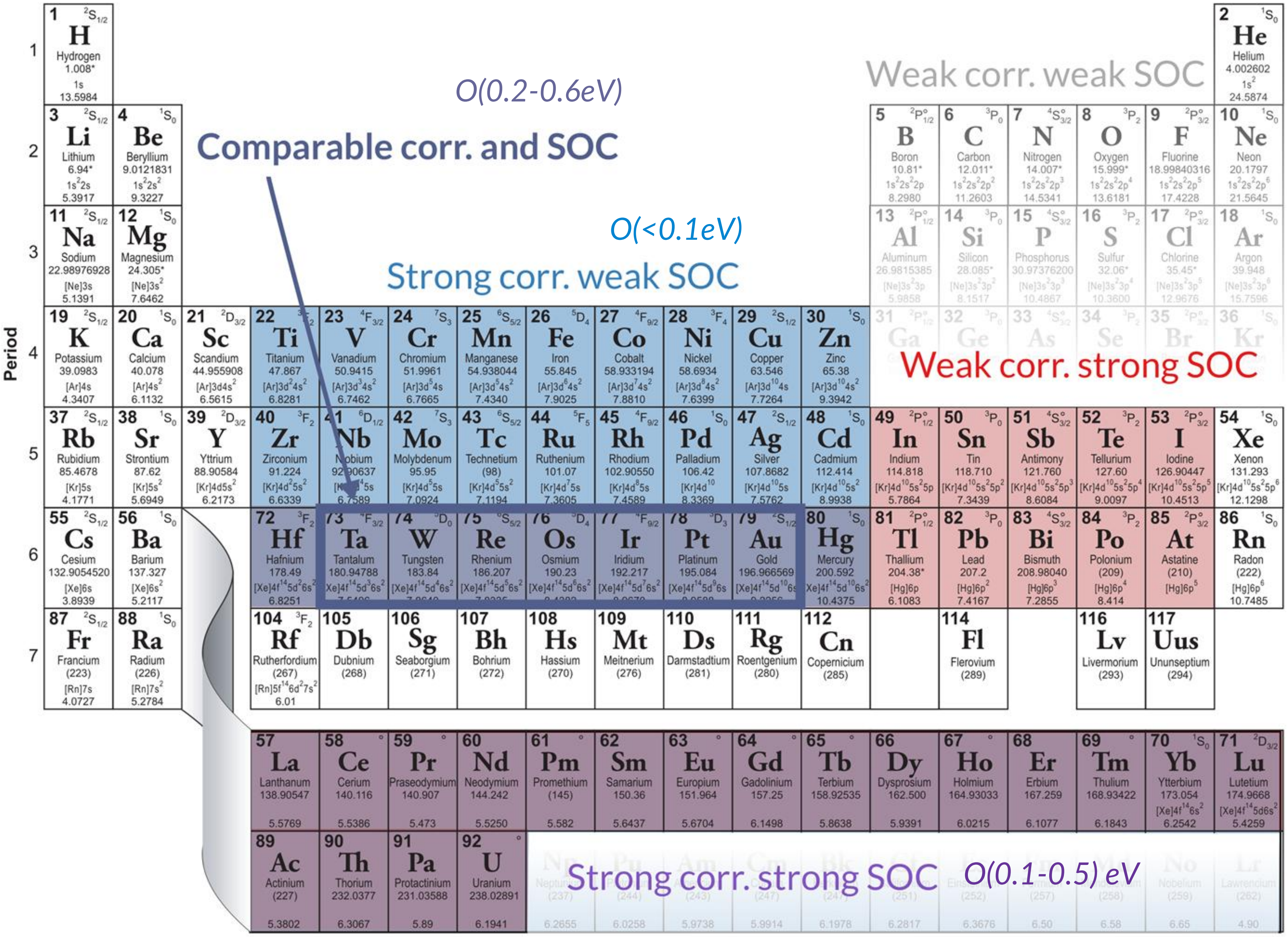
XY $J\sum_{\langle ij\rangle}\left(S_i^xS_j^x + S_i^yS_j^y\right)$

Ising $J\sum_{\langle ij\rangle}S_i^zS_j^z$

Should we expect some simple, robust limits? … or we should get **everything**? Depends on strength of SOC

I. Dzyaloshinskii, J. Phys. Chem. of Solids **4**, 241 (1958), T. Moriya, Phys. Rev. **120**, 91 (1960)

Spin-orbit coupling



Increases with Z

(does **not** scale as Z^4; screening)

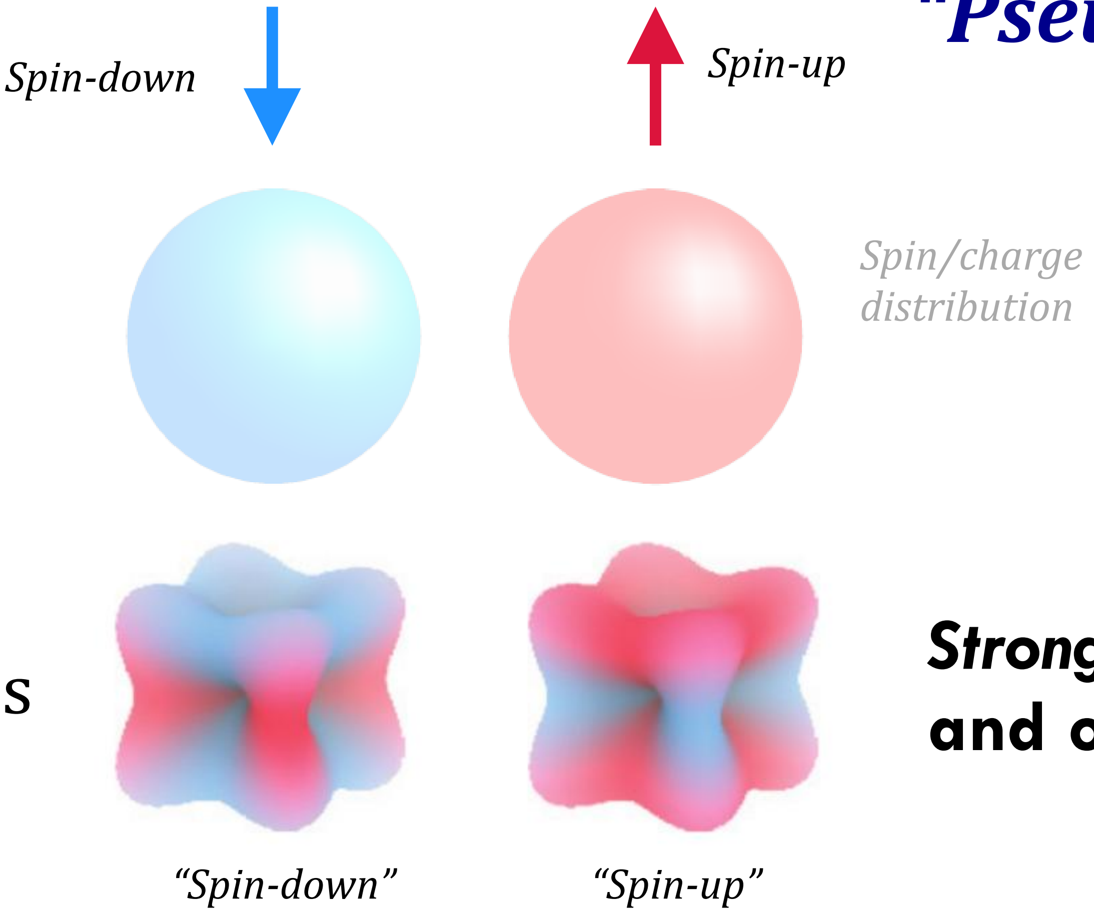
What do we mean by *spin*?

With strong spin-orbit spin & orbital *no longer distinct*

"Pseudo-spin-1/2

So instead of atomic states like this:

... *pseudo-spin-1/2* states can look like this:



***Strongly* mix spin and orbital states**

Protected by Kramers' theorem or spatial symmetries

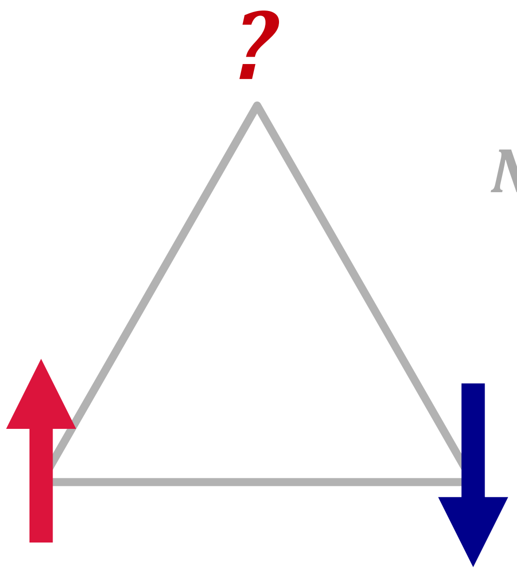
Where to find spin liquids?

(Or: How to get interesting collective behaviour?)

Competition between many states → Complex behaviour

Frustration: Inability to satisfy all interactions simultaneously

Generically leads to ***many competing states***

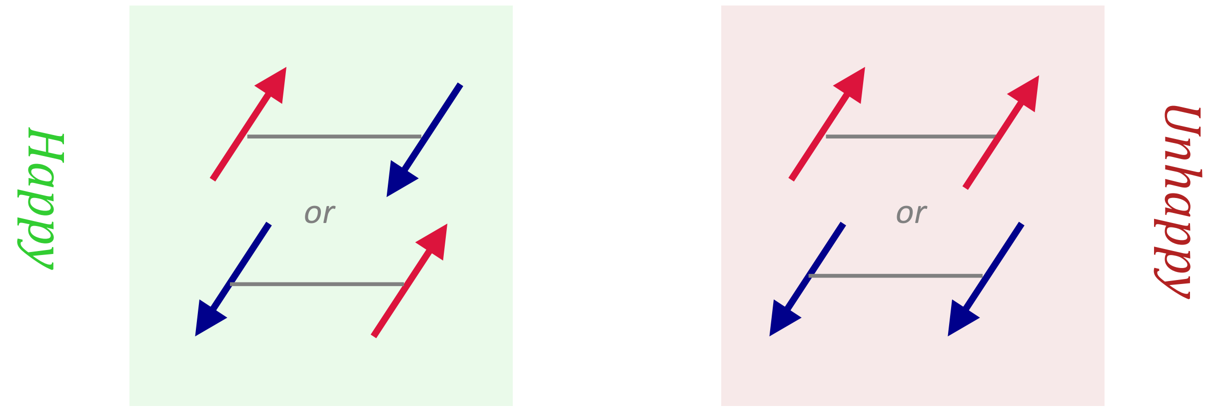


*No choice to satisfy **all** bonds*

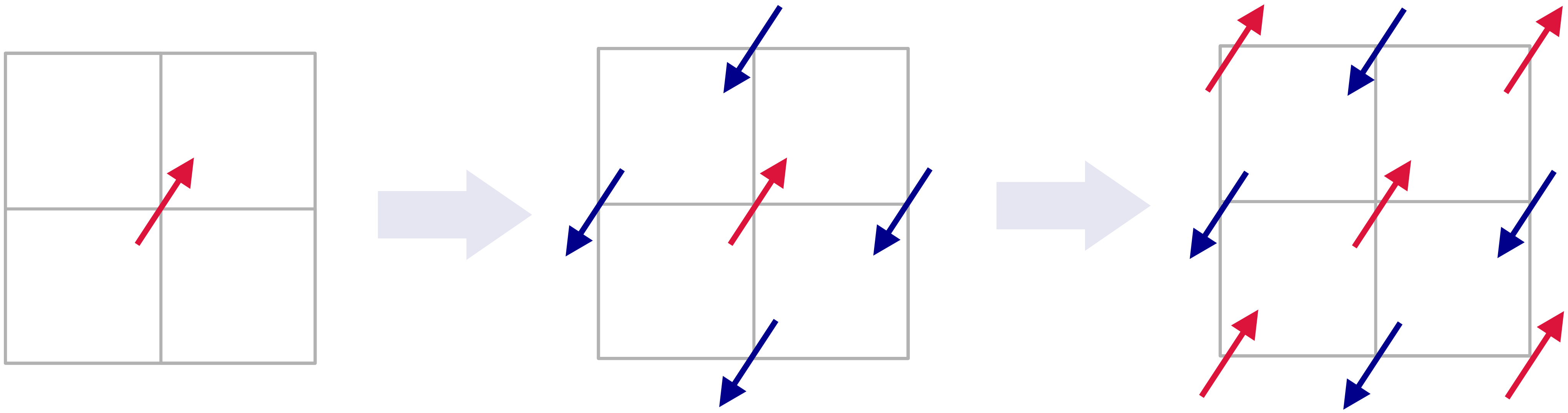
"All happy families are alike; each unhappy family is unhappy in its own way"

– L. Tolstoy

Example of an *unfrustrated anti*-ferromagnet:



Spins tend to anti-align with neighbours

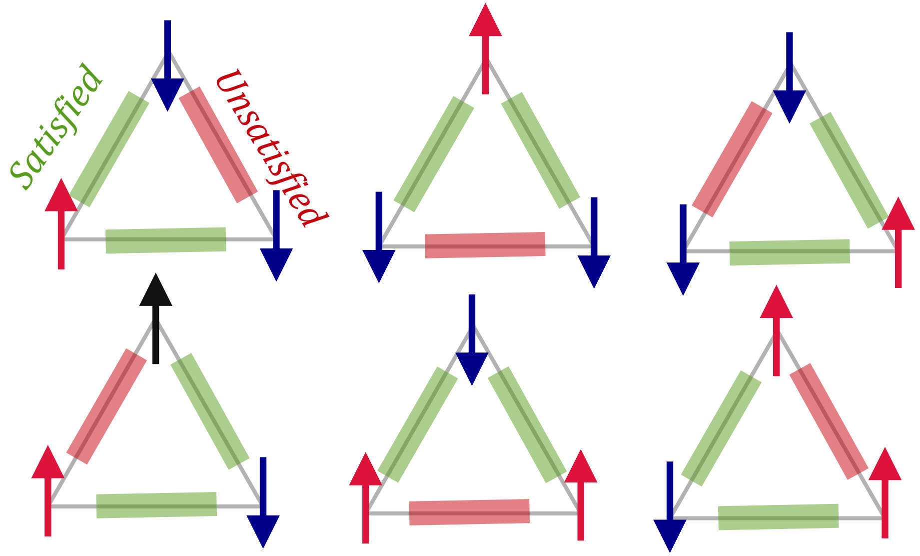


Two intial choices

One way to satisfy all pairs

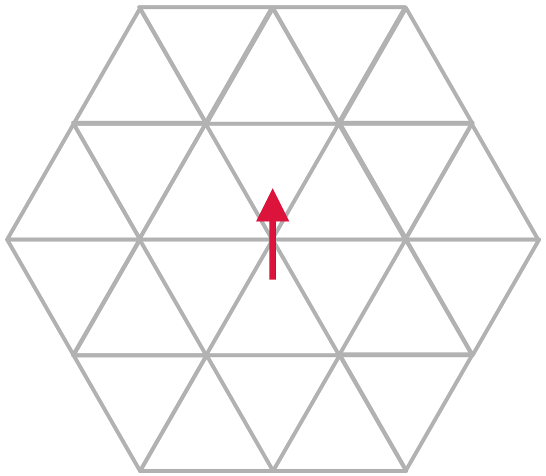
(Essentially) *unique* satisfied state

How does this go for a ***frustrated*** magnet?

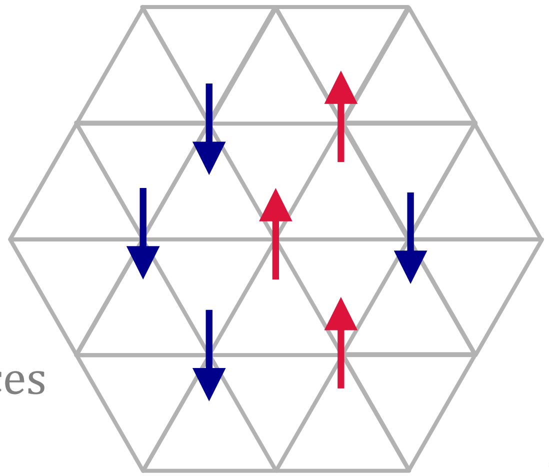


Six *equally unhappy* arrangements on the triangle

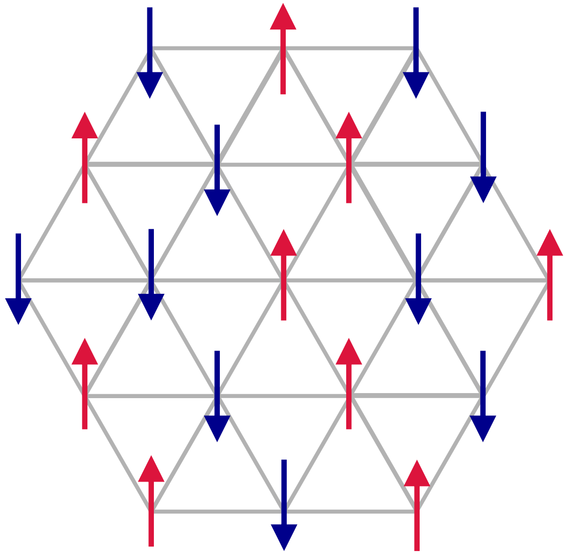
Exponentially many on lattice



Several choices at each step



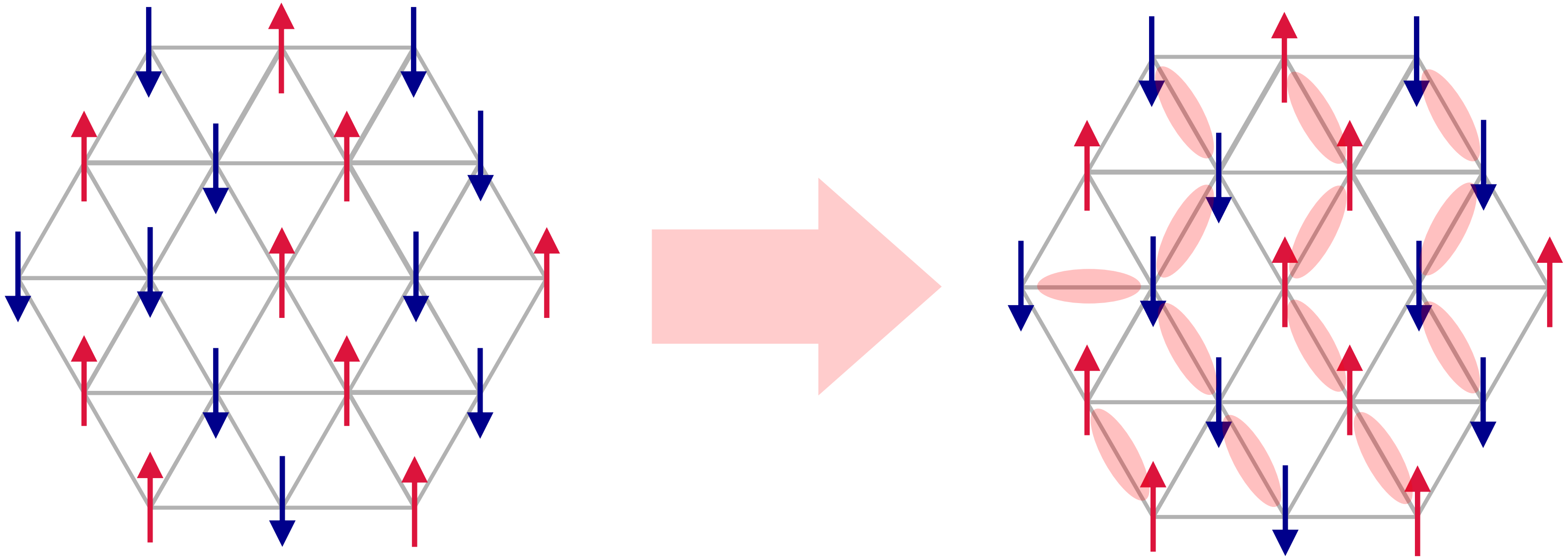
Number of states ~ 1.39^N



This is ***geometric*** frustration

Wannier, Phys. Rev. (1950)

Many, many states – what are their properties?



Triangles share unsatisfied edge

Disordered, like paramagnet

… but still ***correlated***

Example of a *cooperative paramagnet* or

"(Classical) Spin liquid"

More broadly this goes like:

Start here: **Frustrated magnet**

Highly degenerate set of states

Third law

Unconventional

Ordered States

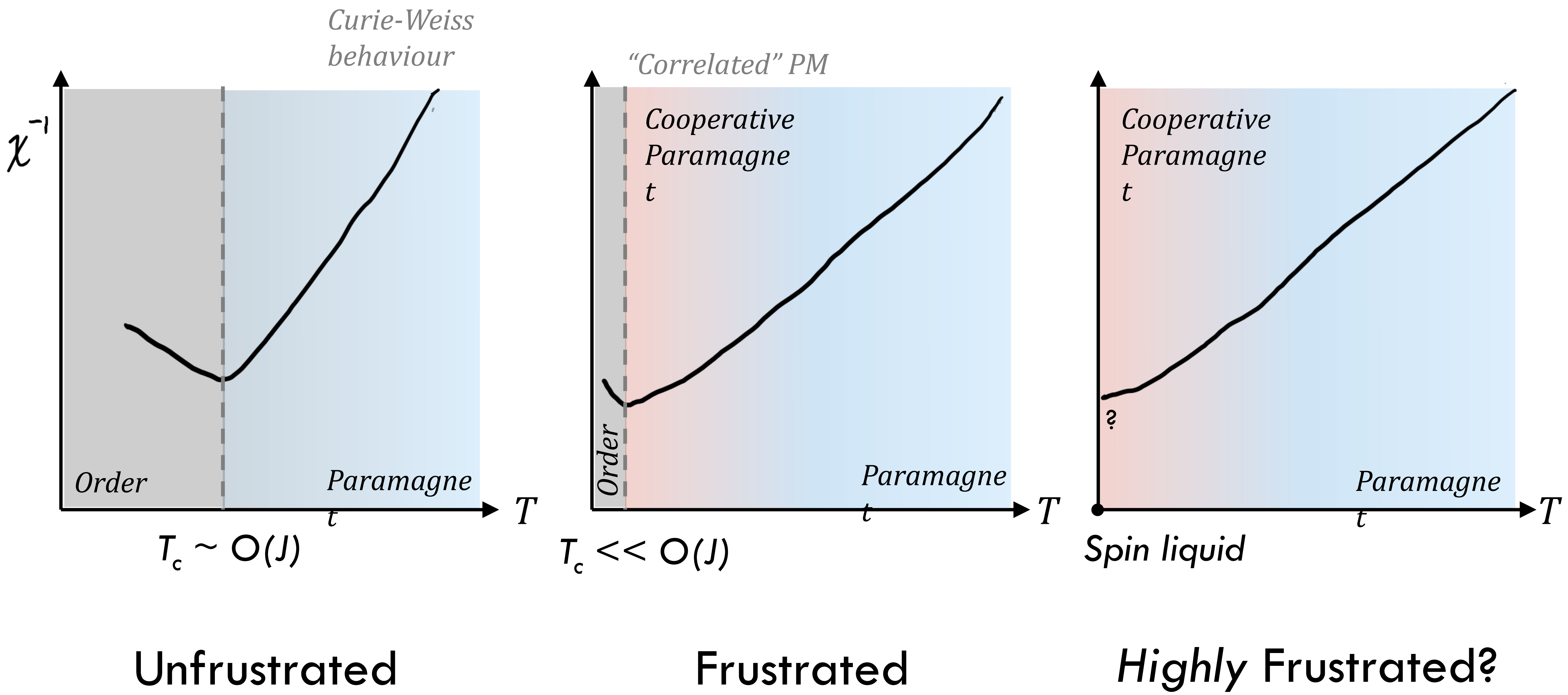
- "Order-by-disorder"
- Incommensurate order
- Skyrmion lattices
- ...

Detail dependent

Disordered States

- Valence bond crystals
- Spin Glasses
- ...
- ***Spin liquids***

"Exotic" phases of matter



Curie-Weiss behaviour
χ^{-1}
Order
Paramagnet
T
$T_c \sim O(J)$
Unfrustrated
"Correlated" PM
Cooperative Paramagnet
Order
Paramagnet
T
$T_c << O(J)$
Frustrated
Cooperative Paramagnet
?
Paramagnet
T
Spin liquid
Highly Frustrated?

Why are spin liquids interesting?

Fractionalized excitations

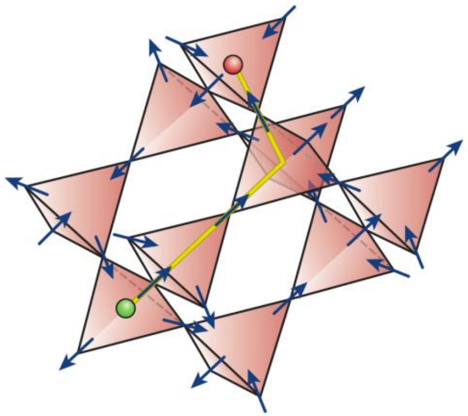
Excitations *split* into new independent parts

Emergent *gauge* theories

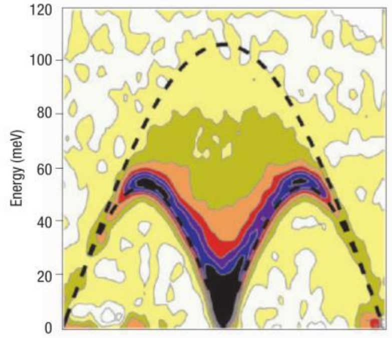
Realizations of electromagnetism, complete with *new* photon

Topological order

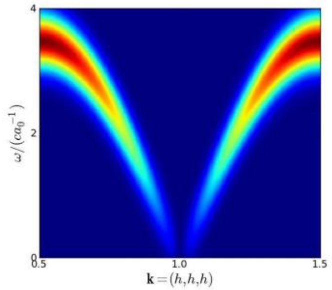
Long-range quantum entangled ground states



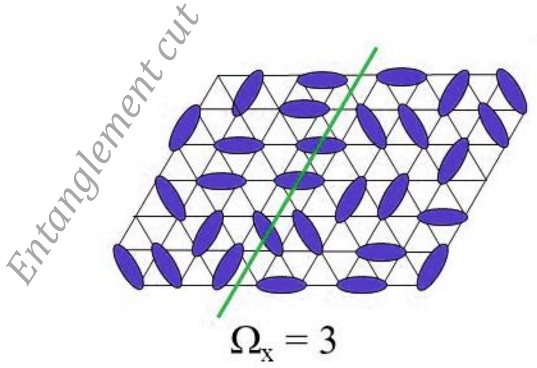
Magnetic monopoles in spin ice

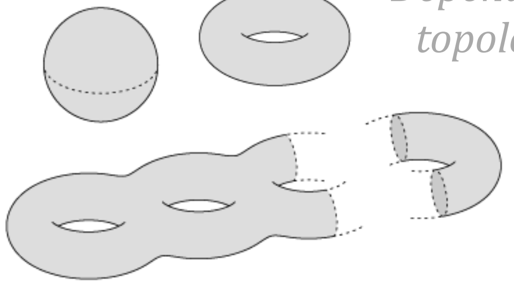


Spinons in a spin chain



Prediction for emergent photon in quantum spin ice

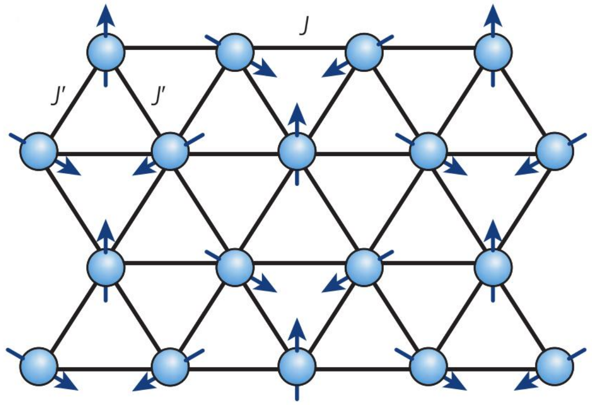


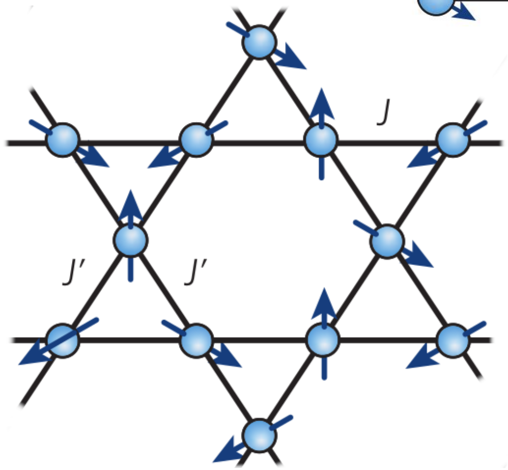


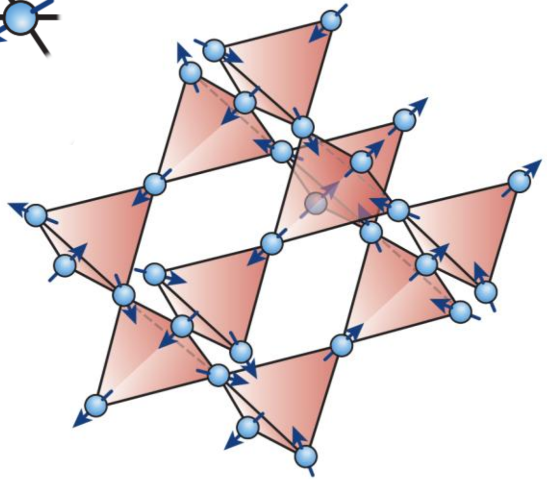
Depends on topology

What kind of models are *known* to have spin liquid ground states?

Lots of triangles







- **Classical models**
  - Triangular Ising AFM
  - Pyrochlore Heisenberg AFM
  - **Spin ice**, …

Extensive ground state manifolds

Quantum

- **Exactly solvable models**
  - Toric code,
  - **Kitaev's honeycomb model**
  - String-net models, …

Hand-crafted interactions

- **Non-solvable models**
  - Kagome anti-ferromagnet
  - **Quantum spin ice**
  - J_1-J_2 models, …

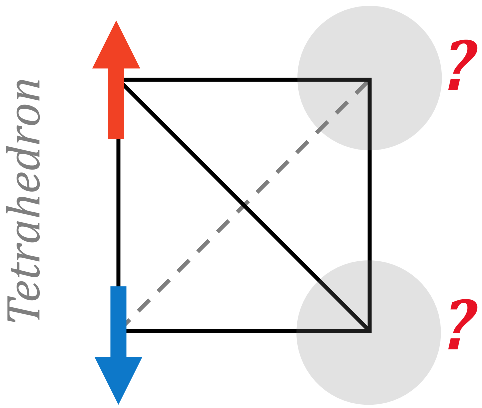
Numerical (mostly)

Quantum Spin Ice

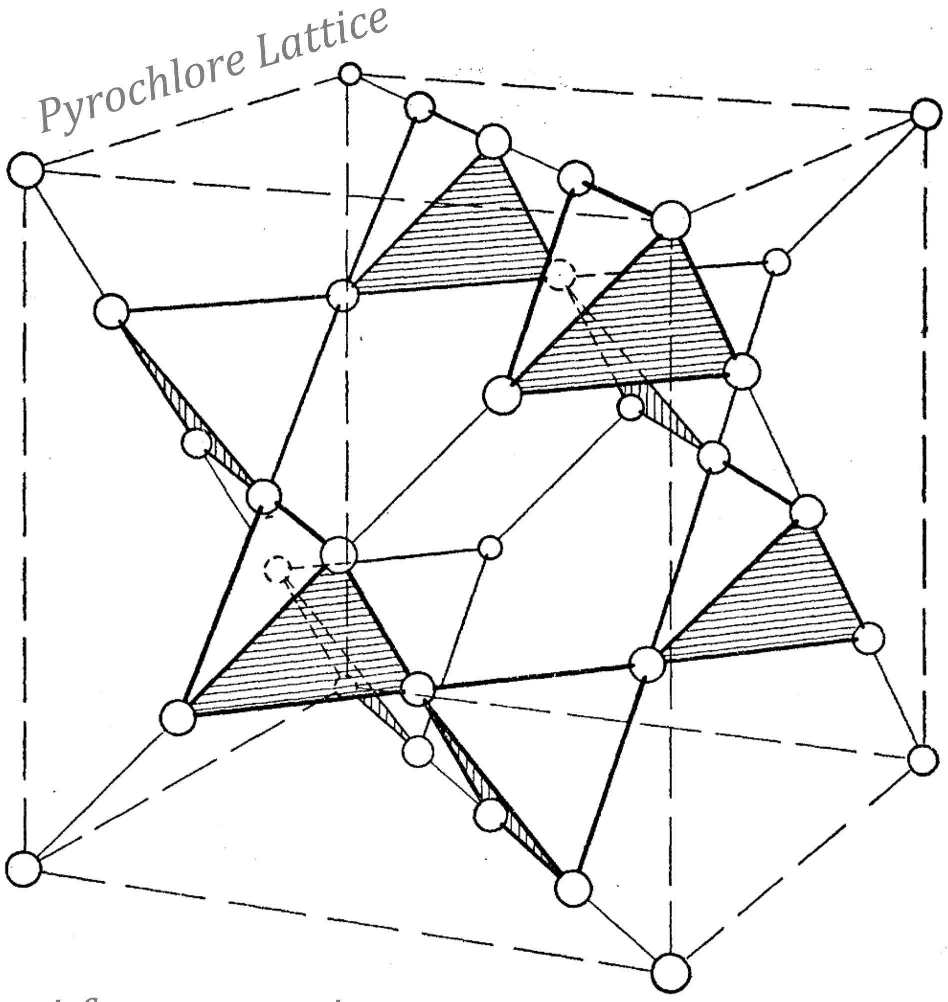
i. Classical Spin Ice
ii. Magnetic Monopoles
iii. Effective Quantum Hamiltonian
iv. Mapping to QED

Classical Spin Ice

- Simplest realization: *Ising model on pyrochlore lattice*
- Lattice of *corner-sharing tetrahedra*
- Four spins, want to **anti-align** with *all others*



No one way to do it!



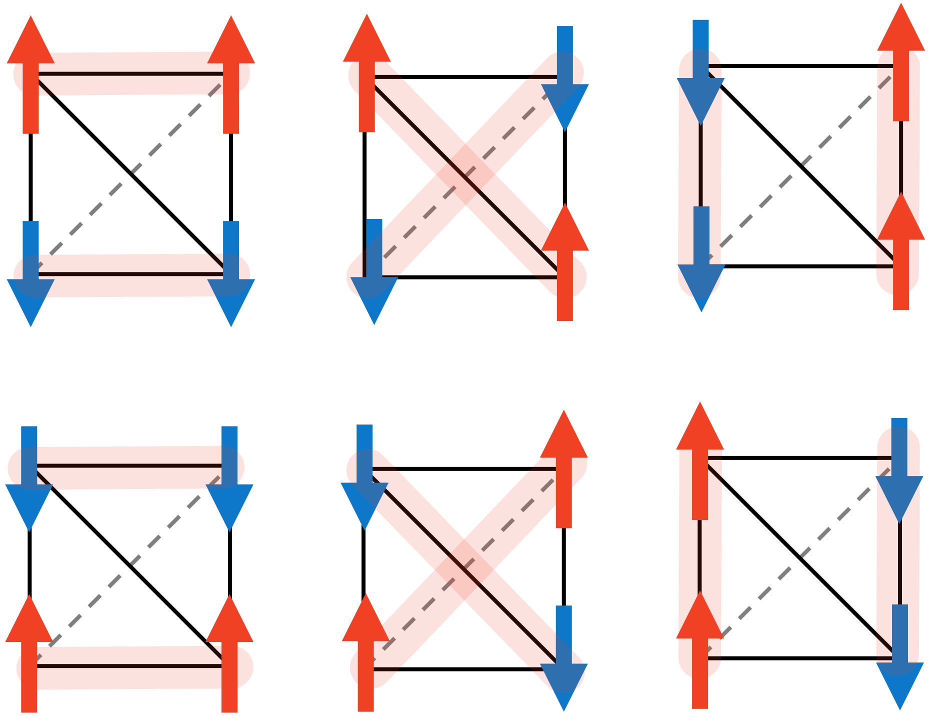
Anti-ferromagnetic exchange

$$E = J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

P. Anderson, Phys. Rev. ***102****, 1008*

… *highly frustrated* model

“Two up and two down”

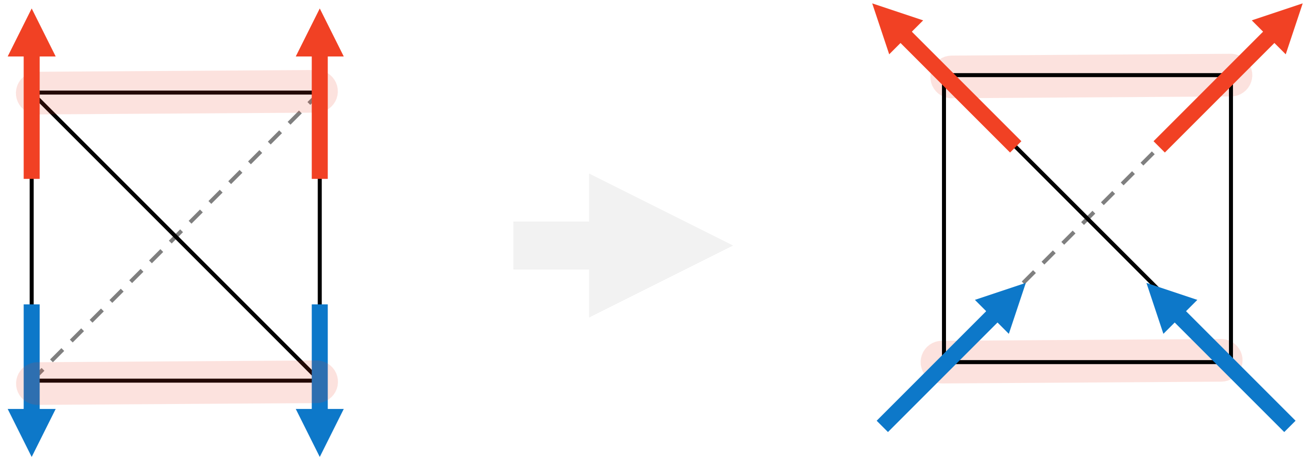


Six ***equally bad*** *ways to arrange*

- We’ll draw our pictures in **two-dimensions**
- Ising model on *checker-board lattice*
- ***“Square Ice”***

… small change in perspective

"Two up / two down"



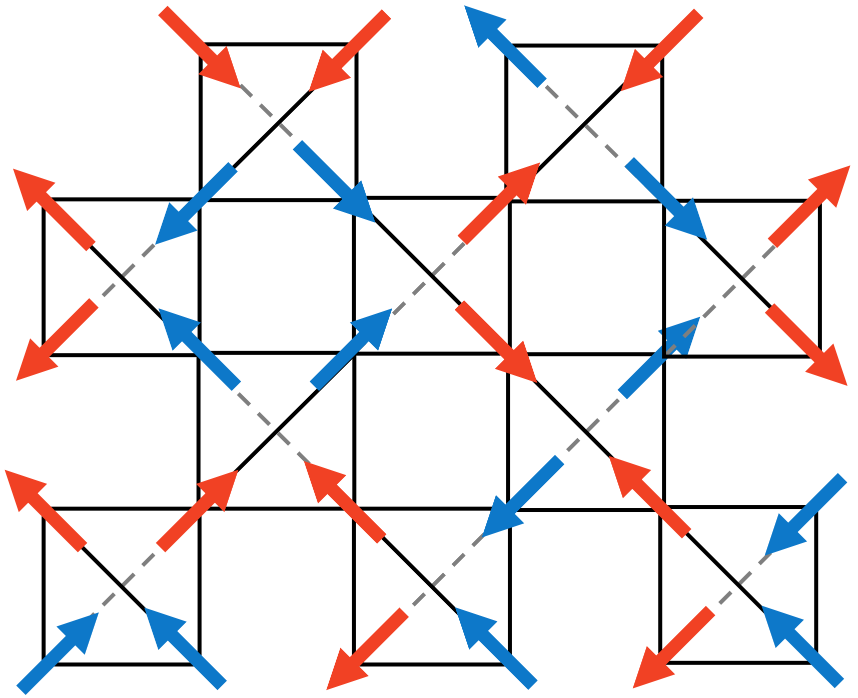
"Two in / Two out"

Closer to how the magnetic dipoles are *really* aligned in materials

When in doubt follow red vs. blue

… does moving to full lattice change this? ***No***

"Checkerboard" lattice



Many, many ways to arrange these

"Square ice" or "Six-vertex model"

- Number of minimal energy states is **exponential** in number of spins:

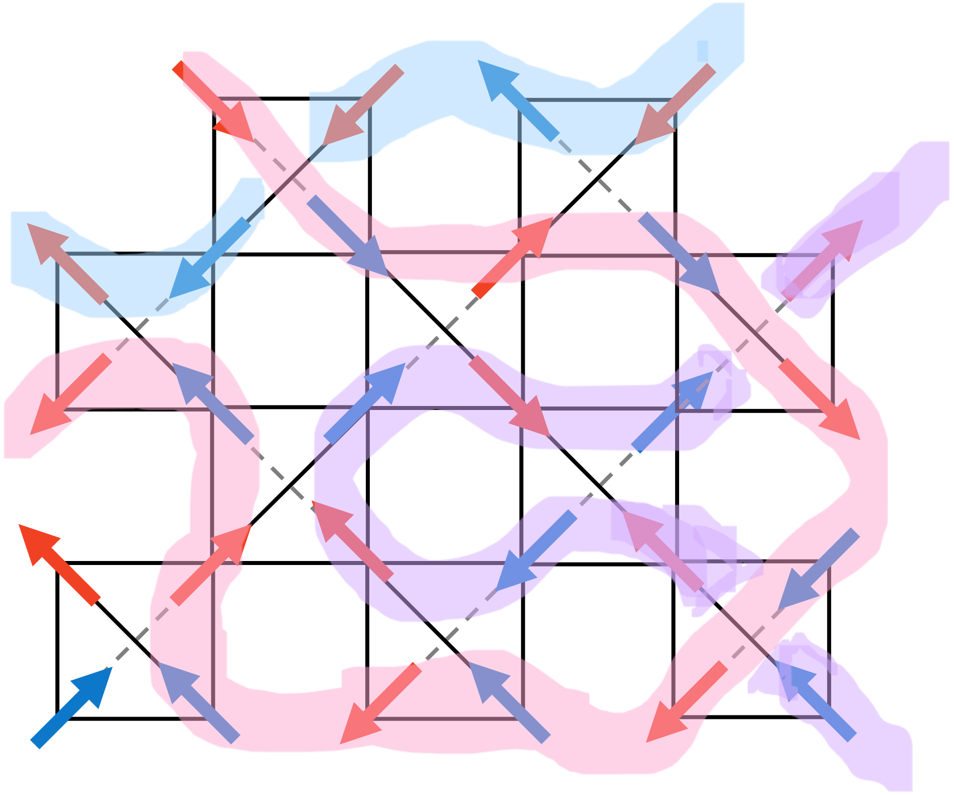
$$\Omega = \left(\frac{4}{3}\right)^{3N/4}$$

- Leads to non-zero, **residual entropy** at *T=0*

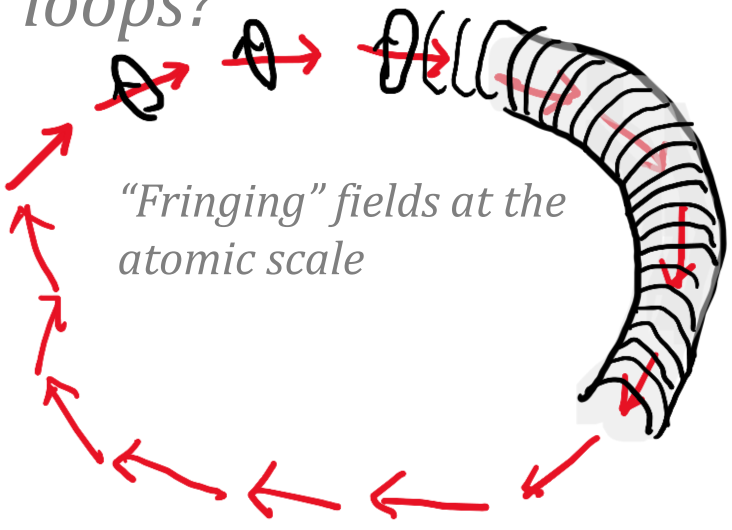
$$S = k_B \log \Omega \approx 0.2157 k_B N$$

E. Lieb, Phys. Rev. ***162****, 162 (1967)*

Loop structure of ice states



Magnetic fields of loops?



Mostly cancel

Chain of magnetic dipoles

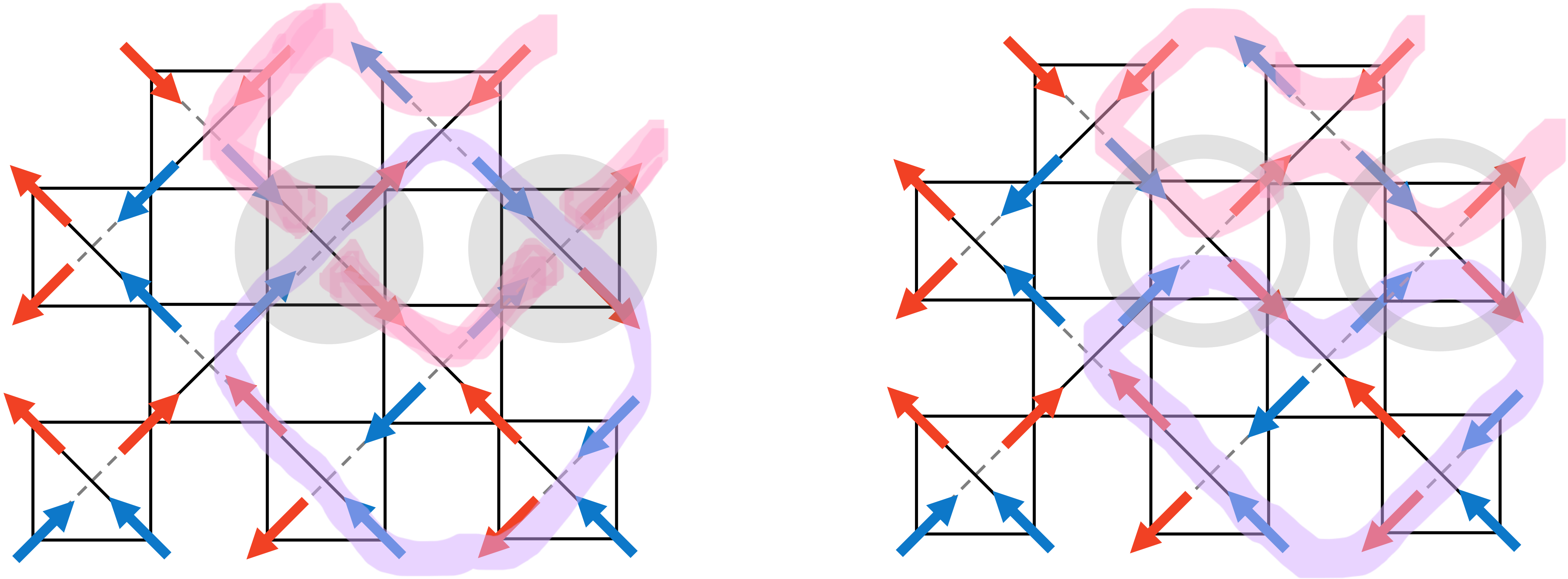
Chain of current loops

Solenoid!

Loop formation is *emergent* version of $\nabla \cdot B = 0$

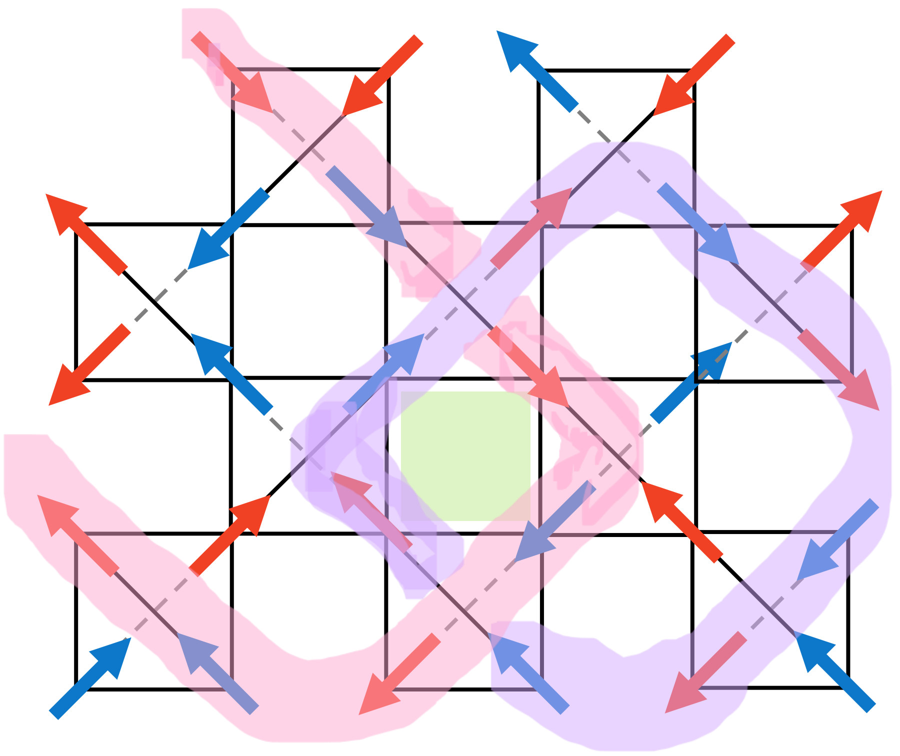
"Field lines form loops"

… these loops are *everywhere*

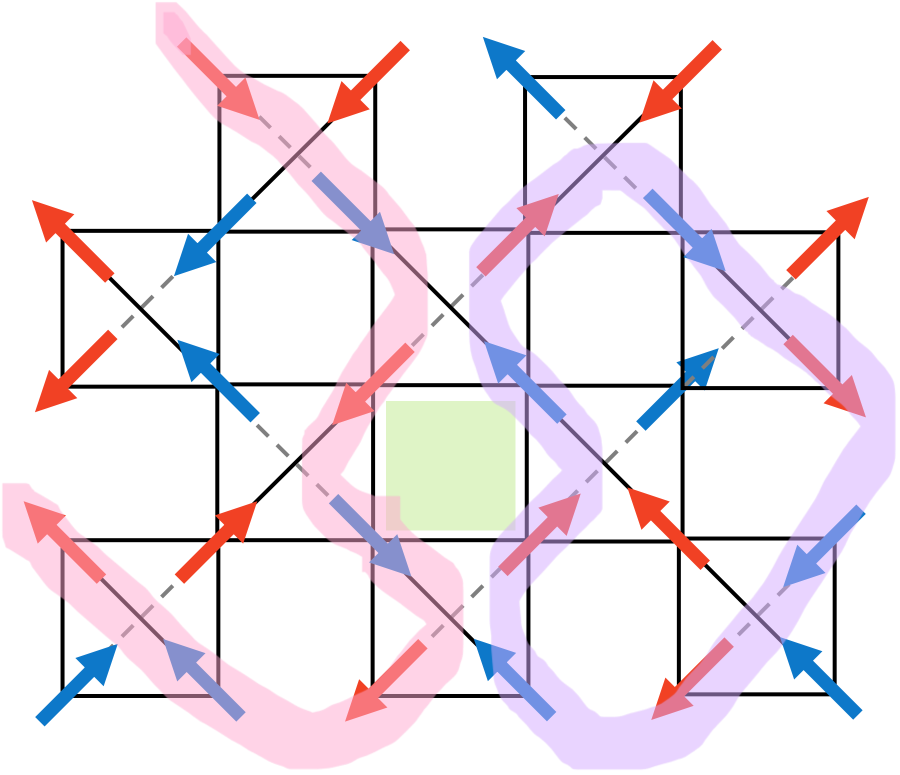


… and *not uniquely tied together*

Further, they can be re-arranged at ***no cost***

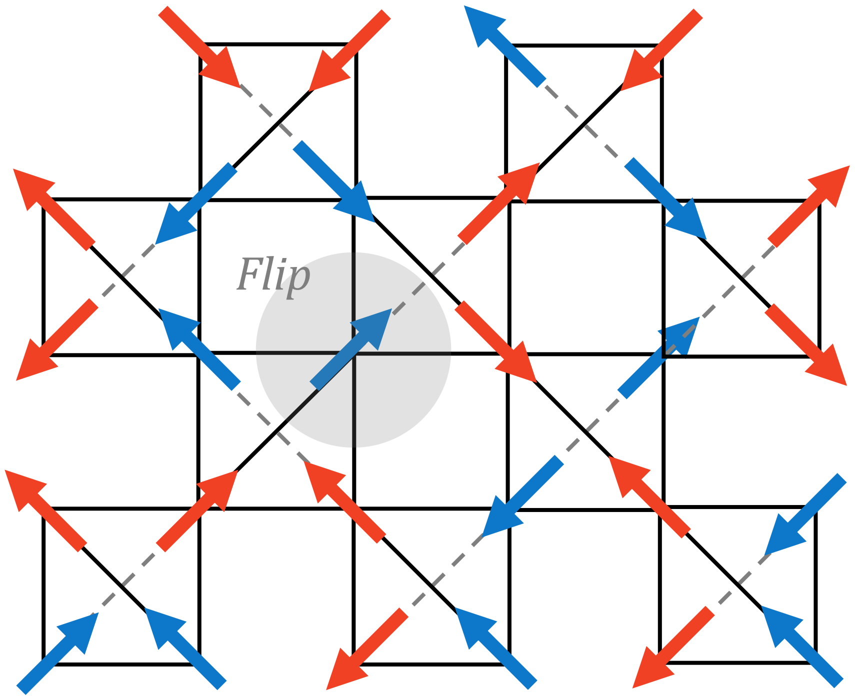


Flip small loop

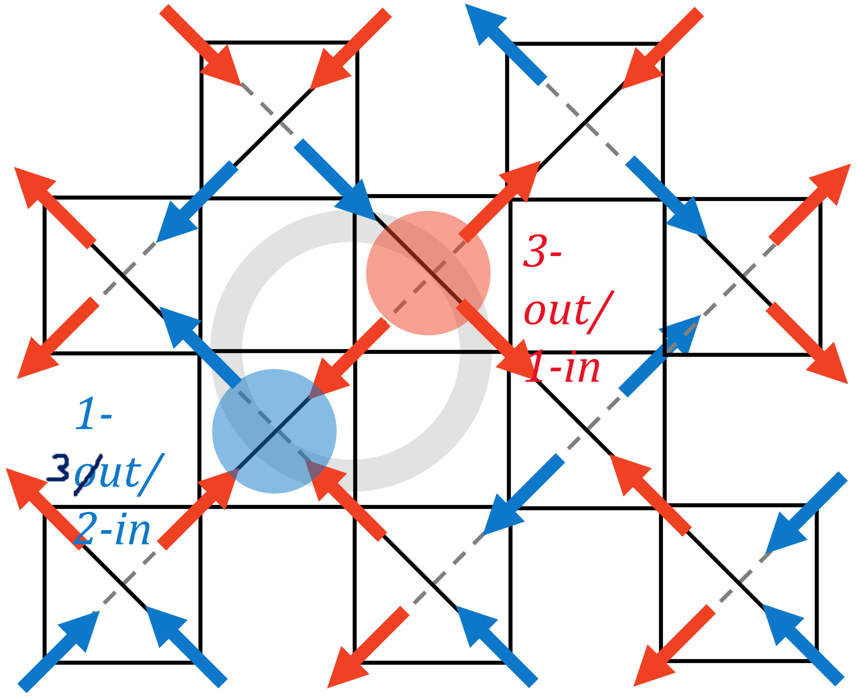


Still minimal energy

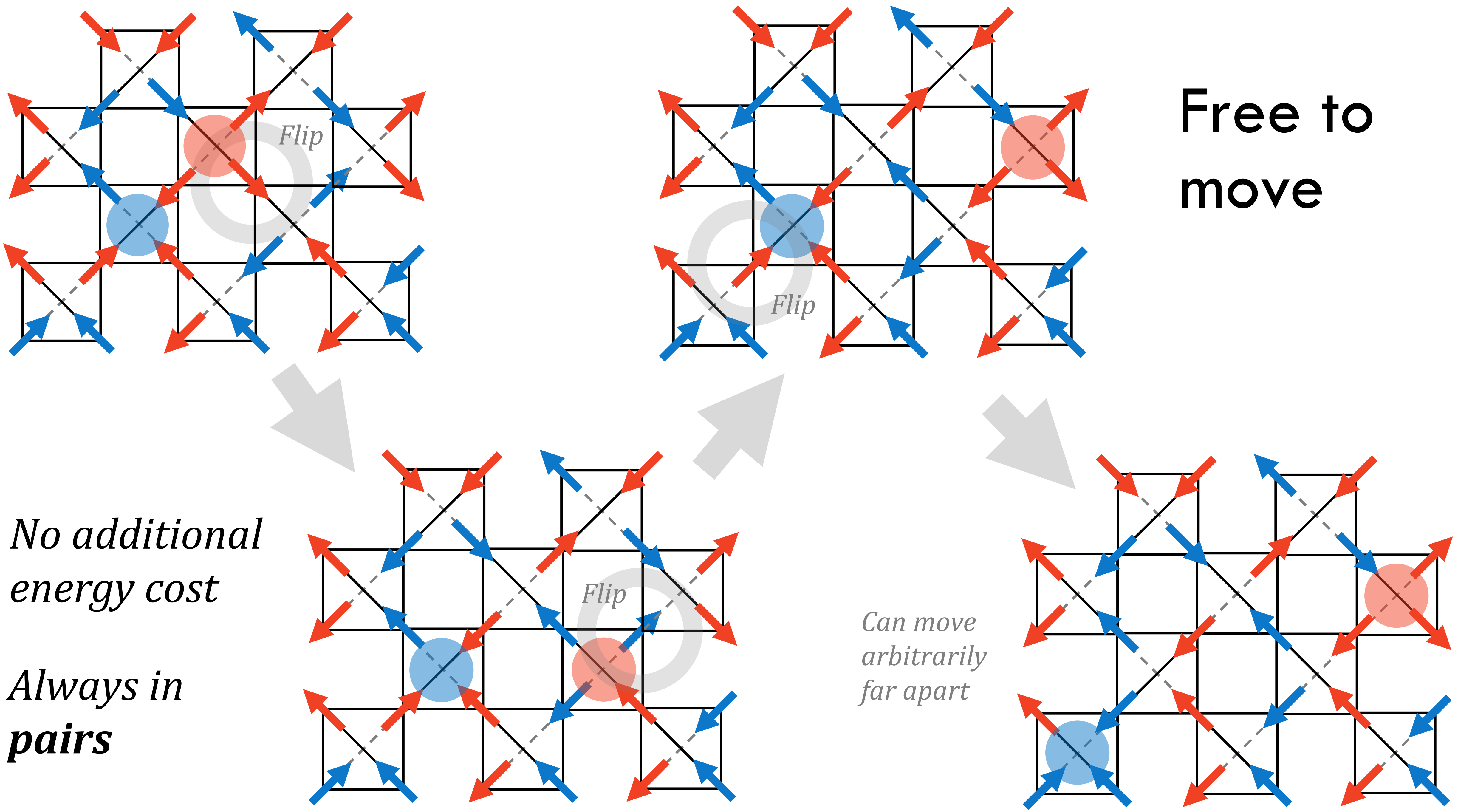
Cut a loop, get a **pair of magnetic monopoles**

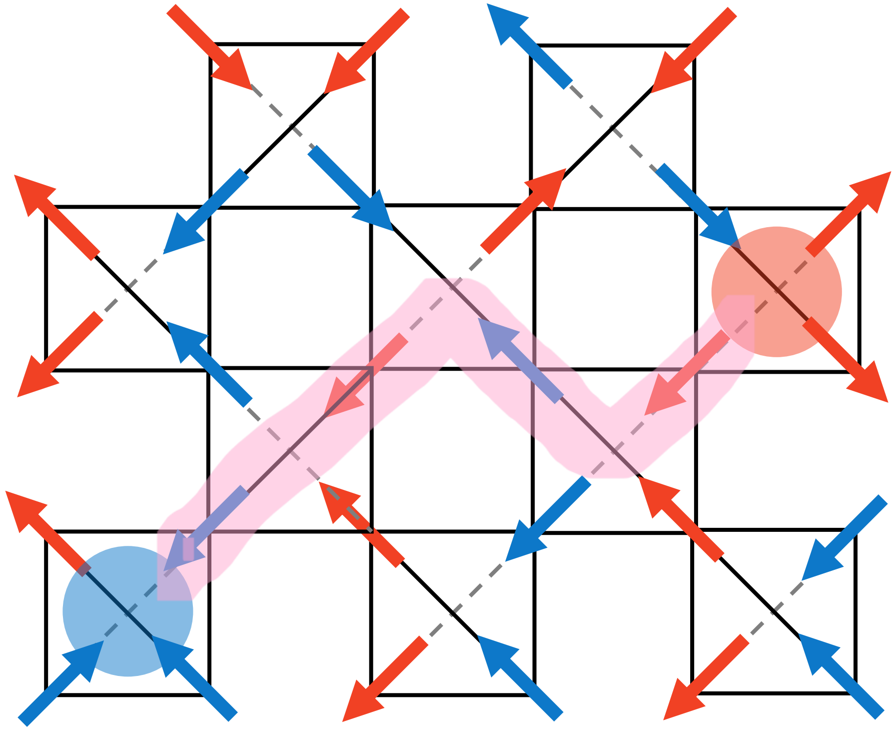


E.g. thermal fluctuations, probes like light, neutrons, …

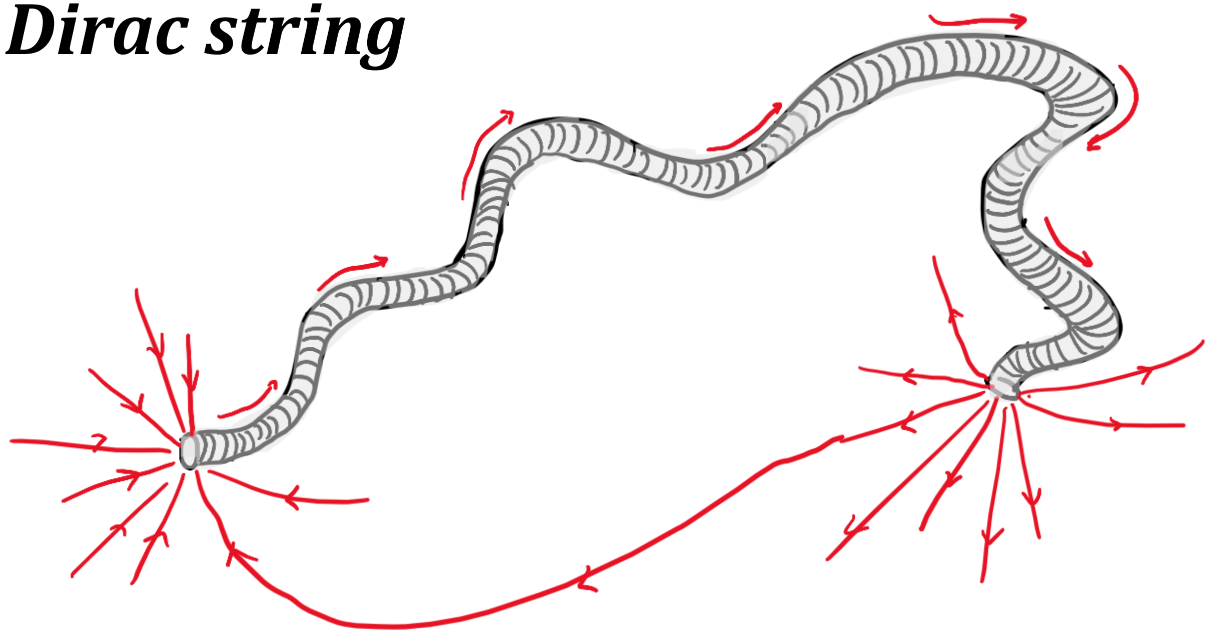


*No longer minimal energy: **Excitation** of system*


Flip
Flip
Flip
Free to move
No additional energy cost
Always in **pairs**
Can move arbitrarily far apart



Compare this to usual
Dirac string

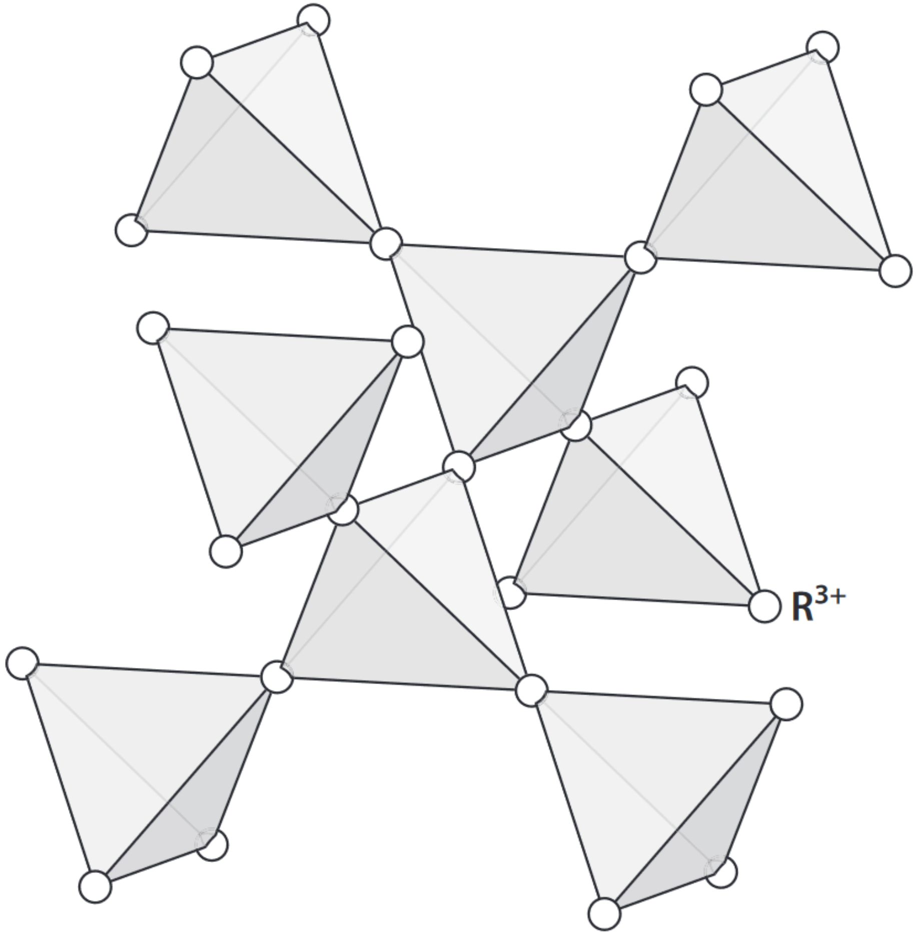


Example of ***fractionalization***

Lowest energy excitations are effectively ***magnetic monopoles***

P. Dirac

Experimental Realizations

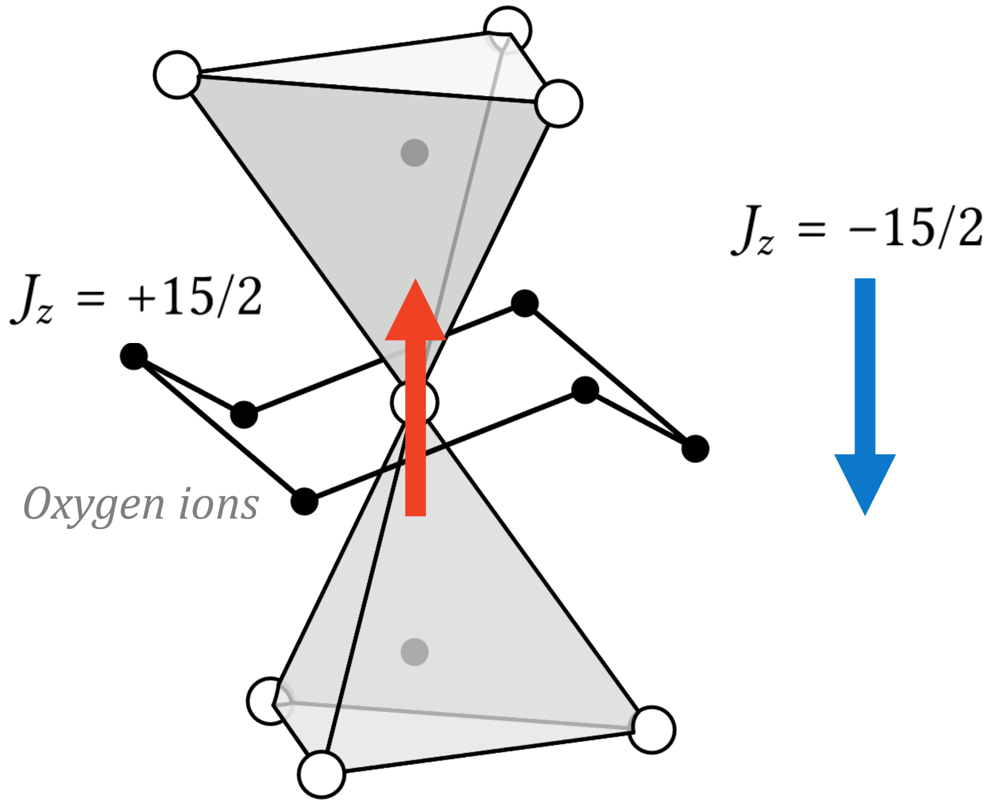


Chemical formula: $\boldsymbol{R_2M_2O_7}$

- Growing family of materials
- Mostly *three-dimensional* **pyrochlore lattice**
  - *Network of corner-sharing tetrahedra*
- Magnetic ion is a trivalent **rare-earth**
  - *Best examples are* $\boldsymbol{Dy_2Ti_2O_7}$ ***and*** $\boldsymbol{Ho_2Ti_2O_7}$

For a review, see: Rev. Mod. Phys. ***82****, 53 (2010)*

Atomic physics



Giant dipole moment

$$\mu \approx 10\mu_B$$

10x that of single electron

- Rare-earth ion has *huge* amount of angular momentum:

$$J = 15/2,\ L = 5,\ S = 5/2$$

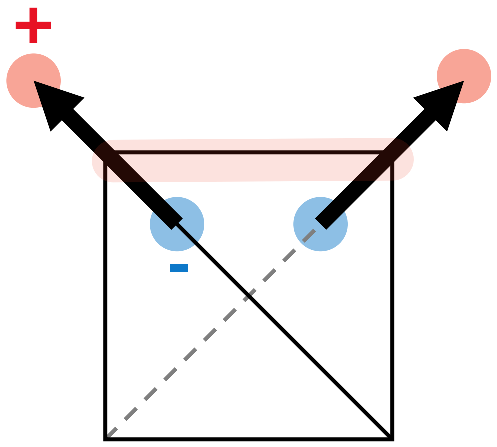
From Hund's Rules

- Both spin *and* orbital contributions
- Surrounding (charged) ions prefer moment ***in*** or ***out*** of the tetrahedron

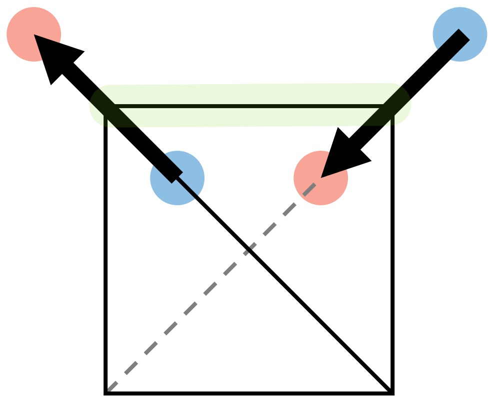
$$|J_z = \pm 15/2\rangle$$

Effect of "crystalline electric field"

… how do they interact? *Mostly* **dipole-dipole**



Charges repel:
Disfavoured



Charges *attract*:
Favoured

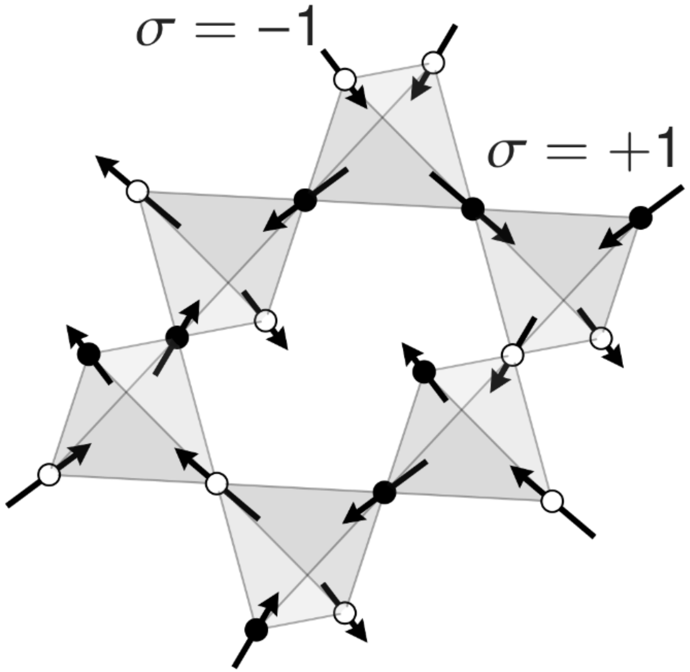
Visualize using “physical” dipoles

- *Just like* our “toy” model from earlier – wants **two-in/two-out** on each tetrahedron

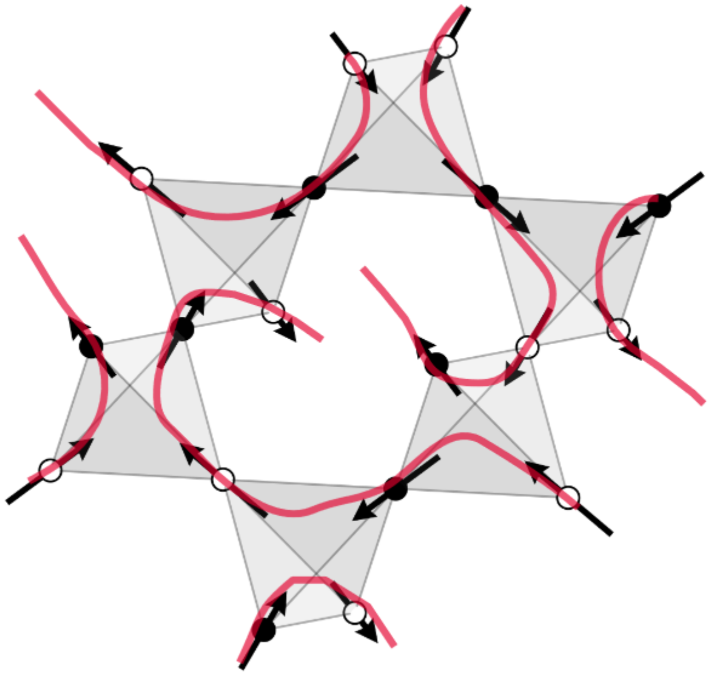
- Full picture *significantly* more complicated
  - *Super-exchange between the 4f electrons is **large***
  - *Multipole interactions must be considered*
- **Final result unaffected**

*JGR and M. Gingras, Phys. Rev. B **92**, 144417 (2015)*

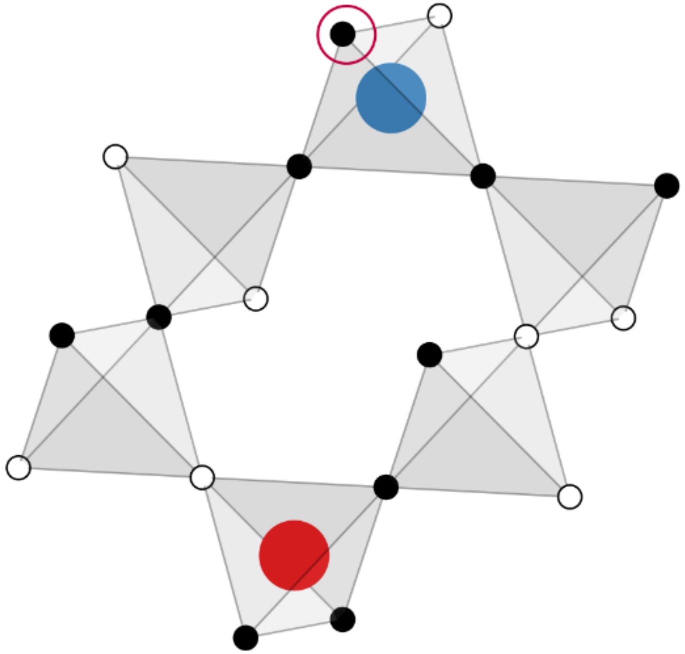
… can draw *precisely* same picture as before



Many, many minimal energy configurations



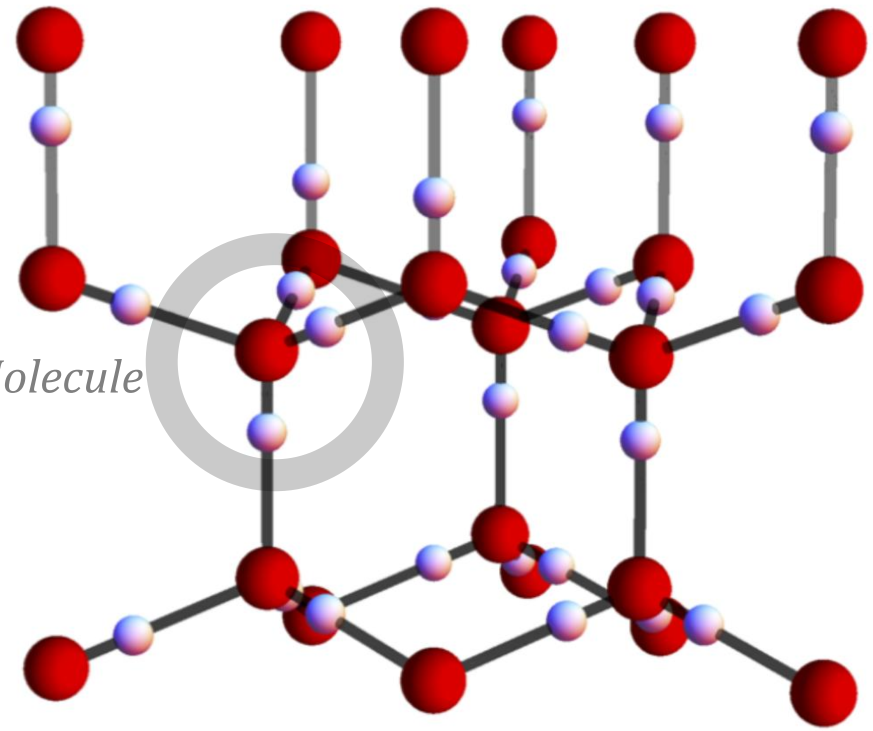
Magnetic dipoles form *loops*



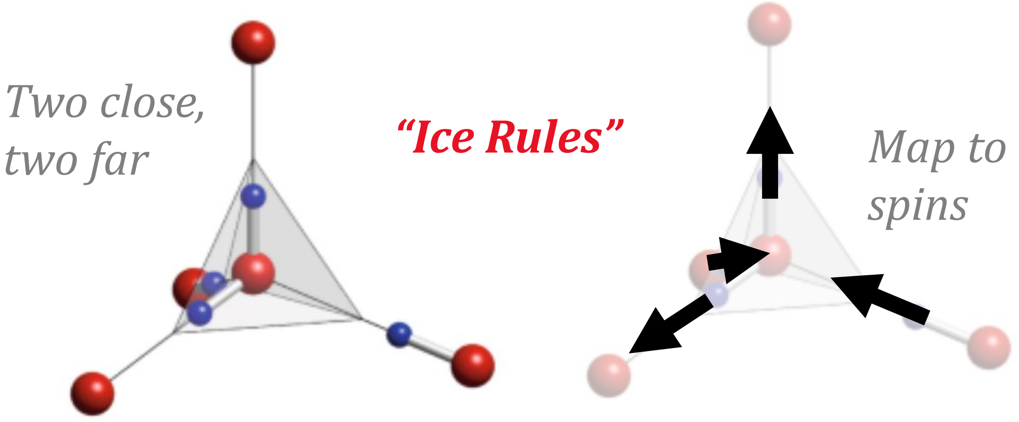
Excitations break them: ***Magnetic monopoles***

Some history: *Proton Disorder in* Water Ice

Hexagonal (I_h) Water Ice

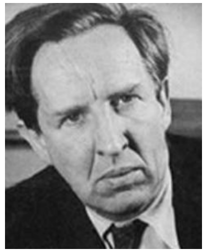


Many, many ways to orient the water molecules



Nearly the same physics!

J. Bernal



R. Fowler

L. Pauling

Key signatures

- Many, many ground states

  Finite, residual entropy at T=0

- Closed loops of magnetic dipoles

  "Pinch-points" in spin-spin correlations

Question:
Are these seen in materials?

Together these tell would tell us the *excitations* are ***magnetic monopoles***

Signature #1: Residual Entropy

- Access via heat capacity:

Experimentally measurable

$$S(T) - S(0) = \int_0^T dT' \frac{C(T')}{T'}$$

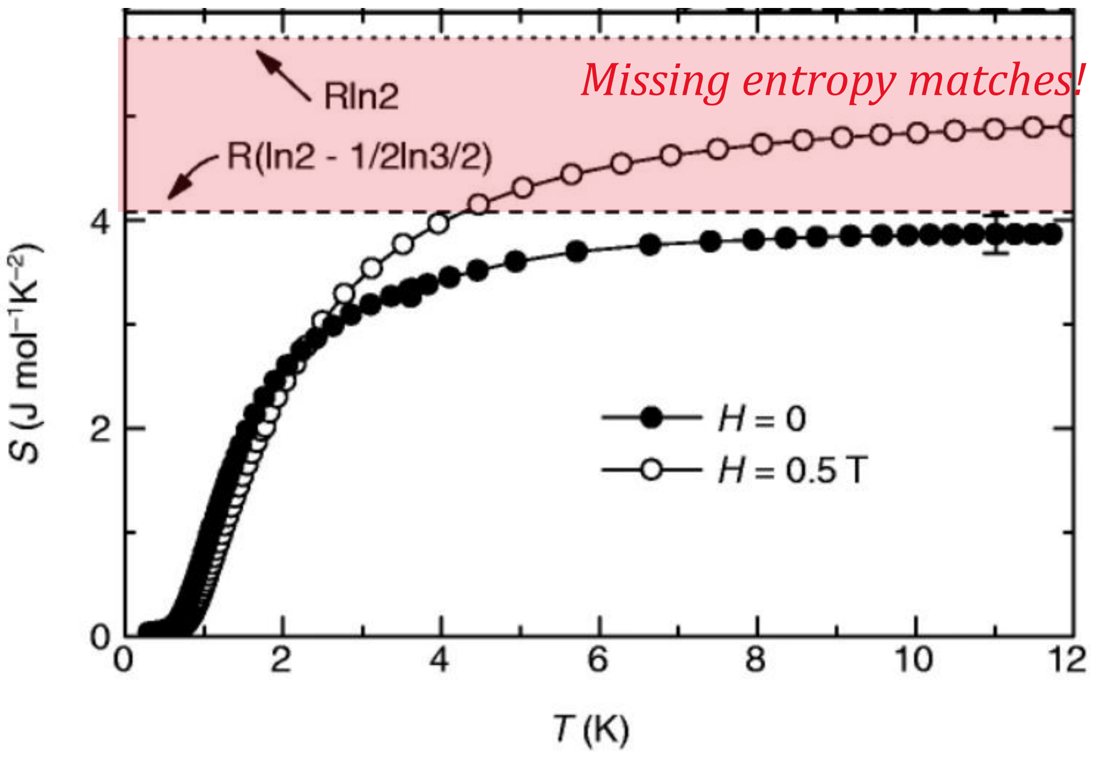
Should be Rlog(2) at high temperature

- Get "missing" amount at high temperature

$$S(0) \approx \frac{R}{2} \log\left(\frac{3}{2}\right) \approx 0.202R$$

"Pauling" Entropy

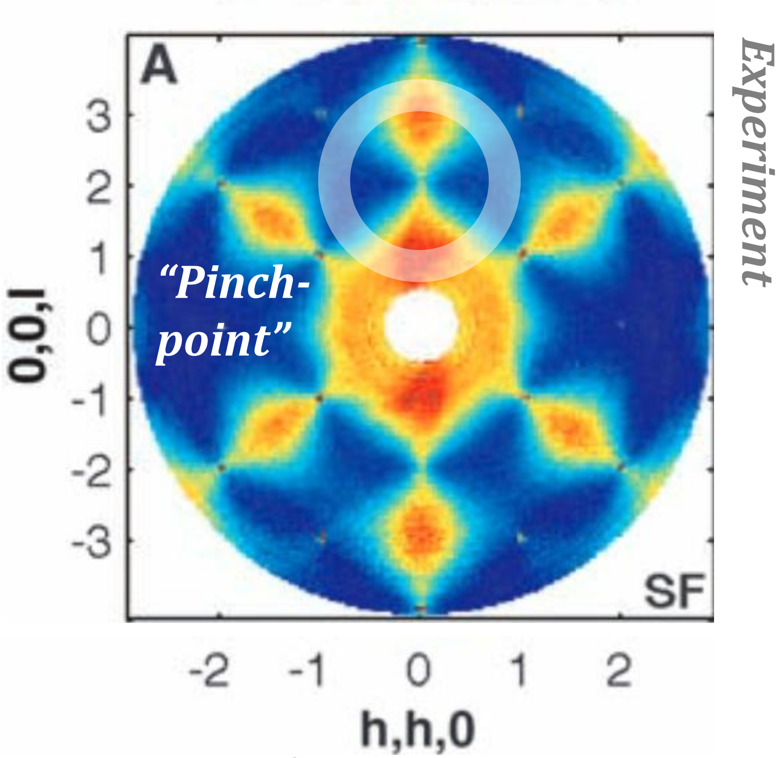
Entropy of $Dy_2Ti_2O_7$ at low temperature



*Ramirez et al, Nature **399**, 333-335 (1999)*

Signature #2: "Loops"

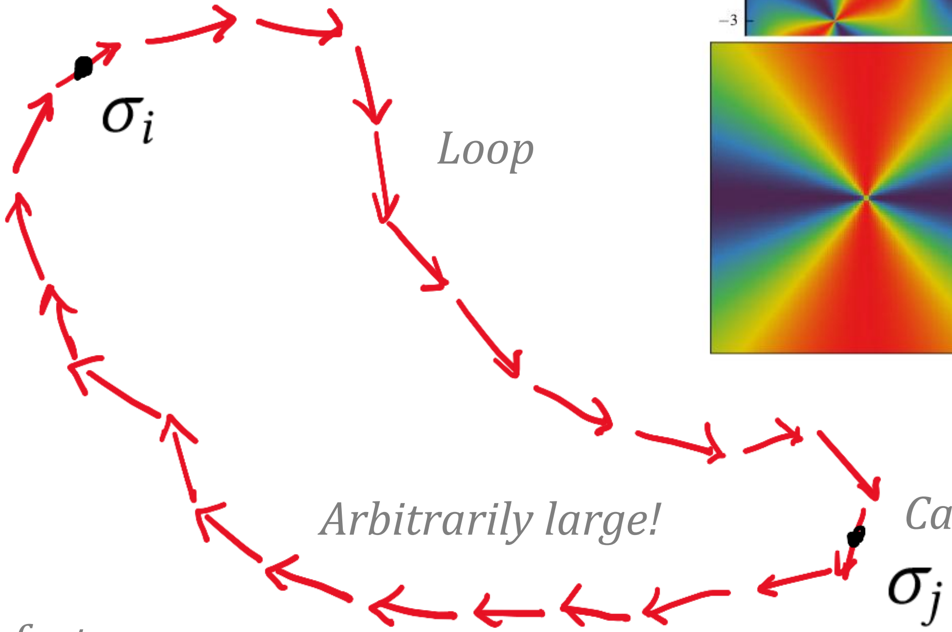
Diffuse neutron scattering on



$$S(\boldsymbol{k}) = \frac{1}{N}\sum_{ij} \langle \sigma_i \sigma_j \rangle \, e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}$$

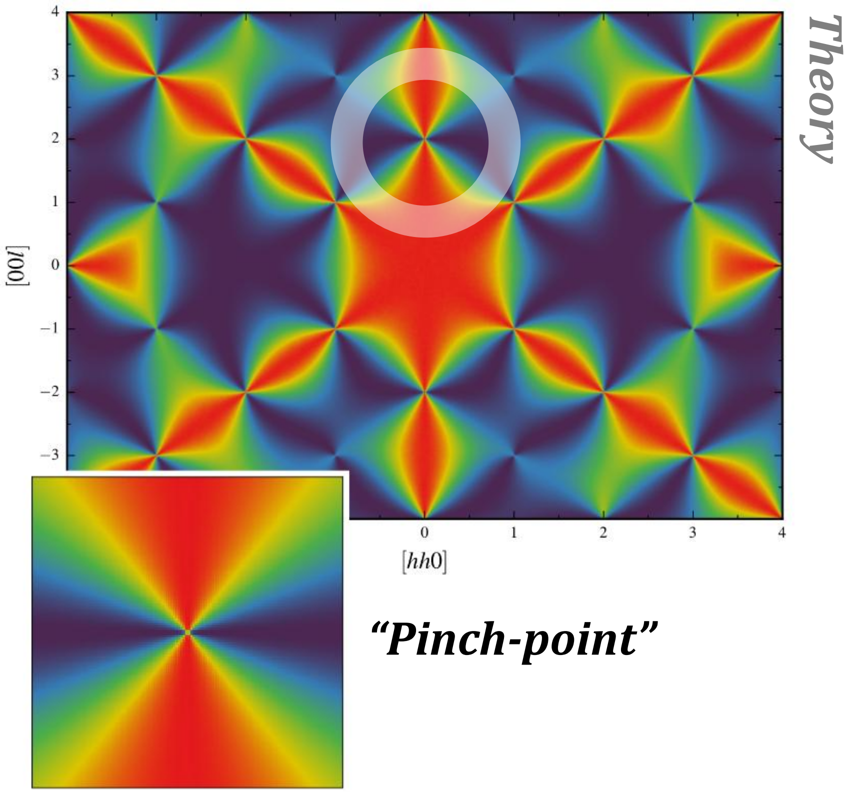
… measures something like the static structure factor

- Since spins form *loops*, the spins on the *same* loop are **highly correlated**



Can't be

Result from simplest version of

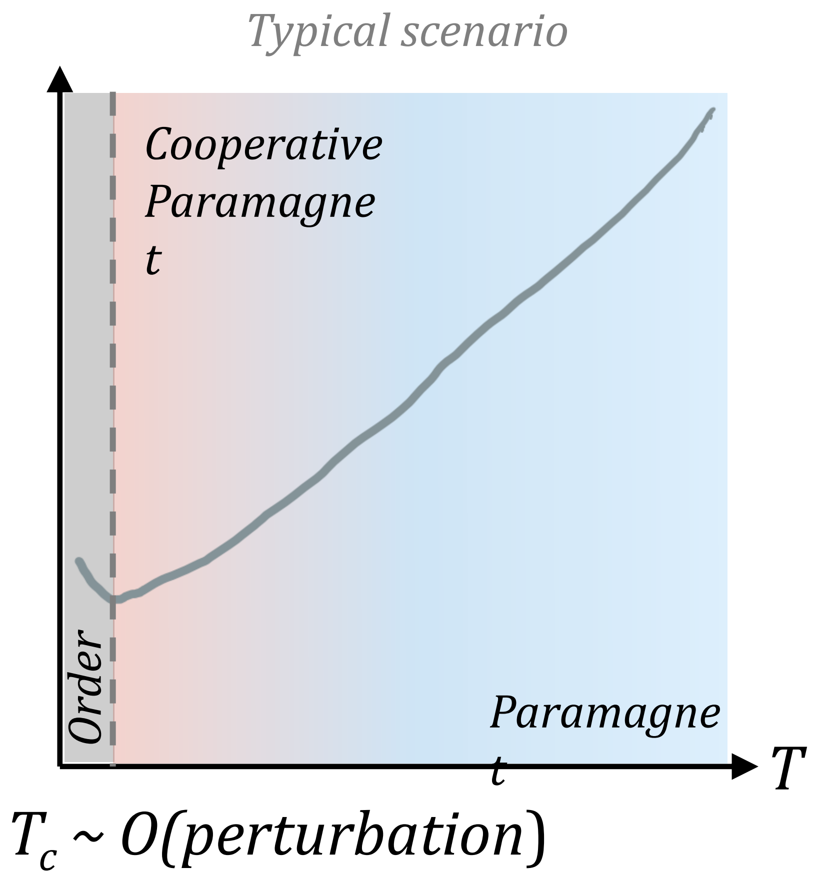


*Fennell et al., Science **326**, 415-417*

Stability?

Classical spin liquids are **unstable to small perturbations,** always *"fine-tuned"*

- "Third-law": Can't have finite entropy density *generically*
- Perturbations that lift degeneracy set ordering scale



Instability *can* be toward *quantum* spin liquid

Quantum Fluctuations

- Perturbations to Ising model: **Anisotropic exchange**

$$H = J_{zz} \sum_{\langle ij \rangle} S_i^z S_j^z - J_{\pm} \sum_{\langle ij \rangle} \left(S_i^+ S_j^- + \text{h.c.} \right)$$
$$+ J_{\pm\pm} \sum_{\langle ij \rangle} \left(\gamma_{ij} S_i^+ S_j^+ + \text{h.c.} \right) + J_{z\pm} \sum_{\langle ij \rangle} \left(\zeta_{ij} \left[S_i^z S_j^+ + S_i^+ S_j^z \right] + \text{h.c.} \right)$$

Ising Exchange

Transverse Exchange

Need $J_{z\pm}$ to be << than other transverse exchanges

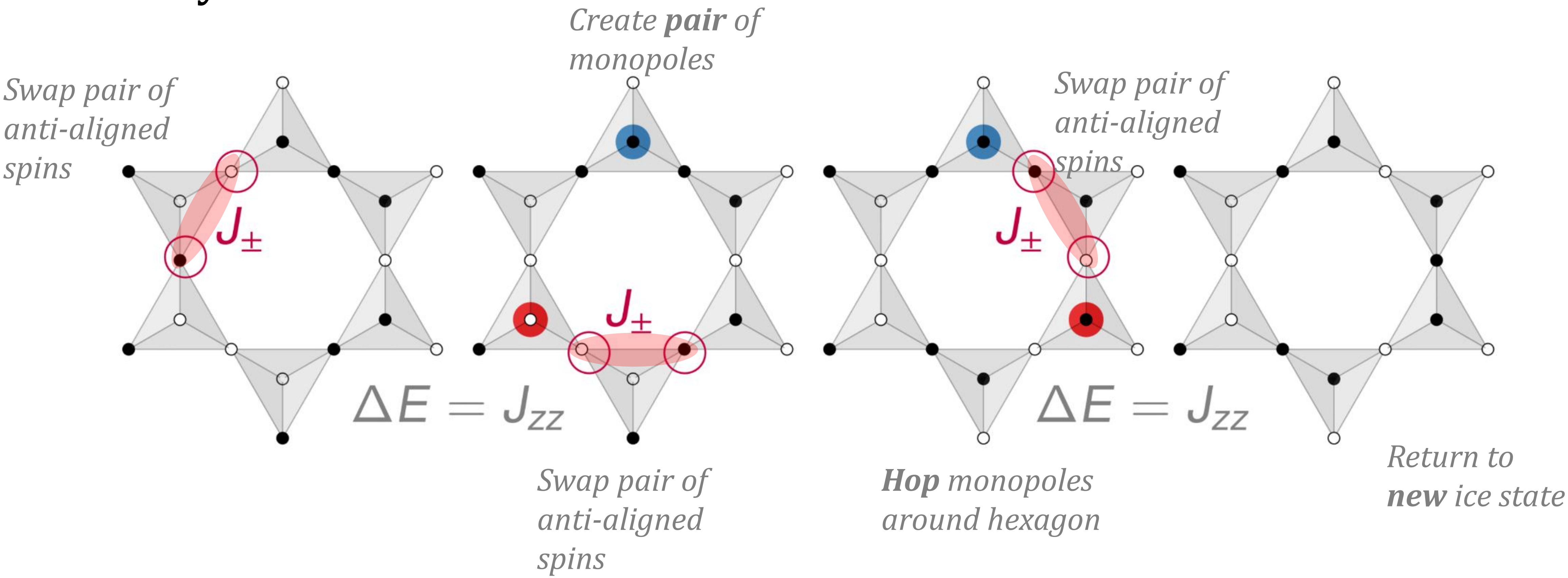
Depending on nature of atomic states: may have $J_{z\pm}$ = 0 and/or trivial phases $\zeta = \gamma = 1$

- Focus on the $J_{\pm}$ part; the other terms have same *qualitative* physics
- **Degenerate perturbation theory** within the manifold of ice states

For a review: *Ann. Rev. Cond. Mat. Phys.* ***10****, 357-386 (2019)*

Degenerate Perturbation Theory

- First non-trivial contribution at **third order** in perturbation theory



*Hermele et al, Phys. Rev. B **69**, 064404 (2004)*

Effective Model

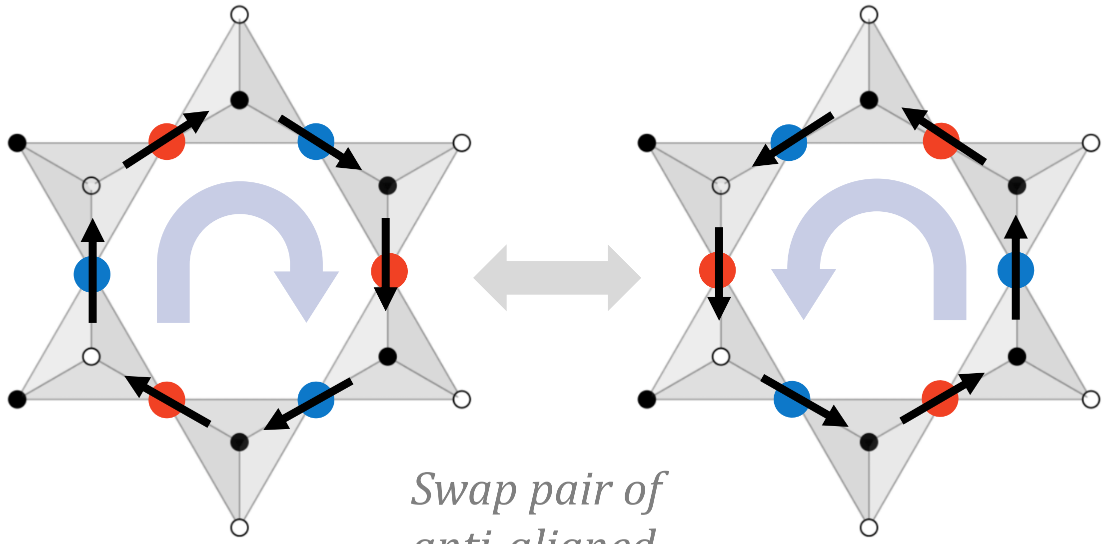
- Six-spin “loop flip” term in effective Hamiltonian

Flux lines become dynamical

$$H_{\text{eff}} = -\frac{2J_{\pm}^2}{J_{zz}}N - \frac{12J_{\pm}^3}{J_{zz}^2}\sum_{\text{hexagons}} P_{\text{ice}}\left(S_1^+S_2^-S_3^+S_4^-S_5^+S_6^- + \text{h.c.}\right)P_{\text{ice}}$$

- Energy scale of dynamics in ice manifold is:

$$g \equiv \frac{12J_{\pm}^3}{J_{zz}^2} \ll J_{\pm} \ll J_{zz}$$



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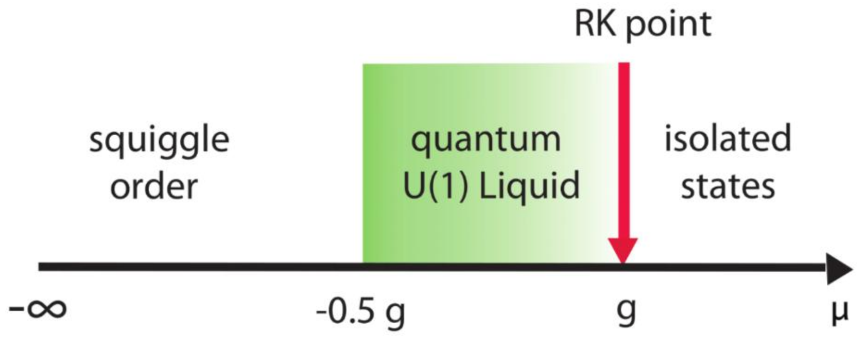
Effective Model (cont.)



Tunnelling term from 3rd order process

$$-g \sum_{\text{hexagons}} \left(|\circlearrowright\rangle\langle\circlearrowleft| + |\circlearrowleft\rangle\langle\circlearrowright| \right)$$

$$+\mu \sum_{\text{hexagons}} \left(|\circlearrowright\rangle\langle\circlearrowright| + |\circlearrowleft\rangle\langle\circlearrowleft| \right)$$

*Added **by hand**; original model has μ = 0*

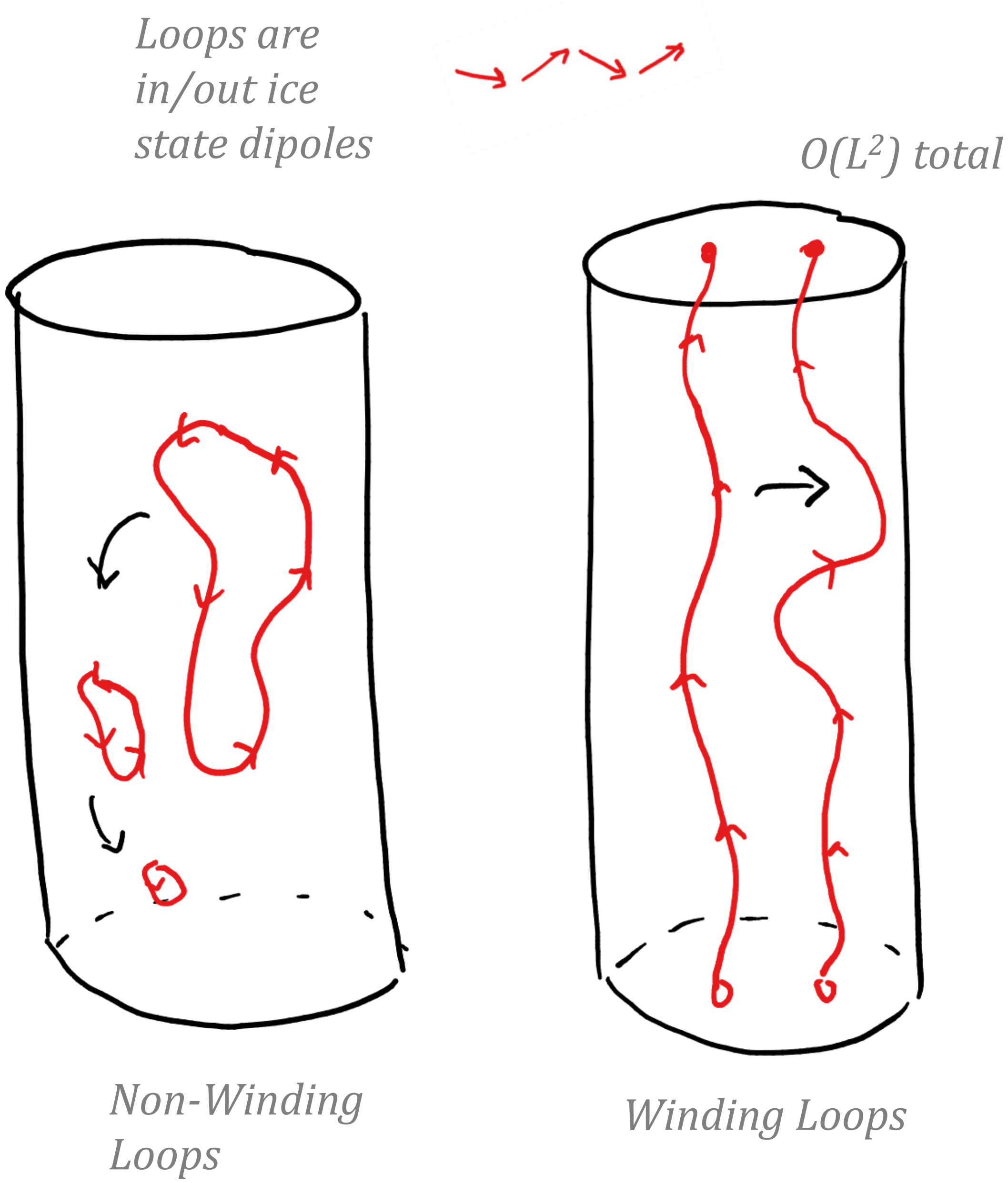
- Augment loop "flip" with loop "*potential*"
- **Rohksar-Kivelson model**
- *Exactly solvable point* when two terms are equal
- Ground state? *Equal superposition of ice states:*

$$|RK\rangle \sim \frac{1}{\sqrt{N_{\text{ice}}}} \sum_{\sigma \in \text{ice}} |\sigma_1 \cdots \sigma_N\rangle$$

*Shannon et al, Phys. Rev. Lett **108**, 067204 (2012)*

Topological Sectors?

- If it traverse the periodic boundaries any loop can be deformed into any other by “flips”
- **Loops that wind through the periodic direction cannot**
- # of winding loops defines *topological sector*



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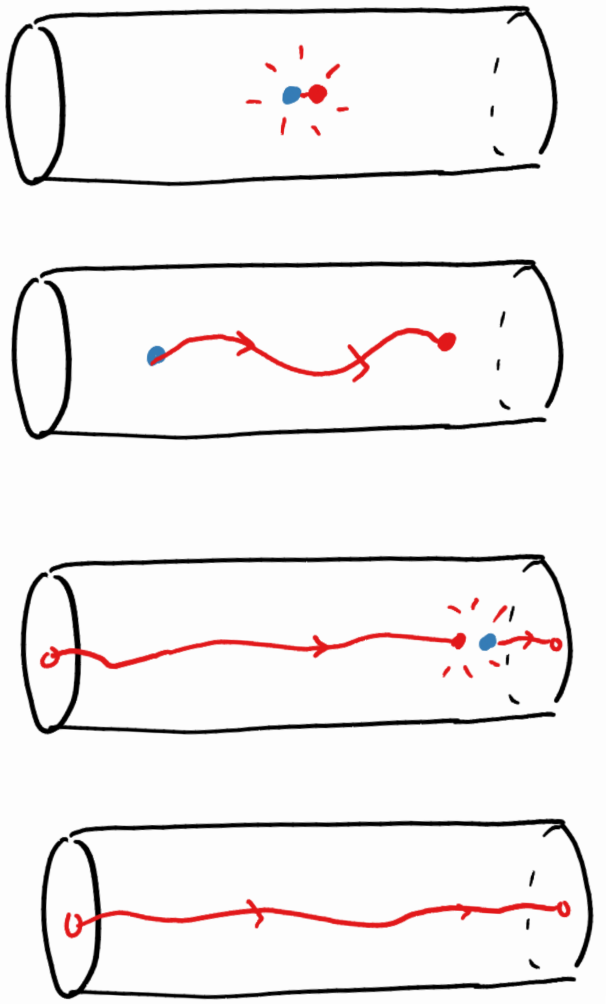
Topological Sectors (cont.)

- Can only remove by *creating monopole pair and annihilating across boundary*

- Tunnelling is *exponentially suppressed* ~ $O(e^{-L})$
- **Think:** *trapping magnetic flux* in the periodic “holes” of the lattice



Make pair

Pull apart

Pull ***through*** *boundary*

Annihilate

Hermele et al, Phys. Rev. B ***69****, 064404 (2004)*

Mapping to Lattice Gauge Theory

- Make connection to electromagnetism explicit:
- **Map spins to O(2) "rotors"**
- Constraint: $n_i = 0$ or 1

Rotor Representation

$$S_i^z = \left(n_i - \tfrac{1}{2}\right),$$

Raising operator

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$$[\theta_i, n_j] = i\delta_{ij}.$$

$$\frac{U}{2}\sum_i (n_i - 1/2)^2 - 2g\sum_{\hexagon}\cos(\theta_1 - \theta_2 + \theta_3 - \theta_4 + \theta_5 - \theta_6).$$

"Softened" constraint; fixes n=0,1 for large values of U

*Factors of n drop when acting on **flippable** hexagons (only non-zero there)*

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- Use these to define **electric** and **magnetic fields** on the diamond (dual-diamond) lattice

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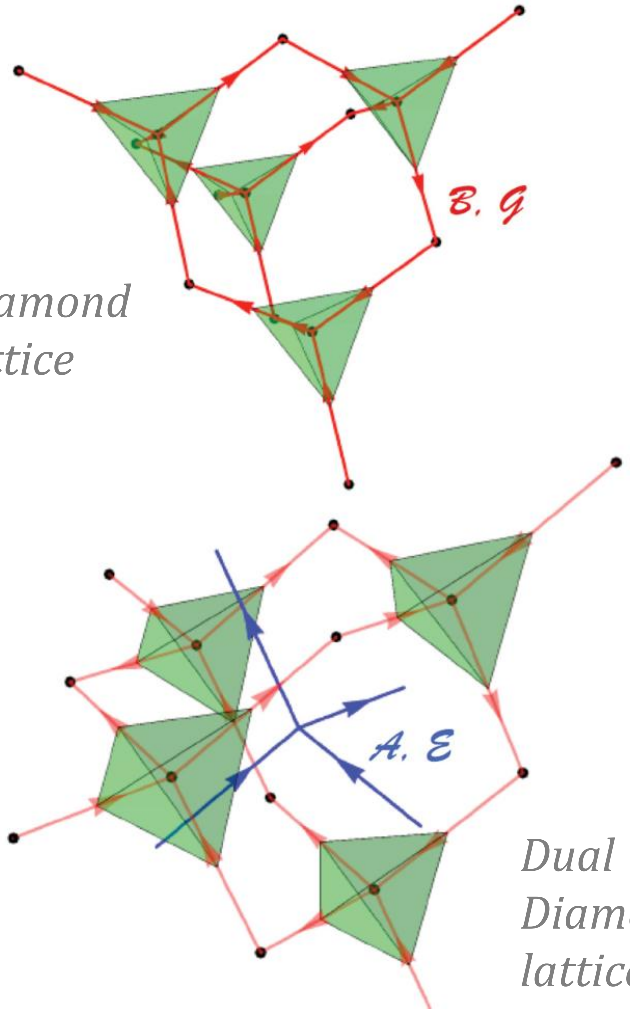
Diamond lattice



Dual Diamond lattice

- These give the representation:

$$\frac{U}{2}\sum_{\langle\mathbf{rr'}\rangle}\mathcal{B}^2_{\mathbf{rr'}} - 2g\sum_{\langle\mathbf{ss'}\rangle}\cos\left(\mathcal{E}_{\mathbf{ss'}}\right),$$

Lattice Gauge Theory

- Coarse-grain to remove strict large U limit; assume *E*-field small; Taylor expand

→ **Emergent Quantum Electrodynamics**

*Hermele et al, Phys. Rev. B **69**, 064404 (2004); Benton et al, Phys. Rev. B **86**, 075154 (2012)*

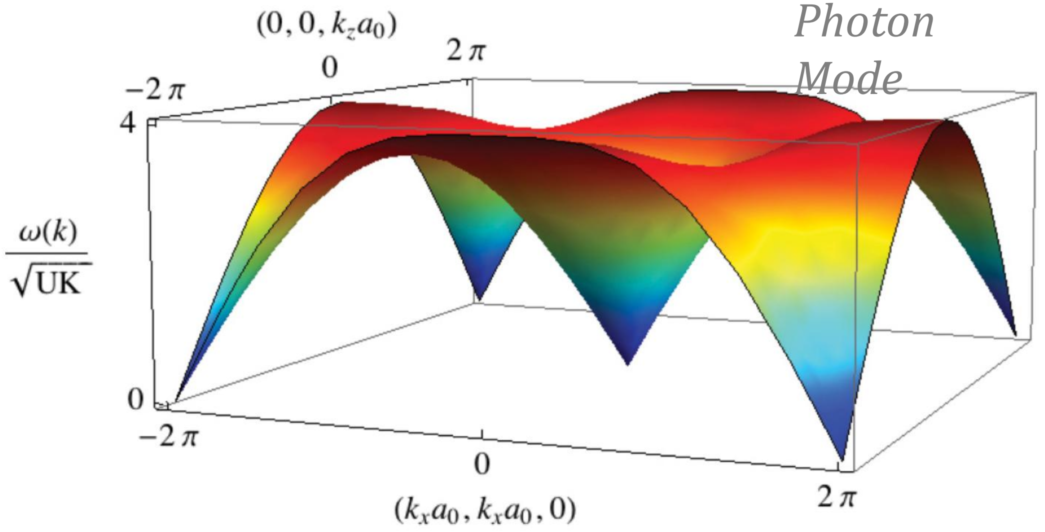
Photon and Emergent Electrodynamics

- Gauge theory can be solved:

$$\sum_{\mathbf{k}} \sum_{\lambda=1}^{2} \omega(\mathbf{k}) \left[a_\lambda^\dagger(\mathbf{k}) a_\lambda(\mathbf{k}) + \frac{1}{2} \right],$$

Gauge boson

- Linearly dispersing **photon mode** near *k ~ 0*



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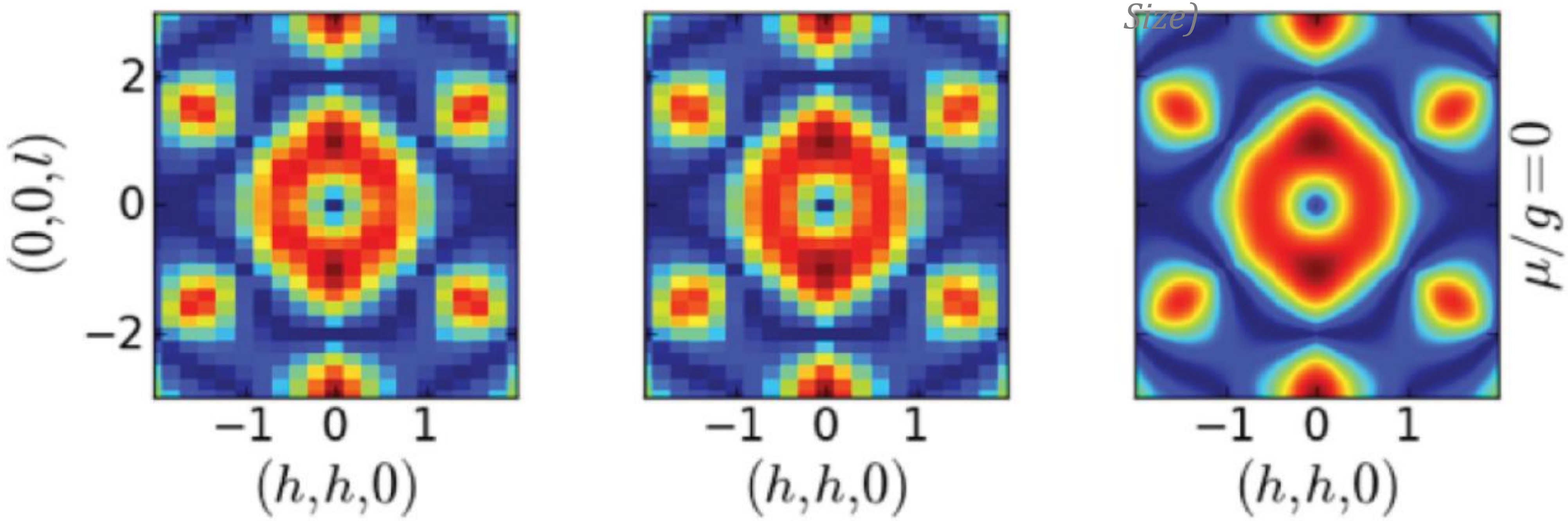

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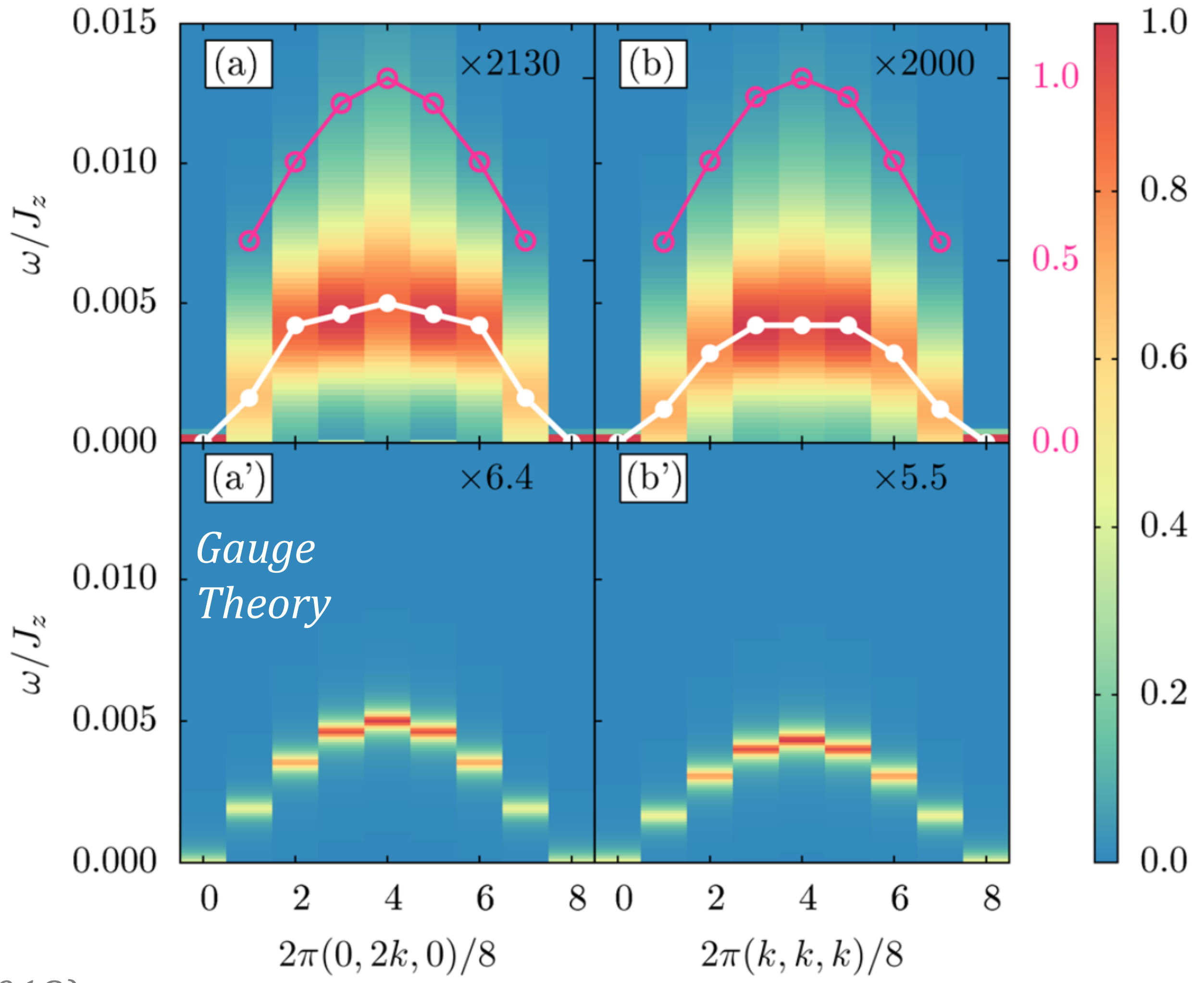

Huang, Deng, Wan, Meng, Phys. Rev. Lett. ***120****, 167202 (2018)*

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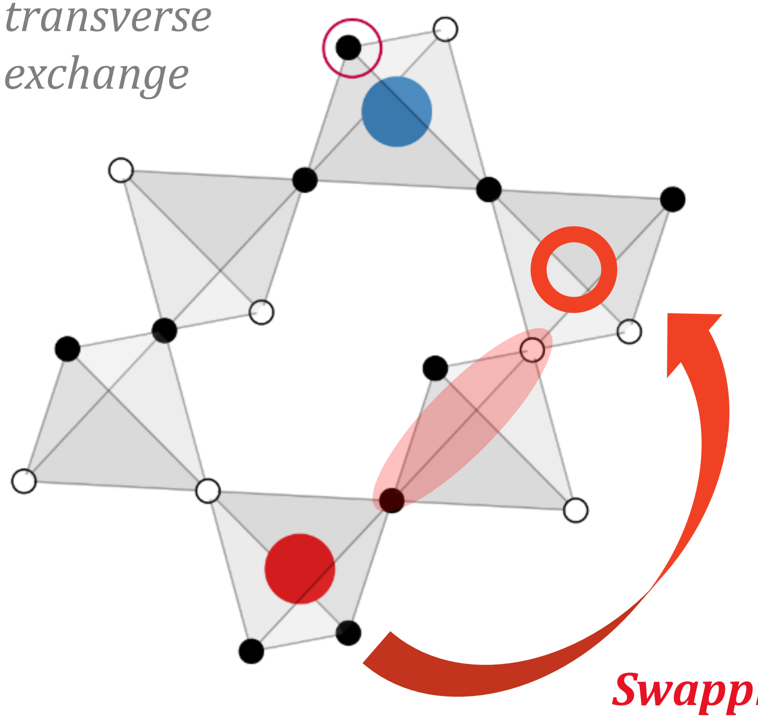
- Transverse exchange **hops** monopoles *at first order in the coupling*

$$g \equiv \frac{12J_{\pm}^3}{J_{zz}^2} \ll J_{\pm} \ll J_{zz}$$

Photon energy scale — ***Monopole hopping*** — *Monopole cost*

- Monopoles are **fast** relative to the photons



Wan et al, Phys. Rev. Lett. ***116*** *167202 (2016)*

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- **Simplest picture:** Monopoles are *free particles* hopping on diamond lattice
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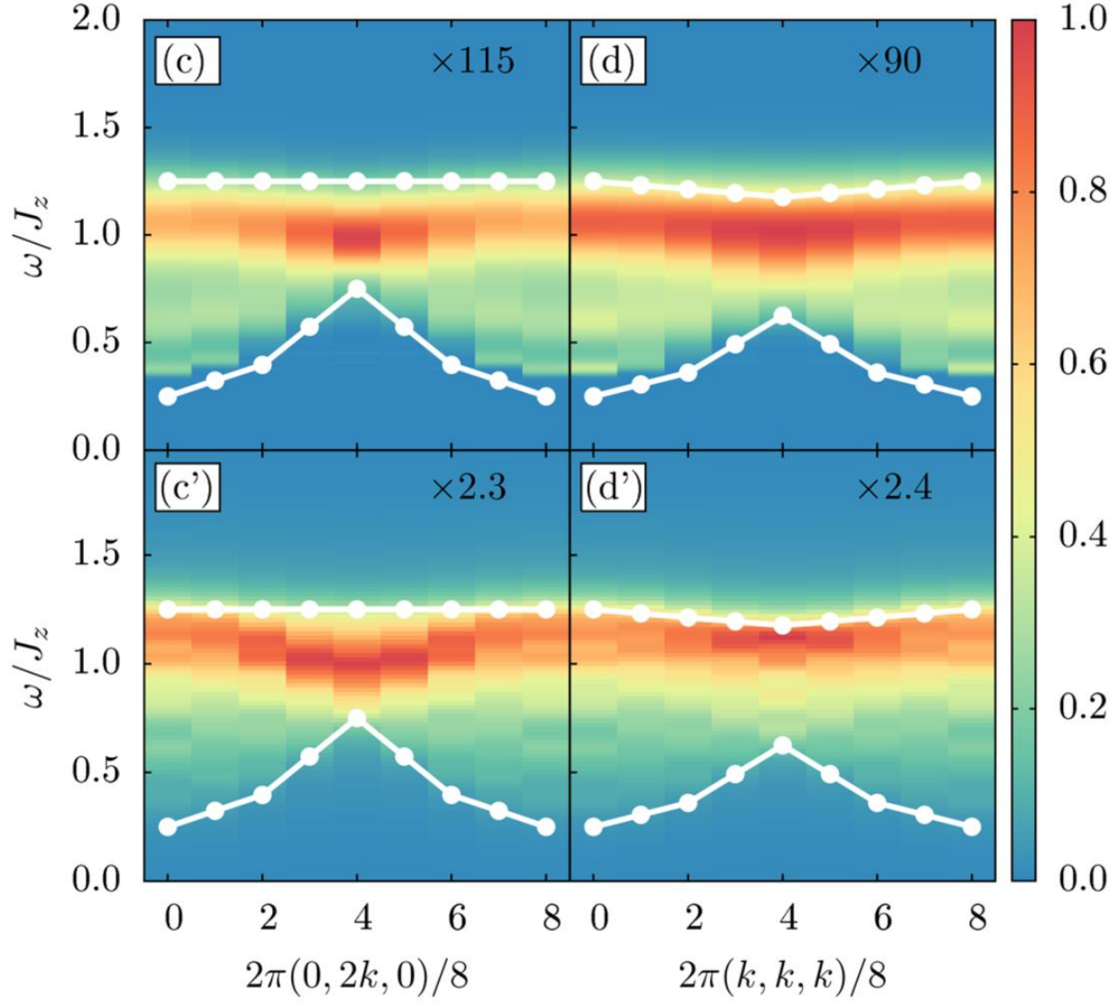

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- **Fine-structure constant**
- Can relate *spacing of flux sectors* to *photon-matter coupling*
- Eq

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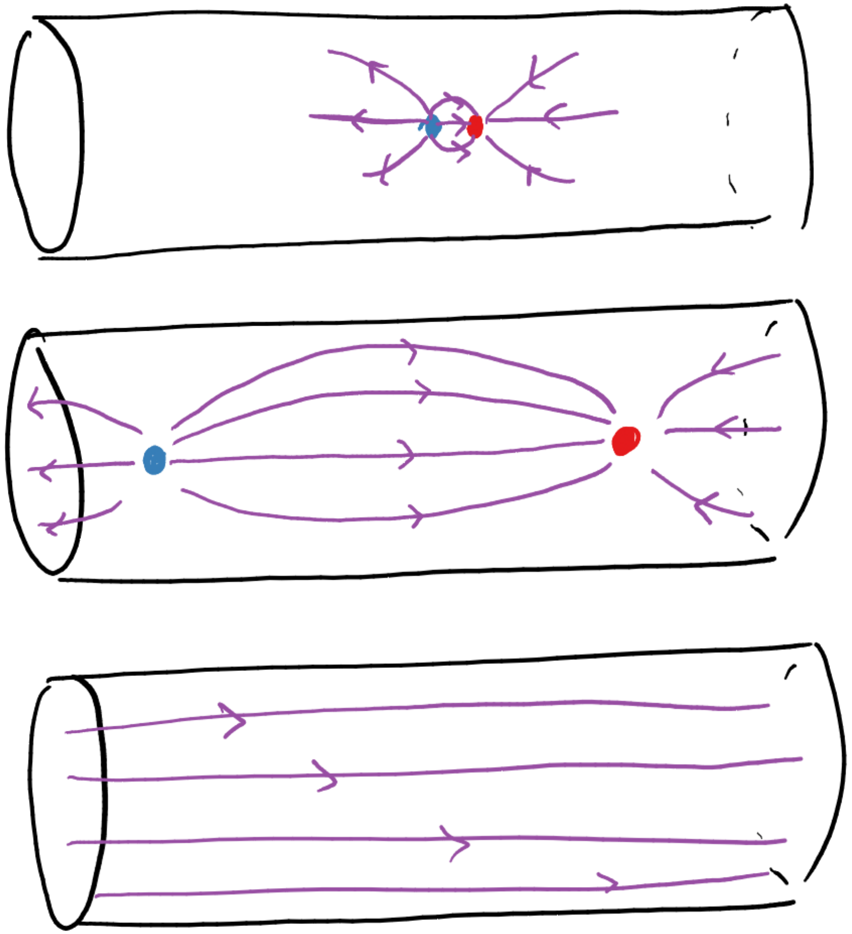

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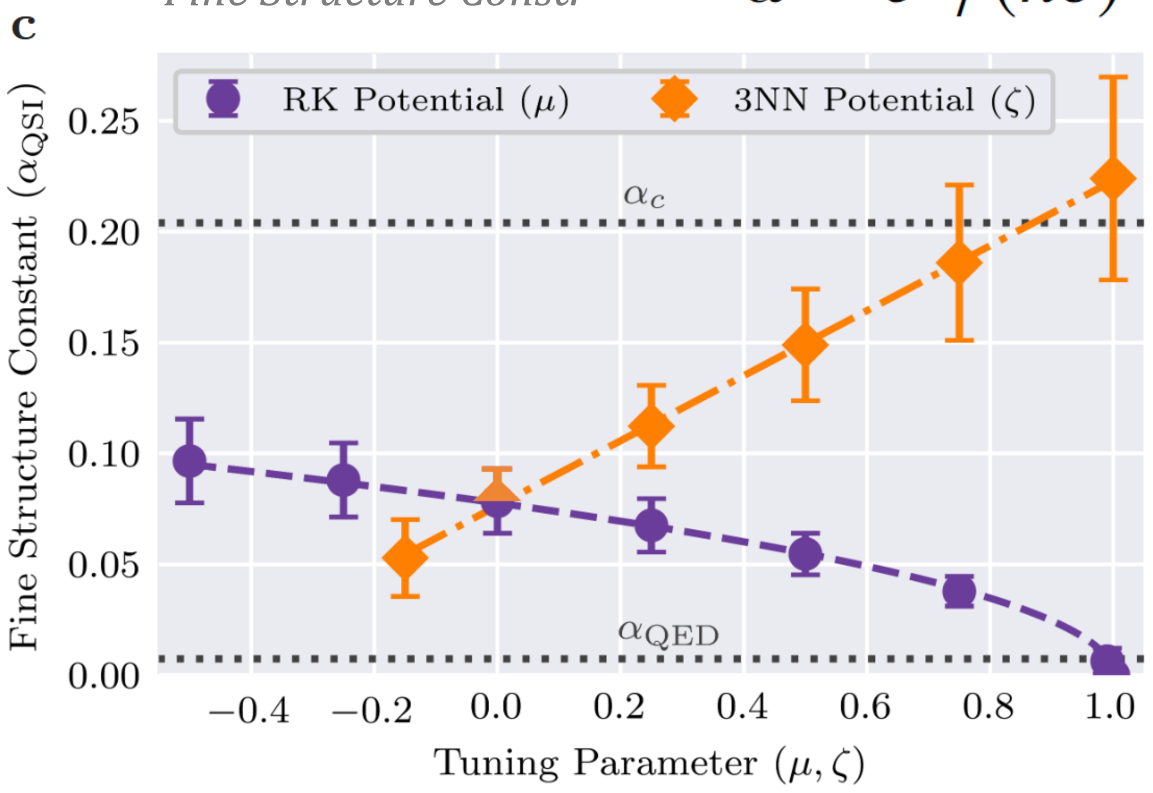

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Summary

Quantum Spin Liquids

- Magnet that doesn't order down to zero temperature and is distinct from a trivial paramagnet
- Can exhibit: Fractionalized excitations, emergent gauge theories, topological order

Quantum *Spin Ice*:

- Classical spin ice + quantum fluctuations gives a quantum spin liquid state
- Emergent realization of QED, complete with gapless photon and fractionalized (magnetic) charges
- Explores regime not accessible in usual QED

Thank you for your attention

Next time:

Kitaev's honeycomb model

i. Definition & Solution
ii. Properties of the Kitaev Spin Liquid
iii. Effect of a Magnetic Field
iv. Generalizations (3D, disorder, …)

Tutorial:
Quantum Spin Liquids (Part II)

Jeffrey G. Rau
University of Windsor

NCTS Summer School on Frontier Topics in Strongly Correlated Electron Systems

University of Windsor

Reminder:

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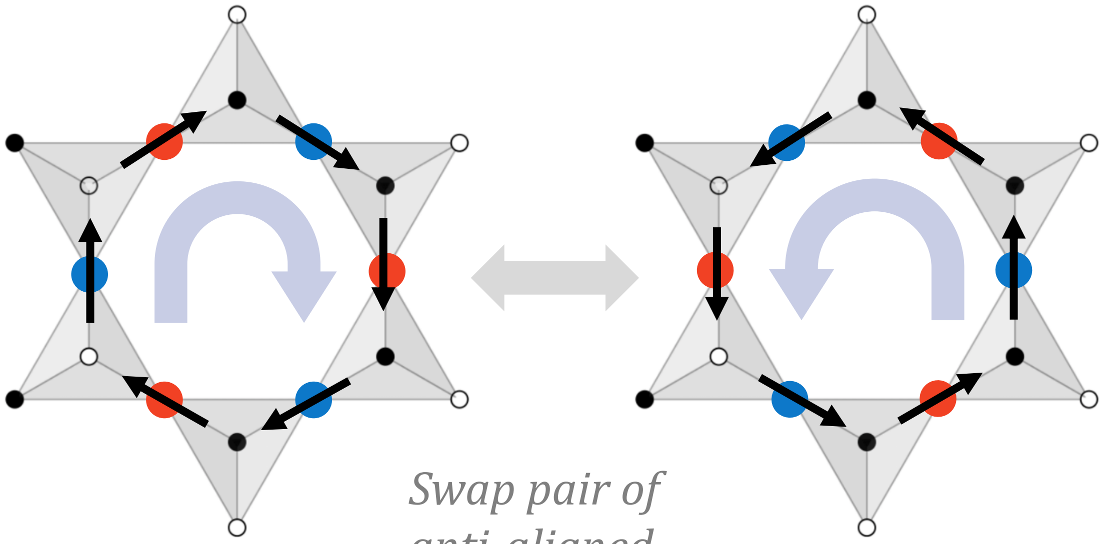

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*Defined on **links** of diamond lattice*

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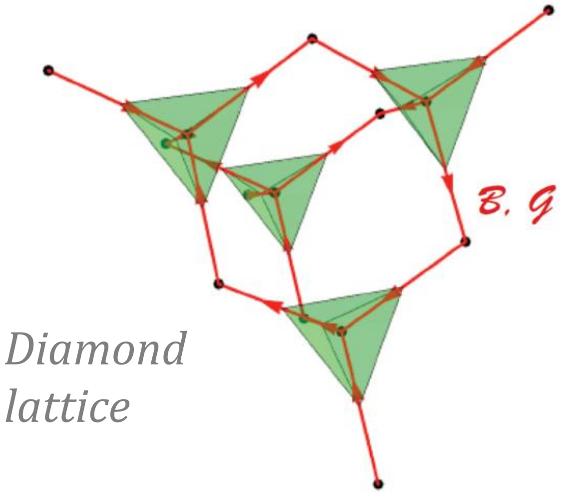

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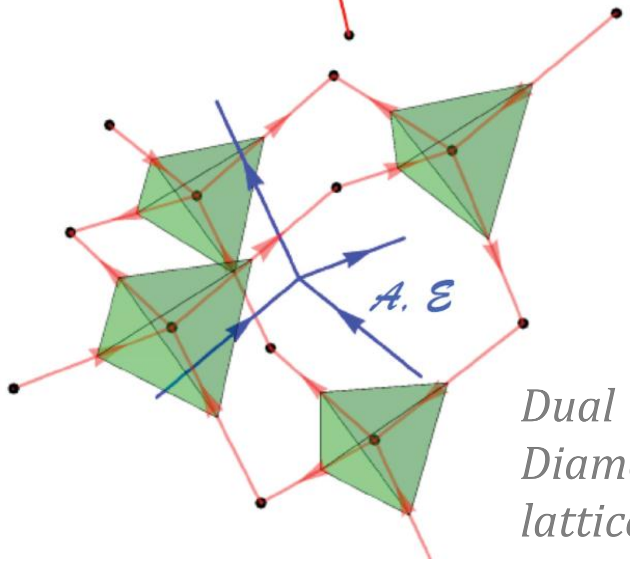

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Ice rule constraint

$$\sum_{\langle \mathbf{r'}\rangle} \mathcal{B}_{\mathbf{rr'}} = 0,$$

Assume E-field is small, Taylor expand

$$\frac{\mathcal{U}}{2}\sum_{\langle rr'\rangle} \mathcal{B}^2_{rr'} + \frac{\mathcal{K}}{2}\sum_{\langle ss'\rangle} \mathcal{E}^2_{ss'}$$

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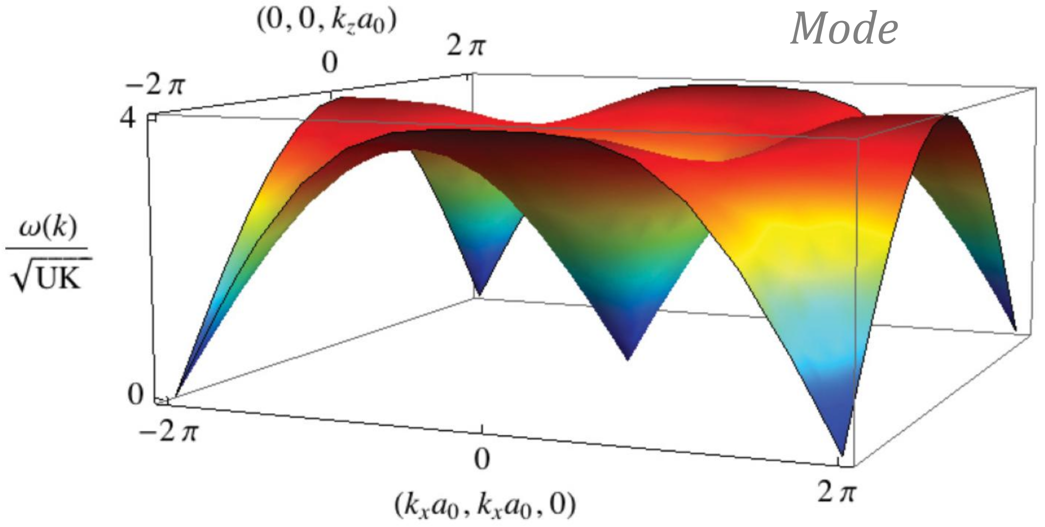

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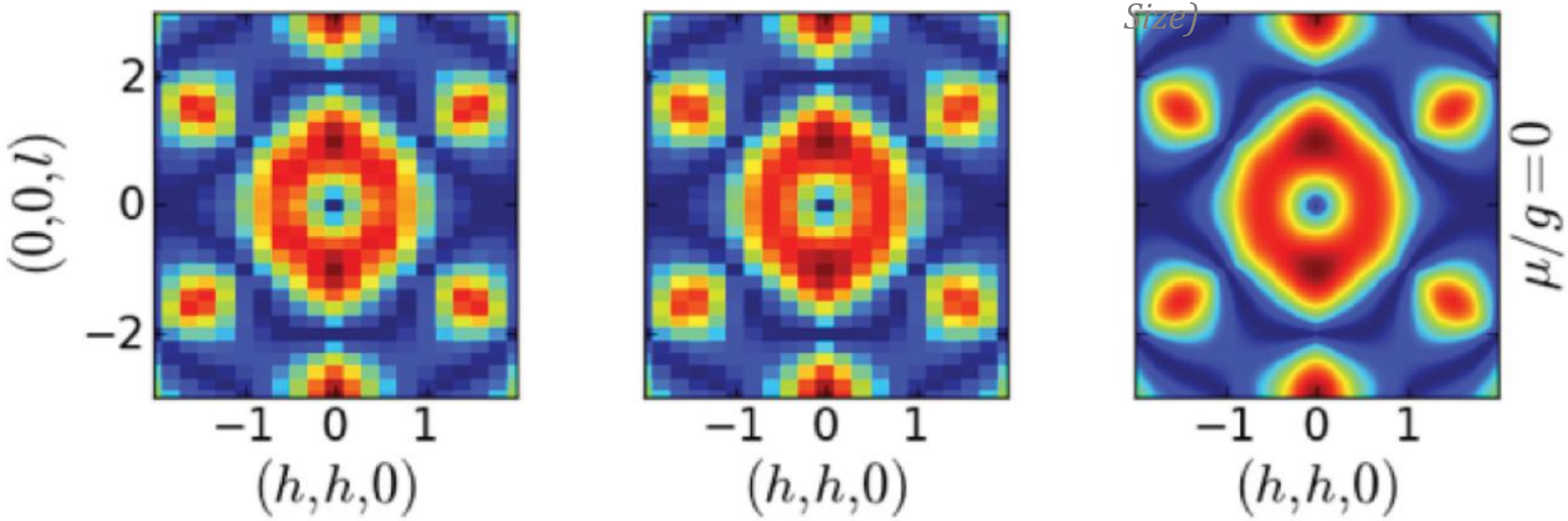

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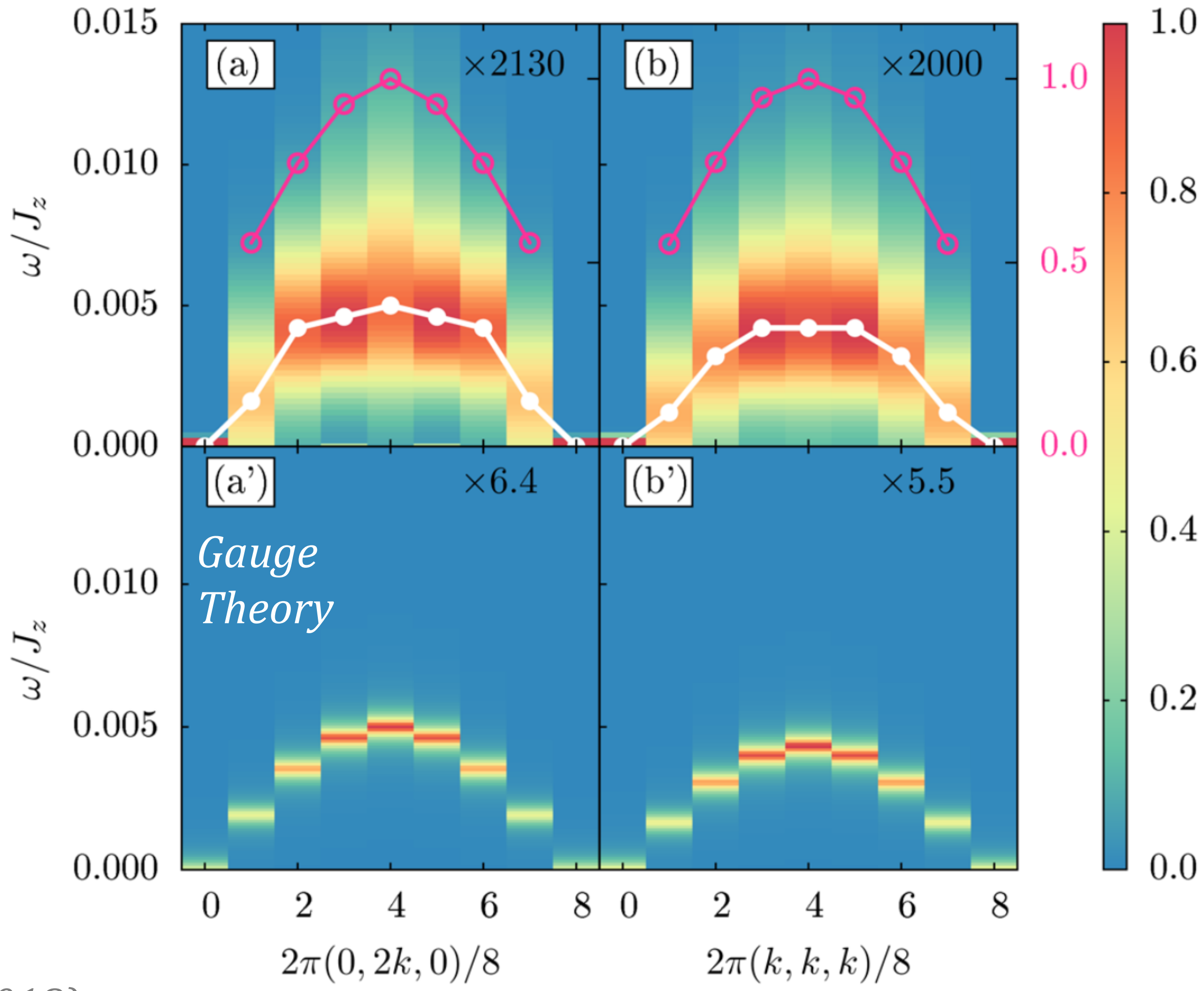

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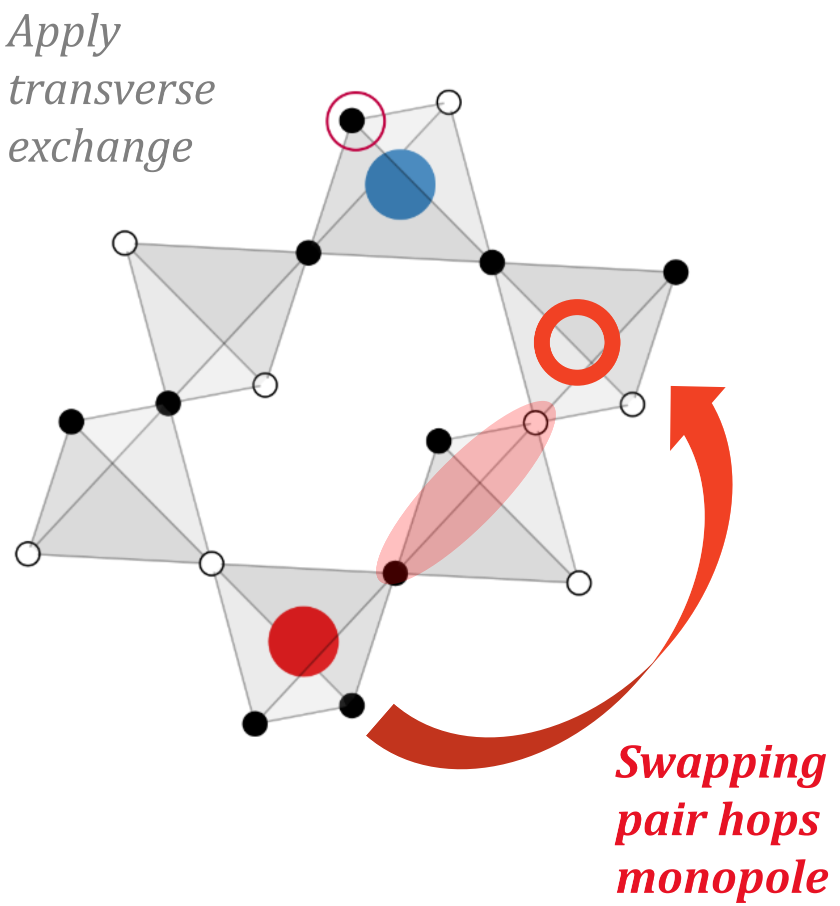

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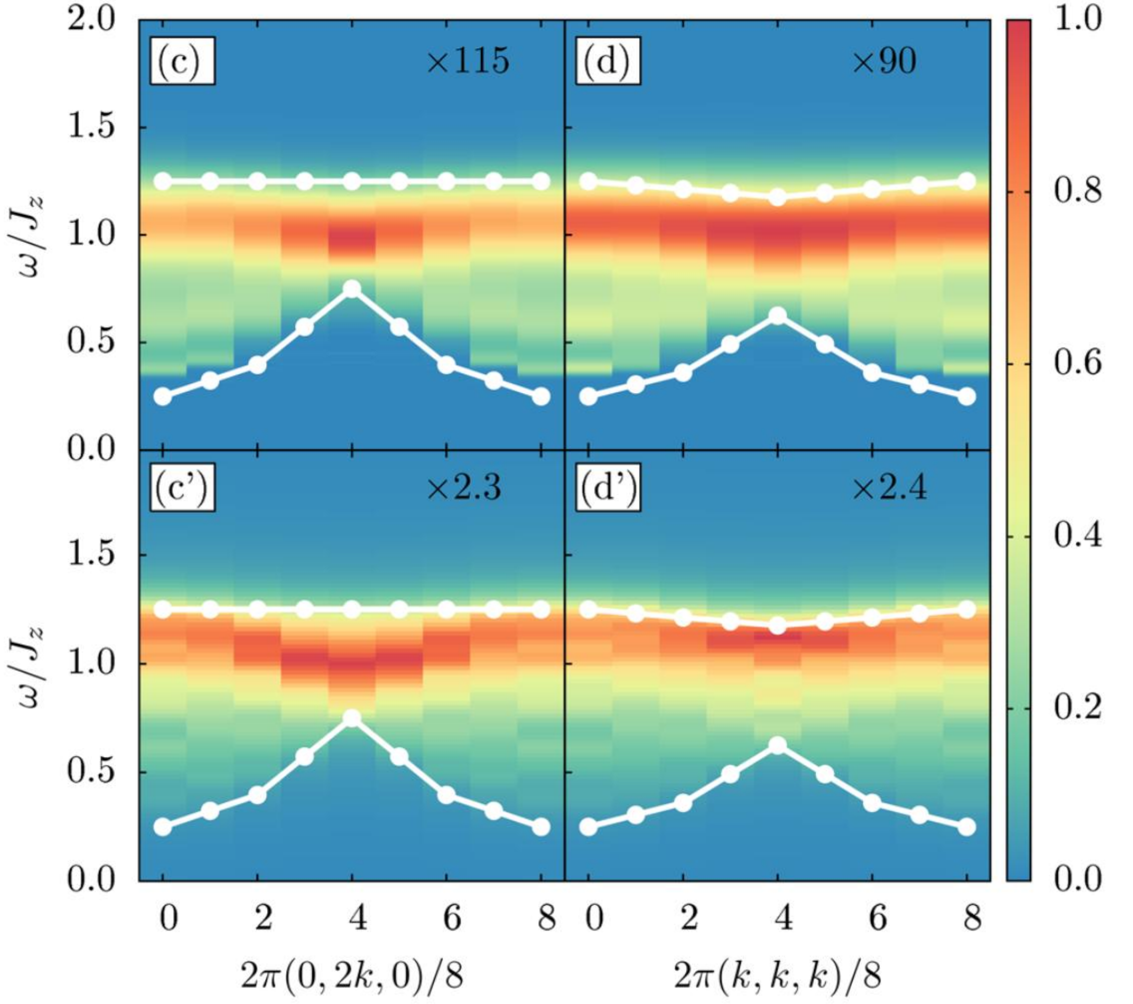

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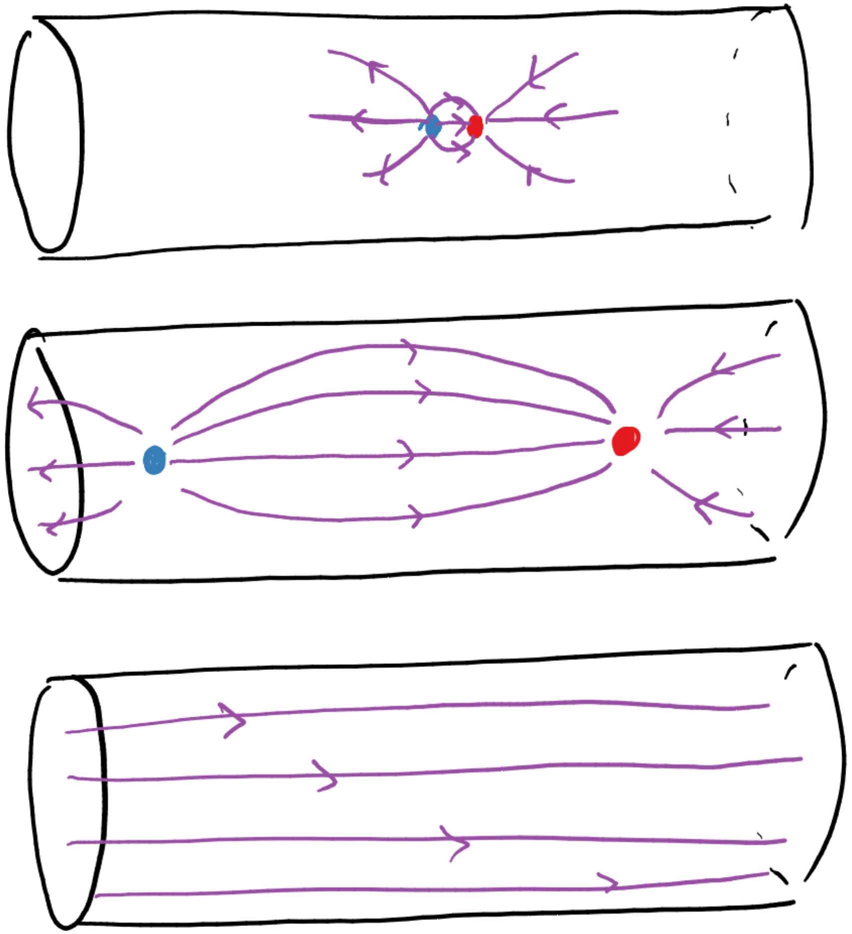

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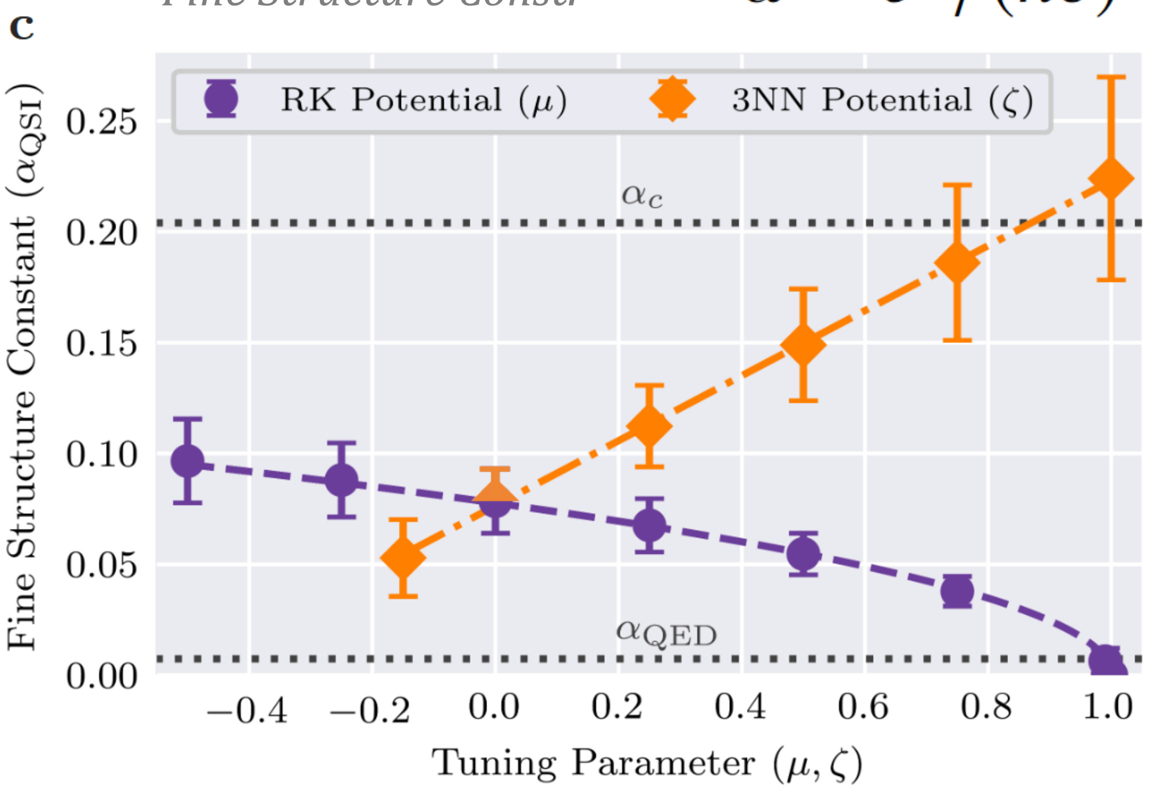

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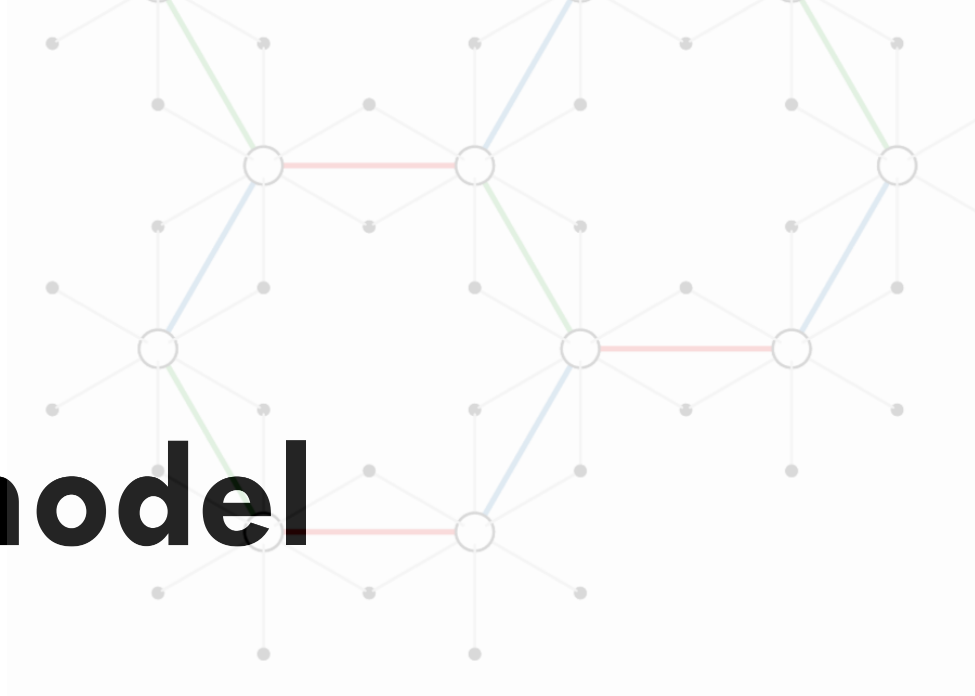
Kitaev's honeycomb model



i. Definition & Solution

ii. Properties of the Kitaev Spin Liquid

iii. Generalizations (3D, disorder, …)

Kitaev's Honeycomb Model

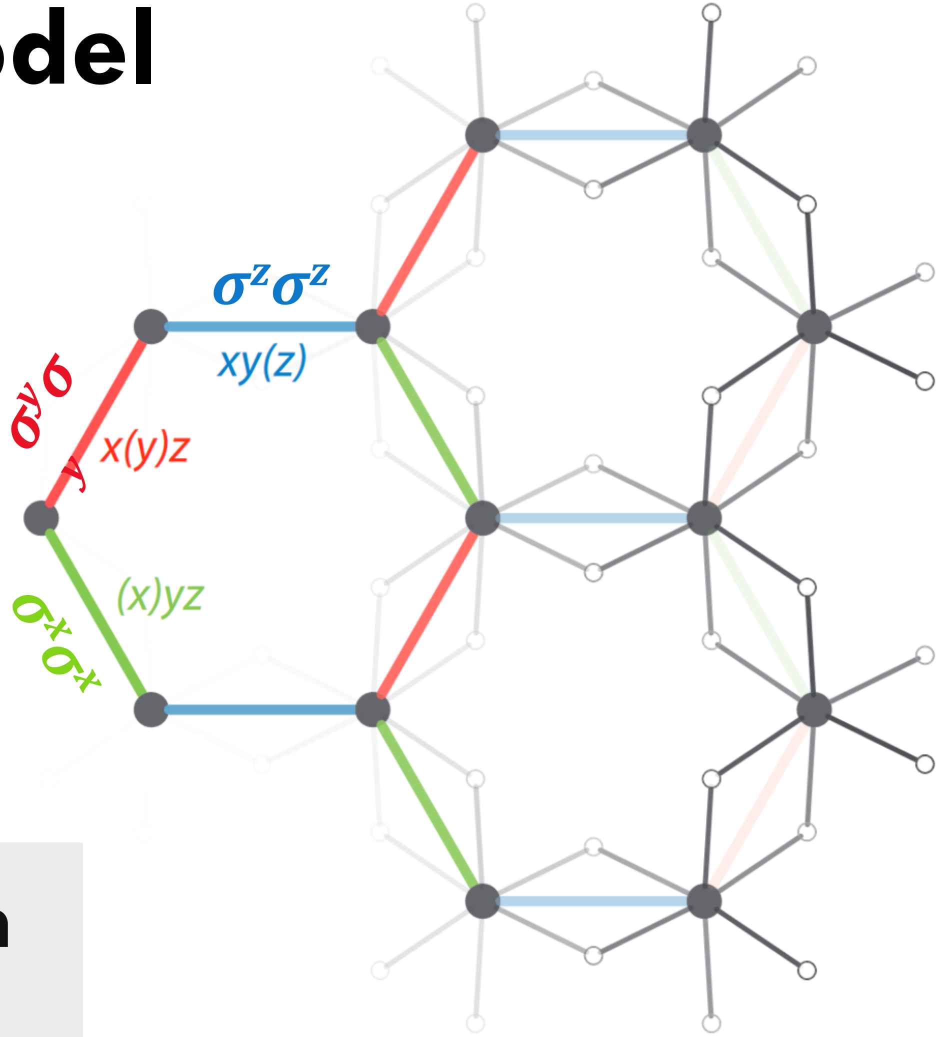
- Frustrated spin-1/2 model on honeycomb lattice

$$-J\sum_{\langle ij\rangle_\gamma}\sigma_i^\gamma\sigma_j^\gamma$$

Two-spin interactions only

- Frustration by *interactions* not geometry

Exactly solvable of a **quantum spin liquid** with *emergent Majorana fermion excitations*



Kitaev, Ann. Phys. **321**, 2

Plaquette symmetries

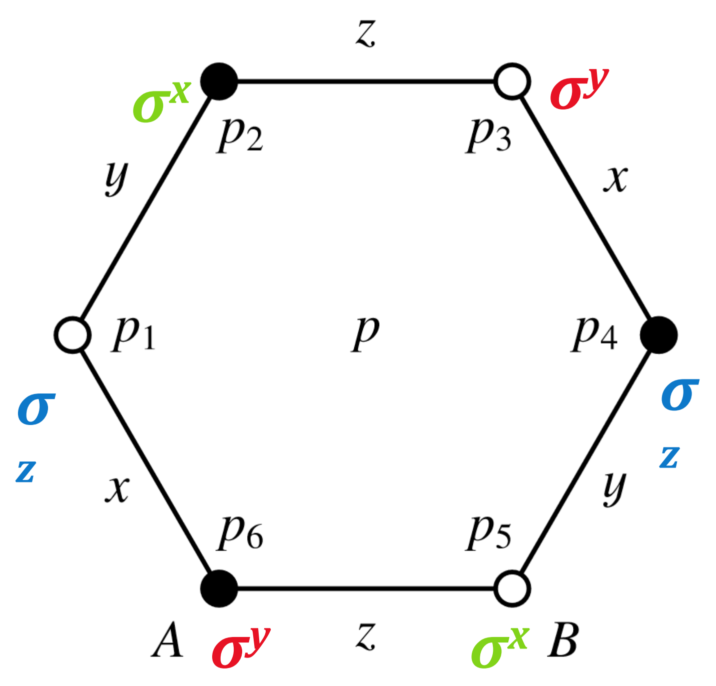
- *Infinite* number of conserved quantities

$$W_p = \sigma^z_{p_1}\sigma^x_{p_2}\sigma^y_{p_3}\sigma^z_{p_4}\sigma^x_{p_5}\sigma^y_{p_6}$$

- Commute with Hamiltonian *and* each other

$$[H, W_p] = 0 \qquad [W_p, W_{p'}] = 0$$

- Eigenvalues +1, -1:
  - *$2^{N/2}$ sectors each of size $2^{N/2}$*



For N sites, there are N/2 plaquettes

Kitaev, Ann. Phys. ***321****, 2*

Absence of magnetic order

- Plaquette symmetries imply **no magnetic order**

$$\{\sigma_i^\mu, W_p\} = 0$$

there exists

Anti- *commutation relation*

- *Elitzur's theorem:* Can't spontaneously break local symmetries

$$\langle \boldsymbol{\sigma}_i \rangle = 0$$

- Also valid for higher-*S* Kitaev models

$$\langle \Psi_0 | \sigma_i^\mu | \Psi_0 \rangle$$

$W_p^2 = 1$

$$\langle \Psi_0 | \sigma_i^\mu W_p^2 | \Psi_0 \rangle$$

$\{\sigma_i^\mu, W_p\} = 0$

$$-\langle \Psi_0 | W_p \sigma_i^\mu W_p | \Psi_0 \rangle$$

Eigenstate of plaquette operators

$$-\langle \Psi_0 | \sigma_i^\mu | \Psi_0 \rangle$$

Exact solution: Plan

$D_i \equiv b_i^x b_i^y b_i^z c_i = 1$

$U_{ij} \equiv i b_i^\gamma b_j^\gamma$

$$-J \sum_{\langle ij \rangle_\gamma} \sigma_i^\gamma \sigma_j^\gamma \;\rightarrow\; iJ \sum_{\langle ij \rangle_\gamma} \left(i b_i^\gamma b_j^\gamma \right) c_i c_j \;\rightarrow\; iJ \sum_{\langle ij \rangle_\gamma} U_{ij} c_i c_j$$

$$\boldsymbol{\sigma}_i \equiv i \boldsymbol{b}_i c_i$$

$u_{ij} = \pm 1$

$u_{ij} = +1$

$$\text{Free fermions (solvable)} \;\leftarrow\; H_0 = J \sum_{\langle ij \rangle_\gamma} i c_i c_j \;\leftarrow\; H[u] \equiv J \sum_{\langle ij \rangle_\gamma} i u_{ij} c_i c_j$$

Free
fermions
(solvable)

$w_p = u_{p_1 p_2} u_{p_2 p_3} u_{p_3 p_4} u_{p_4 p_5} u_{p_5 p_6} u_{p_6 p_1}$

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

Majorana representation

- Highly suggestive: *$2^{N/2}$* states per sector, *Majorana fermions?*

$$\boldsymbol{\sigma}_i \equiv i\boldsymbol{b}_i c_i \qquad \boldsymbol{b}_i \equiv (b_i^x, b_i^y, b_i^z)$$

- Represent spin-1/2 as *four* Majoranas, subject to *constraint*

$$D_i \equiv b_i^x b_i^y b_i^z c_i = 1$$

- Satisfy the anti-commutation relations for for Majorana fermions

$$\{c_i, c_j\} = 2\delta_{ij}$$

$$\{c_i, \boldsymbol{b}_j\} = 0$$

$$\{b_i^\mu, b_j^\nu\} = 2\delta_{ij}\delta_{\mu\nu}$$

Relation to SU(2) slave fermions?

- How does the relate to the "usual" representation:

$$\boldsymbol{\sigma}_i = \boldsymbol{f}_i^\dagger \boldsymbol{\sigma} \boldsymbol{f}_i$$

Complex *fermions*

- With constraint: $\boldsymbol{f}_i^\dagger \boldsymbol{f}_i = 1$

- **Equivalent**; just a *change of basis*

$$c = \frac{1}{\sqrt{2}}(f_\uparrow + f_\uparrow^\dagger)$$

$$b^x = \frac{1}{i\sqrt{2}}(f_\downarrow - f_\downarrow^\dagger)$$

$$b^y = -\frac{1}{\sqrt{2}}(f_\downarrow + f_\downarrow^\dagger)$$

$$b^z = \frac{1}{i\sqrt{2}}(f_\uparrow - f_\uparrow^\dagger)$$

One possible way to express Majoranas in terms of complex fermions

*Burnell & Nayak, Phys. Rev. B **84**, 125125 (2011); You et al, Phys. Rev. B **86**, 085145 (2012)*

Hamiltonian in terms of Majoranas

- Substitute these in to Kitaev model:

$$\tilde{H} = iJ \sum_{\langle ij \rangle_\gamma} \left(i b_i^\gamma b_j^\gamma \right) c_i c_j$$

Defined in ***extended*** *space, need to impose constraint*

- If we can solve *this,* and get ground state $|\tilde{\Psi}_0\rangle$ then just need to *project* into physical subspace

Really, ***any*** *eigenstate*

$$|\Psi_0\rangle = P |\tilde{\Psi}_0\rangle$$

Ground state of Kitaev model

Imposes constraint
$D_i \equiv b_i^x b_i^y b_i^z c_i = 1$

Link operators and Z_2 gauge structure

- To solve this, notice that the operators

$$U_{ij} \equiv i b_i^{\gamma} b_j^{\gamma}$$

- Commute with the Hamiltonian *and* with each other: **definite value in energy eigenstate**

Really, ***any*** *eigenstate*

$$U_{ij} |\tilde{\Psi}_0\rangle = u_{ij} |\tilde{\Psi}_0\rangle$$

- Two possible values: $u_{ij} = \pm 1$

$$[\tilde{H}, U_{ij}] = 0$$

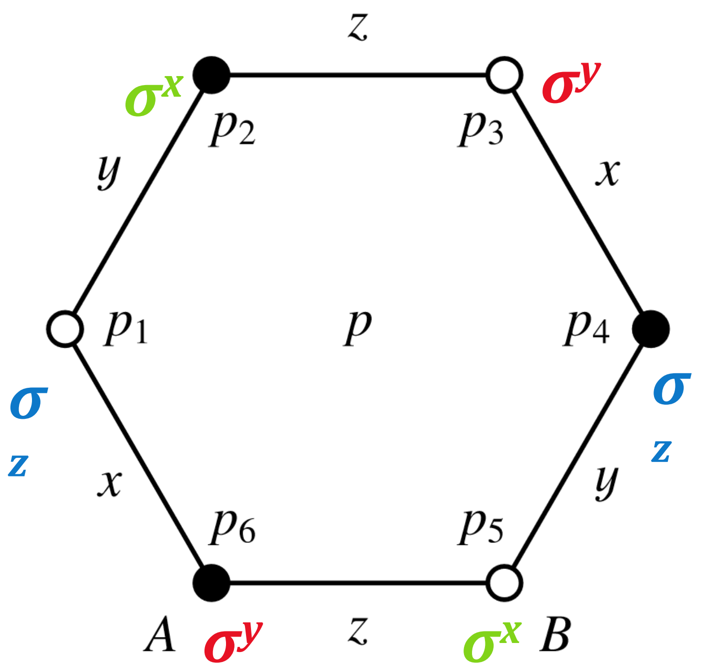
$$[U_{ij}, U_{lk}] = 0$$

$$U_{ij}^2 = 1$$

Defines a $\boldsymbol{Z_2}$ **gauge field** for the *c* Majorana fermions

Z_2 Flux Operators

$$W_p = \sigma^z_{p_1}\sigma^x_{p_2}\sigma^y_{p_3}\sigma^z_{p_4}\sigma^x_{p_5}\sigma^y_{p_6}$$



Under gauge transformation:

Preserves spin-operators $\sigma_i = i b_i c_i$

$$c_i \longrightarrow z_i c_i \qquad z_i = \pm 1$$

$$\boldsymbol{b}_i \longrightarrow z_i \boldsymbol{b}_i$$

$$u_{ij} \longrightarrow z_i z_j u_{ij}$$

- What are the associated **Z_2 flux** operators?

$$w_p = u_{p_1p_2}u_{p_2p_3}u_{p_3p_4}u_{p_4p_5}u_{p_5p_6}u_{p_6p_1}$$

Product of link variables around hexagon

$$W_p\,|\tilde{\Psi}_0\rangle = w_p\,|\tilde{\Psi}_0\rangle$$

± 1

- *Gauge invariant* quantities

Flux sectors

- Gauge field is **static**: fluxes (and links) have *fixed* values
- Each of the $2^{N/2}$ choices of u_{ij} defines **flux sector**

$$H[u] \equiv J \sum_{\langle ij \rangle_\gamma} i u_{ij} c_i c_j$$

Independent "block" of Hamiltonian

Size of block = $2^{N/2}$

- Each flux sector is a *free fermion* problem! (efficiently solvable)

Cost is $O(N^3)$

Ground state? Need to find flux sector with *lowest possible energy*.

Ground state flux sector & Lieb's Theorem

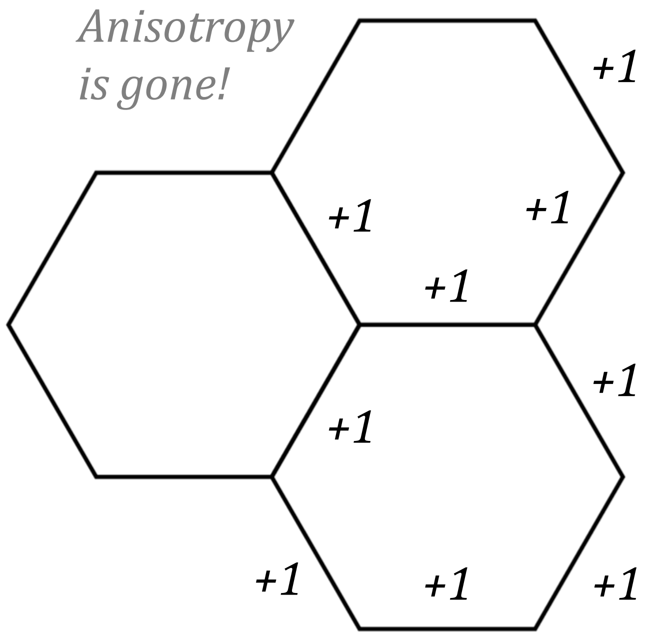
- Could brute force minimize; instead can use **Lieb's theorem:**

Ground sector state is **flux-free**

Depends on lattice structure

Simplest gauge choice

$$u_{ij} = +1$$



- Description is *free Majoranas* hopping on honeycomb lattice

$$H_0 = J \sum_{\langle ij \rangle_\gamma} i c_i c_j$$

Lieb, Phys. Rev. Lett. ***73,*** *2158 (1994)*

Solution in flux-free sector

$$c_{\boldsymbol{r},\alpha} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} c_{\boldsymbol{k},\alpha}$$

- Now problem is simple: *Fourier transform, then diagonalize*

$$H_0 = J \sum_{\langle ij \rangle_\gamma} i c_i c_j = \frac{1}{2} \sum_{\boldsymbol{k}>0} (c_{-\boldsymbol{k},A}\ c_{-\boldsymbol{k},B}) \begin{pmatrix} 0 & f(\boldsymbol{k}) \\ f(\boldsymbol{k})^* & 0 \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{k},A} \\ c_{\boldsymbol{k},B} \end{pmatrix}$$

$$f(\boldsymbol{k}) \equiv 2iJ\left(1 + e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_1} + e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_2}\right)$$

- Final dispersion has two bands:

$$\epsilon(\boldsymbol{k}) \equiv \pm |f(\boldsymbol{k})|$$

- Defines the ground state wave-function

We are done!

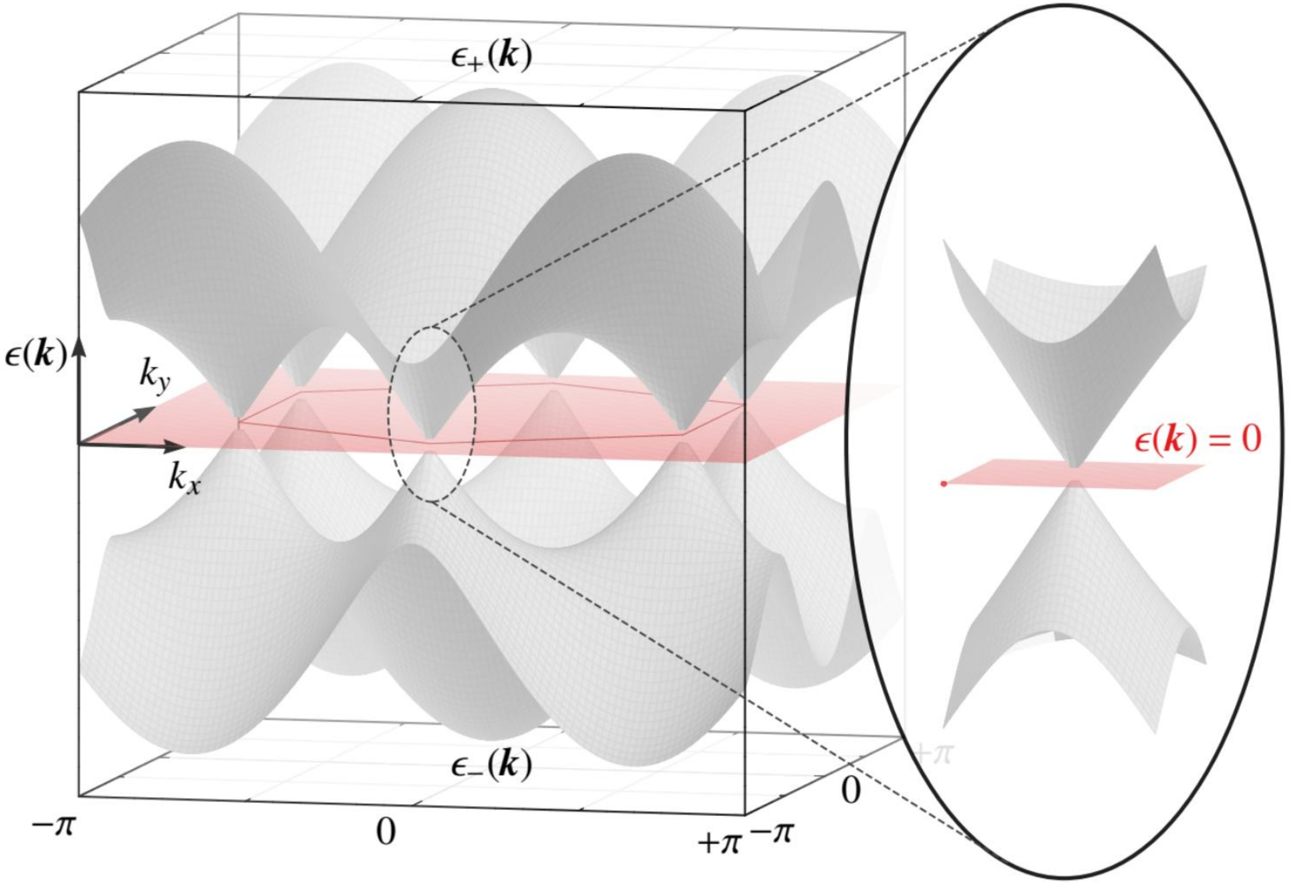
Flux-free spectrum

- What does the dispersion look like?

$$\epsilon(\boldsymbol{k}) \equiv \pm|f(\boldsymbol{k})|$$

$$f(\boldsymbol{k}) \equiv 2iJ\left(1 + e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_1} + e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_2}\right)$$

- **Dirac cones** near the corners
the Brillouin zone
- Same spectrum as graphene



Stable to (symmetric) perturbations

$$\epsilon(\boldsymbol{K} + \boldsymbol{q}) \approx \pm v|\boldsymbol{q}|$$

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

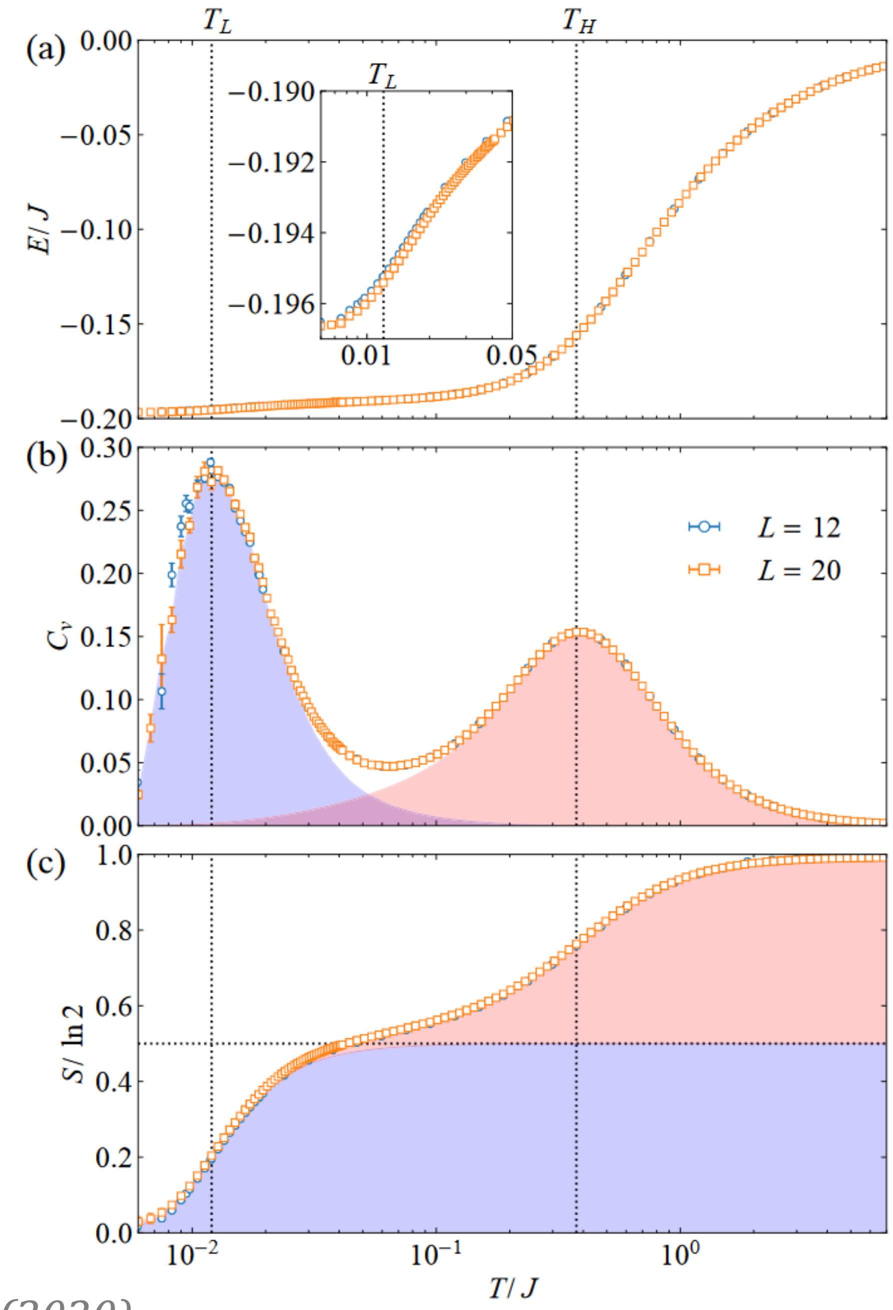
Properties of the Kitaev Spin Liquid

Thermodynamics:

- Structure from exact solution allows for Monte Carlo simulation at *finite temperature*

Roughly: Sample flux sectors, by solving fermionic problem in each sector

- *Note:* Practically uses Jordan-Wigner form of solution



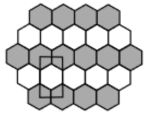
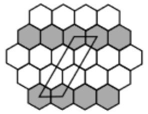
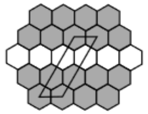
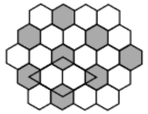
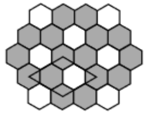
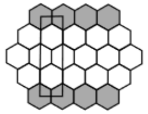
Nasu et al, Phys. Rev. ***92*** *115122 (2015); Motome & Nasu, JPSJ* ***89*** *012002 (2020)*

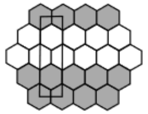
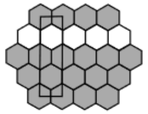
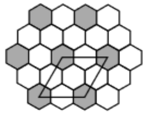
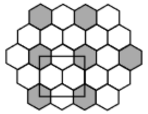
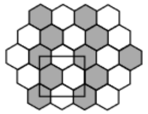
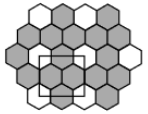
Excitations

- Two classes of excitations
  1. **Majorana excitations:** Governed by dispersion in that flux sector
  2. **Flux Excitations:** *Add* non-zero fluxes to system

- *Intertwined:* Majoranas depends on the flux sector, flux sector energy depends on Majoranas

$E_{\text{vortex}} \approx 0.1536$, $\Delta E\Big($  $\Big) \approx -0.04$, $\Delta E\Big($  $\Big) \approx -0.07$.

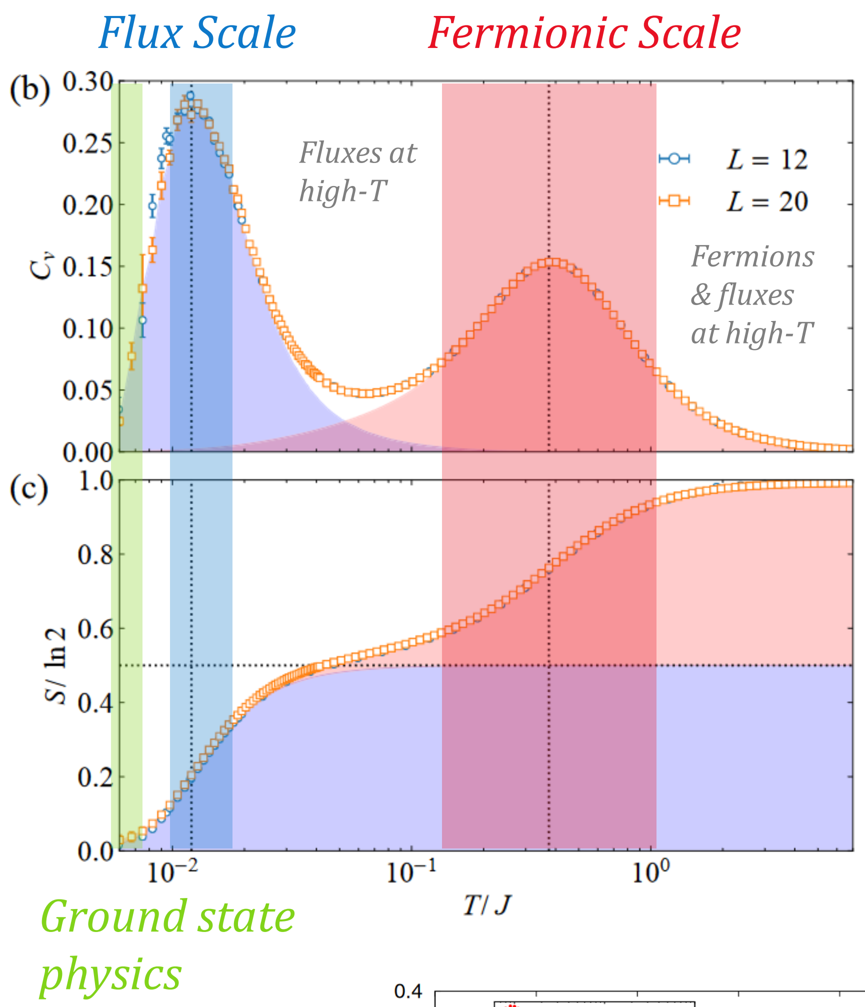
	Phase	Vortex density	Energy per ⬡ and per vortex
1		$\frac{1}{1}$	0.067 0.067
2		$\frac{1}{2}$	0.052 0.104
3		$\frac{1}{3}$	0.041 0.124
4		$\frac{2}{3}$	0.054 0.081
5		$\frac{1}{3}$	0.026 0.078
6		$\frac{2}{3}$	0.060 0.090
7		$\frac{1}{4}$	0.034 0.136

	Phase	Vortex density	Energy per ⬡ and per vortex
8		$\frac{2}{4}$	0.042 0.085
9		$\frac{3}{4}$	0.059 0.078
10		$\frac{1}{4}$	0.042 0.167
11		$\frac{3}{4}$	0.074 0.099
12		$\frac{1}{4}$	0.025 0.101
13		$\frac{2}{4}$	0.046 0.092
14		$\frac{3}{4}$	0.072 0.096

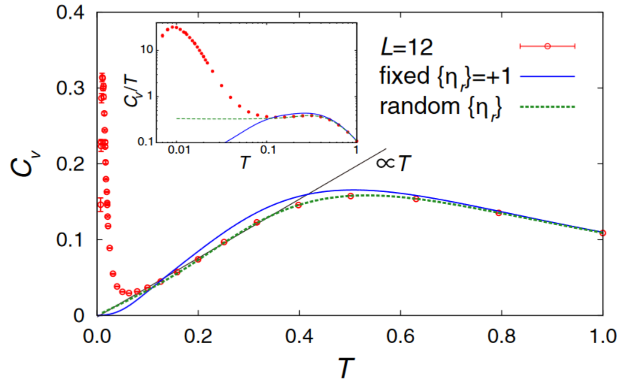
Kitaev, Ann. Phys. ***321****, 2 (2006)*

Thermodynamics (cont.):

- Can understand in terms of two energy scales:
    1. **Fermionic scale:** Spins have fractionalized into Majoranas, fluxes are *disordered* ~ *O(J)*
    2. **Flux scale:** Flux excitations no longer populated, settle into flux-free sector ~ *O(flux gap)*
- At *each* of these, release ~ log(2)/2 entropy per spin



Looks like Majoranas in random flux background



Nasu et al, Phys. Rev. ***92*** *115122 (2015); Motome & Nasu, JPSJ* ***89*** *012002 (2020)*

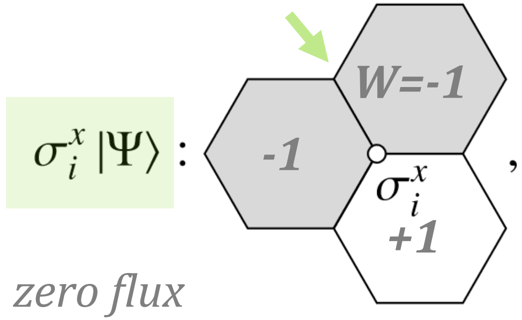
Spin correlations:

- *Static* spin-spin correlations are **ultra-short range**

$$\langle \sigma_i^\gamma \sigma_j^\gamma \rangle = \begin{cases} \neq 0, & \langle ij \rangle \in \gamma \\ = 0, & \langle ij \rangle \notin \gamma \end{cases}$$

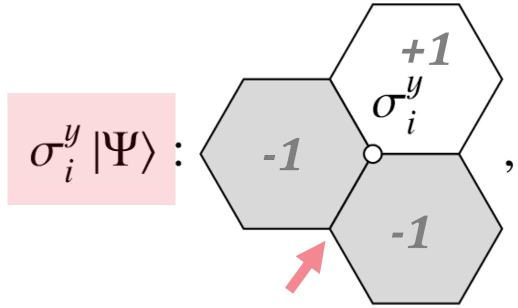
- Consequence of *plaquette symmetries*
- At isotropic point? *single correlation function*
- Also holds for **dynamical** correlator

$$\langle \sigma_i^\gamma(t) \sigma_j^\gamma \rangle$$

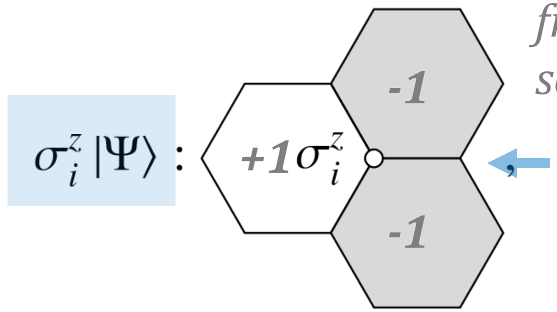


Act on zero flux state, with W=+1

Create pair of flux excitations



Only one way back to flux-free sector



Baskaran et al, Phys. Rev. Lett. ***98****, 247201*

Dynamics?

- Can compute from exact solution; **hard**, must deal with two-flux excitations

Remove flux pair + c-fermion

Evolve with fluxes

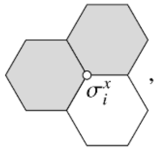
Add flux pair + c-fermion

$$\langle \sigma_i^\gamma(t)\sigma_j^\gamma \rangle = e^{iE_0 t}\langle \Psi_0 | \sigma_i^\gamma e^{-iHt} \sigma_j^\gamma | \Psi_0 \rangle$$

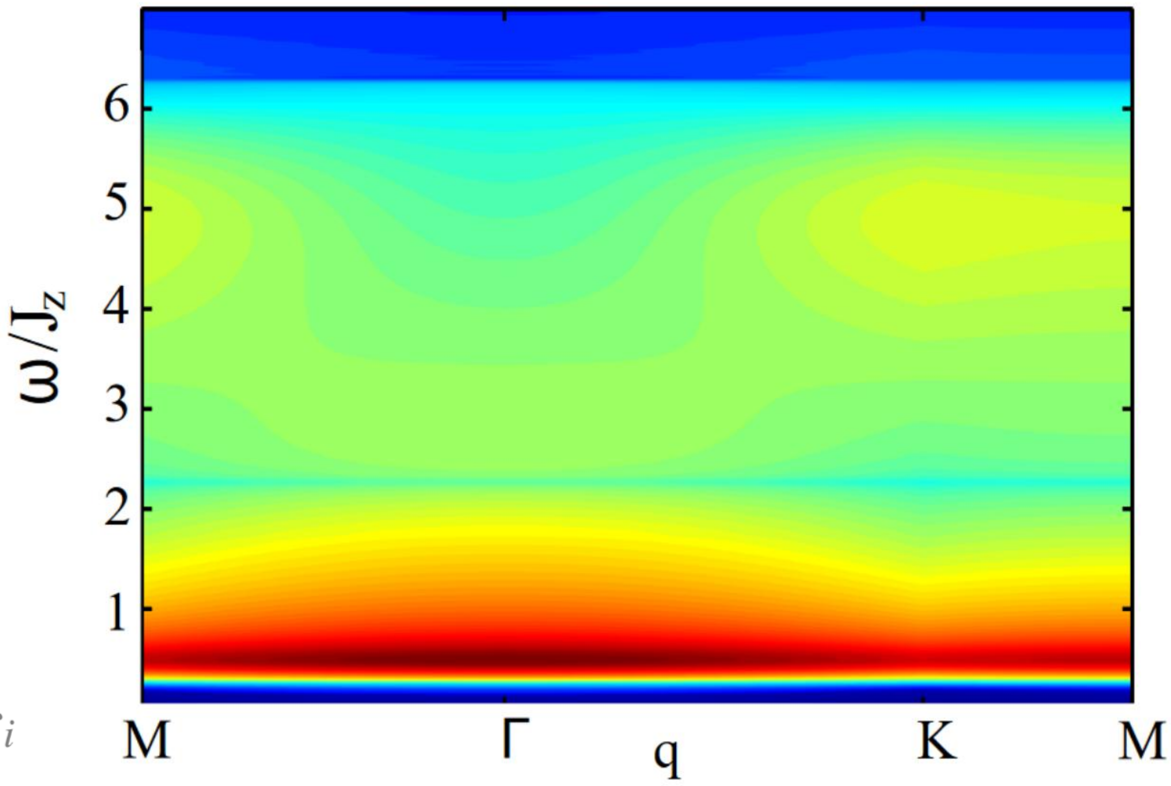
$\boldsymbol{\sigma}_i \equiv i\boldsymbol{b}_i c_i$

$$= e^{iE_0 t}\langle \tilde{\Psi}_0 | c_i e^{-iH[u_{\text{pair}}]t} c_j | \tilde{\Psi}_0 \rangle$$

Sector with pair of fluxes



- Related to *X-ray edge problem*



$$S(\boldsymbol{q},\omega) \propto \sum_\gamma \sum_{ij} \int dt\, e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j) - i\omega t} \langle \sigma_i^\gamma(t)\sigma_j^\gamma \rangle$$

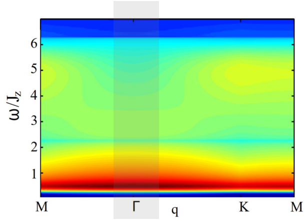
Fourier-transform of spin-spin correlator

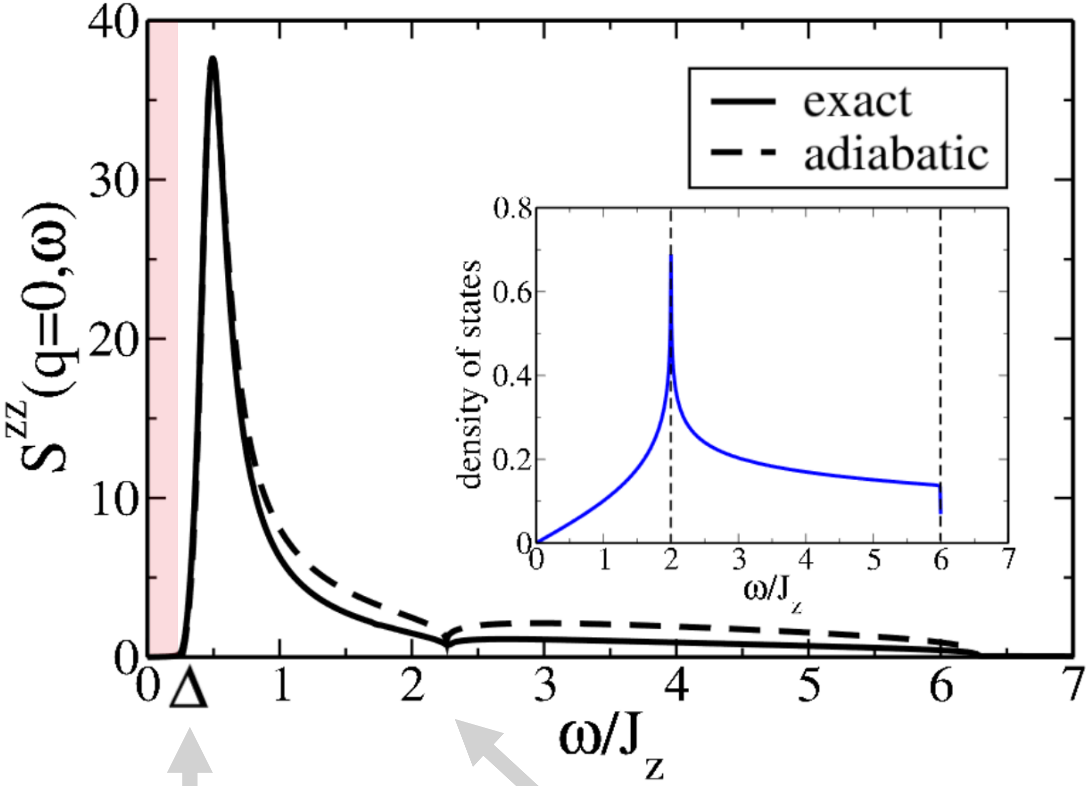
Knolle et al, Phys. Rev. Lett ***112*** *207203 (2014)*

Dynamics (cont.):

- Dirac cones *not* directly visible, no flux change
- Clear **gap** corresponding to energy cost to create pair of flux excitations
- **Continuum** of intensity going out energies of ~*O(J)*

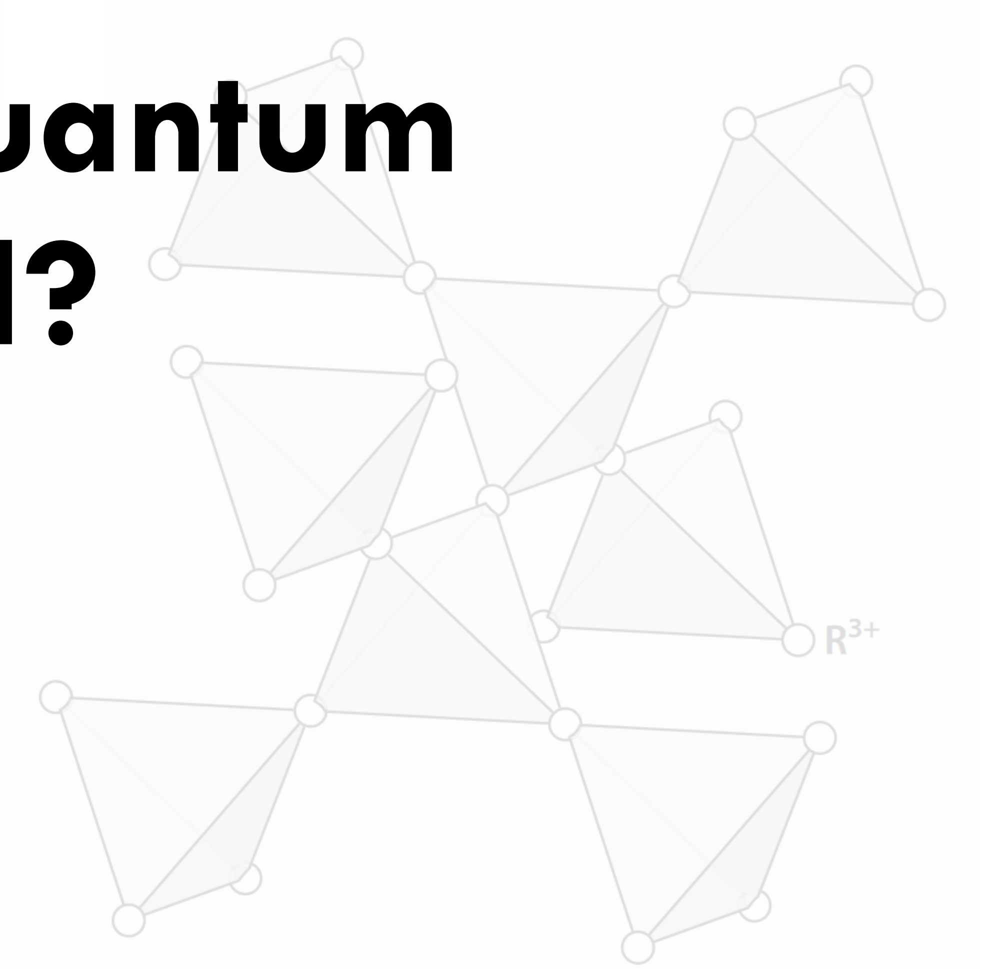
Energy scale of Majorana dispersion





Knolle et al, Phys. Rev. Lett ***112*** *207203 (2014)*

How to *find* a quantum spin liquid?



Signatures of spin liquids

- Lack of magnetic order
- Shows broad excitation spectrum

Fractionalization ?

- Still *dynamic* at very low temperature
- Topological response

e.g. Emergent photon, quantized gravitational response, …

Is disorder playing a role?

Is temperature/energy low enough?

Conventional route?

Stability?

Stability is possible!

- Kitaev? *Time-reversal symmetry*
- Quantum spin ice? ***Any** perturbation*

- Still need to worry about **energy scales**

Effective model of QSI

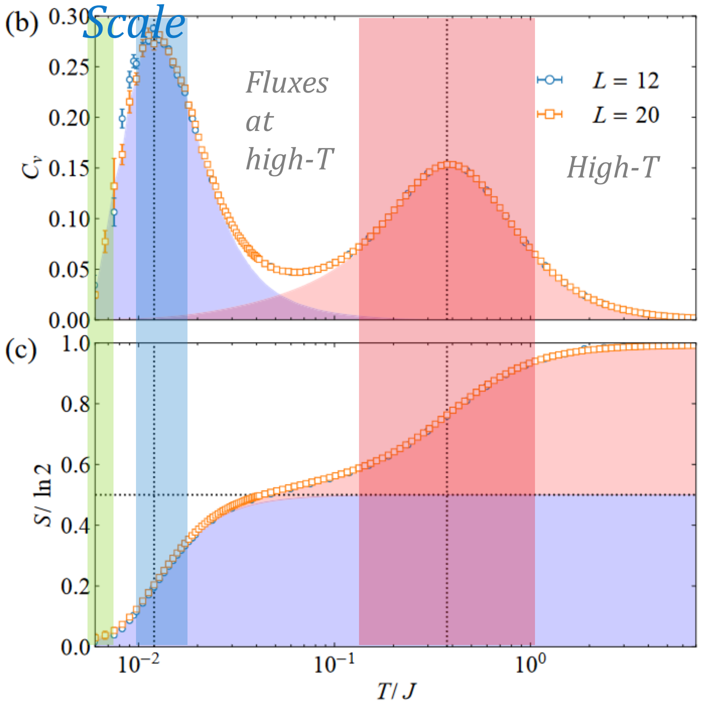
$$-\frac{12J_{\pm}^3}{J_{zz}^2}\sum_{\text{hexagons}} P_{\text{ice}}\left(S_1^+S_2^-S_3^+S_4^-S_5^+S_6^- + \text{h.c.}\right)P_{\text{ice}}$$

*Temperature/perturbations must be compared to **this***

*Kato & Onoda, Phys. Rev. Lett. **115** 077202 (2015);*
*Motome & Nasu, JPSJ **89** 012002 (2020)*

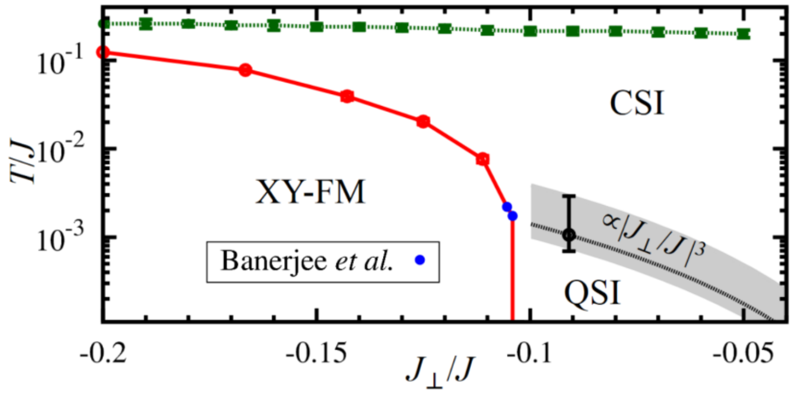
Flux Scale *Fermionic Scale*

Ground state physics



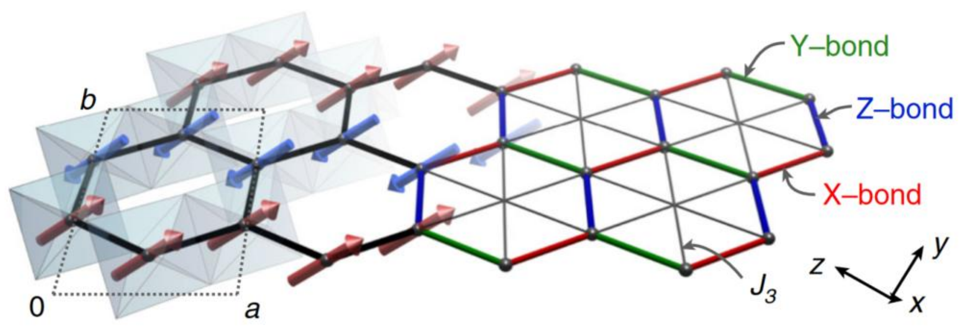
Thermodynamics of Kitaev Model

Phase diagram of QSI



... temperatures *order of magnitude* or two **smaller than**

Example: $RuCl_3$



- Kitaev spin liquid is *stable,* **but …**
- … sub-dominant perturbations large enough to **destroy the spin liquid**

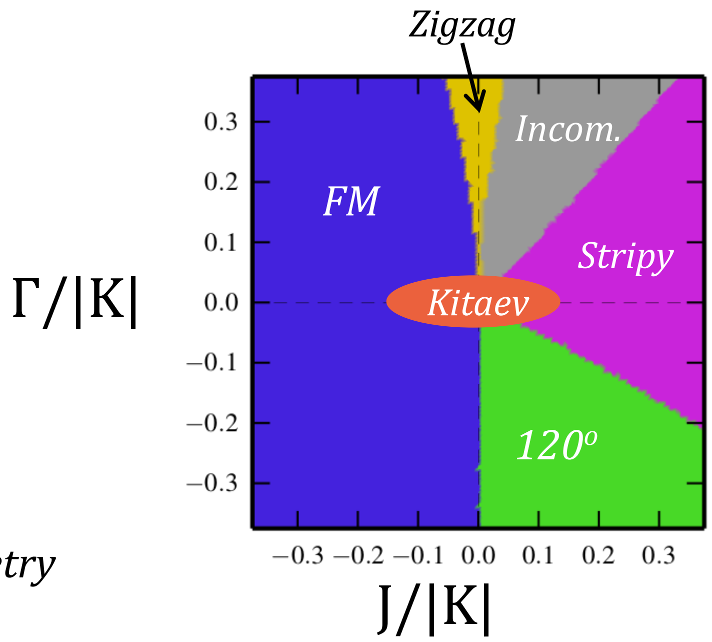
$$\sum_{\langle ij\rangle \in \alpha\beta(\gamma)} \left[J\mathbf{S}_i \cdot \mathbf{S}_j + K S_i^{\gamma} S_j^{\gamma} + \Gamma \left(S_i^{\alpha} S_j^{\beta} + S_i^{\beta} S_j^{\alpha} \right) \right]$$

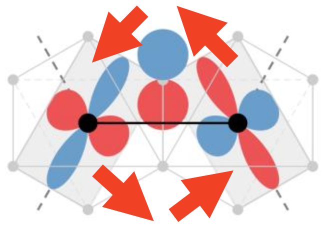
Jackeli/Khaliullin

From direct d-d overlap

Cross-term

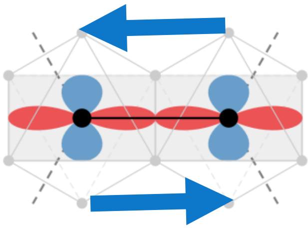
***Generic** symmetry allowed model*





Ligand mediated

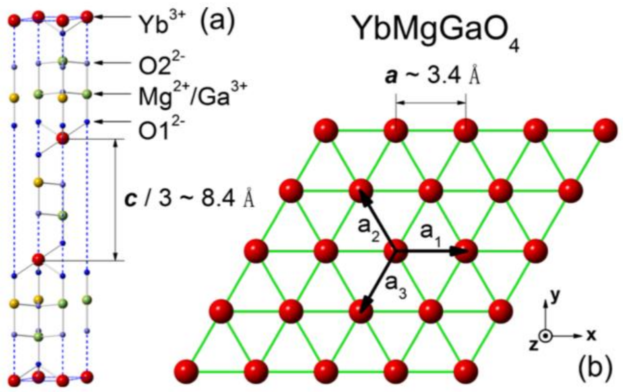
Direct overlap

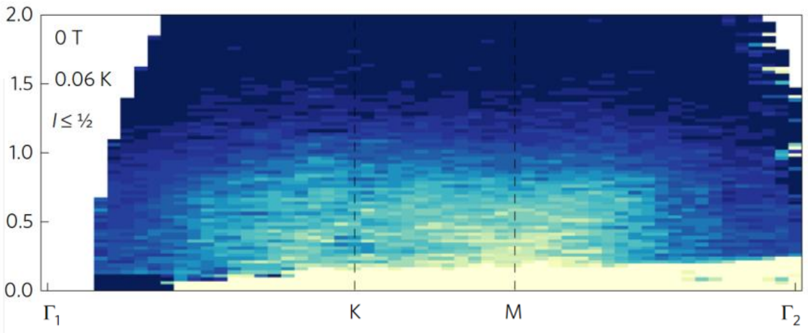


Katakuri et al., New. J. Phys. ***16,*** *013056 (2014)*
Rau, Lee & Kee, Phys. Rev. Lett. ***112,*** *077204 (2014)*

Disorder?

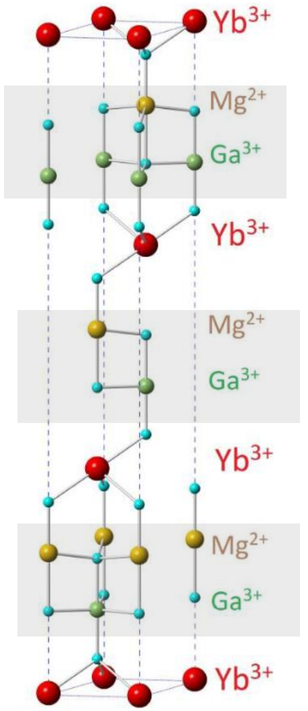
- Key signature of spin liquid: **fractionalization of excitation spectrum**
- Broad, indistinct excitations instead of sharp quasiparticles
- **Problem:** How to disentangle from effects of *structural disorder*?



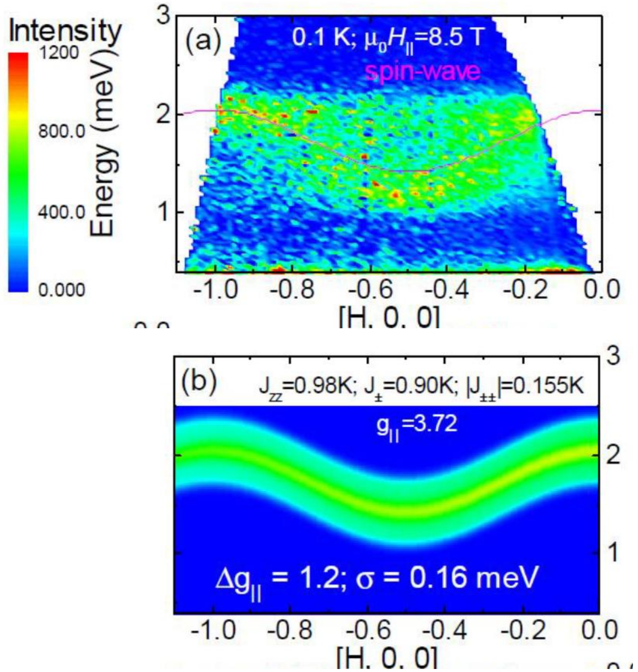


... this disorder can explain some of the broadness of spectrum

Mg/Ga layers are ***disordered***



Charge *disorder, 2+ vs. 3+*



Lake et al, Phys. Rev. Lett. ***111*** *137205*

Broader Questions:

How does disorder affect frustrated magnets?

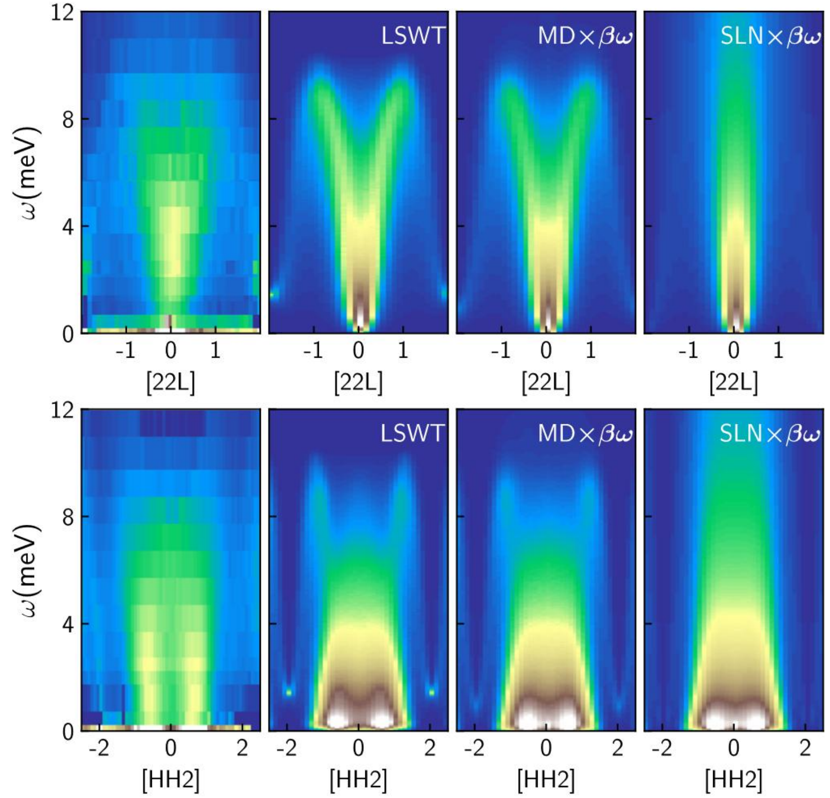
- Always destructive?
- Disorder induced/stabilized spin liquids?

How to distinguish *trivially* disordered states from spin liquids *with* disorder?

- Fractionalization obscured

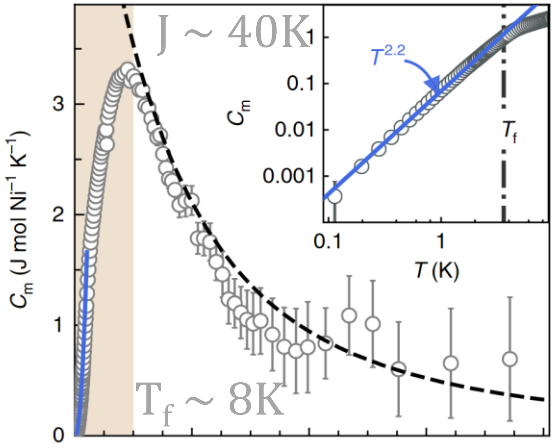
$NaCaNi_2F_7$

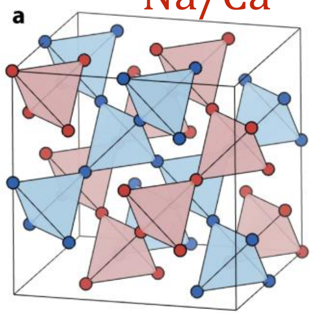
Exp. Theory



Inelastic neutron scattering

Heat Capacity

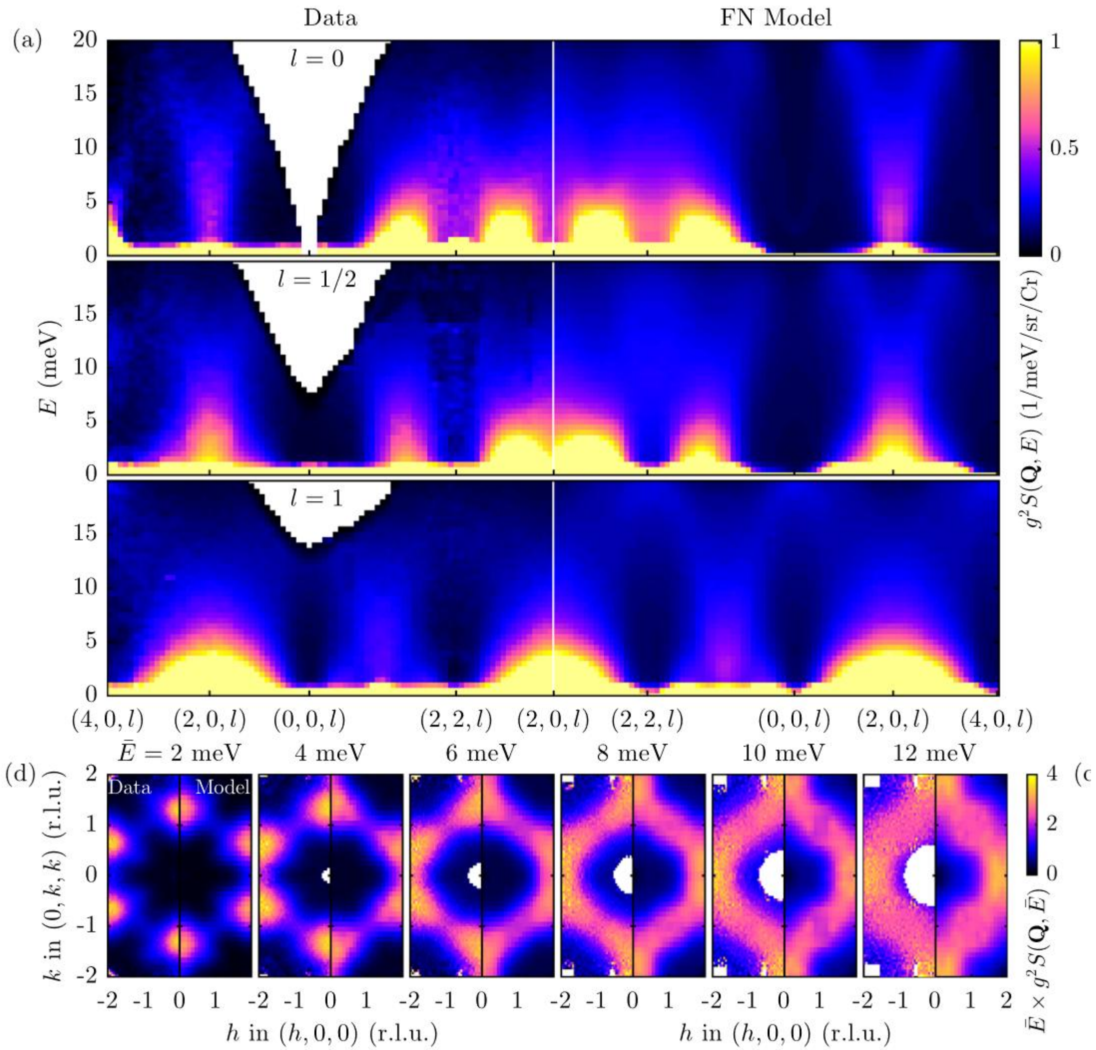




Plumb et al, Nat. Phys. ***15*** *54 (2019); Zhang et al, Phys. Rev. Lett.* ***122*** *167203 (2019)*

Fractionalization?

- … once we've eliminated and/or understood disorder **still need understand of continua**
  - Some unexpected success of semi-classics
- Source?
  - **Genuine spin liquid**
  - Quasi-particle decay (general *broadening)*
  - Phase coexistence or competition
  - …



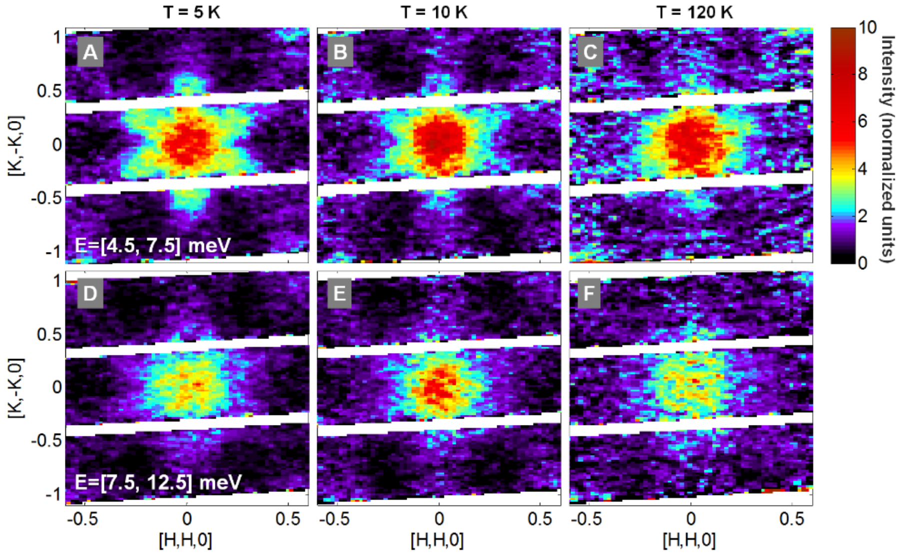
Neutron scattering on $MgCr_2O_4$

Broader Questions:

How to better understand *unconventional* excitations in frustrated magnets?

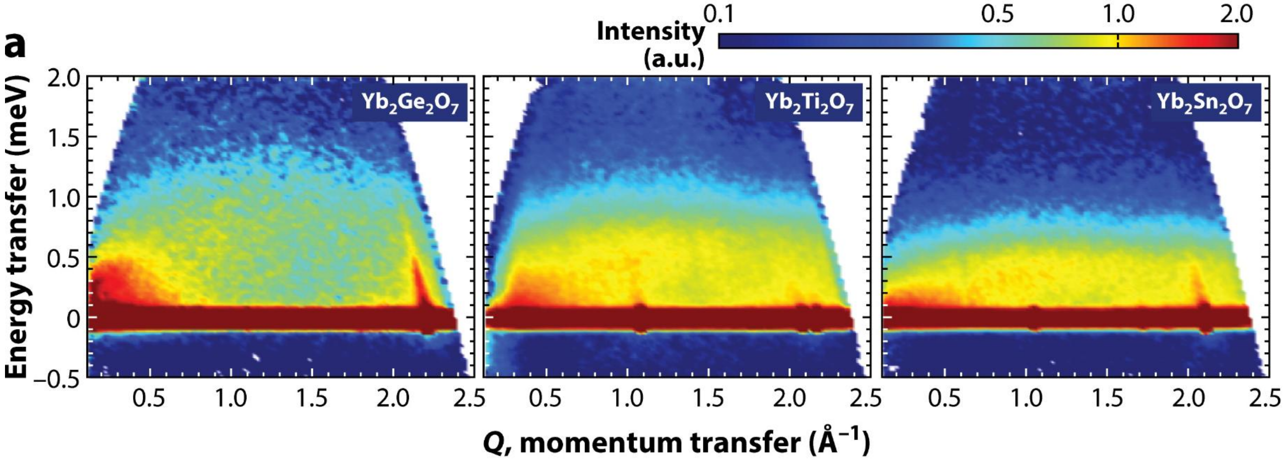
- Imprint of proximate fractionalized phases?
- Distinguish from conventional broadening?
- What role can semi-classical ideas play?

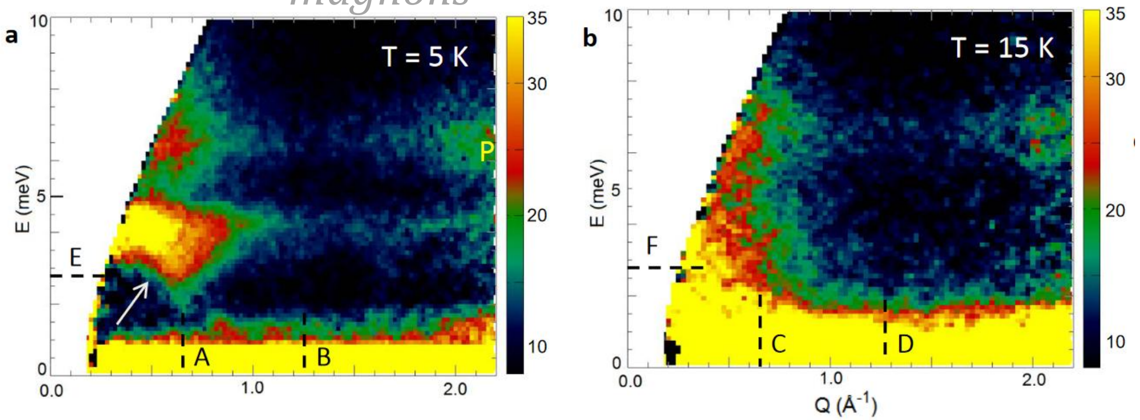
High-energy structure persists?



Low-energy features: magnons

$RuCl_3$





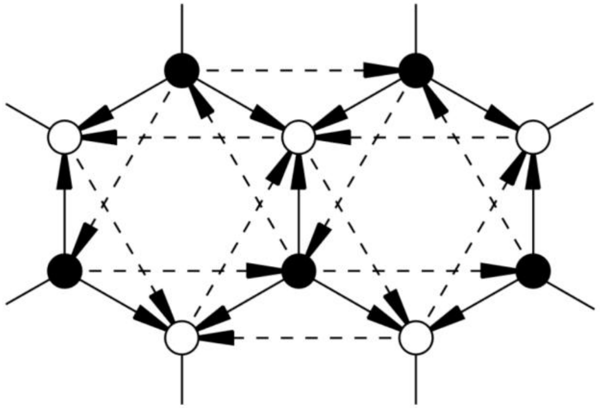
Hallas et al, ARCMP (2018)

Banerjee et al, Nat. Mat. (2016); Banerjee et al, Science (2017)

Topological Response?

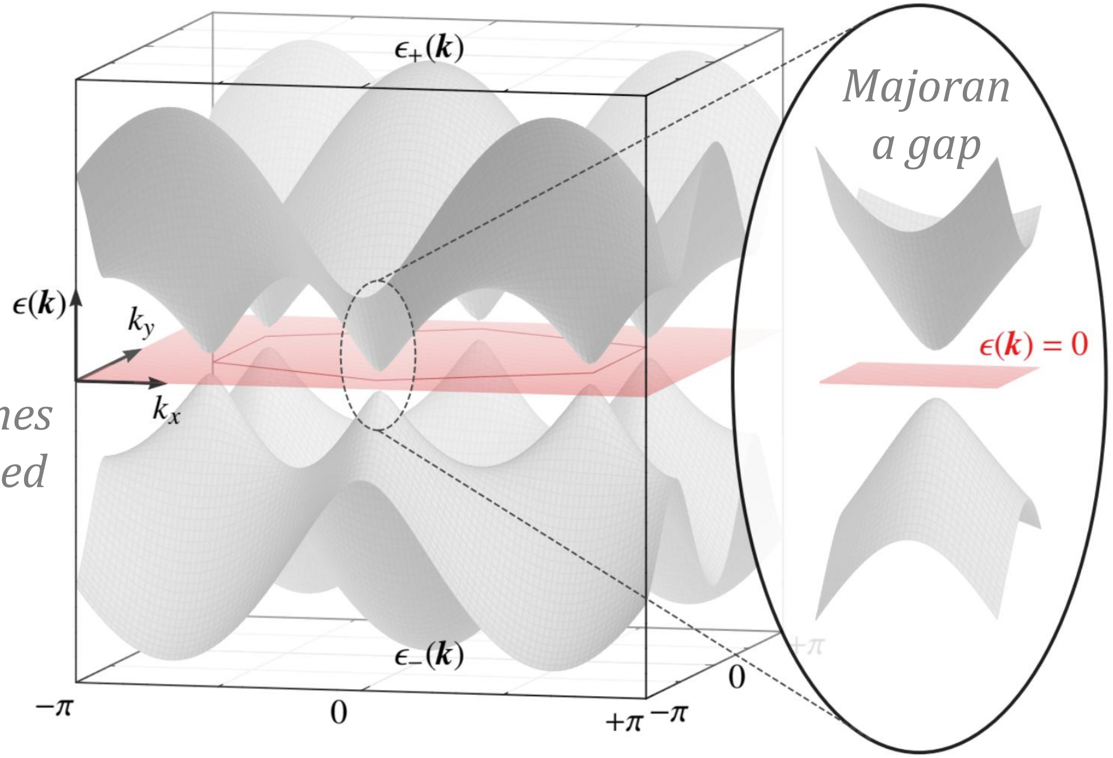
$$\Delta \sim \frac{h_x h_y h_z}{J^2}$$

- Field appears at 3rd order as *second-neighbour hopping*



- *Identical* in form to Haldane-type model
- *Topological bands;* ***chiral Majorana edge modes***

Dirac cones are gapped out



Spectrum near cones

$$\varepsilon(\mathbf{q}) \approx \pm\sqrt{3J^2\,|\delta\mathbf{q}|^2 + \Delta^2}$$

Majorana "mass"

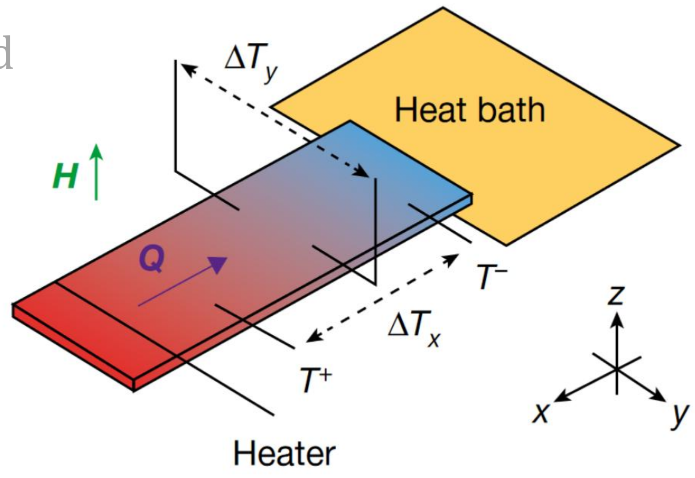
Haldane, Phys. Rev. Lett. ***61*** *2015 (1988); Kitaev, Ann. Phys.* ***321****, 2*

Broader Questions:

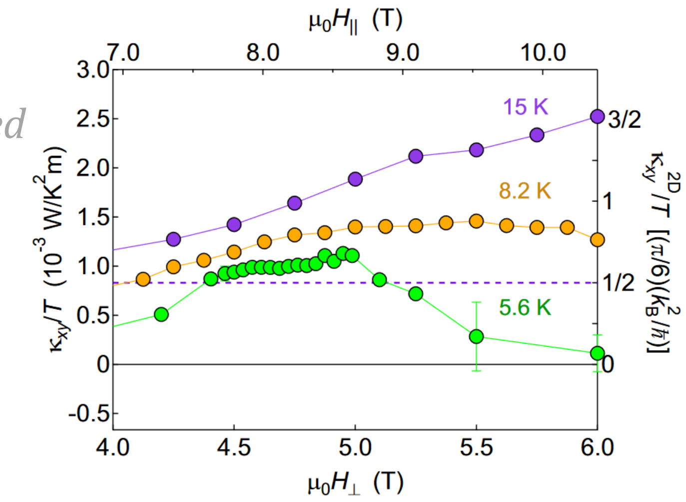
Do we understand thermal transport in frustrated* magnets?

- From spinons, magnons, monopoles, etc?
- At high/intermediate temperatures?
- Interplay with phonon transport?

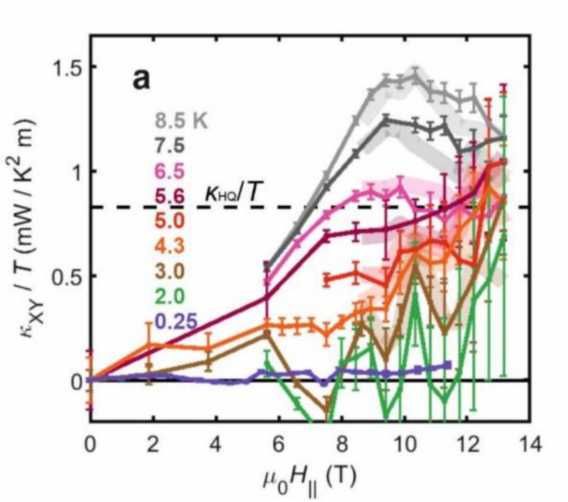
**Not just frustrated magnets*



Half-quantized



Kasahara et al, Nature (2018)



Not half-quantized?

$$\frac{\kappa_{xy}}{T} = q\frac{\pi}{6}\frac{k_B^2}{\hbar}$$

(Chiral) central charge of edge modes

Three ~~questions~~ "answers"

1. What *is* a spin liquid? → Magnet that *doesn't order* down to zero temperature **and** is *distinct from a trivial paramagnet*

2. How to *stabilize* a spin liquid? → Look for highly frustrated models (e.g. extensive degeneracy), minimize any perturbations

3. How to *detect* a spin liquid?

→ Go to low enough energy, be *mindful* of disorder, look for fractionalized excitations and/or topological responses