

Tutorial: Quantum Pyrochlore Magnets

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Three Questions

1. What are the spins?

What's possible for single-ion physics?

2. How do they interact?

What kind of exchange interactions do we have?

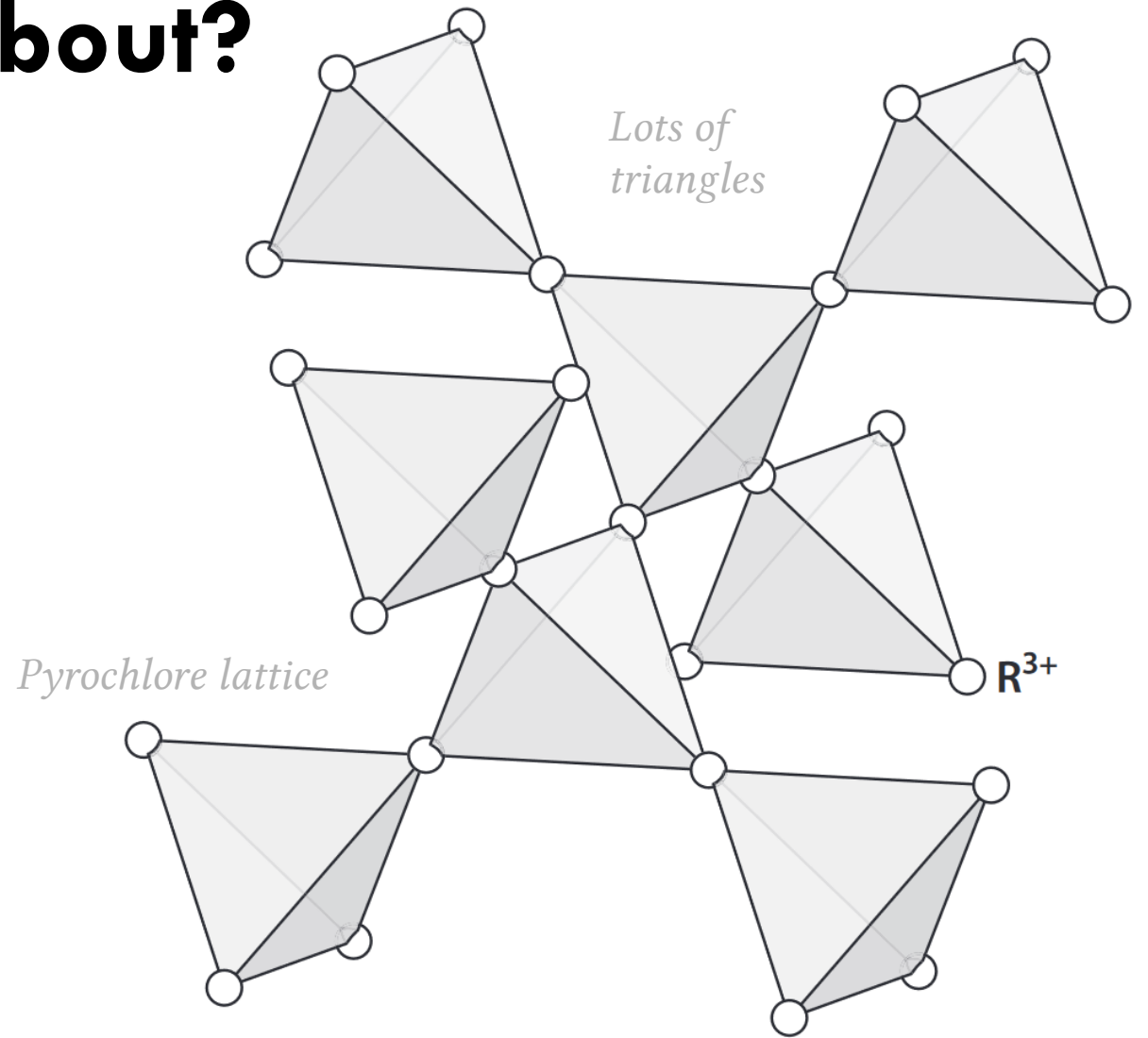
3. Where to look for interesting *quantum* phases?

Where do ordered phases breakdown?

What are we talking about?

- Corner-sharing tetrahedra
- Canonical 3D **frustrated** lattice
- Materials:
 - $R_2M_2O_7$ *Pyrochlore oxides*
 - AR_2X_4 *Spinels*
 - ...
- **R** = Rare-earth, **M** = Transition Metal
- Strong insulators

*Will
focus on
this case*



Atomic Physics?

Spin-orbit coupling

Period

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Free-ion Physics

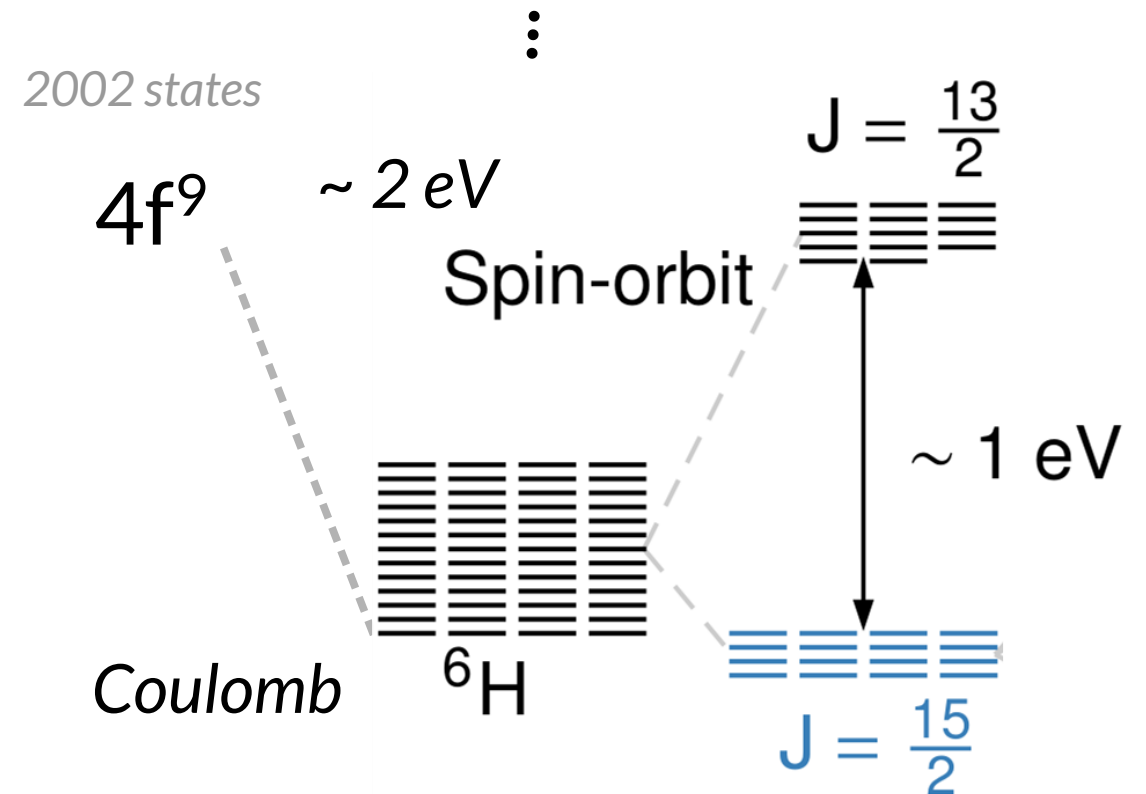
- For 4f electrons: in most cases many atomic states
- Only **free-ion ground state** is relevant

Hund's rules:

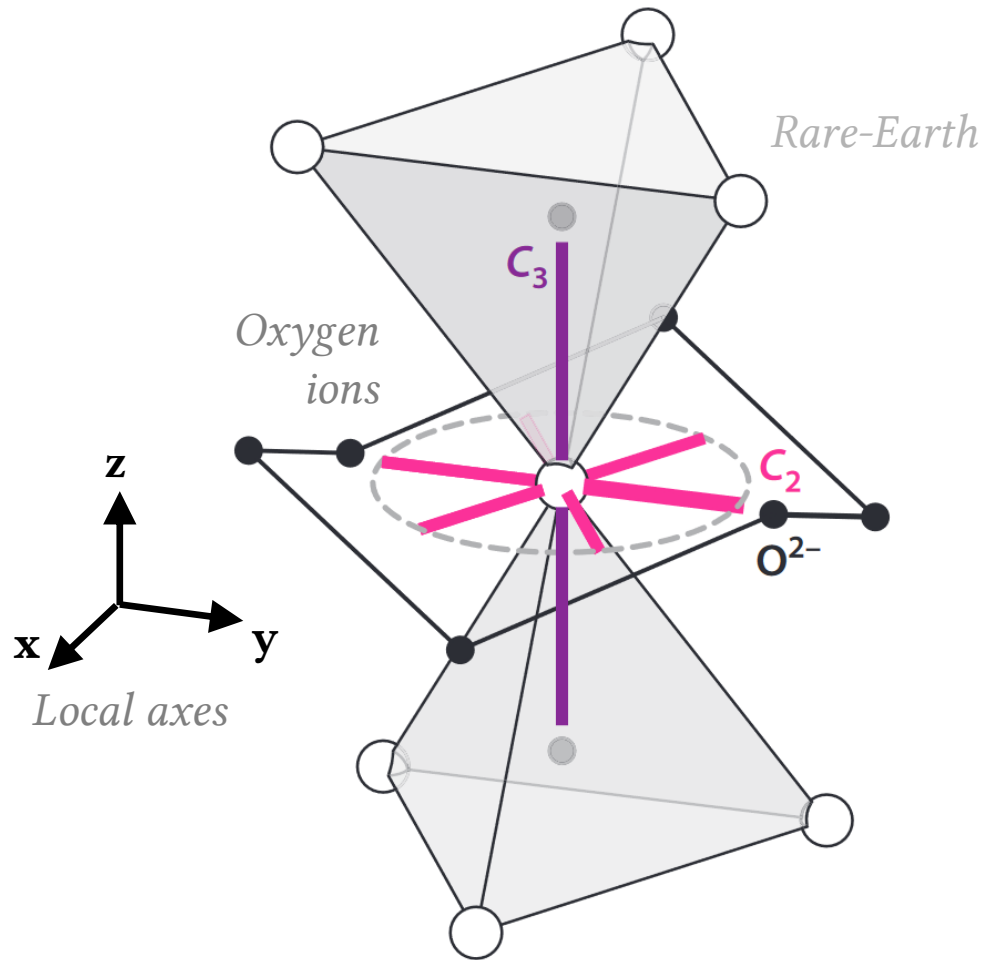
1. Maximize S
2. Maximize L
3. Maximize J ($n < 7$)
Minimize J ($n > 7$)

- For 4f series:
 - $5/2 \leq J \leq 8, 0 \leq L \leq 6$

Example: $\text{Dy}^{3+}, 4f^9$
 $L=5, S=5/2 \rightarrow J=15/2$



Crystalline Electric Field



Local environment for RE in $R_2M_2O_7$

- Atomic manifold split by electric fields from surrounding ions
- Local symmetry: D_{3d}
 - C_3 axis (local z)
 - C_2 axis (local y)
 - Inversion
- Reduces degeneracy (e.g. from $2j+1$) to **singlet or doublet**

Form of CEF ground state?

Crystalline Electric Field (cont.)

- Classify states by **local symmetry**: label by irreducible representations of (site-symmetry group) D_{3d}

- **Kramers** (*odd* number of electrons)

- Γ_4 irrep. \rightarrow pseudo-spin doublet

Case #1

- $\Gamma_{5,6}$ irrep. \rightarrow dipolar-octupolar doublet

Case #3

- **non-Kramers** (*even* number of electrons)

- A_{1g} or A_{2g} irrep. \rightarrow singlet (non-magnetic)

- E_g irrep. \rightarrow non-Kramers doublet

Case #2

Case #1: Pseudo-Spin Kramers Doublet (Γ_4)

- Simplest case, doublet **protected by time-reversal**

Doublet states

$$|\pm\rangle = \alpha |\pm 1/2\rangle + \beta |\mp 5/2\rangle + \dots \quad \text{Differ by multiples of 3 in } J_z$$

- Effective spin operators (S_x, S_y, S_z) **all represent magnetic dipoles**

Effective spin-1/2 operators

- Two** g-factors generically:

Local axes

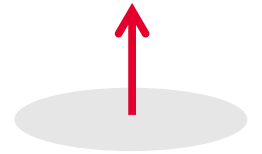
$$\boldsymbol{\mu}_i \equiv \mu_B [g_{\pm} (\hat{\mathbf{x}}_i S_i^x + \hat{\mathbf{y}}_i S_i^y) + g_z \hat{\mathbf{z}}_i S_i^z],$$

Magnetic dipole moment

- Transforms in same way as spin-1/2** under spatial symmetries of pyrochlore lattice

$$\langle S_z \rangle \neq 0$$

- Time-reversal odd
- Breaks C_2



$$\langle S_{\pm} \rangle \neq 0$$

- Time-reversal odd
- Breaks C_2, C_3



Case #2: Non-Kramers Doublet (E_g)

- Not protected by time-reversal

$$|\pm\rangle = \alpha |\pm 4\rangle + \beta |\pm 1\rangle + \dots$$

*Doublet
states*

- Strongly anisotropic

- S_z transforms as **magnetic dipole** along local z
- S_x, S_y transform as **electric quadrupoles**

- Magnetic probes couple **only** to S_z directly

$$\mu_i = \mu_B g_z S_i^z \hat{\mathbf{z}}_i$$

Single g-factor

- Sensitive to non-magnetic disorder, couples directly to elastic degrees of freedom, ...

$$\langle S_z \rangle \neq 0$$

- Time-reversal odd
- Breaks C_2



$$\langle S_{\pm} \rangle \neq 0$$

- Time-reversal **even**
- Breaks C_2, C_3



~xz, yz orbital

Case #3: Dipolar-Octupolar Doublet ($\Gamma_{5,6}$)

- State unrelated under spatial symmetry, connected **only by time-reversal**

$$|\pm\rangle = \alpha |\pm 3/2\rangle + \beta |\mp 9/2\rangle + \dots$$

At least 3 to flip

- Canonical basis choice: magnetic moment proportional to S_z

$$\mu_i = \mu_B g_z S_i^z \hat{\mathbf{z}}_i \quad (\text{By construction})$$

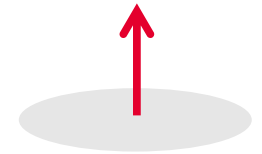
- **Strongly anisotropic**

- Both S_x and S_z transform like **magnetic dipoles** along the **local z axis**
- S_y transforms like **magnetic octupole** – invariant under *all* D_{3d} symmetries

$$\langle S_z \rangle, \langle S_x \rangle \neq 0$$

.Time-reversal
odd

.Breaks C_2



$$\langle S_y \rangle \neq 0$$

.Only breaks time-reversal!



Aside: Multipolar Content of Spin

- Can project multipole into CEF ground doublet

$$\text{Projection into ground doublet} \quad PO_{KQ}(\mathbf{J})P = \sum_{\mu} C_{KQ}^{\mu} S_{\mu} \quad \text{Akin to multipolar "g" factors}$$

- **Any** multipole can contribute to effective spin so long as symmetries match

- **Pseudo-spin:** dipole, octupole, ... (odd ranks) $\sim A_{2g}, E_g$

- **Dipolar-Octupolar:**

$\sim A_{2g}$ S_x, S_z : dipole, octupole, ... (odd ranks)

$\sim A_{1g}$ S_y : octupole, ... (odd ranks)

- **Non-Kramers:**

$\sim A_{2g}$ $S_z \rightarrow$ dipole, octupole, ... (odd ranks)

$\sim E_g$ $S_x, S_y \rightarrow$ quadrupole, hexadecapole ... (even ranks)

"Singlet" A_{1g}, A_{2g} even rank multipoles project to nothing

Summary of Single-Ion Physics

- Three **doublet** types under D_{3d} symmetry:
 pseudo-spin, dipolar-octupolar, non-Kramers

Irrep.	g_z	g_{\pm}	Time. rev.	C_3	C_2	States	Examples
Γ_4	$\neq 0$	$\neq 0$	$\mathbf{S} \rightarrow -\mathbf{S}$	$S^z \rightarrow S^z$ $S^{\pm} \rightarrow e^{\pm \frac{2\pi i}{3}} S^{\pm}$	$S^z \rightarrow -S^z$ $S^{\pm} \rightarrow S^{\mp}$	$ \pm \frac{1}{2}\rangle, \pm \frac{5}{2}\rangle, \dots$	Er ₂ Ti ₂ O ₇ , Yb ₂ Ti ₂ O ₇
$\Gamma_5 \oplus \Gamma_6$	$\neq 0$	0	$\mathbf{S} \rightarrow -\mathbf{S}$	$\mathbf{S} \rightarrow \mathbf{S}$	$S^z \rightarrow -S^z$ $S^{\pm} \rightarrow S^{\mp}$	$ \pm \frac{3}{2}\rangle, \pm \frac{9}{2}\rangle, \dots$	Dy ₂ Ti ₂ O ₇
E_g	$\neq 0$	0	$S^z \rightarrow -S^z$ $S^{\pm} \rightarrow S^{\mp}$	$S^z \rightarrow S^z$ $S^{\pm} \rightarrow e^{\pm \frac{2\pi i}{3}} S^{\pm}$	$S^z \rightarrow -S^z$ $S^{\pm} \rightarrow S^{\mp}$	$ \pm 1\rangle, \pm 4\rangle, \mp 5\rangle, \dots$	Ho ₂ Ti ₂ O ₇ , Tb ₂ Ti ₂ O ₇

Interactions?



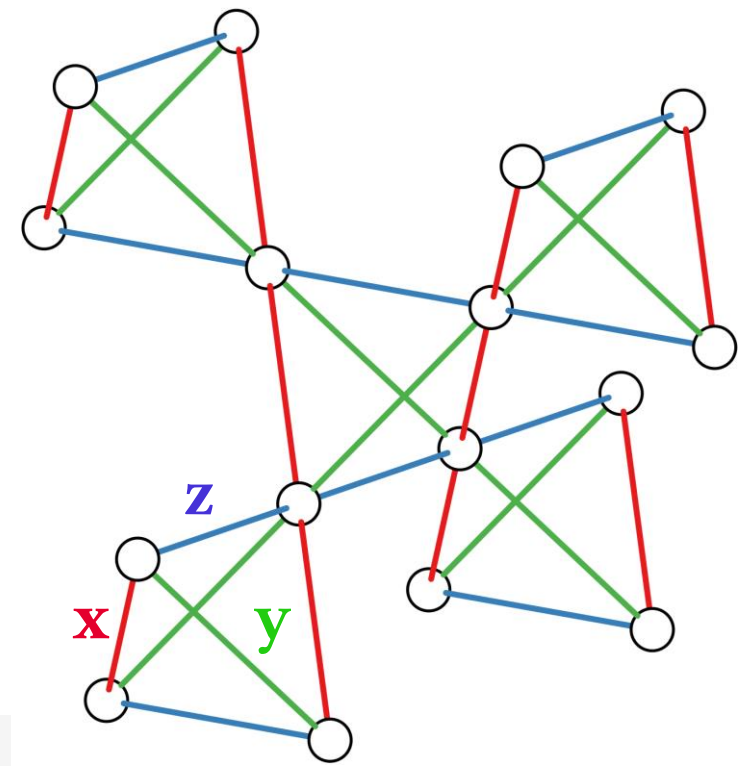
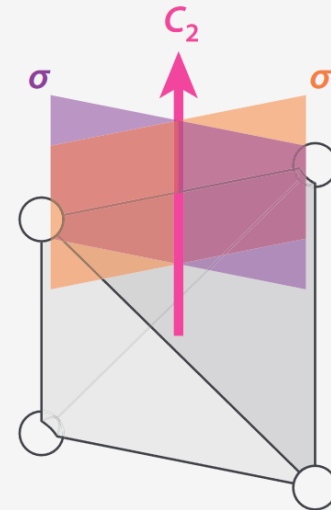
How do these interact?

Two-ion physics

- How do these doublets **interact**?
- Consider neighbours
- Strongly constrained by symmetry of lattice

Symmetry of bond:

- C_2 axis *Nearest neighbour bond*
- Reflection σ
- Reflection σ'
- Connect other bonds using C_3 :
 $\mathbf{x} \rightarrow \mathbf{y} \rightarrow \mathbf{z}$



Three types of bond

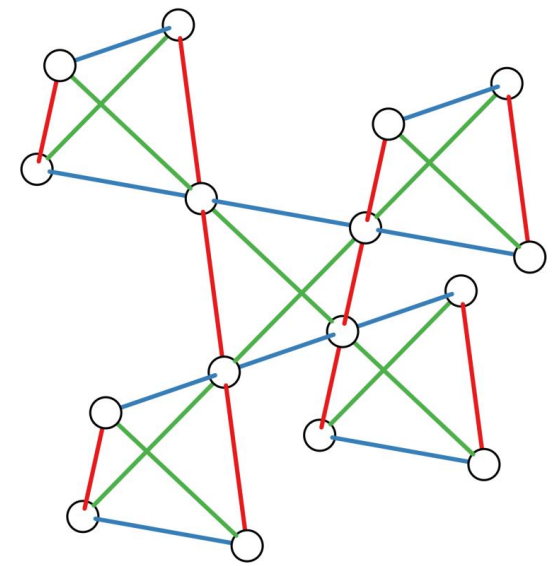
Anisotropic exchange model

- Symmetry constrained model takes the form:

$$\begin{aligned}
 & \sum_{\langle ij \rangle} [J_{zz} S_i^z S_j^z - J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+) + J_{\pm\pm} (\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-)] \\
 & + J_{z\pm} (\zeta_{ij} [S_i^z S_j^+ + S_i^+ S_j^z] + \zeta_{ij}^* [S_i^z S_j^- + S_i^- S_j^z])
 \end{aligned}$$

XXZ model
Bond dependent phases

Zero for non-Kramers
Bond dependent phases



Three or four independent exchange parameters

Cases: $\zeta_{ij} = -\gamma_{ij}^*$

- Pseudo-spin: $\gamma_x = 1, \gamma_y = e^{2\pi i/3}, \gamma_z = e^{-2\pi i/3}$
- Non-Kramers: $\gamma_x = 1, \gamma_y = e^{2\pi i/3}, \gamma_z = e^{-2\pi i/3}$ $J_{z\pm} = 0$
- Dipolar-Octupolar: $\gamma_{ij} = 1$

Origin of exchange?

Origin of Exchange interactions?

- Lots of ways to generate exchange interactions

- **Magneto- and electro-statics** *Rare-Earths*

- *Direct exchange*

- **Super-exchange (ligand-mediated)** *Transition Metals, Rare-earths*

- Exchange via higher orbitals (5d, 6s)

- Exchange via inter-shell interactions

- Magneto-elastic couplings

- Virtual crystal field interactions

- Many competing mechanisms, small energy scales, hard to estimate

Complicated ...

Special Cases?

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

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

Heisenberg – Align or Anti-align *In weak SOC limit $\hbar \gg D \gg \Gamma$* *Γ is a symmetric 3x3 matrix*

Dzyaloshinskii-Moriya (DM) interaction *Symmetric anisotropy (pseudo-dipolar, Ising, etc)*

- Transition metal with weak SOC:** Expect leading terms to be Heisenberg + D.M.
- Spin-Only Moment (Fe^{3+} , Gd^{3+} , Eu^{2+} , ...):** Expect Heisenberg dominant (& possibly dipolar interactions)
- Large ΔJ in CEF doublet:** Ising-like interactions

“Standard” limits:

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

XY $J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y)$

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

Strong SOC? No prescribed form!

Summary of Two-Ion Physics

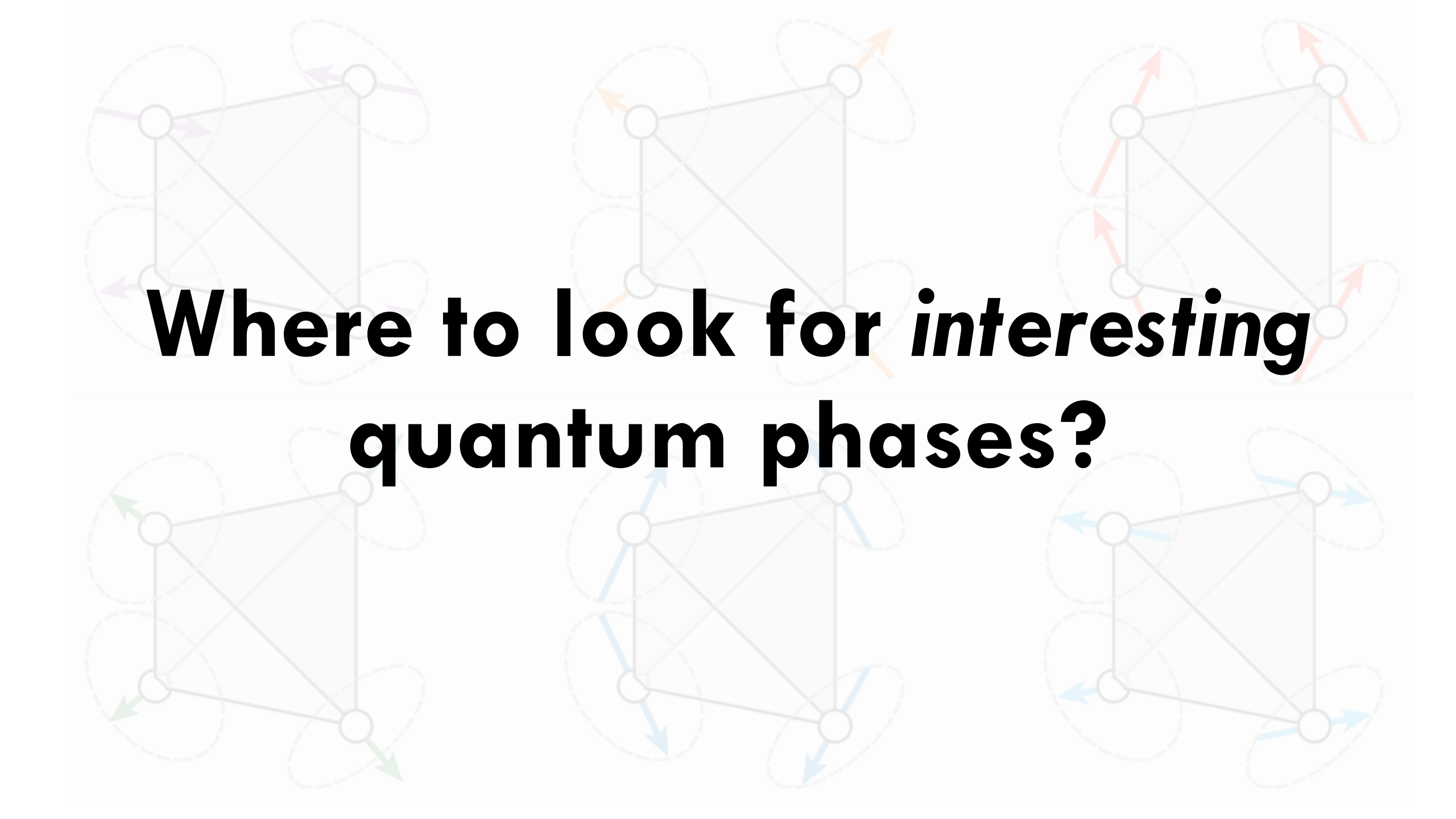
	Irrep.	g_z	g_{\pm}	Time. rev.	C_3	C_2	States	Examples
Pseudo-spin	Γ_4	$\neq 0$	$\neq 0$	$\mathbf{S} \rightarrow -\mathbf{S}$	$S^z \rightarrow S^z$ $S^{\pm} \rightarrow e^{\pm \frac{2\pi i}{3}} S^{\pm}$	$S^z \rightarrow -S^z$ $S^{\pm} \rightarrow S^{\mp}$	$ \pm \frac{1}{2}\rangle, \pm \frac{5}{2}\rangle, \dots$	$\text{Er}_2\text{Ti}_2\text{O}_7$, $\text{Yb}_2\text{Ti}_2\text{O}_7$
Dipolar-octupolar	$\Gamma_5 \oplus \Gamma_6$	$\neq 0$	0	$\mathbf{S} \rightarrow -\mathbf{S}$	$\mathbf{S} \rightarrow \mathbf{S}$	$S^z \rightarrow -S^z$ $S^{\pm} \rightarrow S^{\mp}$	$ \pm \frac{3}{2}\rangle, \pm \frac{9}{2}\rangle, \dots$	$\text{Dy}_2\text{Ti}_2\text{O}_7$
Non-Kramers	E_g	$\neq 0$	0	$S^z \rightarrow -S^z$ $S^{\pm} \rightarrow S^{\mp}$	$S^z \rightarrow S^z$ $S^{\pm} \rightarrow e^{\pm \frac{2\pi i}{3}} S^{\pm}$	$S^z \rightarrow -S^z$ $S^{\pm} \rightarrow S^{\mp}$	$ \pm 1\rangle, \pm 4\rangle, \mp 5\rangle, \dots$	$\text{Ho}_2\text{Ti}_2\text{O}_7$, $\text{Tb}_2\text{Ti}_2\text{O}_7$

$$\sum_{\langle ij \rangle} [J_{zz} S_i^z S_j^z - J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+) + J_{\pm\pm} (\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-) + J_{z\pm} (\zeta_{ij} [S_i^z S_j^+ + S_i^+ S_j^z] + \zeta_{ij}^* [S_i^z S_j^- + S_i^- S_j^z])]]$$

$$\zeta_{ij} = -\gamma_{ij}^*$$

$$\gamma_x = 1, \gamma_y = e^{2\pi i/3}, \gamma_z = e^{-2\pi i/3} \quad \gamma_{ij} = 1$$

$$\gamma_x = 1, \gamma_y = e^{2\pi i/3}, \gamma_z = e^{-2\pi i/3} \quad J_{z\pm} = 0$$

The background of the slide features a repeating pattern of six tetrahedra arranged in two rows of three. Each tetrahedron is represented by a light gray wireframe with a semi-transparent gray face. At each of the four vertices of a tetrahedron, there is a small white circle. From each circle, a colored arrow points outwards, perpendicular to the face of the tetrahedron. The colors of the arrows vary by tetrahedron: the top-left and bottom-left tetrahedra have purple and green arrows; the top-middle and bottom-middle tetrahedra have orange and blue arrows; and the top-right and bottom-right tetrahedra have red and light blue arrows. The arrows on the top and bottom tetrahedra of each pair point in opposite directions.

**Where to look for *interesting*
quantum phases?**

Classical Phases

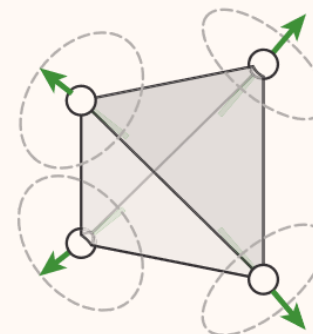
- To find *interesting* regions, identify “boring” ones first:
- Start from *classical* limit

$$\mathbf{S}_i \approx \langle \mathbf{S}_i \rangle$$

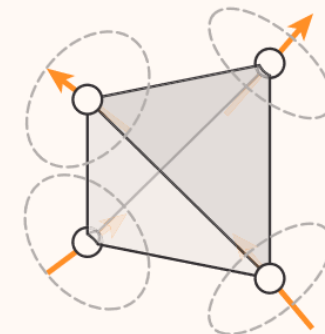
- Energy minimization finds only orders within the unit cell ($\mathbf{Q}=\mathbf{0}$)
- *Six* classes of order

e.g. Yan et al, Phys. Rev. B **95** 094422 (2017)

Ising-like
orders

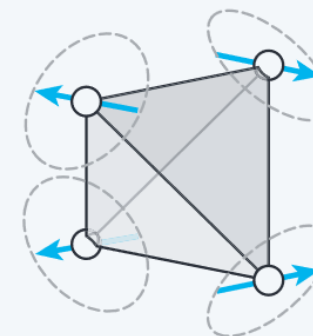


AIAO (A_{2g})

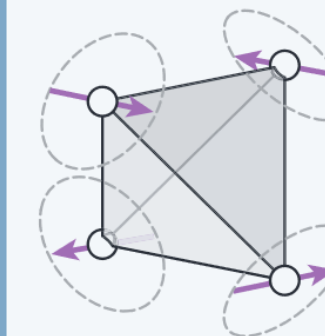


SI (T_{1g})

XY-like
orders

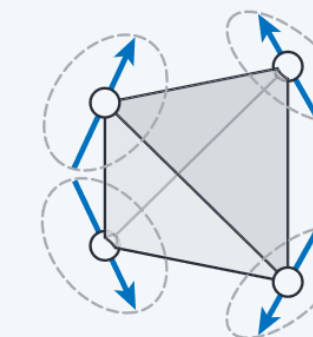


ψ_3 (E_g)

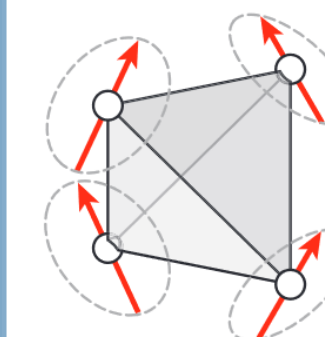


PC (T_{2g})

$U(1)$
Manifold



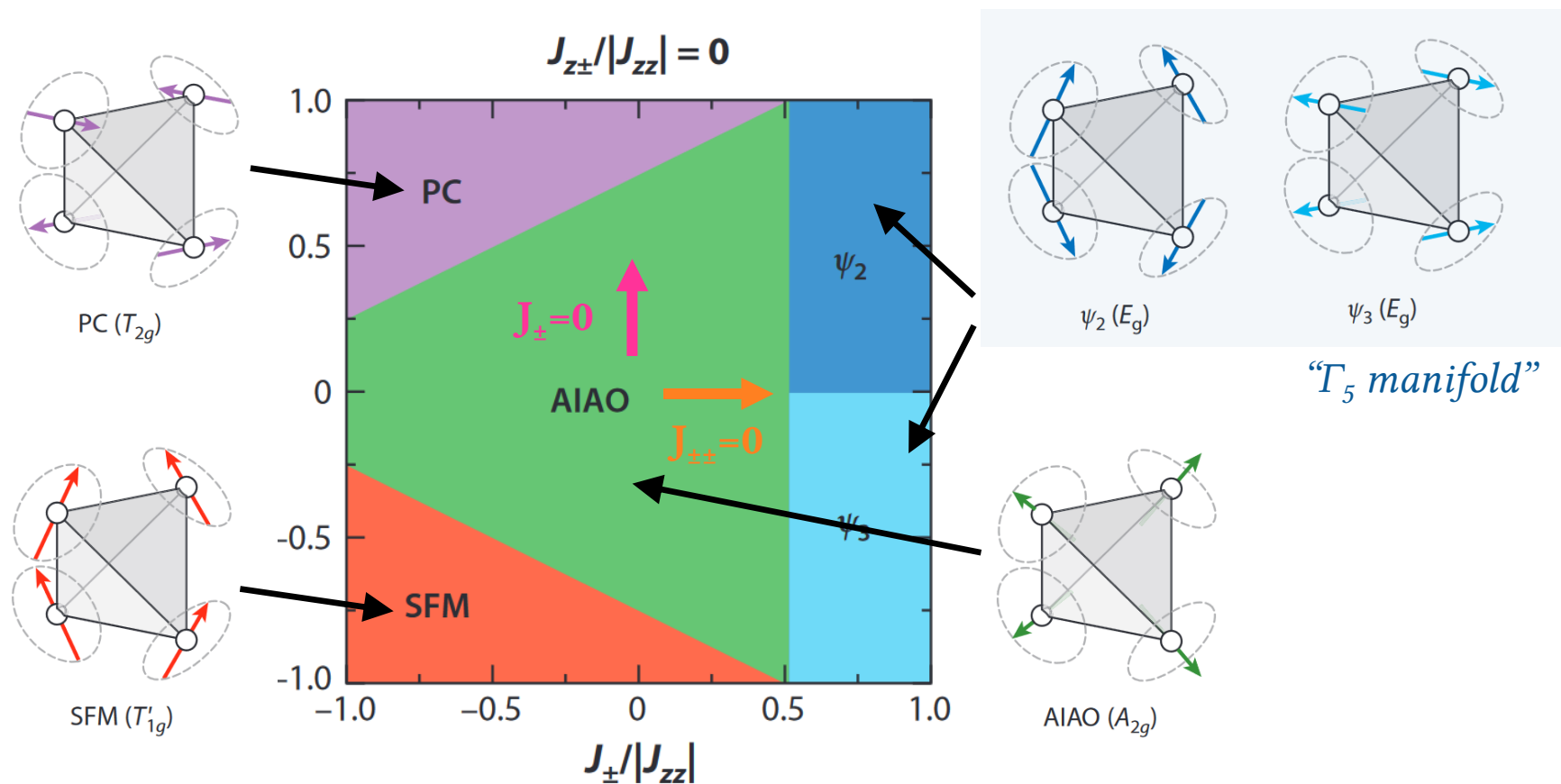
ψ_2 (E_g)



SFM (T'_{1g}) *Mixed*

Simplest limit:

$$J_{zz} < 0 \text{ and } J_{z\pm} = 0$$



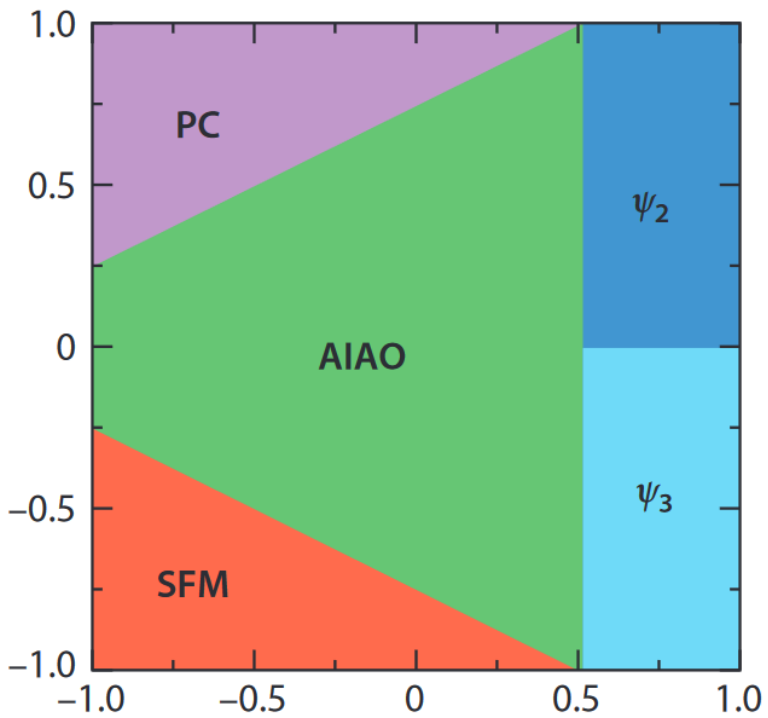
Negative

$$\sum_{\langle ij \rangle} [J_{zz} S_i^z S_j^z - J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+) + J_{\pm\pm} (\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-)]$$

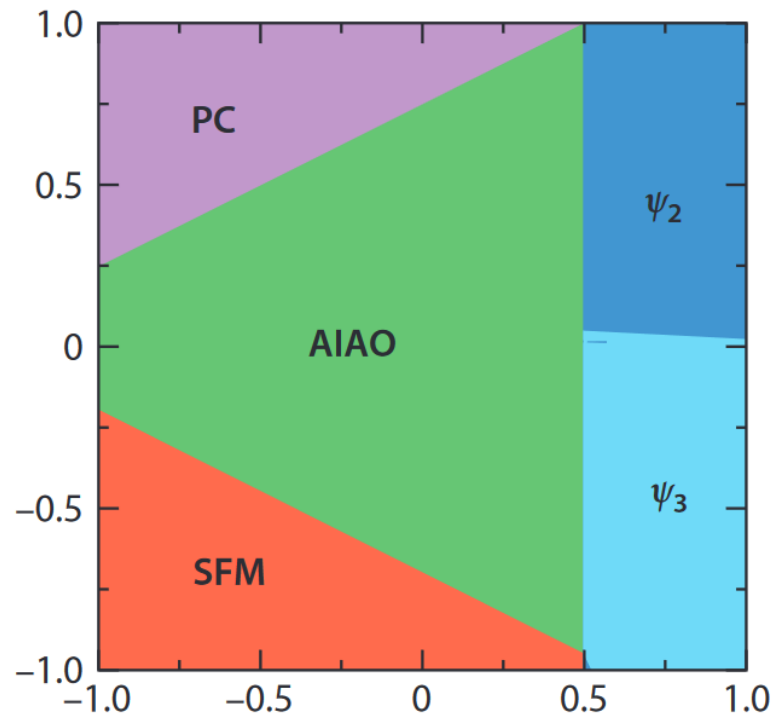
$$+ J_{z\pm} (\zeta_{ij} [S_i^z S_j^+ + S_i^+ S_j^z] + \zeta_{ij}^* [S_i^z S_j^- + S_i^- S_j^z])$$

Setting $J_{z\pm} = 0$ is required
in the non-Kramers case

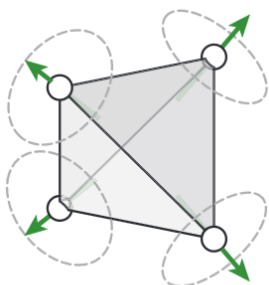
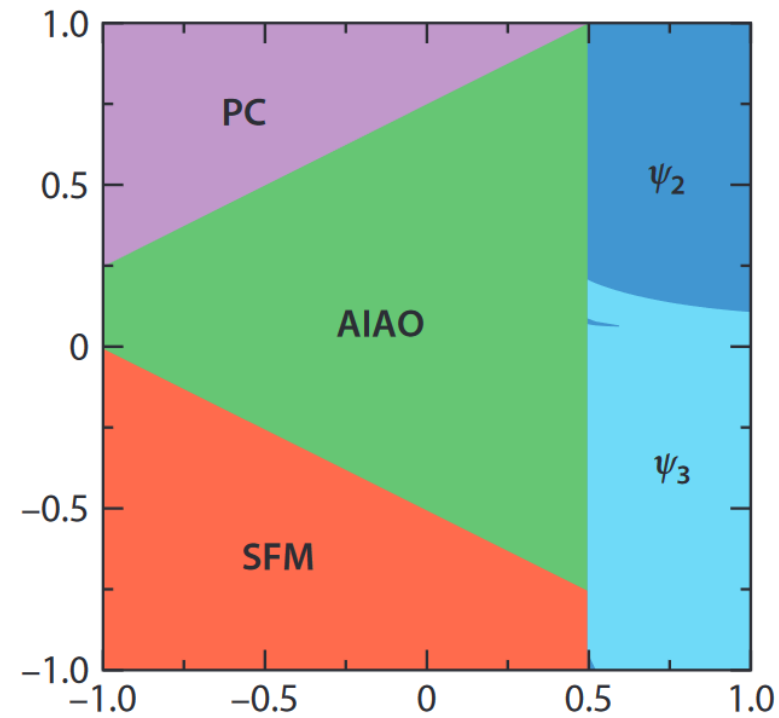
$$J_{z\pm}/|J_{zz}| = 0$$



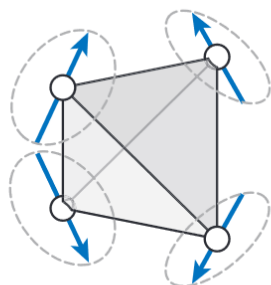
$$J_{z\pm}/|J_{zz}| = 1/4$$



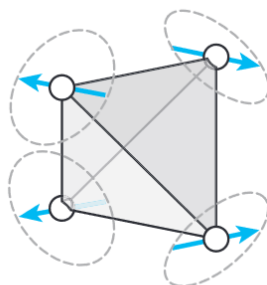
$$J_{z\pm}/|J_{zz}| = 1/2$$



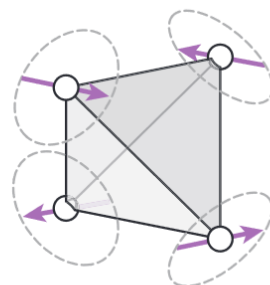
AIAO (A_{2g})



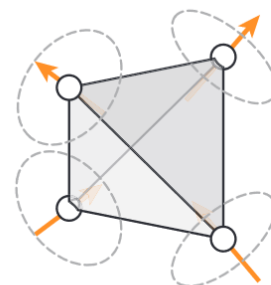
ψ_2 (E_g)



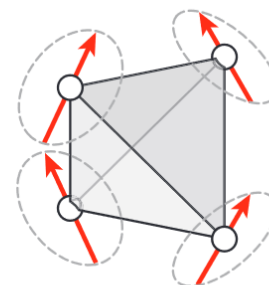
ψ_3 (E_g)



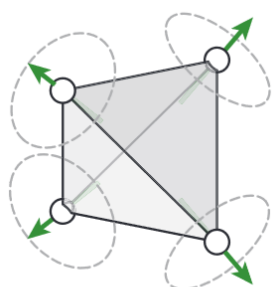
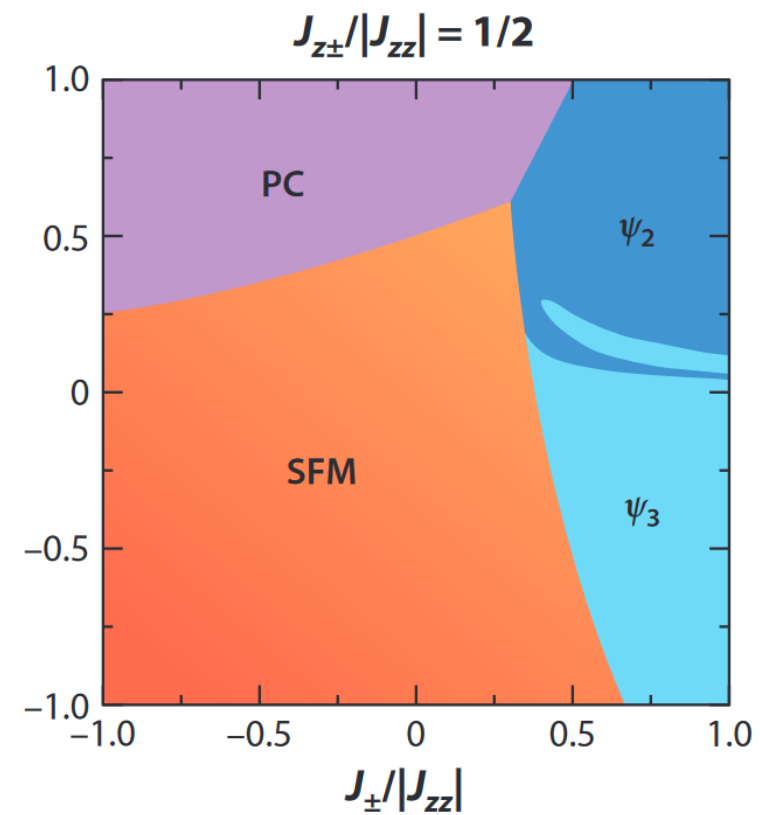
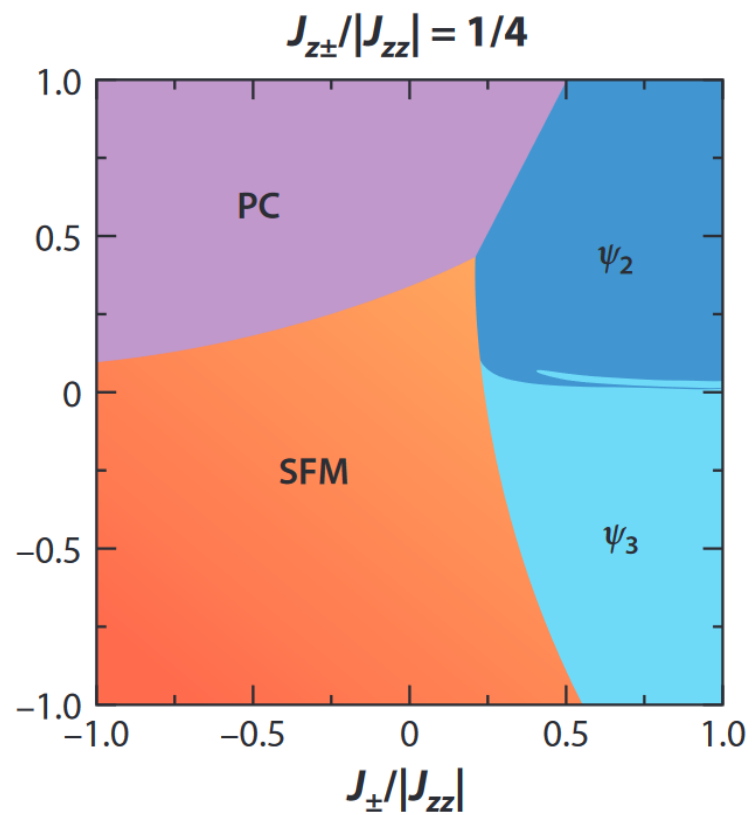
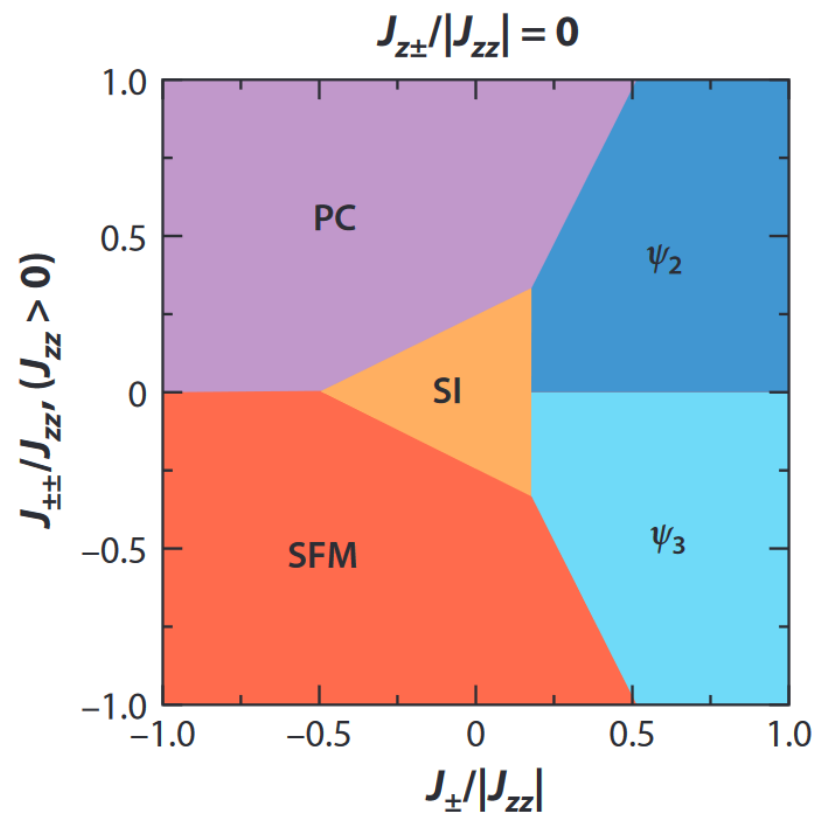
PC (T_{2g})



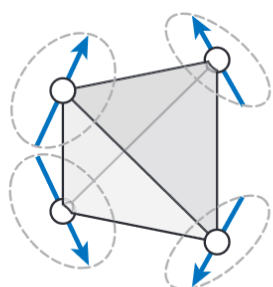
SI (T_{1g})



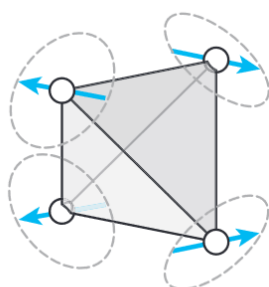
SFM (T'_{1g})



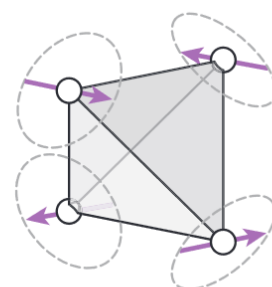
AIAO (A_{2g})



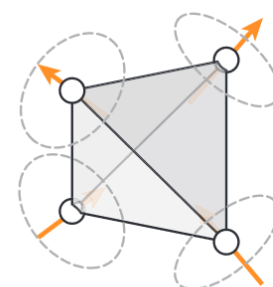
ψ_2 (E_g)



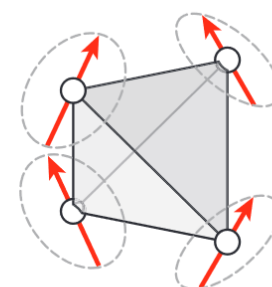
ψ_3 (E_g)



PC (T_{2g})

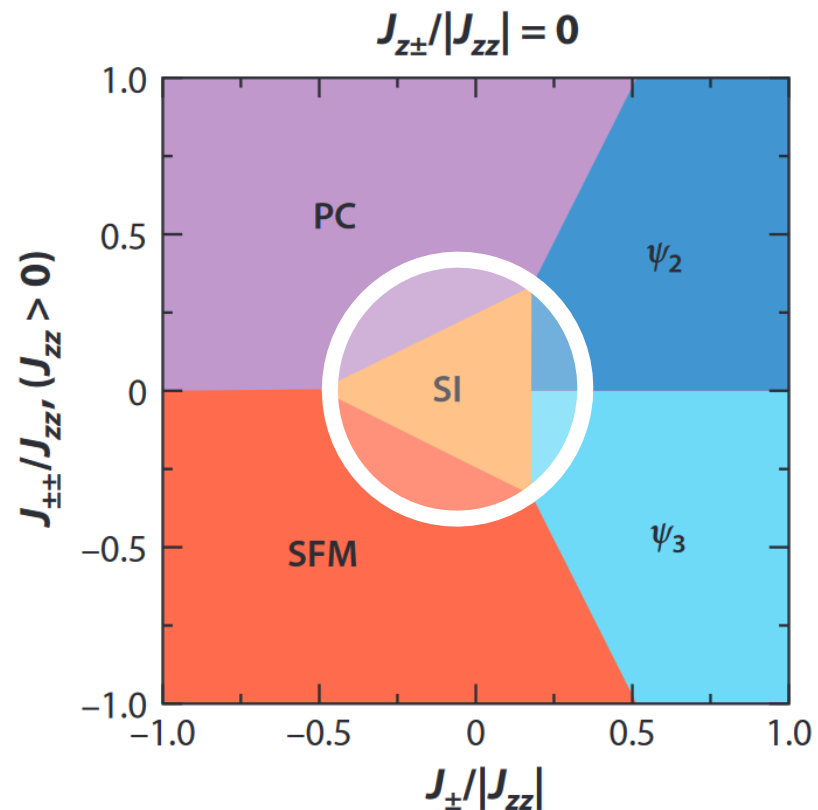


SI (T_{1g})

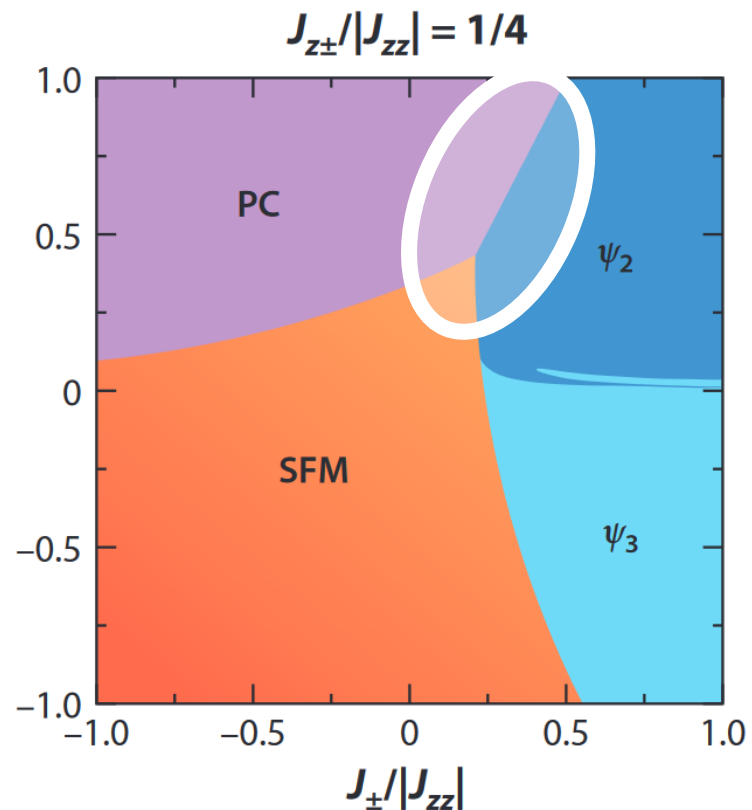


SFM (T'_{1g})

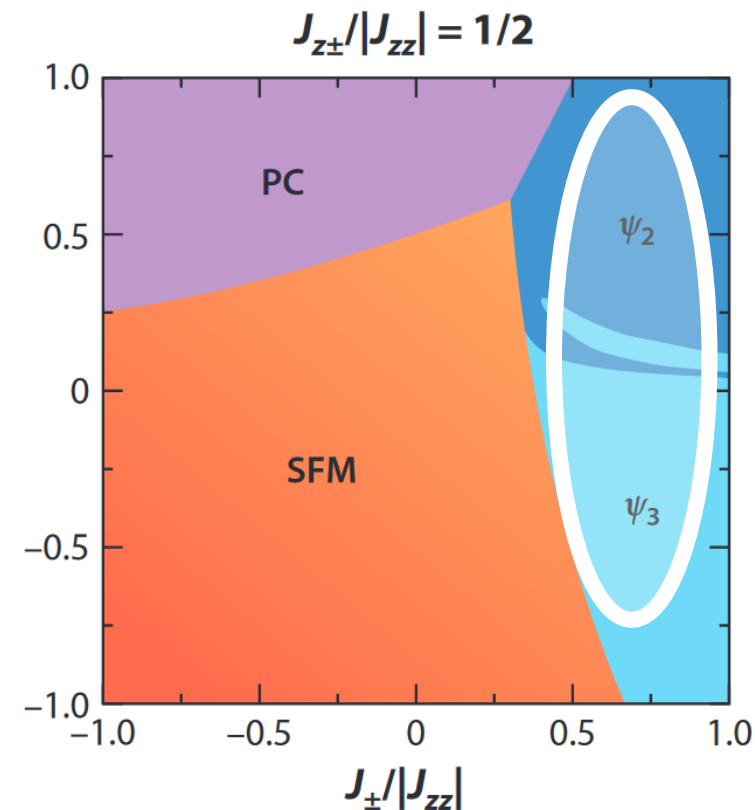
Interesting “Quantum” Regions



Quantum Spin Ice

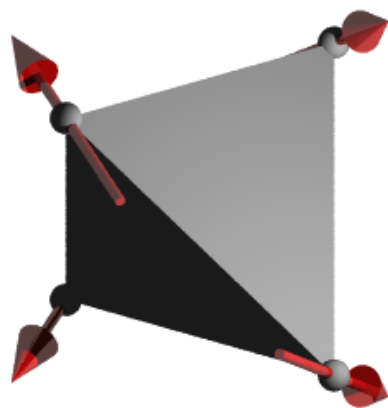


Pinch “lines”?



Order-by-Disorder

Order by Disorder

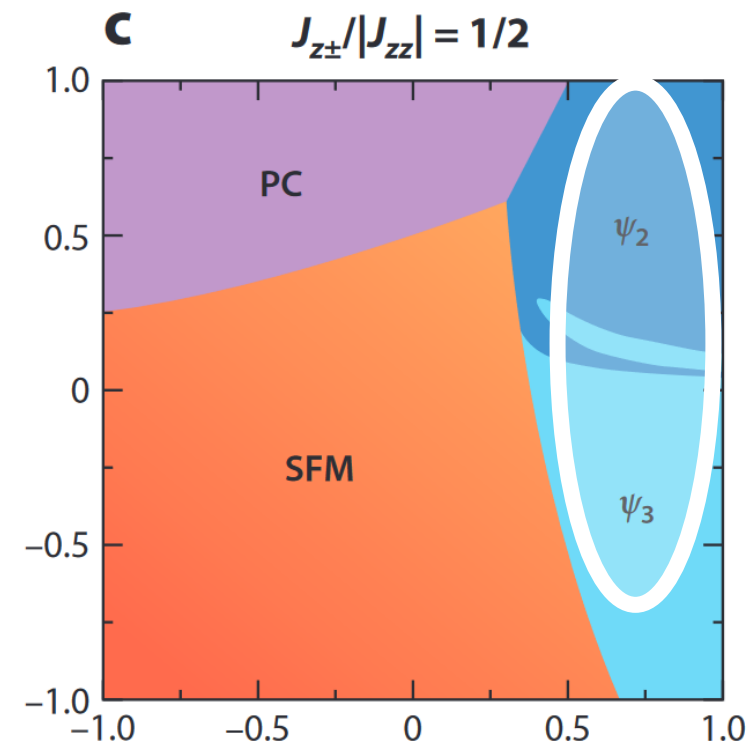


- Classical energy *doesn't distinguish* between ψ_2 and ψ_3 states

U(1) degeneracy: Rotating these states about local z-axes does not change energy

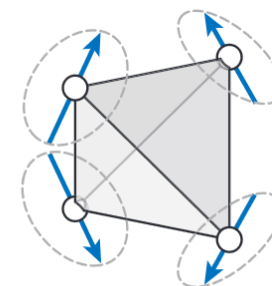
State with minimum energy isn't unique

- Not a symmetry of the Hamiltonian – “accidental”

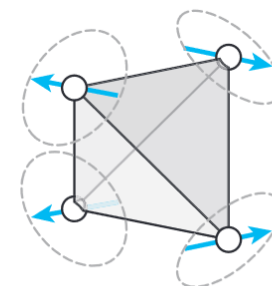


Local x-axis

Local y-axis



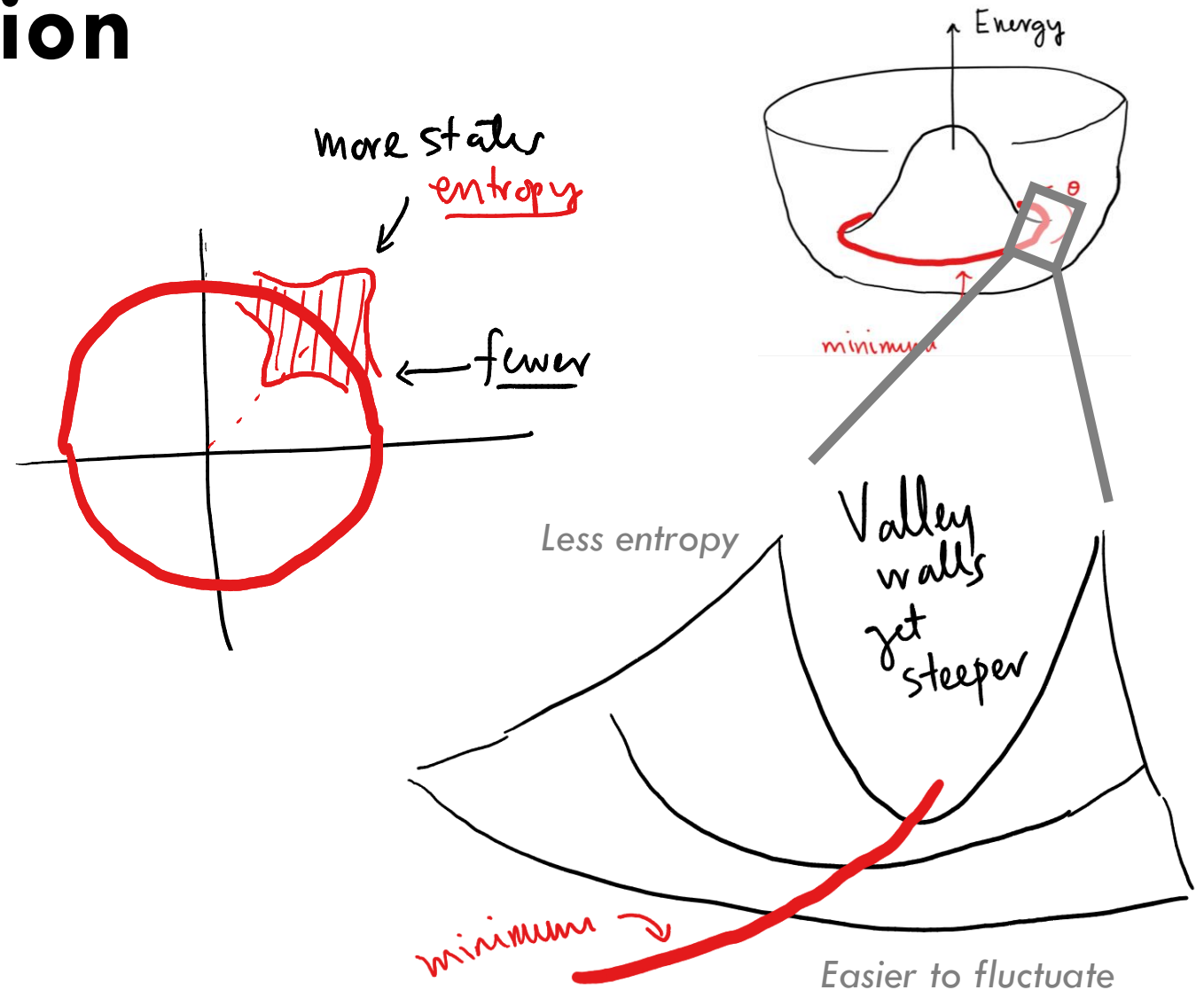
$\psi_2 (E_g)$

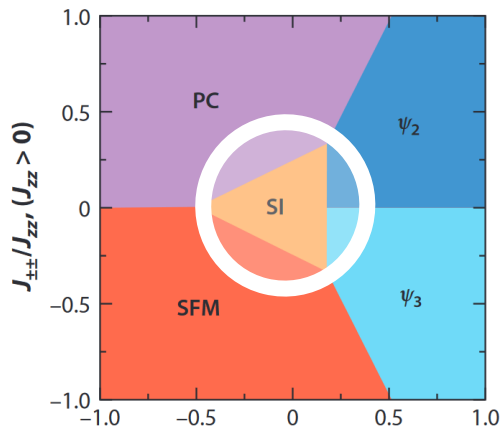


$\psi_3 (E_g)$

Ground State Selection

- Fluctuations *around* the ground states can be different
- **Quantum zero point fluctuations** select a ground state
- **Realized in $\text{Er}_2\text{Ti}_2\text{O}_7$:** ψ_2 ground state is selected by quantum fluctuations





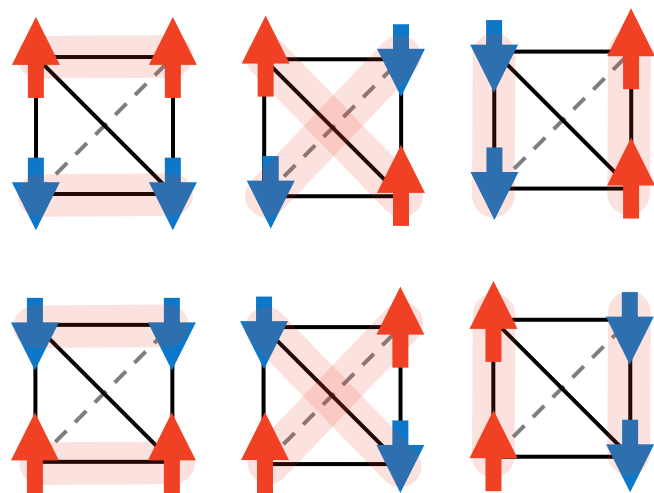
Classical Spin Ice

- Ising model:

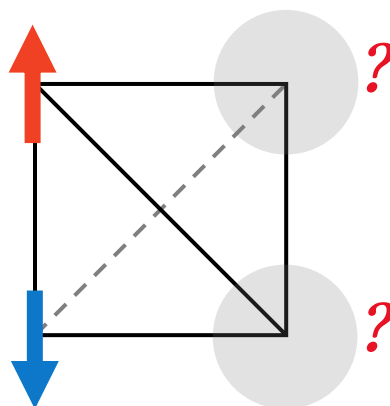
$$J_{zz} \sum_{\langle ij \rangle} S_i^z S_j^z$$

Positive

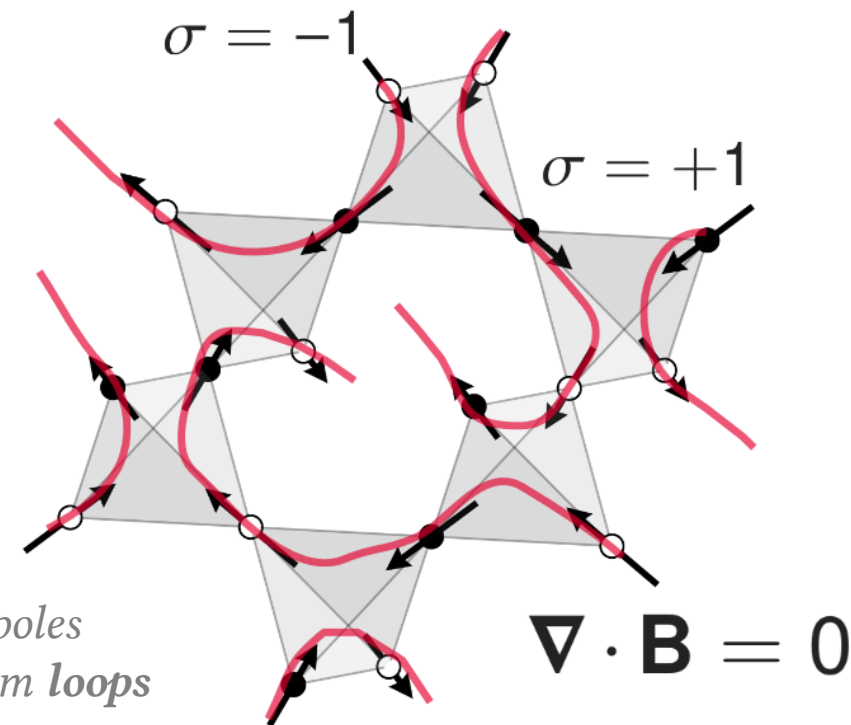
“Two in /
two out”
rule



Six ground states per tetrahedron



Tetrahedron



Dipoles
form *loops*

Corner-sharing tetrahedra

- Extensive ground state degeneracy
- **Classical spin liquid**

Quantum Spin Ice

- Simplest perturbation:

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

Classical spin ice model

Term that induces quantum fluctuations

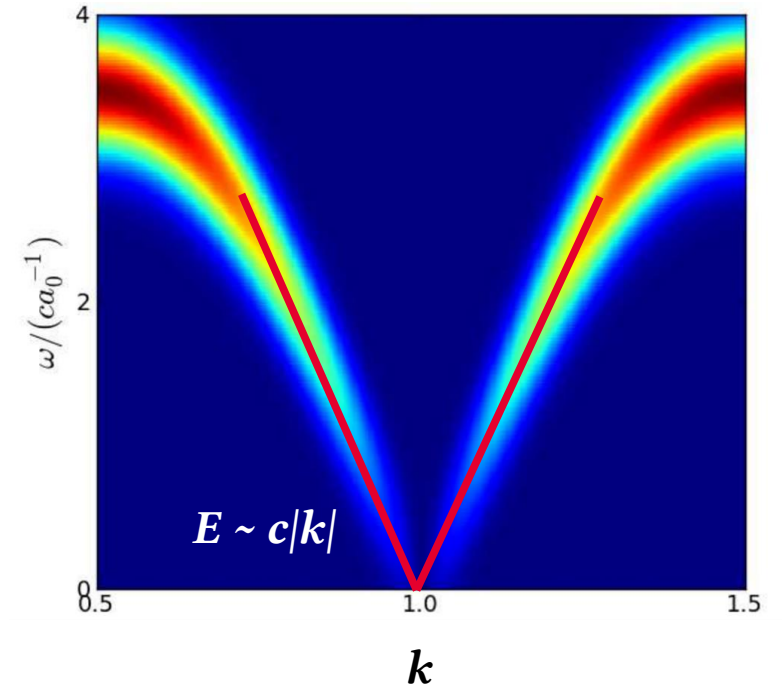
- Effective model:

Perturbative in quantum part

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

Can map to U(1) lattice gauge theory; solve numerically

Emergent photon excitation

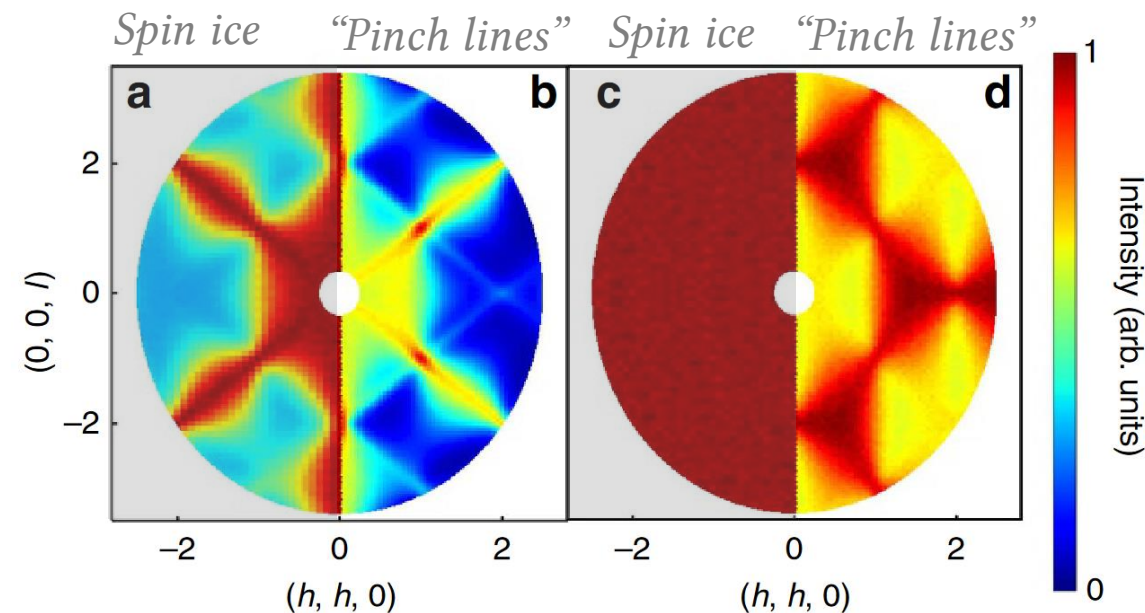
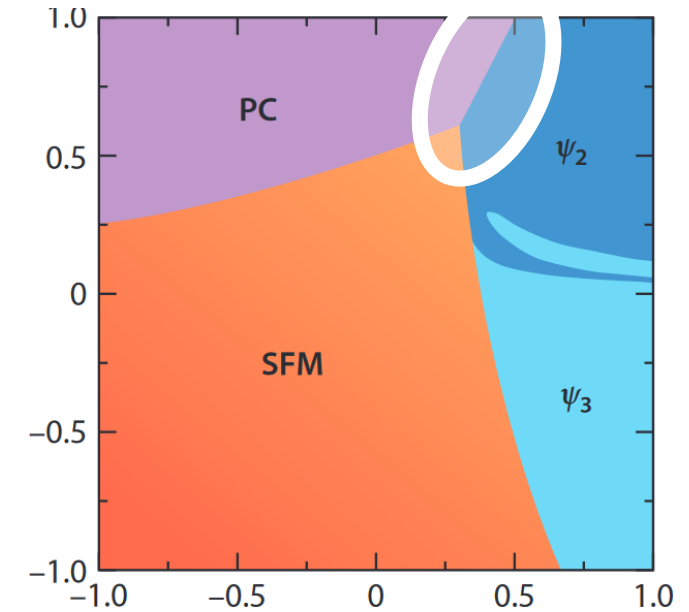


Classical SI: emergent magnetostatics

Quantum SI: emergent electrodynamics

More exotic spin liquids?

- Interesting physics at *other* places multiple phases meet (*away* from ice limit)
- *Classical models* show new kinds of **classical spin liquids** near the points
- “Higher rank” gauge structures
 - What happens in the quantum limit?
- Applications to $\text{Yb}_2\text{Ti}_2\text{O}_7$?



Summary

Quantum Pyrochlores

- Rich variety of degrees of freedom and models
- **Three types of “effective spin”**, each with unique features
- **Up to four anisotropic exchanges**, leading to classical phase diagram with **six (non-collinear) ordered phases**
- *Quantum* effects appear in bulk of phases, at phase boundaries and points where three or more phases meet
 - **Order-by-quantum-disorder**
 - **Quantum spin ice** (classical spin ice limit)
 - Other, *new*, phases along the boundary?

**Thank you
for your
attention**