

# Coulombic Quantum Liquids in Spin-1/2 Pyrochlores

Lucile Savary





# Collaborators



Leon Balents  
(KITP, UCSB)



Kate Ross



Bruce Gaulin

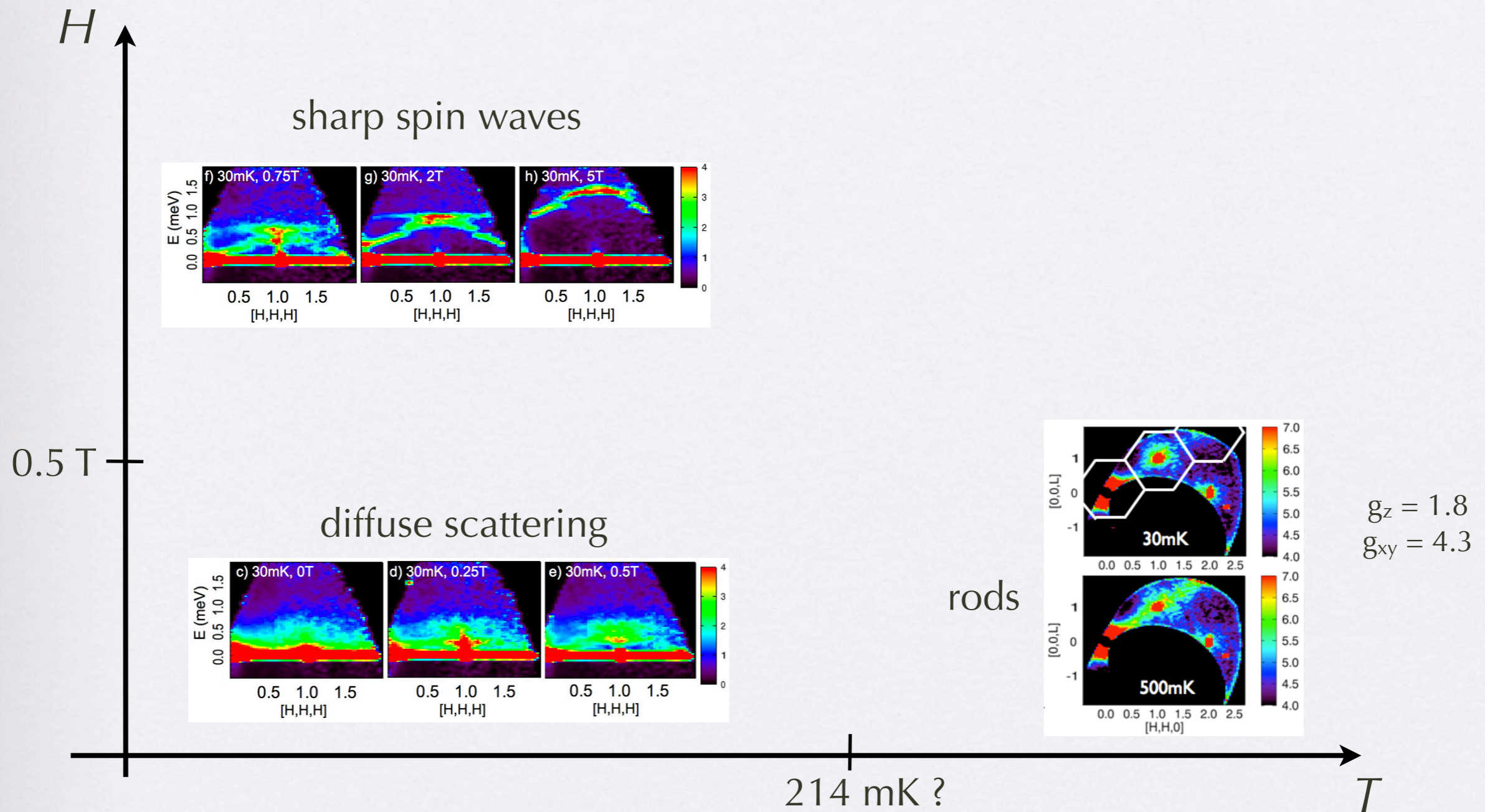
(experiments, Mc Master)

$\text{Yb}_2\text{Ti}_2\text{O}_7$  project

Special thanks to Benjamin Canals and Peter Holdsworth.

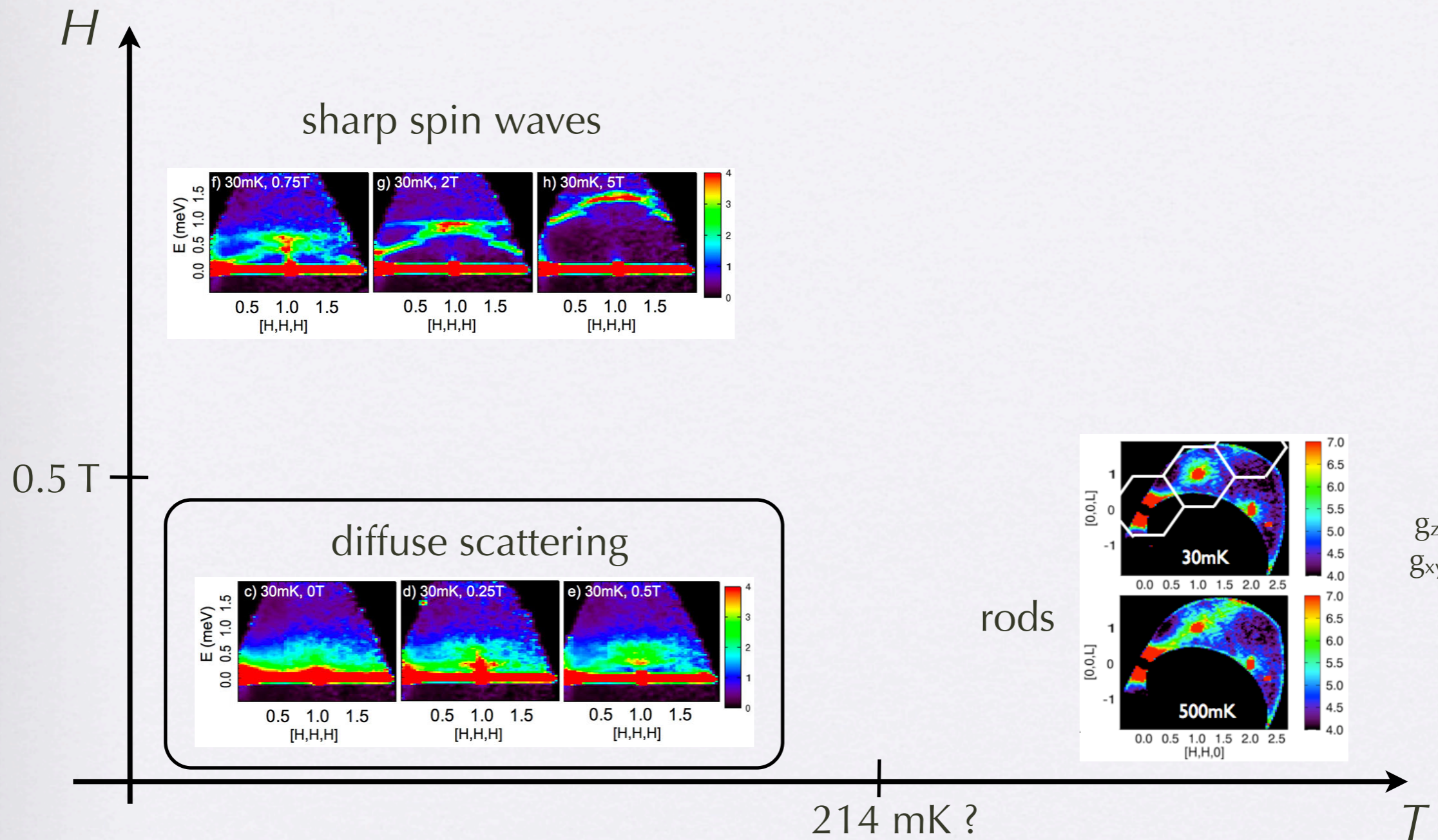


# Yb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>: puzzling experimental features





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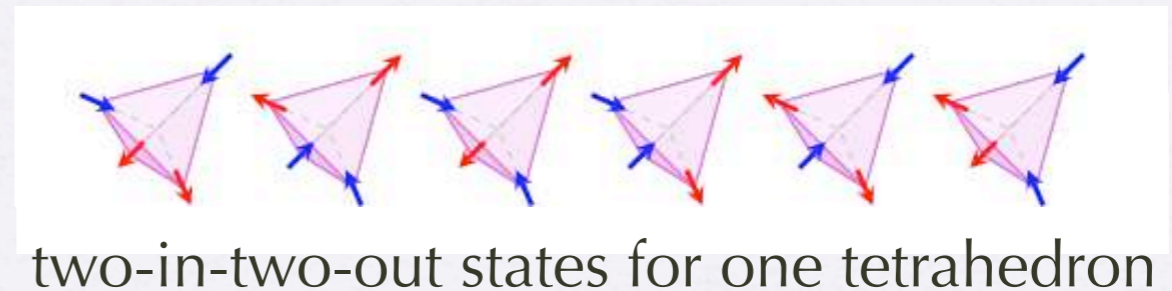
quantum spin liquid regime?



# What we know

- What spin ice is -- Michel's talk this morning

$$H_{\text{SI}} = J_{zz} \sum_{\langle i,j \rangle} S_i^z S_j^z \quad J_{zz} > 0$$



- What the generic definition of a quantum spin liquid is (and that it would be *very* nice to find one in nature) -- Leon's talk yesterday afternoon

- looks trivial:  $\langle \vec{S} \rangle = \vec{0}$  \*history

- but non-trivial correlations & fractional excitations!

} quantum entanglement

- Good place to look for QSLs: frustrated magnets

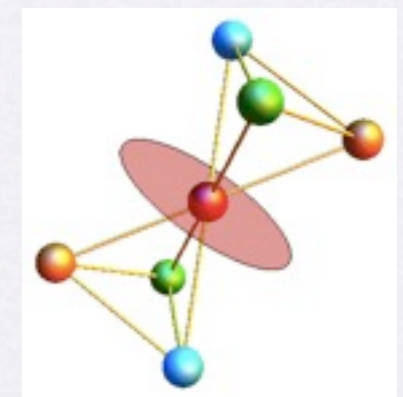


# Rare-earth pyrochlores



- grown rare-earth pyrochlores:  $\text{Ho}_2\text{Ti}_2\text{O}_7$ ,  $\text{Dy}_2\text{Ti}_2\text{O}_7$ ,  $\text{Ho}_2\text{Sn}_2\text{O}_7$ ,  $\text{Dy}_2\text{Sn}_2\text{O}_7$ ,  $\text{Er}_2\text{Ti}_2\text{O}_7$ ,  $\text{Yb}_2\text{Ti}_2\text{O}_7$ ,  $\text{Tb}_2\text{Ti}_2\text{O}_7$ ,  $\text{Er}_2\text{Sn}_2\text{O}_7$ ,  $\text{Tb}_2\text{Sn}_2\text{O}_7$ ,  $\text{Pr}_2\text{Sn}_2\text{O}_7$ ,  $\text{Nd}_2\text{Sn}_2\text{O}_7$ ,  $\text{Gd}_2\text{Sn}_2\text{O}_7$ , ...
- grown rare-earth B-site spinels:  $\text{CdEr}_2\text{S}_4$ ,  $\text{CdEr}_2\text{Se}_4$ ,  $\text{CdYb}_2\text{S}_4$ ,  $\text{CdYb}_2\text{Se}_4$ ,  $\text{MgYb}_2\text{S}_4$ ,  $\text{MgYb}_2\text{S}_4$ ,  $\text{MnYb}_2\text{S}_4$ ,  $\text{MnYb}_2\text{Se}_4$ ,  $\text{FeYb}_2\text{S}_4$ ,  $\text{CdTm}_2\text{S}_4$ ,  $\text{CdHo}_2\text{S}_4$ ,  $\text{FeLu}_2\text{S}_4$ ,  $\text{MnLu}_2\text{S}_4$ ,  $\text{MnLu}_2\text{Se}_4$ , ...

lots of room for diverse behaviors!





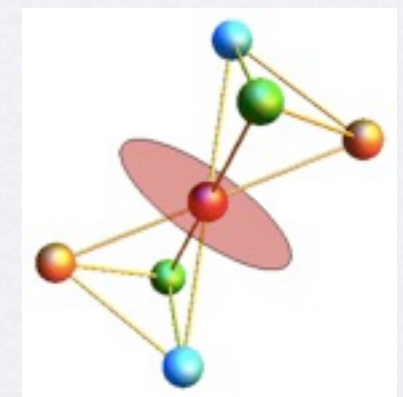
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spin ices

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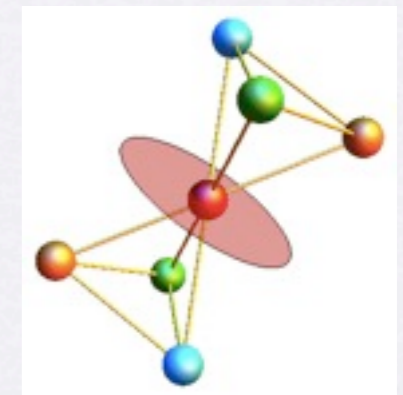
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quantum AFM

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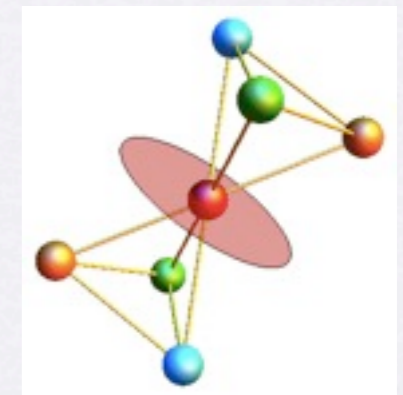
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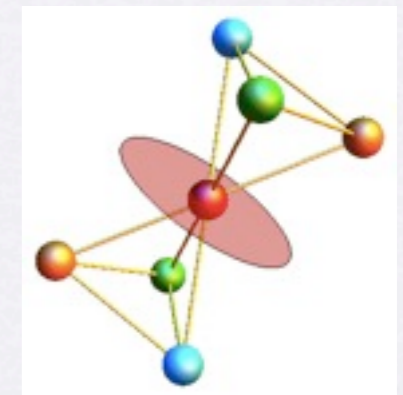


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# Outline

- method
- results
- experimental signatures
- materials

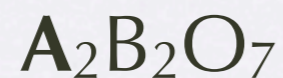
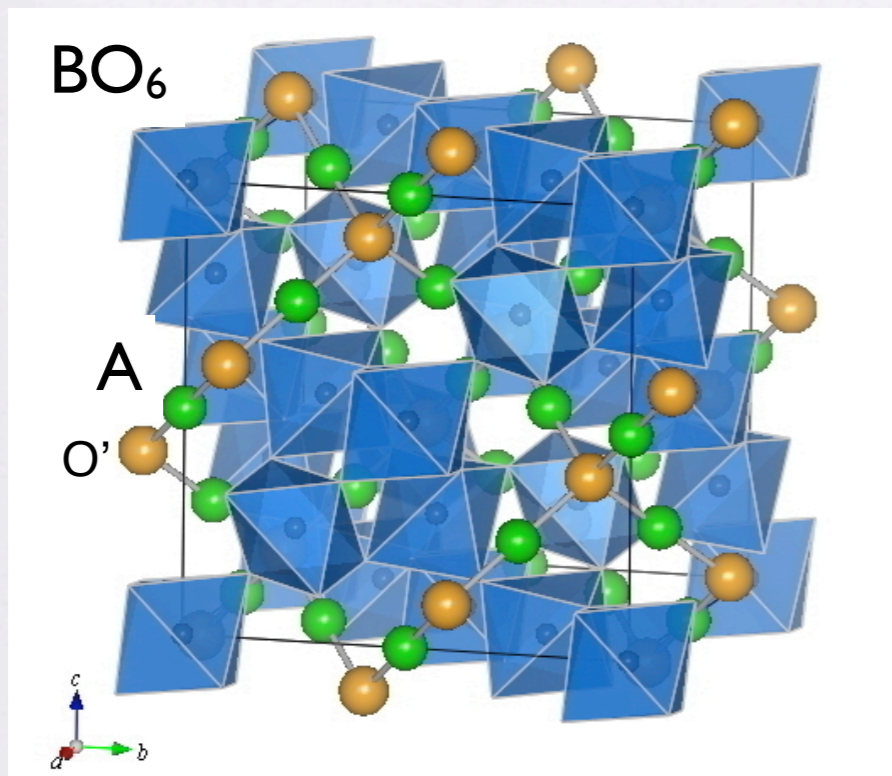


# Symmetries of the Hamiltonian

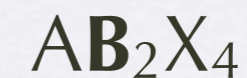
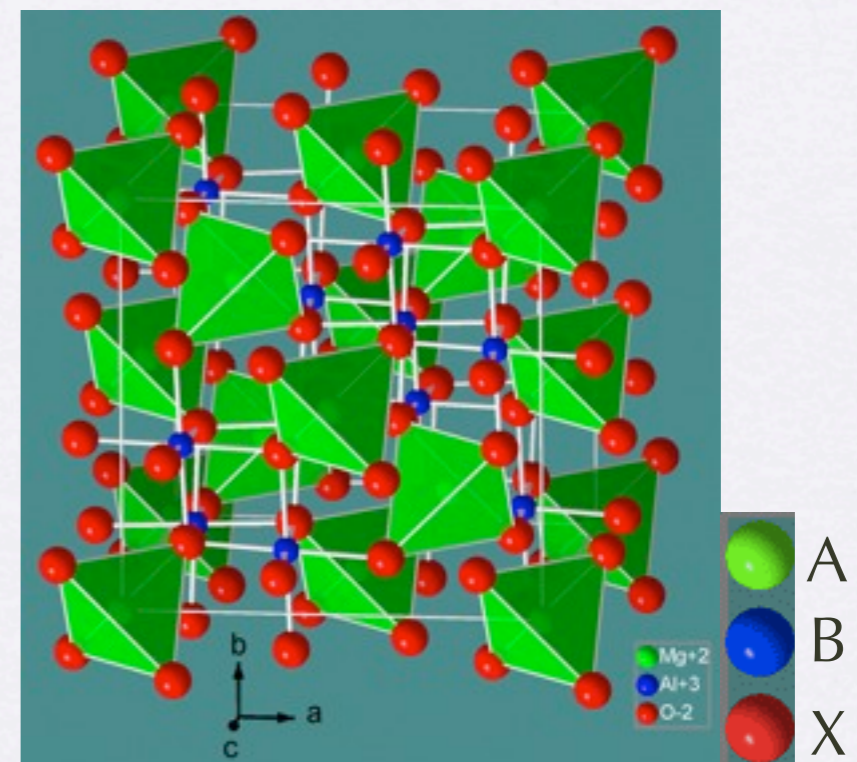
rare-earths : intrinsic strong spin-orbit coupling

→ *discrete cubic symmetries only*

space group:  $Fd-3m$ , i.e. #227 :



"pyrochlore oxides"

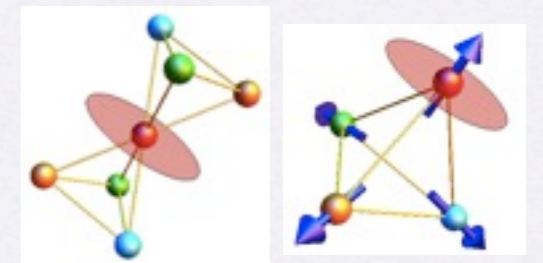
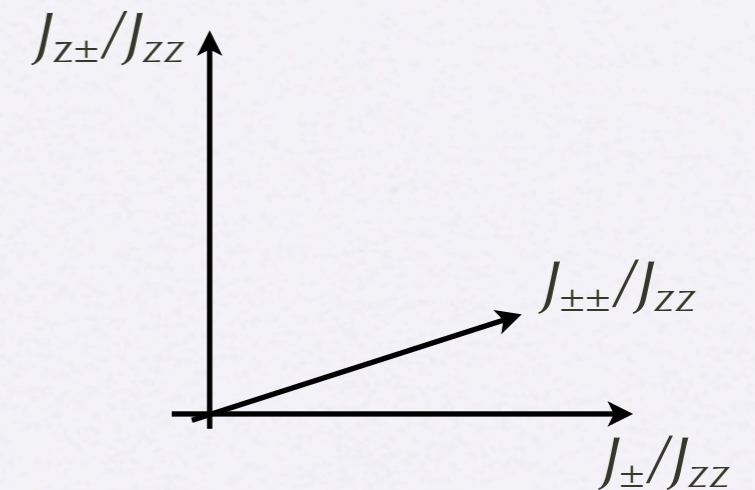


spinel



# General NN exchange Hamiltonian for effective spins 1/2

$$\begin{aligned}
 H = \sum_{\langle ij \rangle} & \left[ J_{zz} S_i^z S_j^z \right. \\
 & - J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+) \\
 & + J_{z\pm} [S_i^z (\zeta_{ij} S_j^+ + \zeta_{ij}^* S_j^-) + i \leftrightarrow j] \\
 & \left. + J_{\pm\pm} [\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-] \right]
 \end{aligned}$$



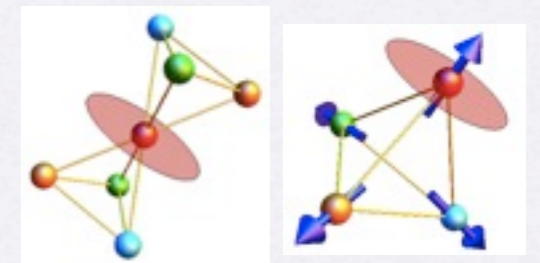
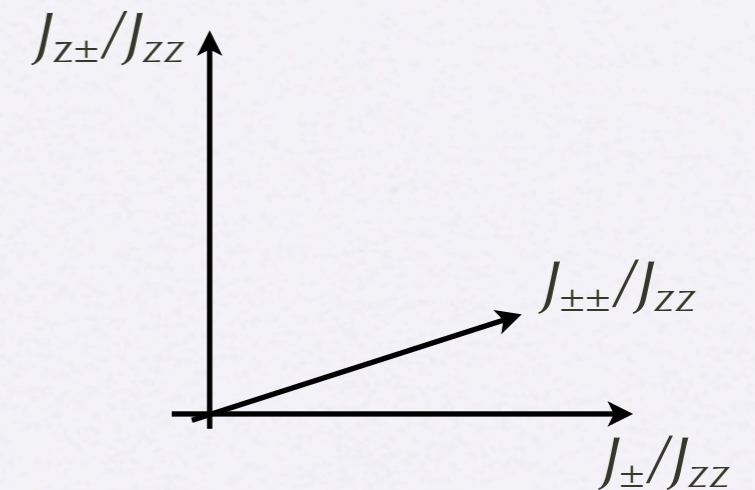
local axes, specific local bases

to each material corresponds a set of  $J$ 's



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local axes, specific local bases

to each material corresponds a set of  $J$ 's

What is the phase diagram ?  
 Are there any exotic phases there ?



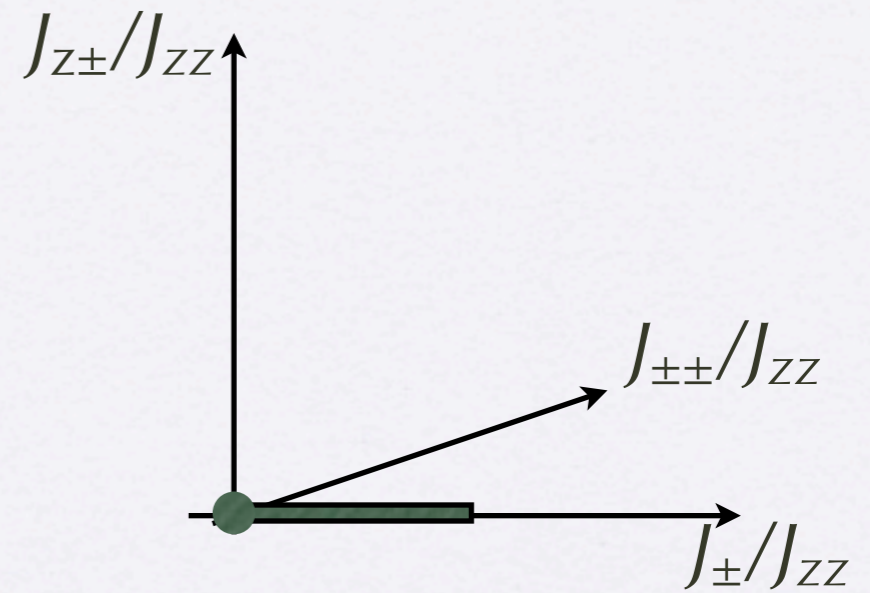
# The Hermele *et al.* QSL

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



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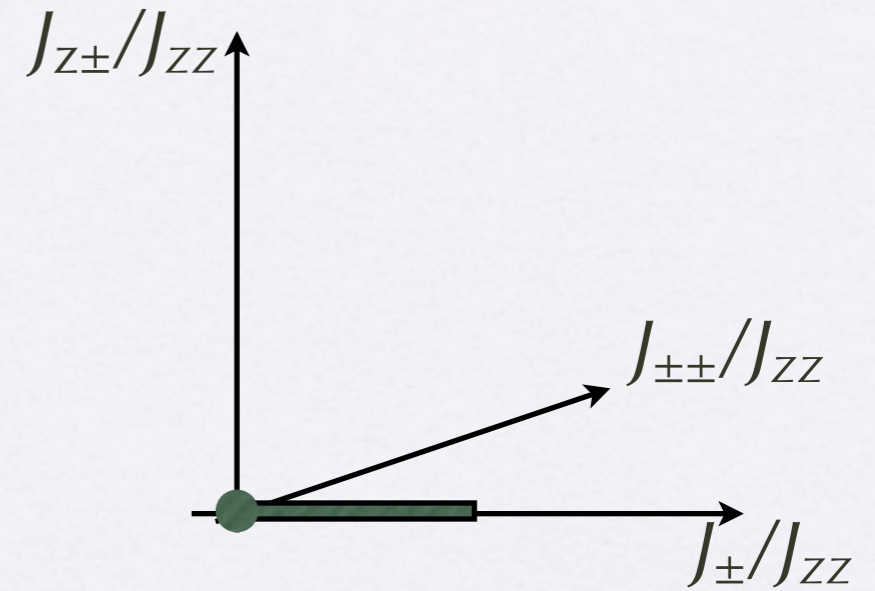


perturbation theory in  $J_{\pm}/J_{zz}$

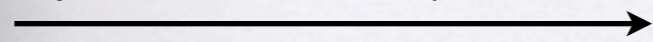


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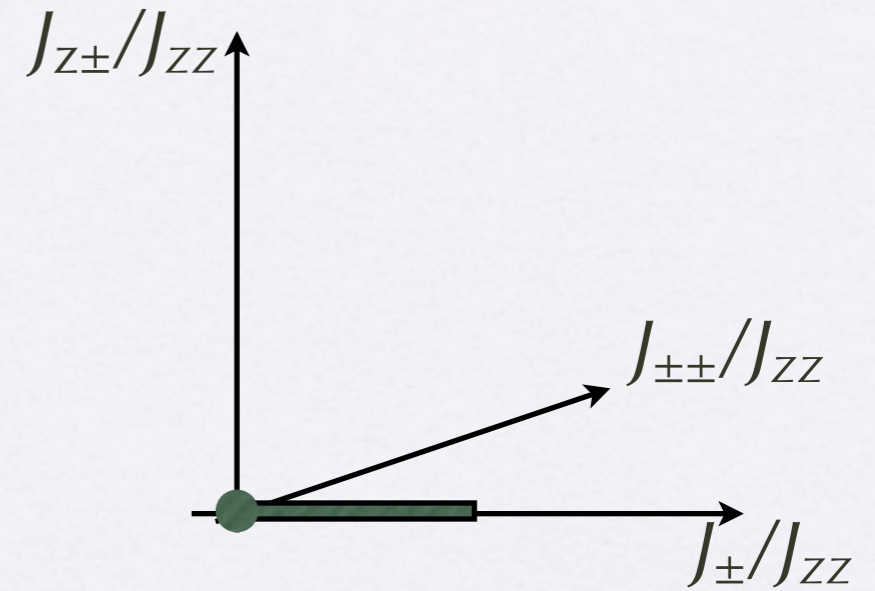


quantum electrodynamics  $H \sim H_{\text{QED}} \sim E^2 + B^2$



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$\xrightarrow{\text{perturbation theory in } J_{\pm}/J_{zz}}$  quantum electrodynamics  $H \sim H_{\text{QED}} \sim E^2 + B^2$

$\Rightarrow$  photon (gapless and linear)  
 particle-hole excitations (gapped)



# Relation to classical spin ice

classical spin ice

U(1) quantum spin liquid

*thermal* spin liquid

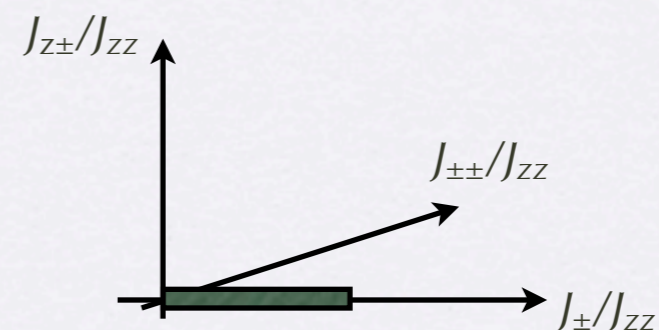
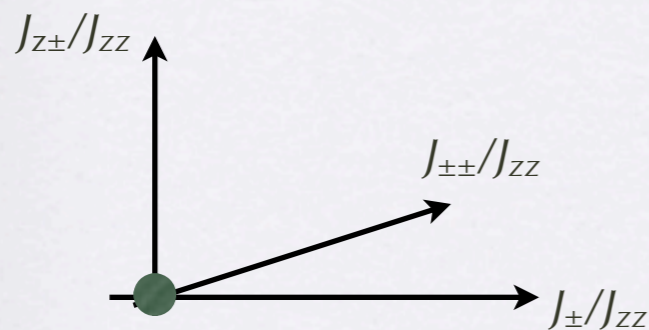
quantum spin liquid

extensively many  
degenerate ground  
states

*one* entangled ground state  
(= vacuum)

magnetic monopoles  
= spinons

spinons  
"electric" monopoles  
gapless photon

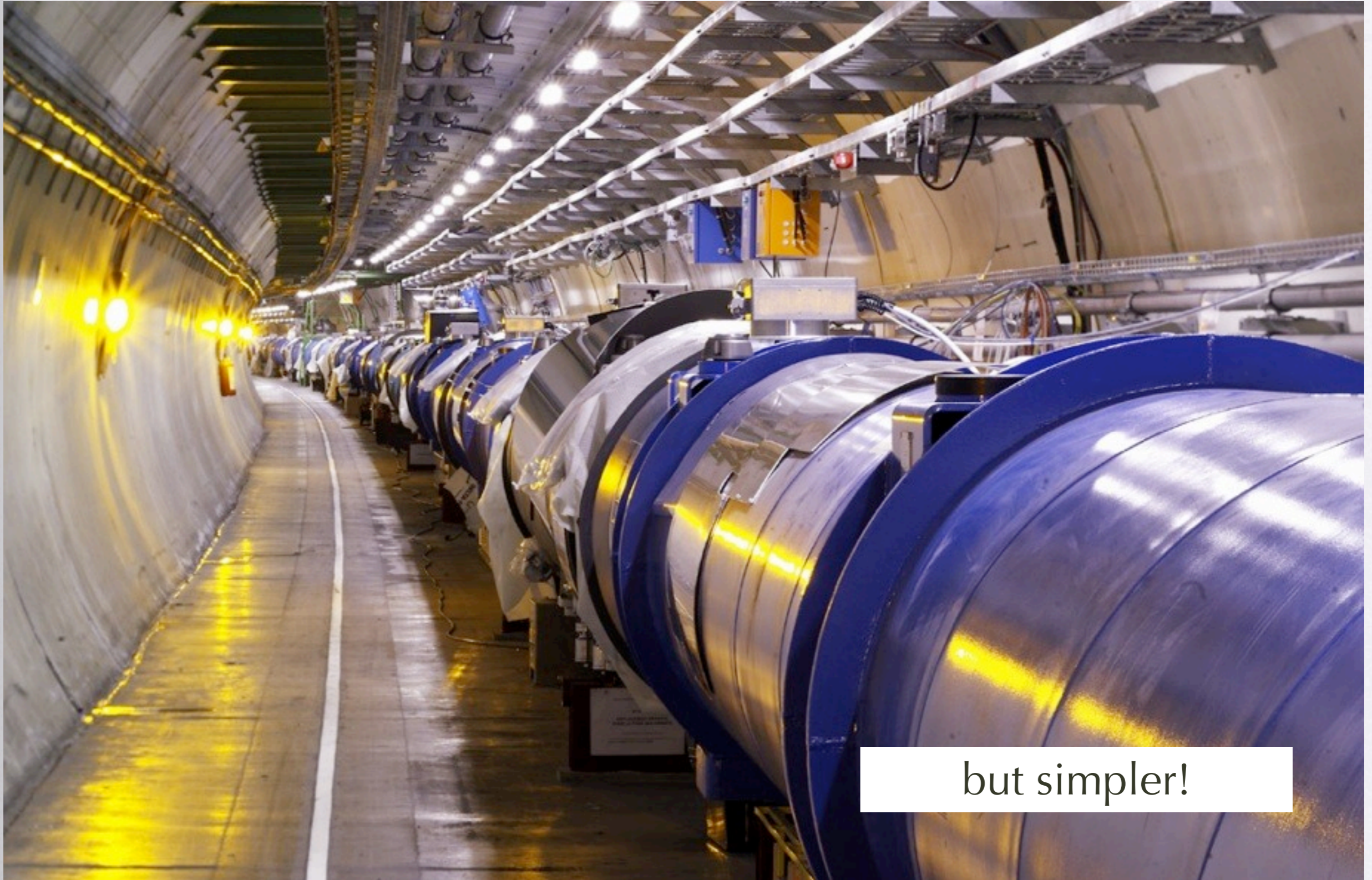




How we do this: compact abelian lattice  
Higgs theory



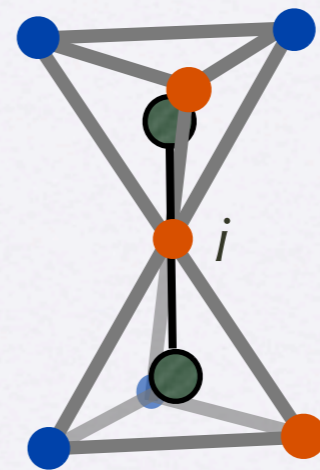
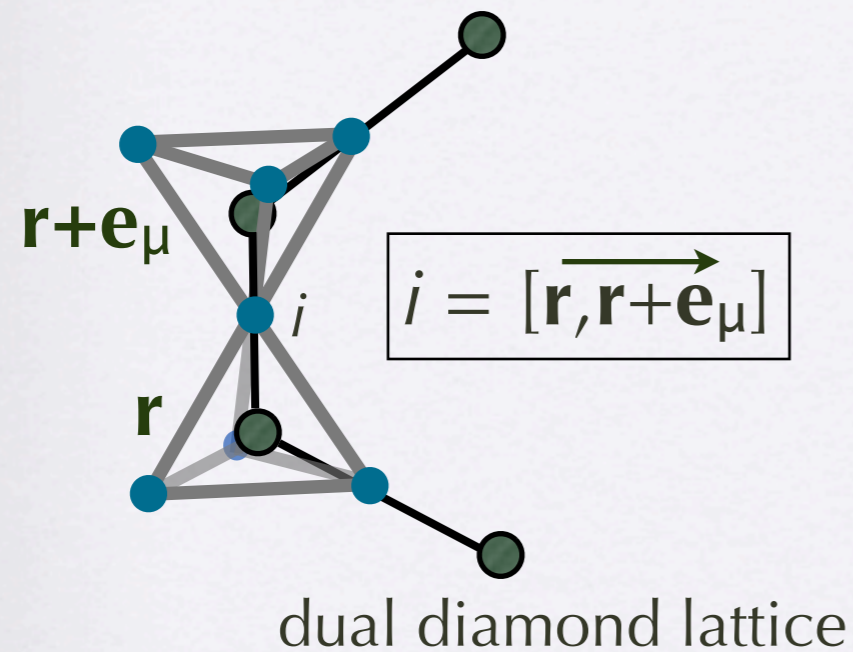
# How we do this: compact abelian lattice Higgs theory



but simpler!

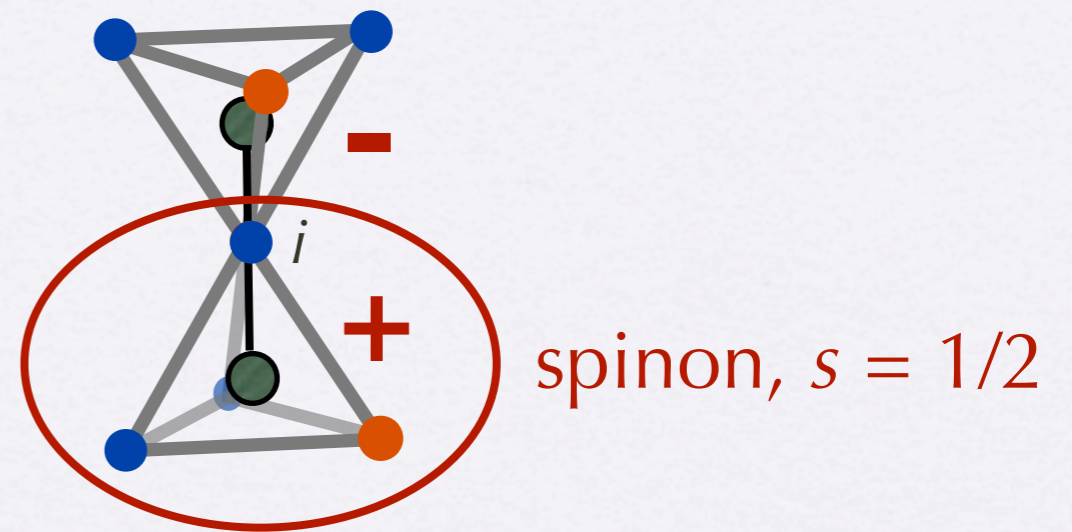
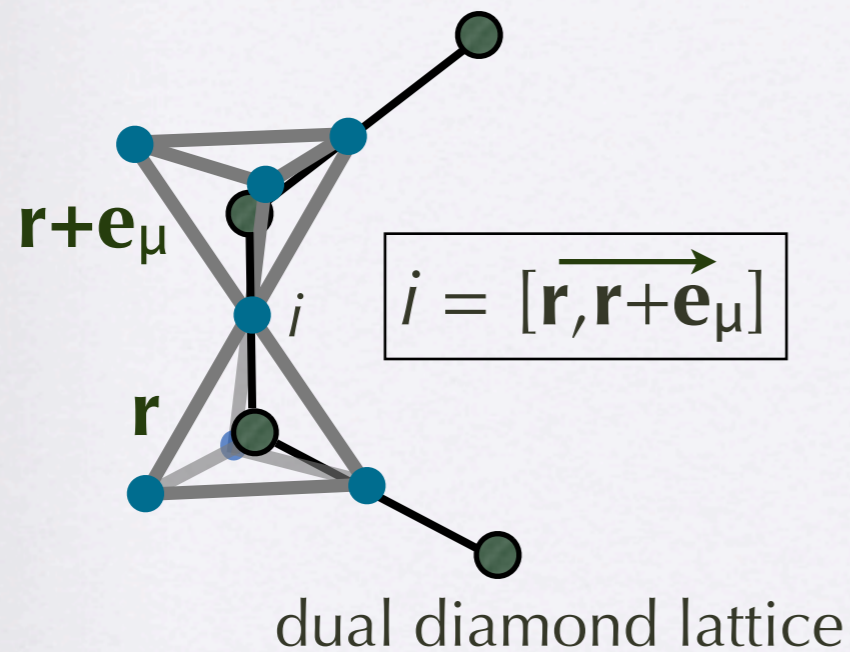


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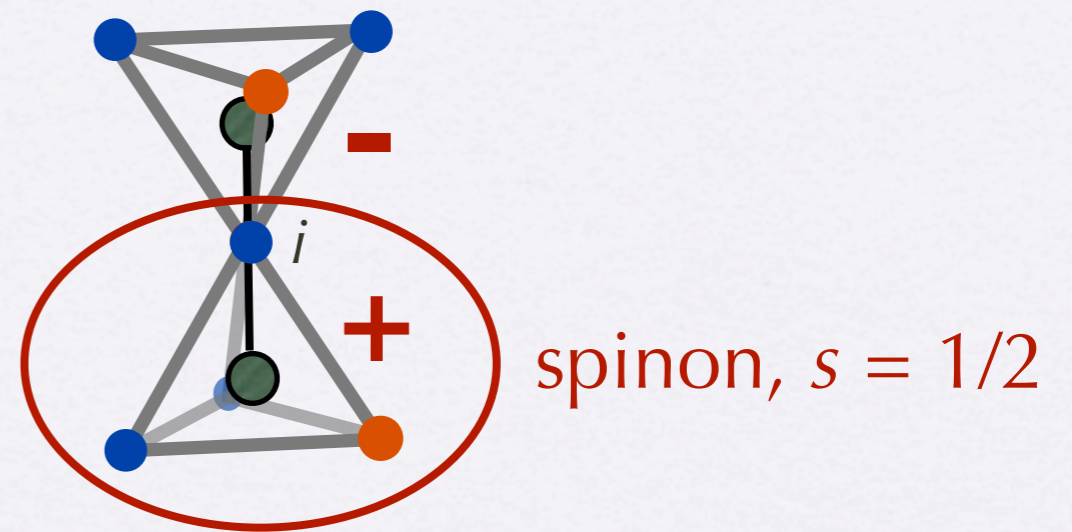
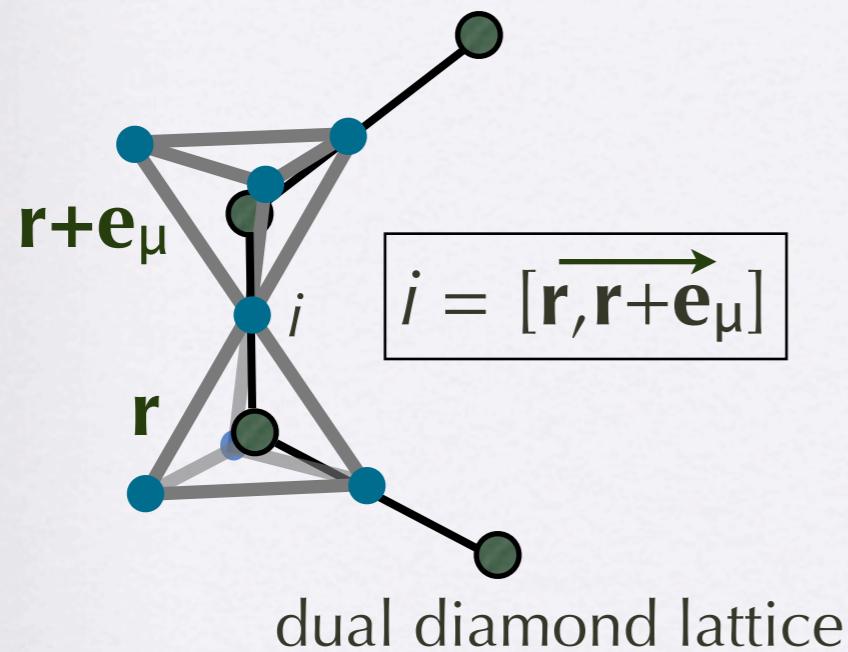


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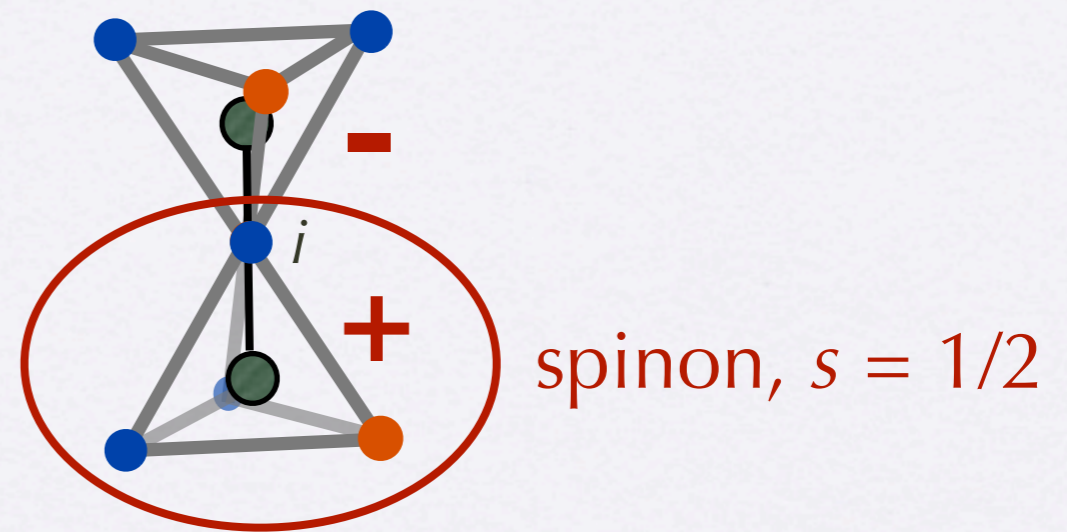
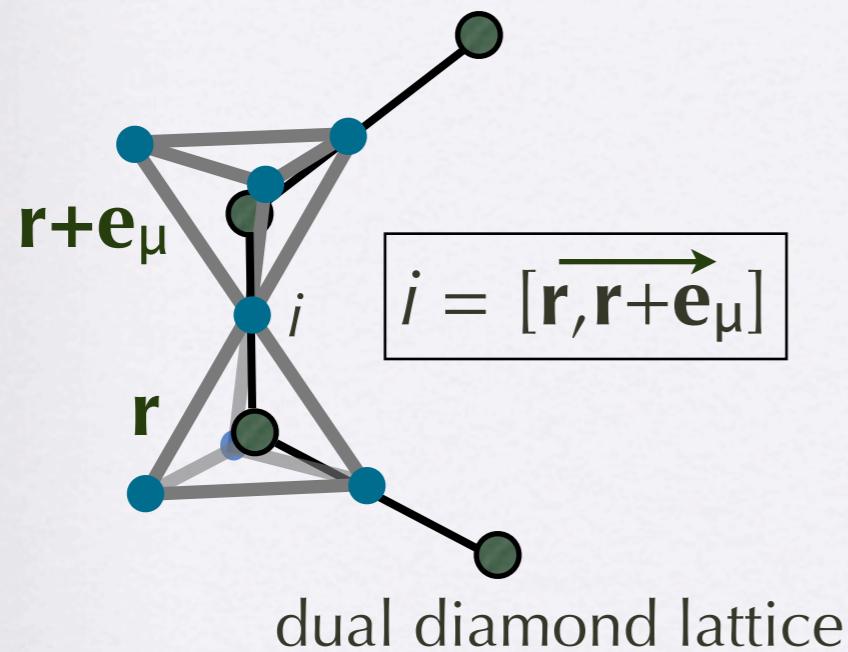


$$S_{\mathbf{r}, \mathbf{r} + \mathbf{e}_\mu}^+ = \Phi_{\mathbf{r}}^\dagger s_{\mathbf{r}, \mathbf{r} + \mathbf{e}_\mu}^+ \Phi_{\mathbf{r} + \mathbf{e}_\mu}$$

$$S_{\mathbf{r}, \mathbf{r} + \mathbf{e}_\mu}^z = s_{\mathbf{r}, \mathbf{r} + \mathbf{e}_\mu}^z$$



# How we do this: compact abelian lattice Higgs theory



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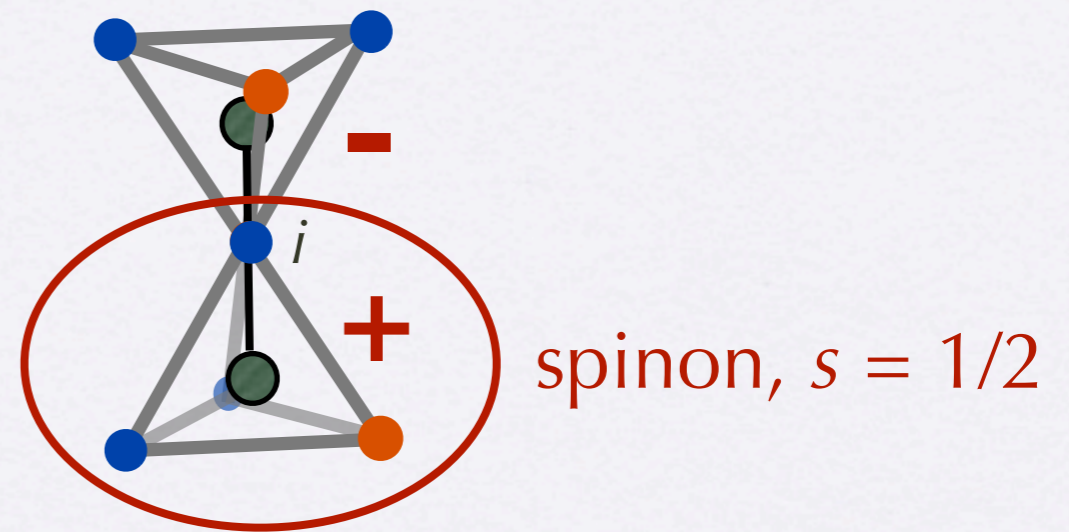
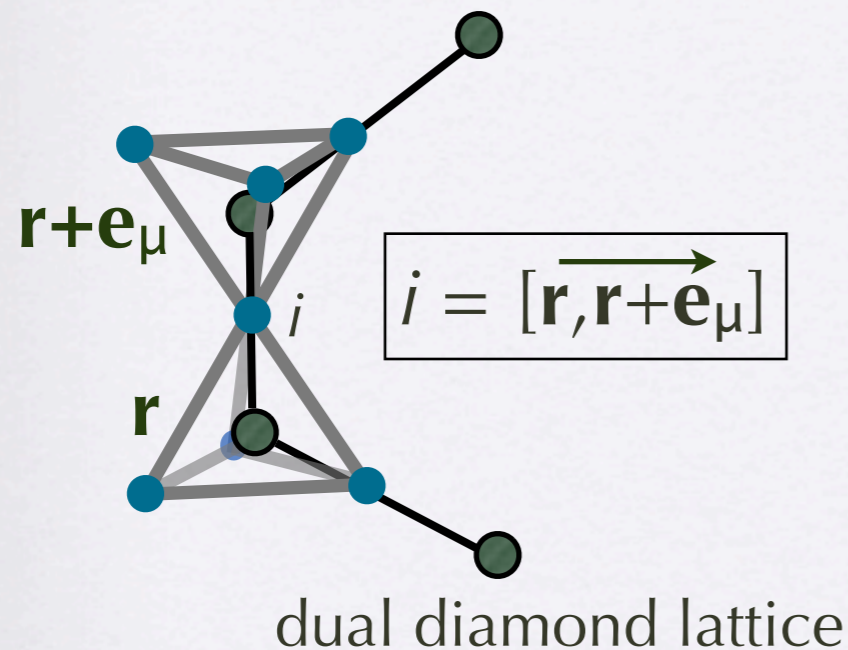
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$$\begin{cases} \Phi_{\mathbf{r}} \rightarrow \Phi_{\mathbf{r}} e^{-i\chi_{\mathbf{r}}} \\ s_{\mathbf{r}\mathbf{r}'}^\pm \rightarrow s_{\mathbf{r}\mathbf{r}'}^\pm e^{\pm i(\chi_{\mathbf{r}'} - \chi_{\mathbf{r}})} \end{cases}$$

U(1) gauge symmetry



# How we do this: compact abelian lattice Higgs theory



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U(1) gauge symmetry

the slave particles have a simple interpretation



# How we do this: compact abelian Higgs U(1) lattice gauge theory

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$$S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^z = s_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^z$$

$$|\Phi_{\mathbf{r}}| = 1$$

$$Q_{\mathbf{r}} = \pm \sum_{\mu} s_{\mathbf{r},\mathbf{r}\pm\mathbf{e}_\mu}^z$$

$$s_{\mathbf{r}\mathbf{r}'}^z = E_{\mathbf{r}\mathbf{r}'}$$

$$s_{\mathbf{r}\mathbf{r}'}^{\pm} = e^{\pm i A_{\mathbf{r}\mathbf{r}'}}$$

our spinons are bosons



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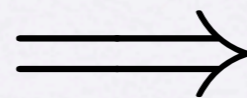
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$$S_{\mathbf{r}\mathbf{r}'}^\pm = e^{\pm i A_{\mathbf{r}\mathbf{r}'}}$$

our spinons are bosons



they can condense

$\langle \Phi \rangle$	phase
$\neq 0$	conventional
$= 0$	exotic



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$$S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^+ = \Phi_{\mathbf{r}}^\dagger S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^+ \Phi_{\mathbf{r}+\mathbf{e}_\mu}$$

$$S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^z = S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^z$$

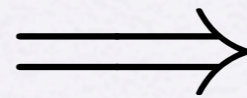
$$|\Phi_{\mathbf{r}}| = 1$$

$$Q_{\mathbf{r}} = \pm \sum_{\mu} S_{\mathbf{r},\mathbf{r}\pm\mathbf{e}_\mu}^z$$

$$S_{\mathbf{r}\mathbf{r}'}^z = E_{\mathbf{r}\mathbf{r}'}$$

$$S_{\mathbf{r}\mathbf{r}'}^\pm = e^{\pm i A_{\mathbf{r}\mathbf{r}'}}$$

our spinons are bosons



they can condense

$\langle \Phi \rangle$	phase
$\neq 0$	conventional
$= 0$	exotic

$$H = \sum_{\mathbf{r} \in \text{I,II}} \frac{J_{zz}}{2} Q_{\mathbf{r}}^2 - J_{\pm} \left\{ \sum_{\mathbf{r} \in \text{I}} \sum_{\mu, \nu \neq \mu} \Phi_{\mathbf{r}+\mathbf{e}_\mu}^\dagger \Phi_{\mathbf{r}+\mathbf{e}_\nu} S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^- S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\nu}^+ + \sum_{\mathbf{r} \in \text{II}} \sum_{\mu, \nu \neq \mu} \Phi_{\mathbf{r}-\mathbf{e}_\mu}^\dagger \Phi_{\mathbf{r}-\mathbf{e}_\nu} S_{\mathbf{r},\mathbf{r}-\mathbf{e}_\mu}^+ S_{\mathbf{r},\mathbf{r}-\mathbf{e}_\nu}^- \right\}$$

$$- J_{z\pm} \left\{ \sum_{\mathbf{r} \in \text{I}} \sum_{\mu, \nu \neq \mu} \left( \gamma_{\mu\nu}^* \Phi_{\mathbf{r}}^\dagger \Phi_{\mathbf{r}+\mathbf{e}_\nu} S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^z S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\nu}^+ + \text{h.c.} \right) + \sum_{\mathbf{r} \in \text{II}} \sum_{\mu, \nu \neq \mu} \left( \gamma_{\mu\nu}^* \Phi_{\mathbf{r}-\mathbf{e}_\nu}^\dagger \Phi_{\mathbf{r}} S_{\mathbf{r},\mathbf{r}-\mathbf{e}_\mu}^z S_{\mathbf{r},\mathbf{r}-\mathbf{e}_\nu}^+ + \text{h.c.} \right) \right\} + \text{const.}$$

$$J_{\pm\pm} = 0$$



# How we do this: compact abelian Higgs U(1) lattice gauge theory

$$S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^+ = \Phi_{\mathbf{r}}^\dagger S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^+ \Phi_{\mathbf{r}+\mathbf{e}_\mu}$$

$$S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^z = S_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}^z$$

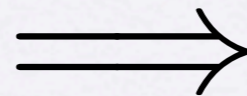
$$|\Phi_{\mathbf{r}}| = 1$$

$$Q_{\mathbf{r}} = \pm \sum_{\mu} S_{\mathbf{r},\mathbf{r}\pm\mathbf{e}_\mu}^z$$

$$S_{\mathbf{r}\mathbf{r}'}^z = E_{\mathbf{r}\mathbf{r}'}$$

$$S_{\mathbf{r}\mathbf{r}'}^\pm = e^{\pm i A_{\mathbf{r}\mathbf{r}'}}$$

our spinons are bosons



they can condense

$\langle \Phi \rangle$	phase
$\neq 0$	conventional
$= 0$	exotic

vacuum: quantum superposition of two-in-two-out states

$H$  = hopping Hamiltonian for spinons in fluctuating background



# gauge Mean Field Theory (gMFT)

$$\Phi^\dagger \Phi s s \rightarrow \Phi^\dagger \Phi \langle s \rangle \langle s \rangle + \langle \Phi^\dagger \Phi \rangle s \langle s \rangle + \langle \Phi^\dagger \Phi \rangle \langle s \rangle s - 2 \langle \Phi^\dagger \Phi \rangle \langle s \rangle \langle s \rangle$$



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$$\Phi^\dagger \Phi s s \rightarrow \Phi^\dagger \Phi \langle s \rangle \langle s \rangle + \langle \Phi^\dagger \Phi \rangle s \langle s \rangle + \langle \Phi^\dagger \Phi \rangle \langle s \rangle s - 2 \langle \Phi^\dagger \Phi \rangle \langle s \rangle \langle s \rangle$$

$$H_s^{\text{MF}} = - \sum_{\mathbf{r}} \sum_{\mu} \vec{h}_{\text{eff},\mu}^{\text{MF}} \cdot \vec{S}_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu}$$

$$H_\Phi^{\text{MF}} = - \sum_{\mathbf{r}} \sum_{\mu \neq \nu} \left[ t_\mu^{\text{MF}} \Phi_{\mathbf{r}}^\dagger \Phi_{\mathbf{r}+\mathbf{e}_\mu} + t'_{\mu\nu}^{\text{MF}} \Phi_{\mathbf{r}}^\dagger \Phi_{\mathbf{r}+\mathbf{e}_\mu-\mathbf{e}_\nu} + \text{h.c.} \right]$$



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$$H_s^{\text{MF}} = - \sum_{\mathbf{r}} \sum_{\mu} \vec{h}_{\text{eff},\mu}^{\text{MF}} \cdot \vec{S}_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu} \quad \text{free (but self-consistent) "spins"}$$

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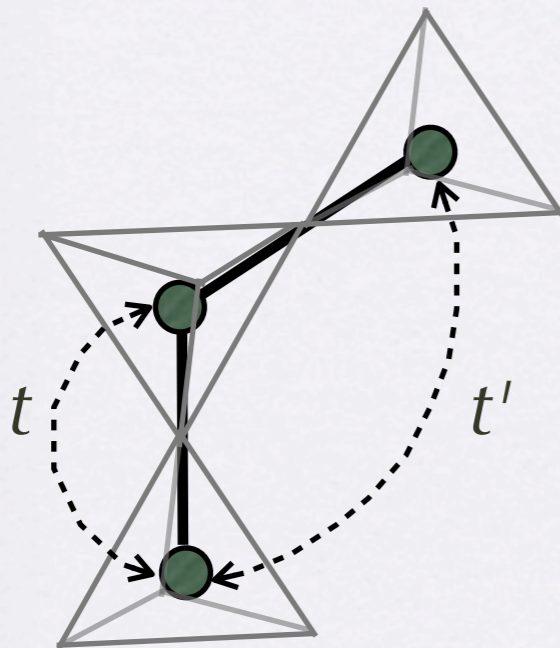
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hopping Hamiltonian for spinons in fixed (but self-consistent) background





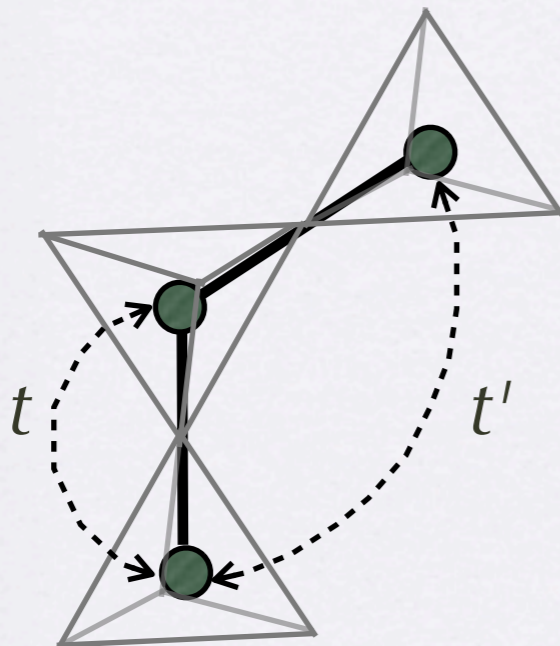
# gauge Mean Field Theory (gMFT)

$$\Phi^\dagger \Phi s s \rightarrow \Phi^\dagger \Phi \langle s \rangle \langle s \rangle + \langle \Phi^\dagger \Phi \rangle s \langle s \rangle + \langle \Phi^\dagger \Phi \rangle \langle s \rangle s - 2 \langle \Phi^\dagger \Phi \rangle \langle s \rangle \langle s \rangle$$

$$H_s^{\text{MF}} = - \sum_{\mathbf{r}} \sum_{\mu} \vec{h}_{\text{eff},\mu}^{\text{MF}} \cdot \vec{S}_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu} \quad \text{free (but self-consistent) "spins"}$$

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hopping Hamiltonian for spinons in fixed (but self-consistent) background



Solve the consistency equations



Now is when you tune  
back in for

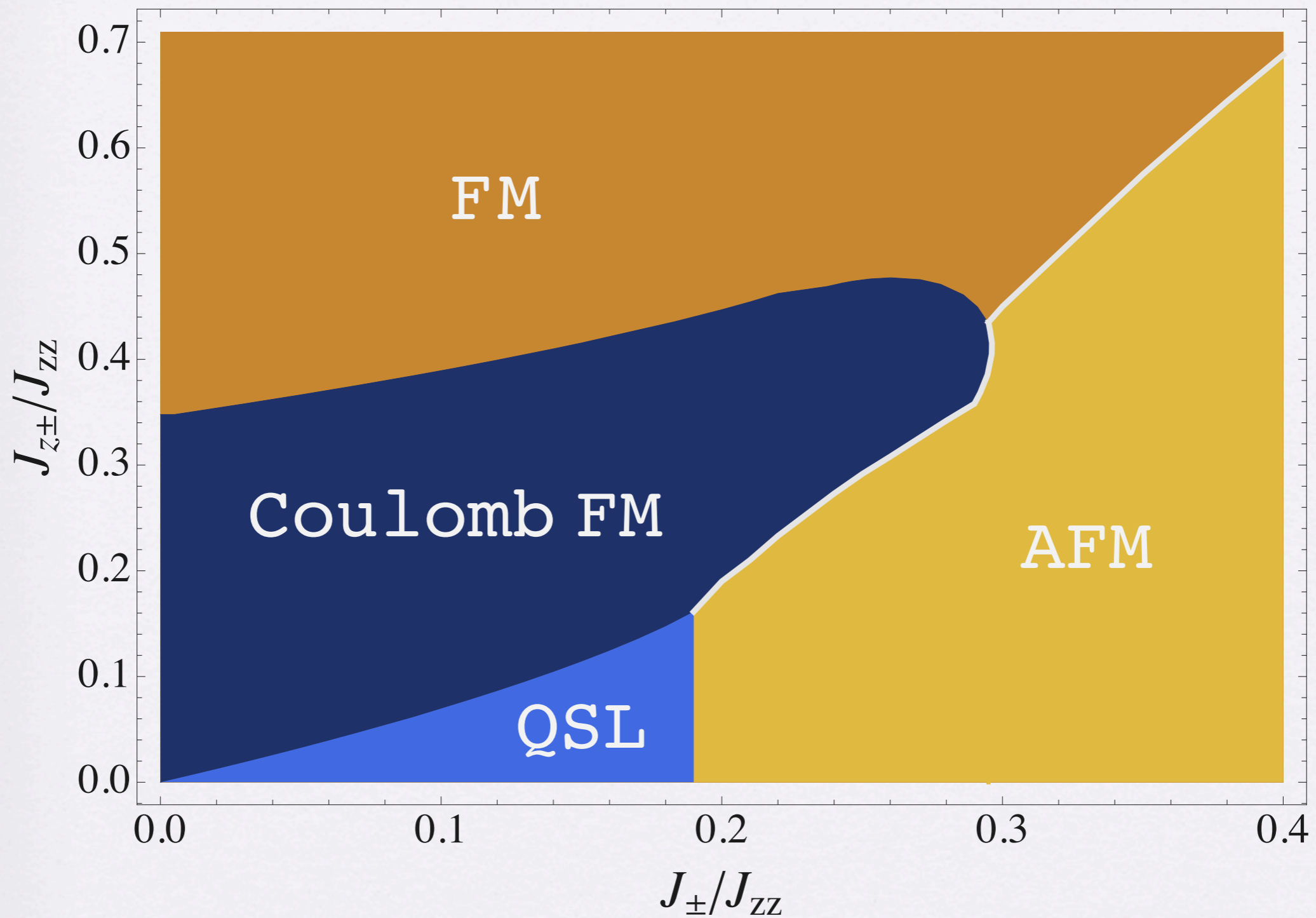




*Quantum spin liquids in quantum spin ices*



# Phase diagram

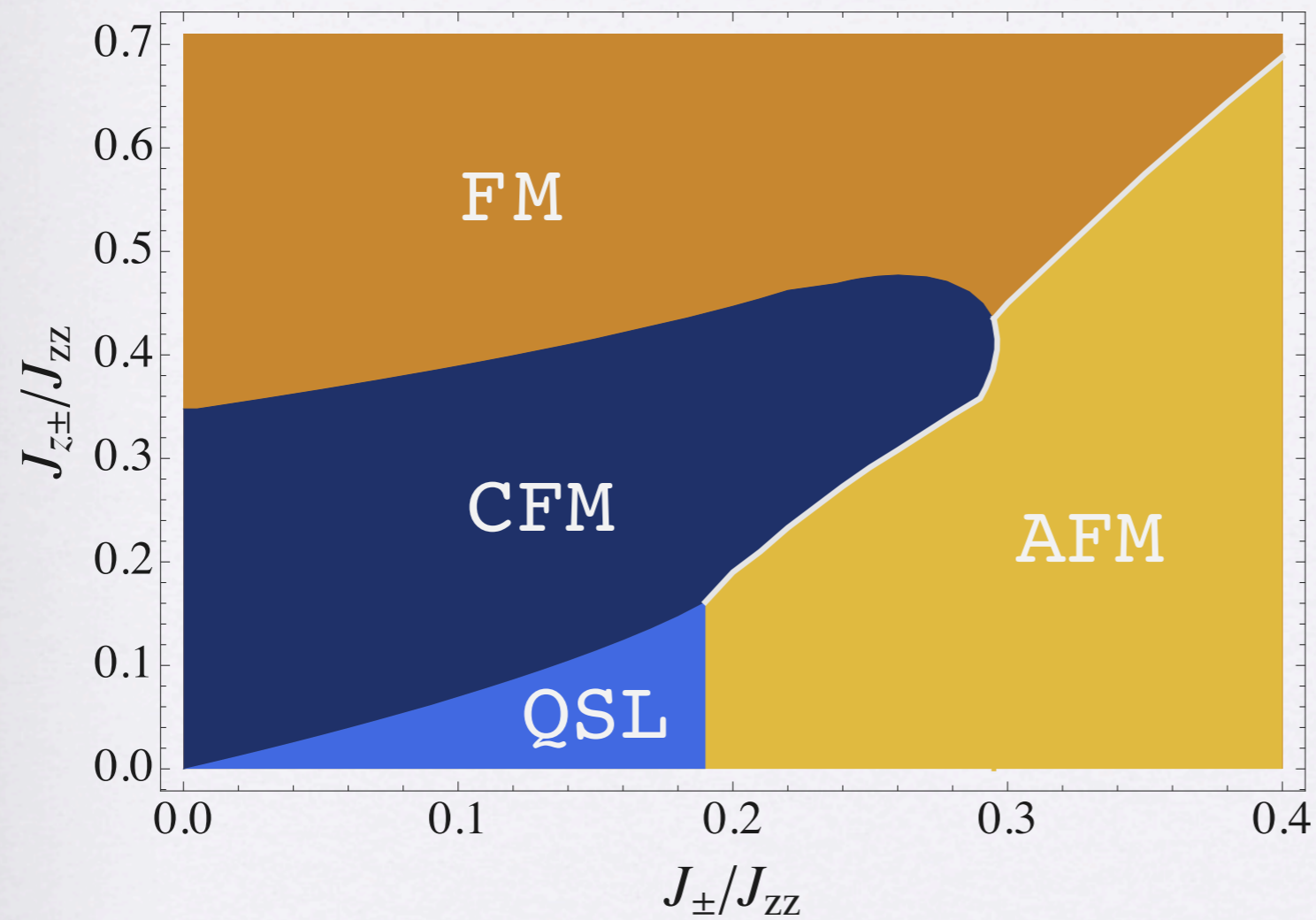


$$J_{\pm\pm} = 0$$



# Phase diagram

$$J_{\pm\pm} = 0$$

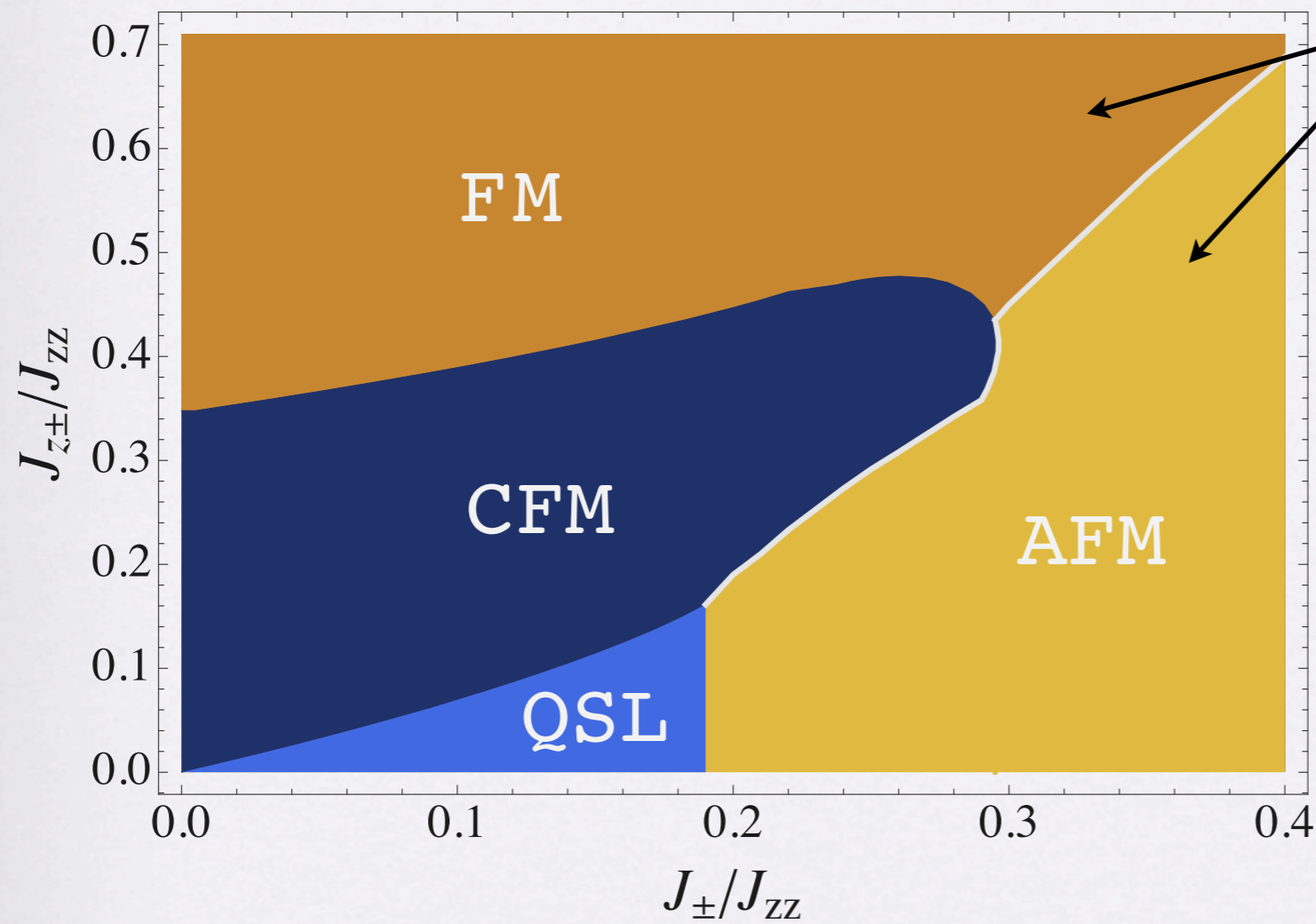


$\langle \Phi \rangle$	$\langle S^z \rangle$	phase
$\neq 0$	$= 0$	AFM
$\neq 0$	$\neq 0$	FM
$= 0$	$= 0$	QSL
$= 0$	$\neq 0$	CFM



# Phase diagram

$$J_{\pm\pm} = 0$$



Higgs  
 = gauge symmetry breaking  
 = condensed  
 = **conventional phases**

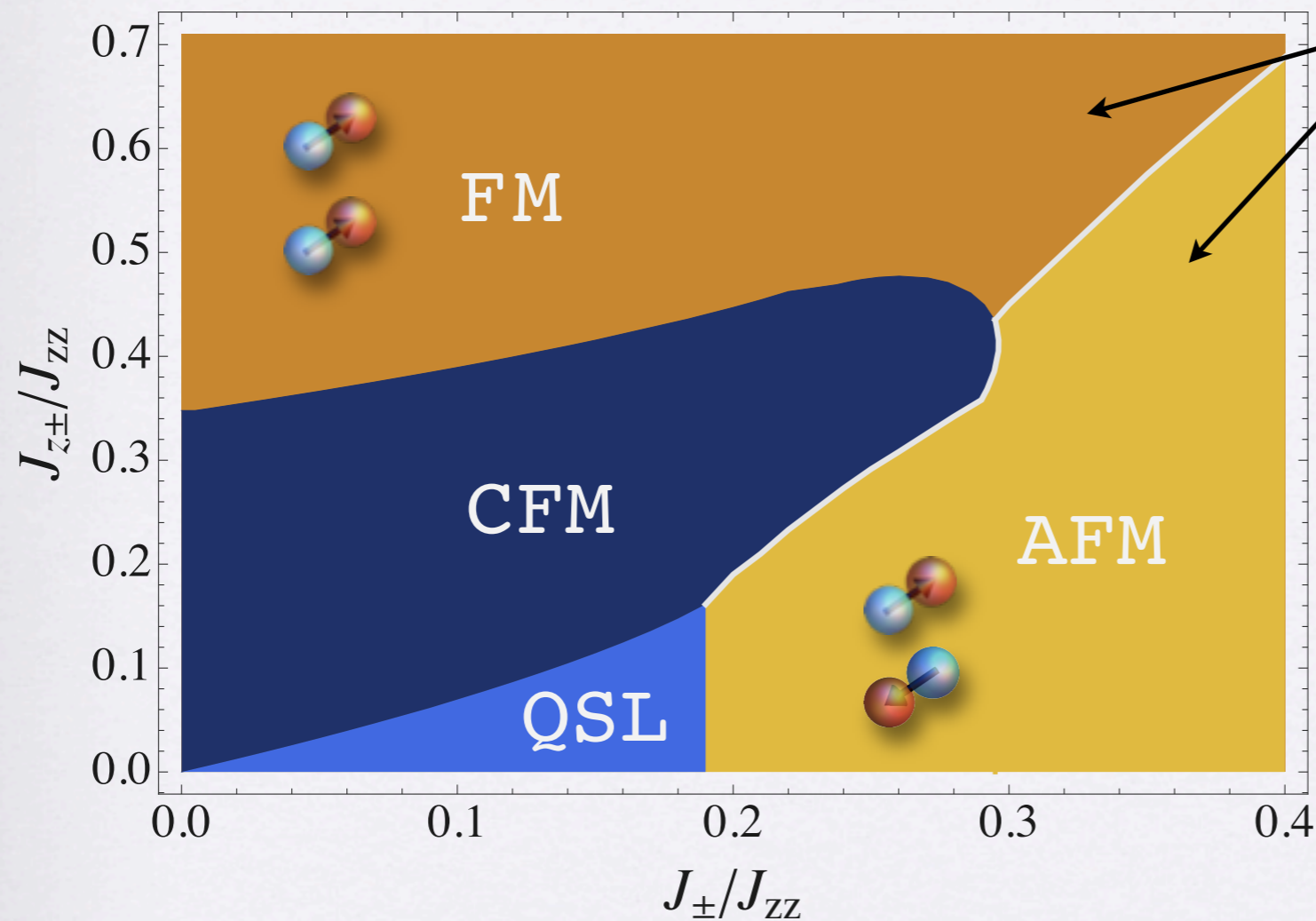
$$\langle \Phi \rangle \neq 0$$

$\langle \Phi \rangle$	$\langle S^z \rangle$	phase
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# Phase diagram

$$J_{\pm\pm} = 0$$



Higgs  
 = gauge symmetry  
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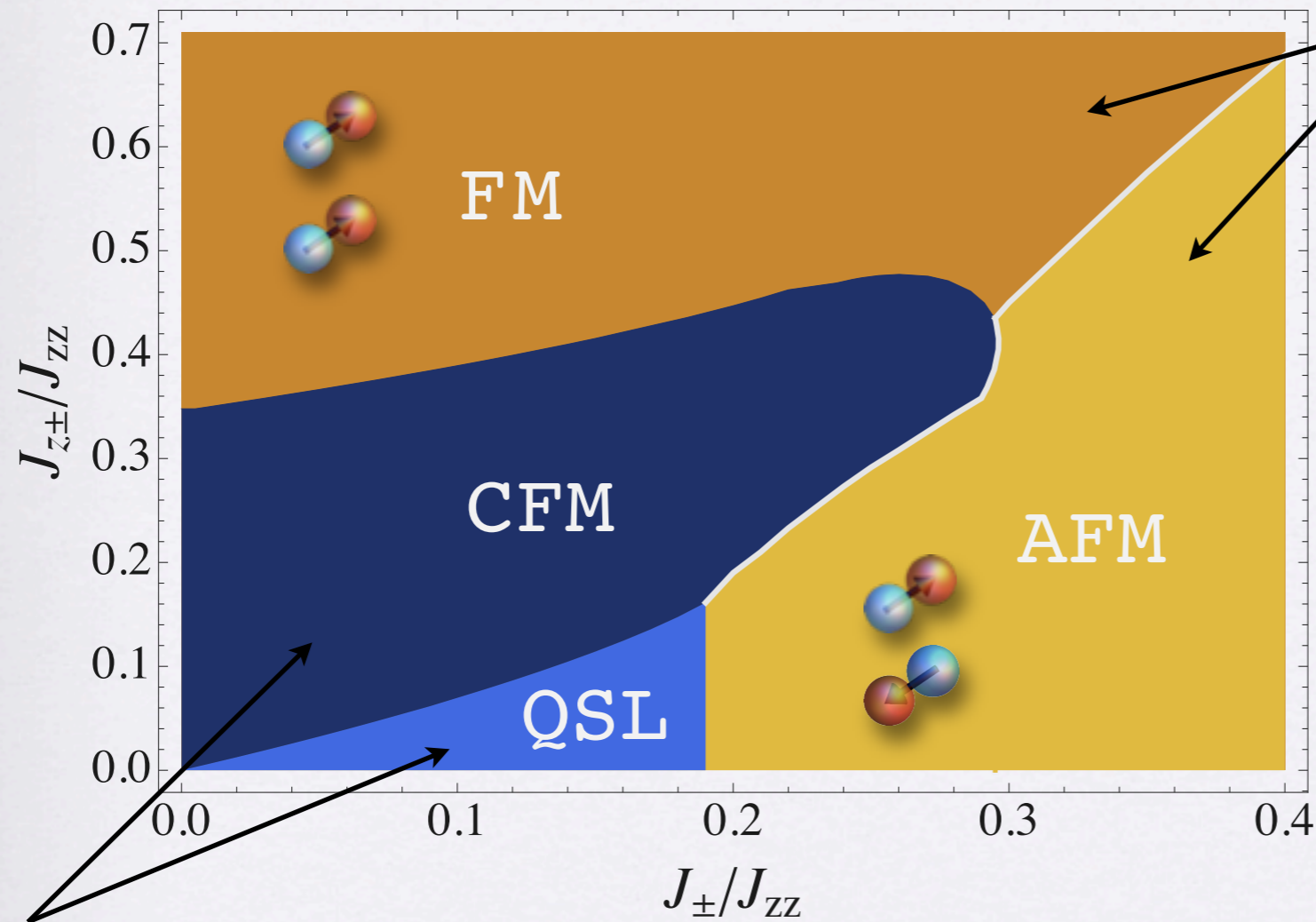
$$\langle \Phi \rangle \neq 0$$

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# Phase diagram

$$J_{\pm\pm} = 0$$



Higgs  
 = gauge symmetry  
 breaking  
 = condensed  
 = **conventional phases**

$$\langle\Phi\rangle \neq 0$$

deconfined  
 = uncondensed  
 = **exotic**

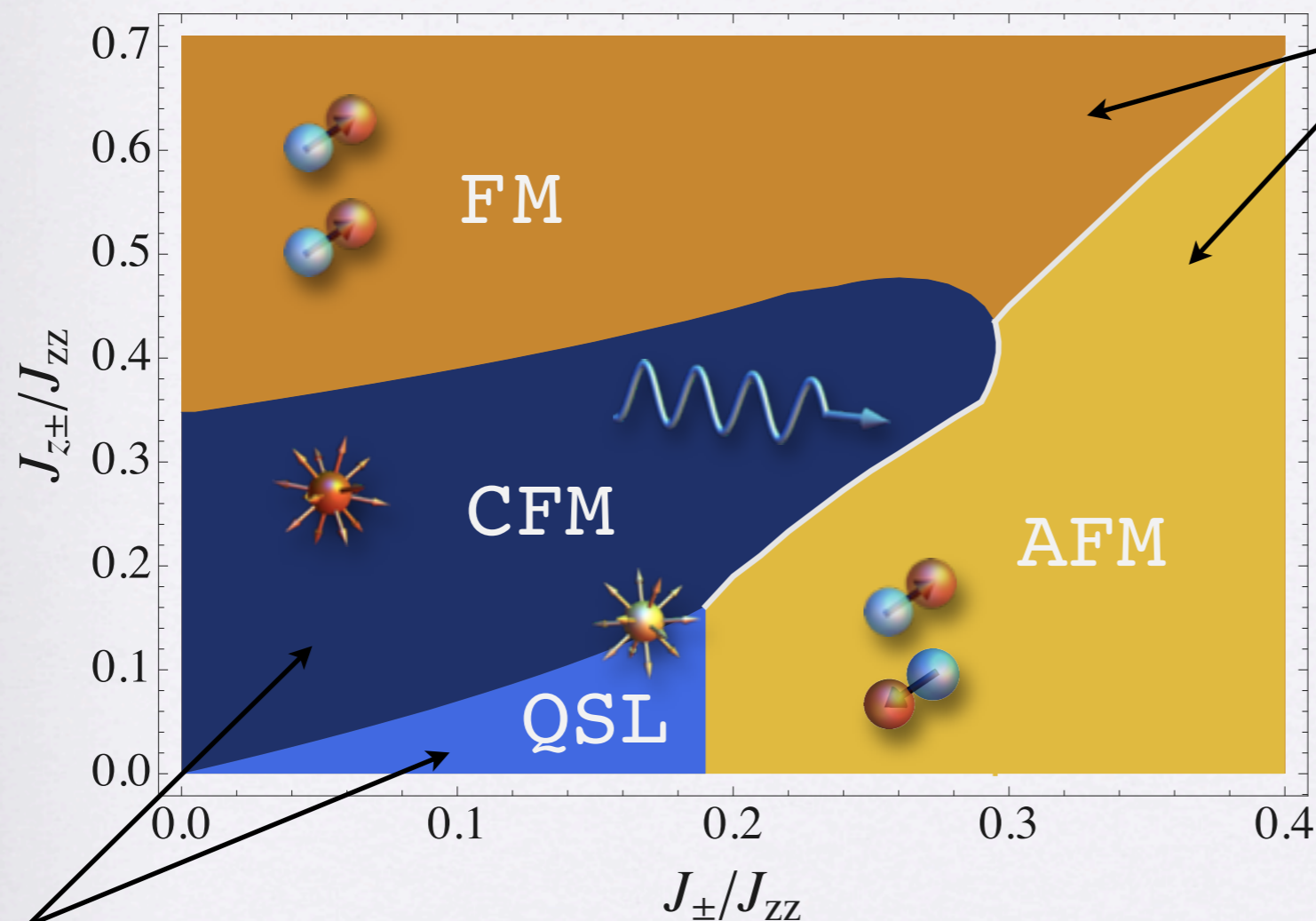
$$\langle\Phi\rangle = 0$$

$\langle\Phi\rangle$	$\langle S^z \rangle$	phase
$\neq 0$	$= 0$	AFM
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# Phase diagram

$$J_{\pm\pm} = 0$$



Higgs  
 = gauge symmetry breaking  
 = condensed  
 = **conventional phases**

$$\langle\Phi\rangle \neq 0$$

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$= 0$	$\neq 0$	CFM



# Insight into the exotic phases

- superposition of states

$|\psi\rangle \sim$  equal-weight quantum superposition of 2-in-2-out states

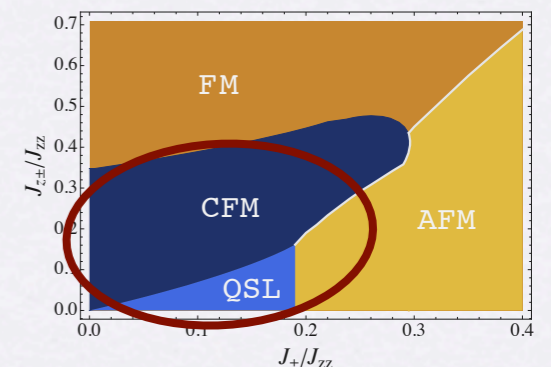
- inelastic structure factor  $\mathcal{S}(\mathbf{k}, \omega) = \sum_{\mu, \nu} \left[ \delta_{\mu\nu} - (\hat{\mathbf{k}})_{\mu} (\hat{\mathbf{k}})_{\nu} \right] \sum_{a, b} \langle m_a^{\mu}(-\mathbf{k}, -\omega) m_b^{\nu}(\mathbf{k}, \omega) \rangle$

$\langle S^z S^z \rangle$  contribution  $\longleftrightarrow$  photon mode

$\langle S^+ S^- \rangle$  contribution  $\longleftrightarrow$  spinon mode

$$S^z |\psi\rangle = |1 \text{ photon} + \text{vacuum}\rangle$$

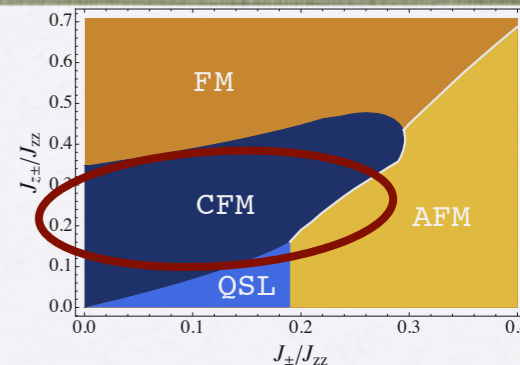
$$S^+ |\psi\rangle = |2 \text{ spinons} + \text{vacuum}\rangle$$





# The Coulomb ferromagnet

(secretly a quantum spin liquid!)

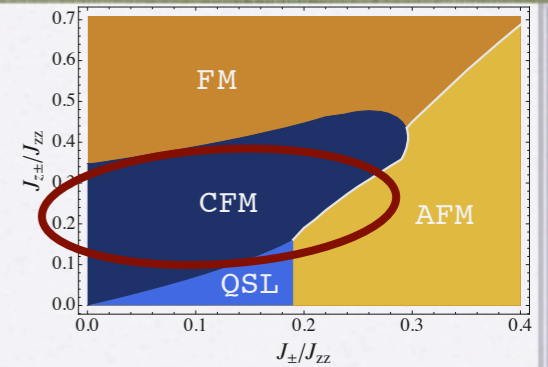


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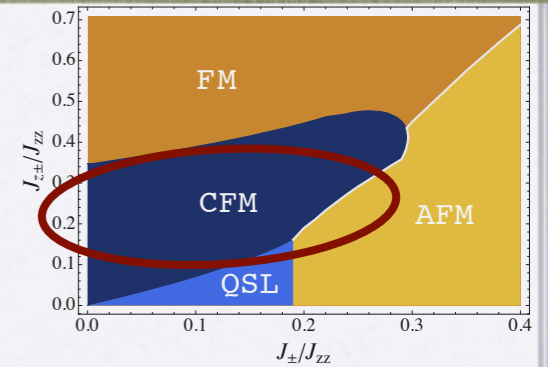
- magnetized

$\langle \Phi \rangle$	$\langle S^z \rangle$	phase
$\neq 0$	$= 0$	AFM
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# The Coulomb ferromagnet

(secretly a quantum spin liquid!)



- magnetized

$$\langle S^z \rangle \neq 0$$



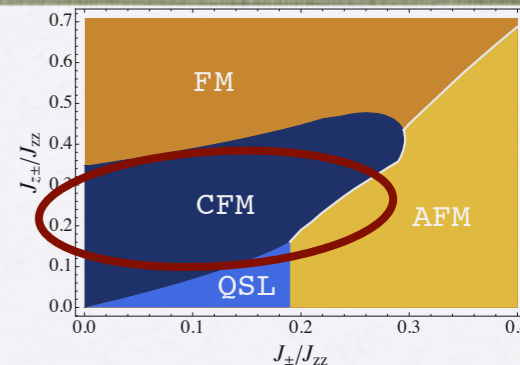
spins with non-zero expectation value

$\langle \Phi \rangle$	$\langle S^z \rangle$	phase
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# The Coulomb ferromagnet

(secretly a quantum spin liquid!)



- magnetized

$$\langle S^z \rangle \neq 0$$

$$\langle S^z \rangle < 1/2$$



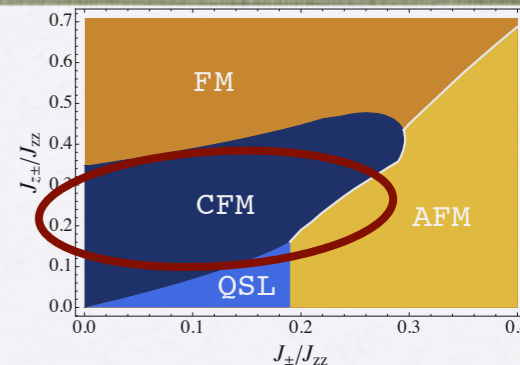
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(secretly a quantum spin liquid!)



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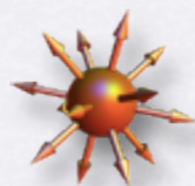
spins with non-zero expectation value

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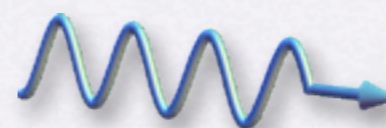
- supports exotic excitations

$$\langle \Phi \rangle = 0$$

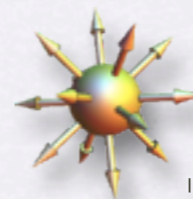
$$\langle S^{\pm} \rangle = 0$$



spinon



gapless photon



"electric" monopole



# Signatures of the deconfined phases



- inelastic neutron scattering:

- photon

- spinon

- specific heat:

- photon

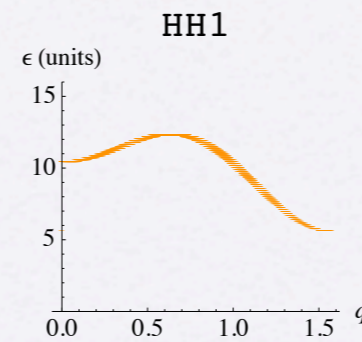
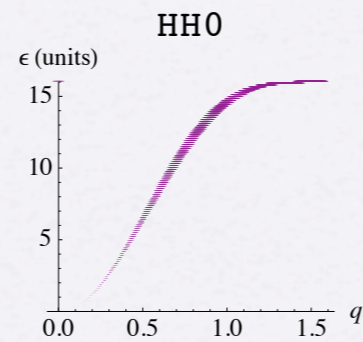
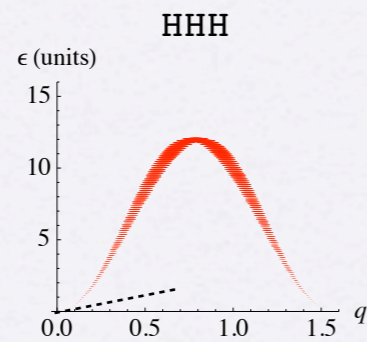


# Signatures of the deconfined phases



- inelastic neutron scattering:

- photon



$$\mathcal{S}(\mathbf{k} \sim \mathbf{0}, \omega) \sim \omega \delta[\omega - v|\mathbf{k}|]$$

- spinon

- specific heat:

- photon

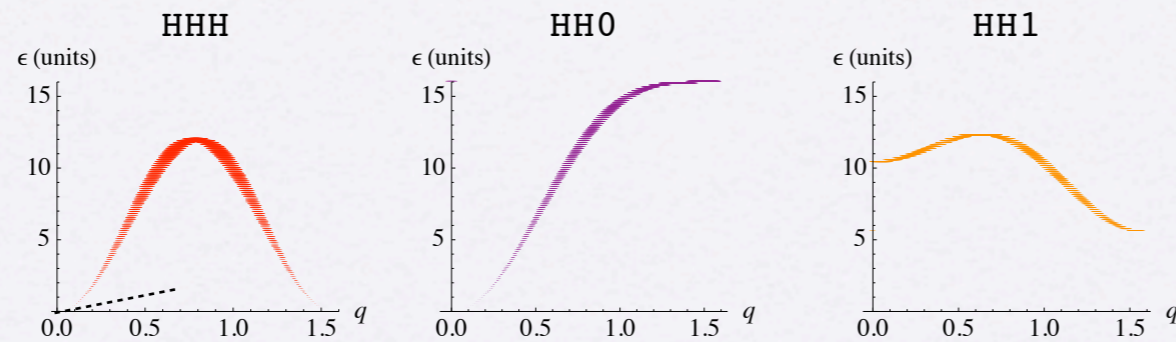


# Signatures of the deconfined phases



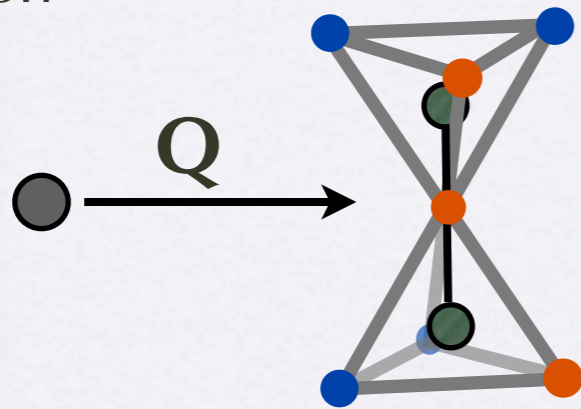
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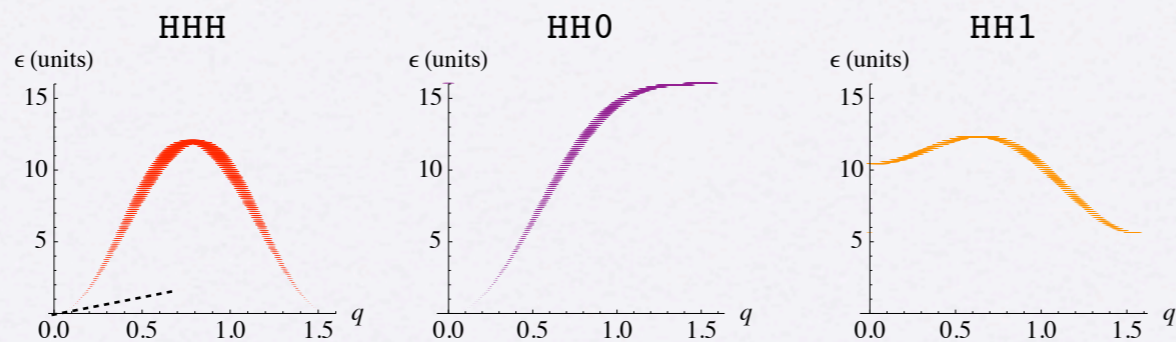


# Signatures of the deconfined phases



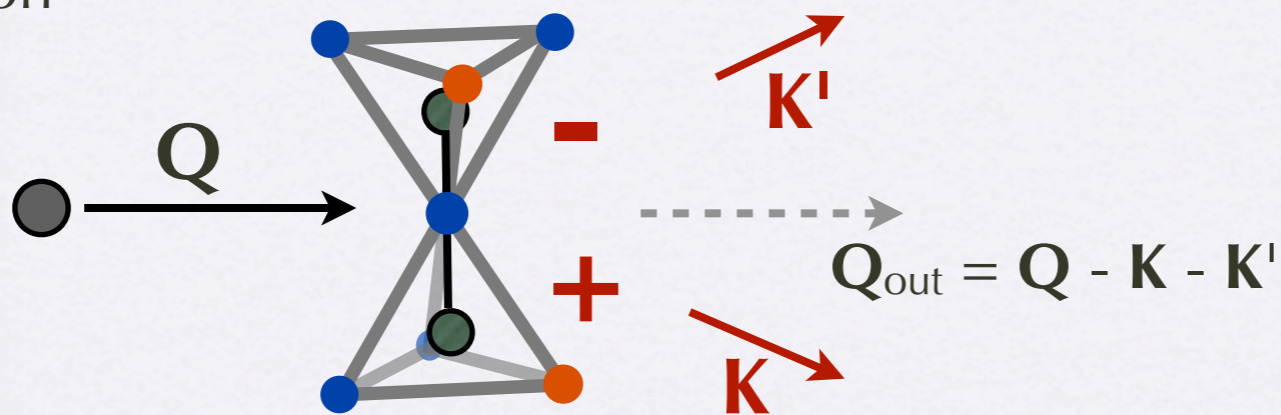
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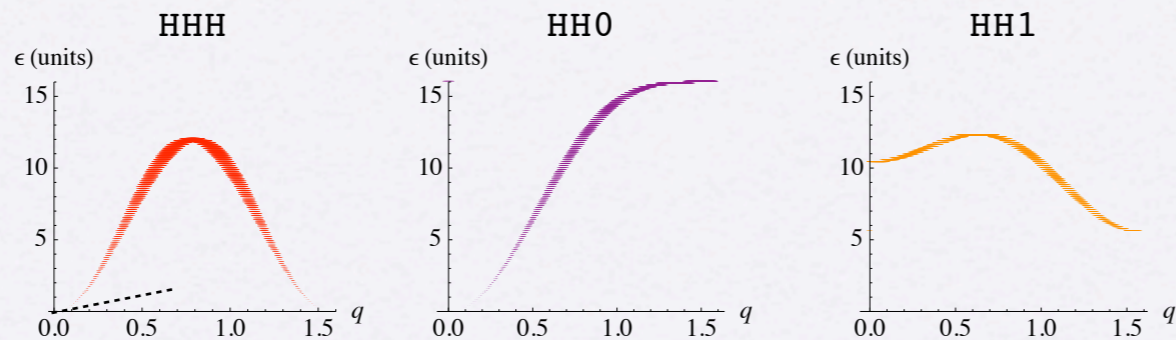


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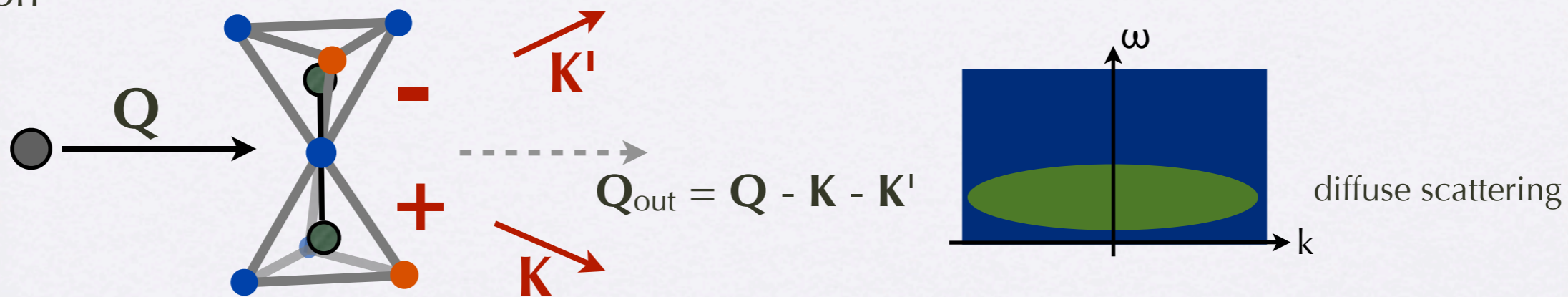
- inelastic neutron scattering:

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$$\mathcal{S}(\mathbf{k} \sim \mathbf{0}, \omega) \sim \omega \delta[\omega - v|\mathbf{k}|]$$

- spinon



- specific heat:

- photon

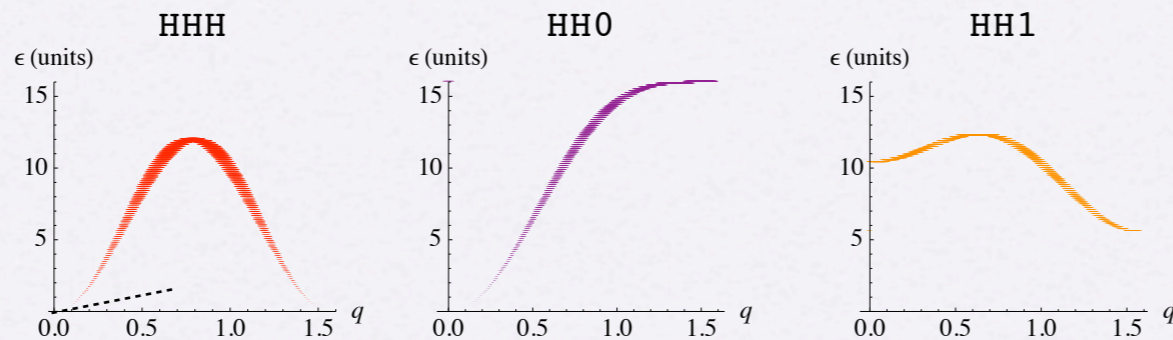


# Signatures of the deconfined phases



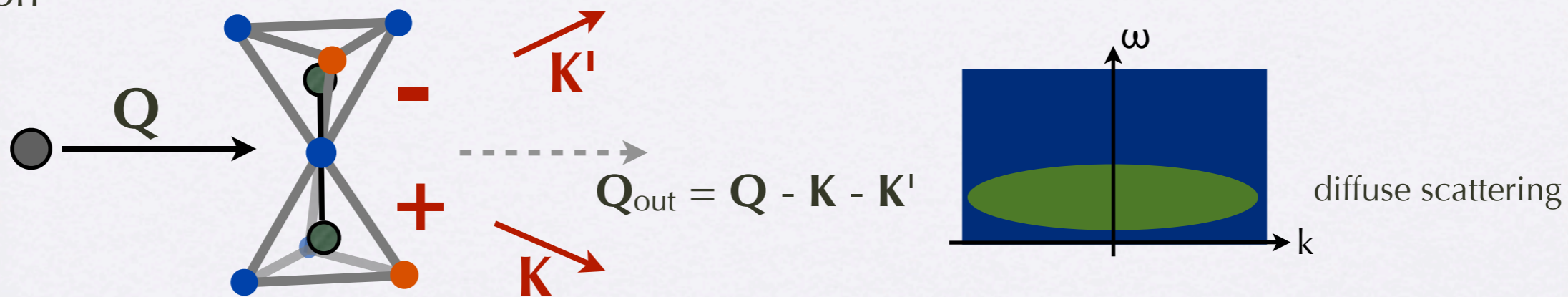
- inelastic neutron scattering:

- photon



$$\mathcal{S}(\mathbf{k} \sim \mathbf{0}, \omega) \sim \omega \delta[\omega - v|\mathbf{k}|]$$

- spinon



- specific heat:

- photon  $C_v^{T \approx 0} \sim B_{\text{photon}} T^3 + B_{\text{phonon}} T^3$

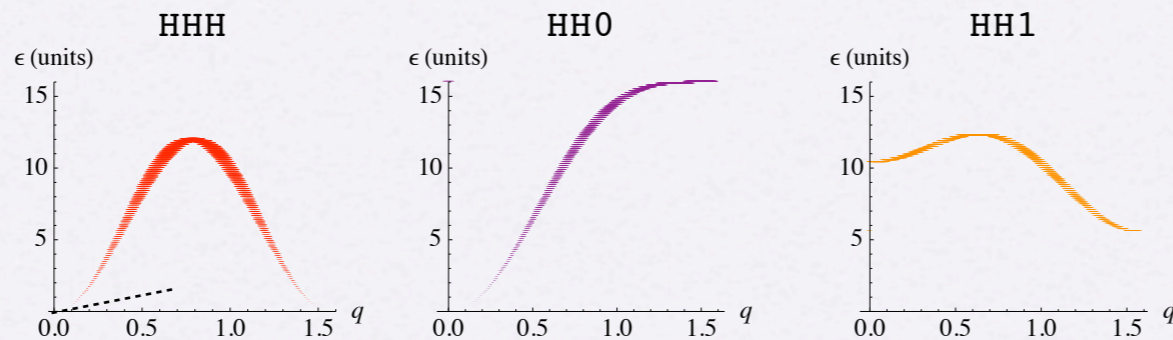


# Signatures of the deconfined phases



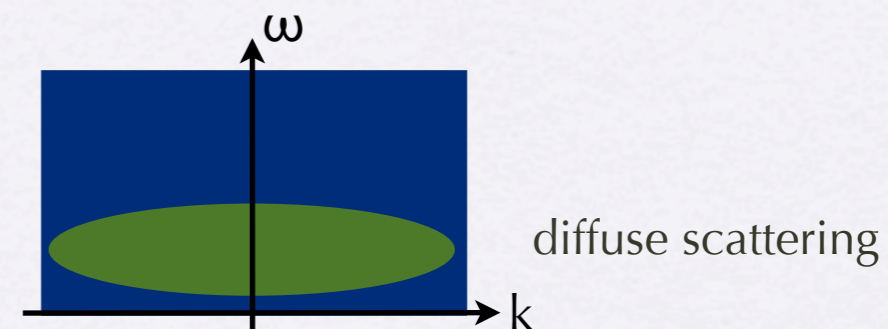
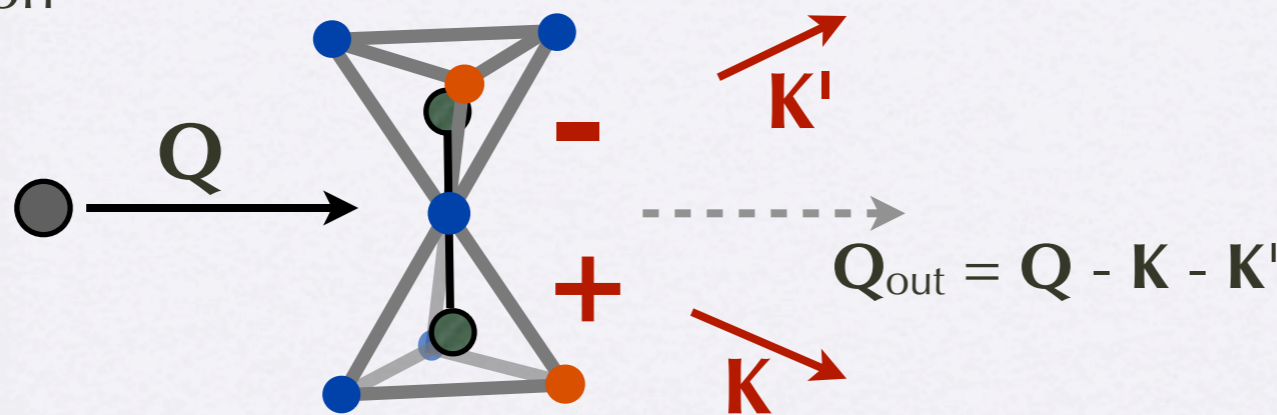
- inelastic neutron scattering:

- photon



$$\mathcal{S}(\mathbf{k} \sim \mathbf{0}, \omega) \sim \omega \delta[\omega - v|\mathbf{k}|]$$

- spinon



- specific heat:

- photon  $C_v^{T \approx 0} \sim B_{\text{photon}} T^3 + B_{\text{phonon}} T^3$

$B_{\text{photon}} \sim 1000 B_{\text{phonon}}$

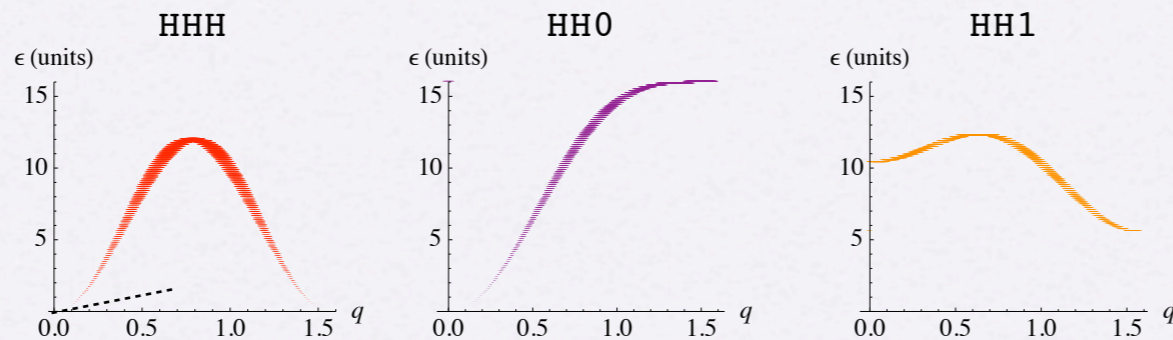


# Signatures of the deconfined phases



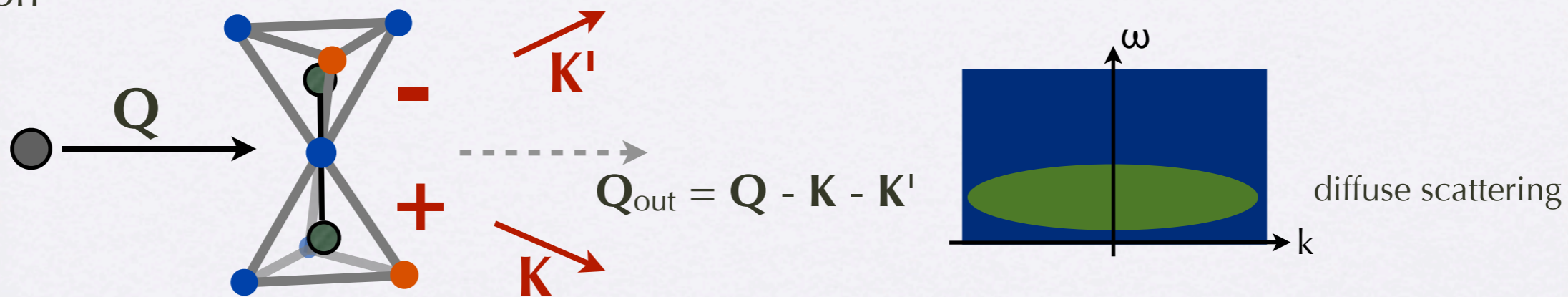
- inelastic neutron scattering:

- photon



$$\mathcal{S}(\mathbf{k} \sim \mathbf{0}, \omega) \sim \omega \delta[\omega - v|\mathbf{k}|]$$

- spinon

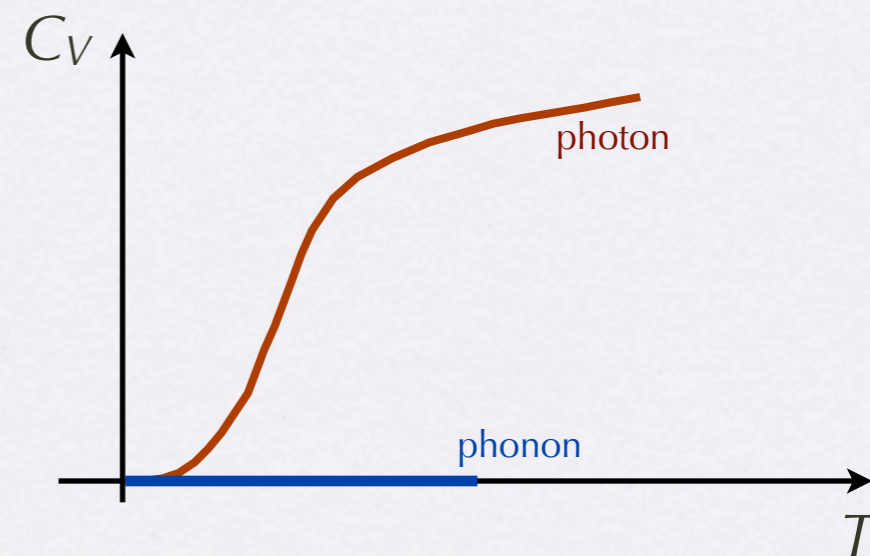


- specific heat:

- photon

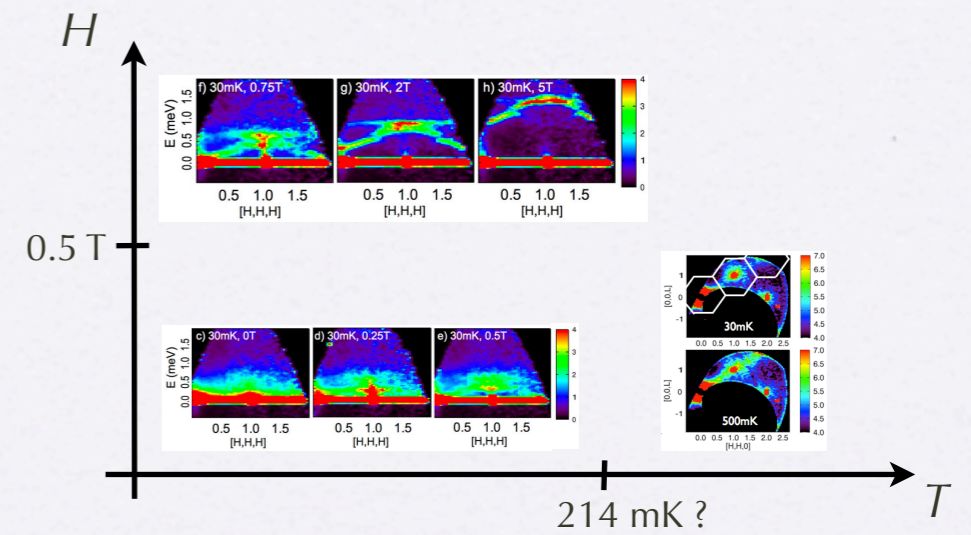
$$C_v^{T \approx 0} \sim B_{\text{photon}} T^3 + B_{\text{phonon}} T^3$$

$$B_{\text{photon}} \sim 1000 B_{\text{phonon}}$$





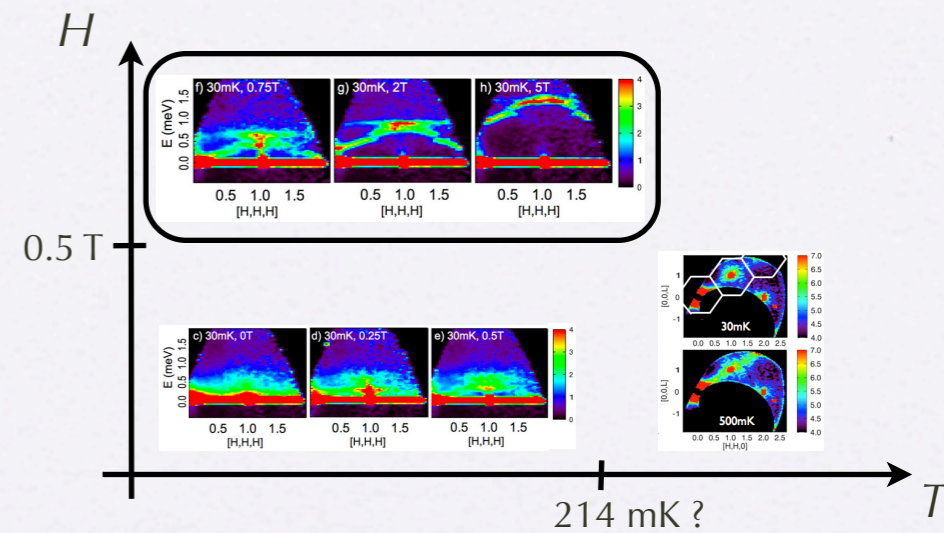
# $\text{Yb}_2\text{Ti}_2\text{O}_7$





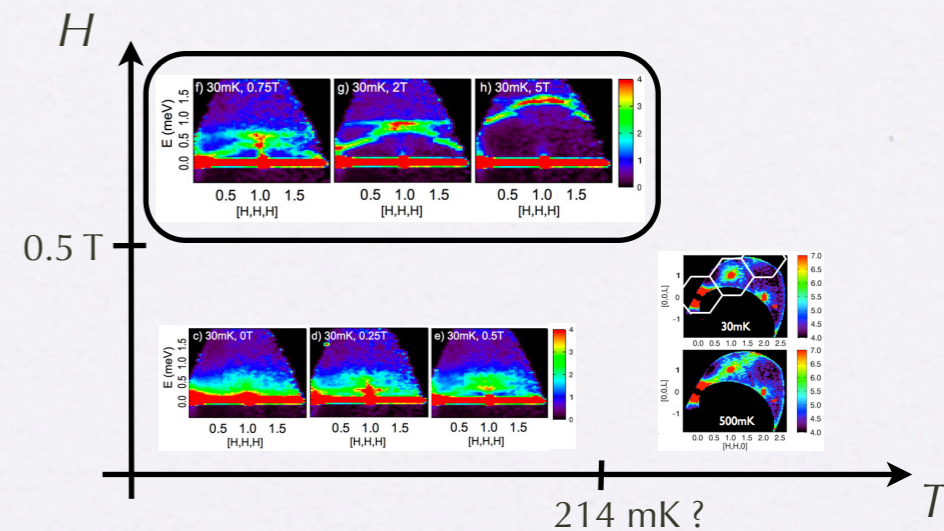
# $\text{Yb}_2\text{Ti}_2\text{O}_7$

high field  $H = 5\text{T}$



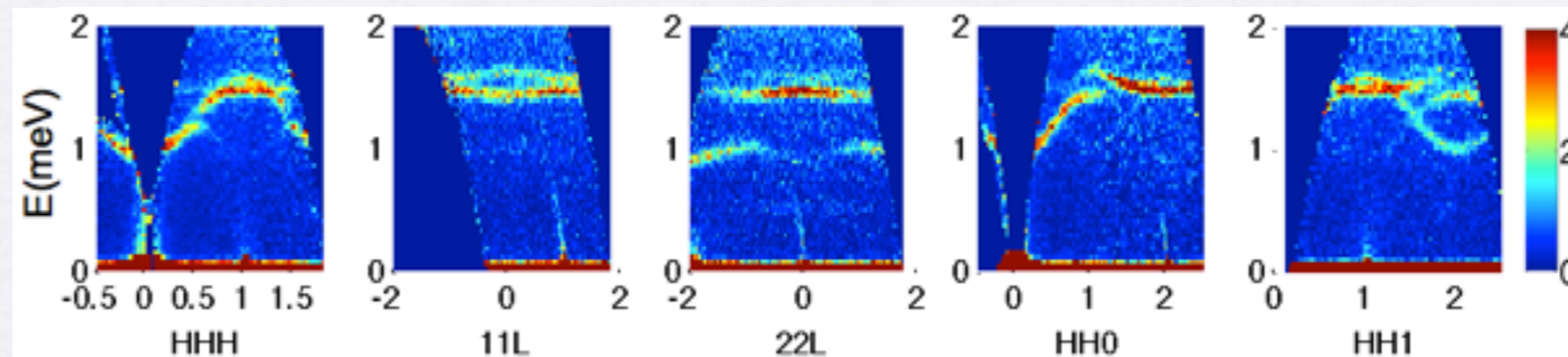


# Yb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>



high field  $H = 5T$

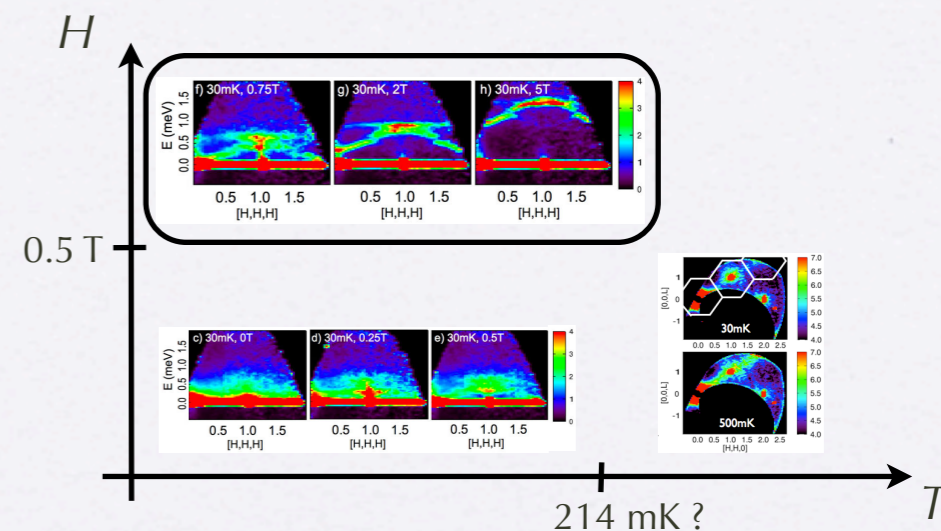
experiment



spin wave theory

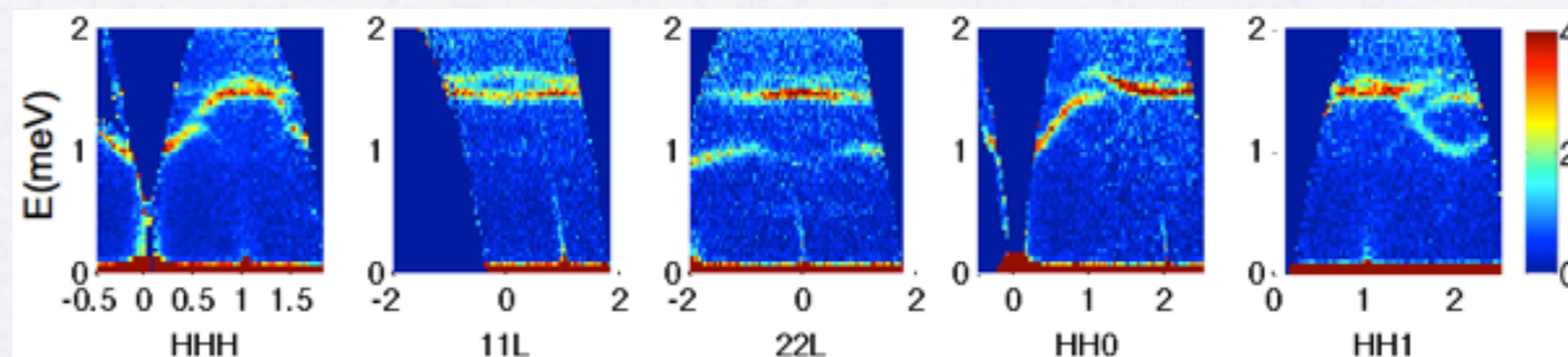


# Yb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>



high field  $H = 5T$

experiment

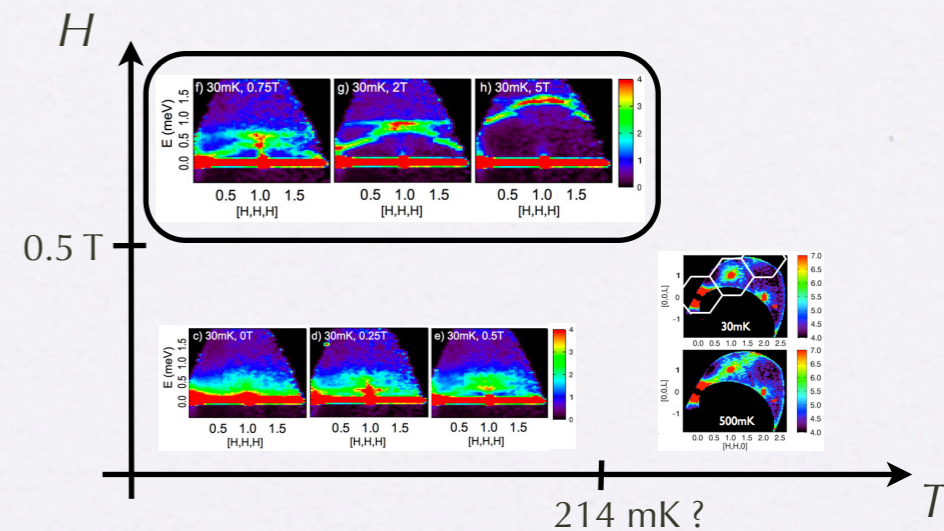


spin wave theory

1. classical high-field ground state
2. Holstein-Primakoff bosons in the spirit of large  $s$
3. calculation of the inelastic structure factor



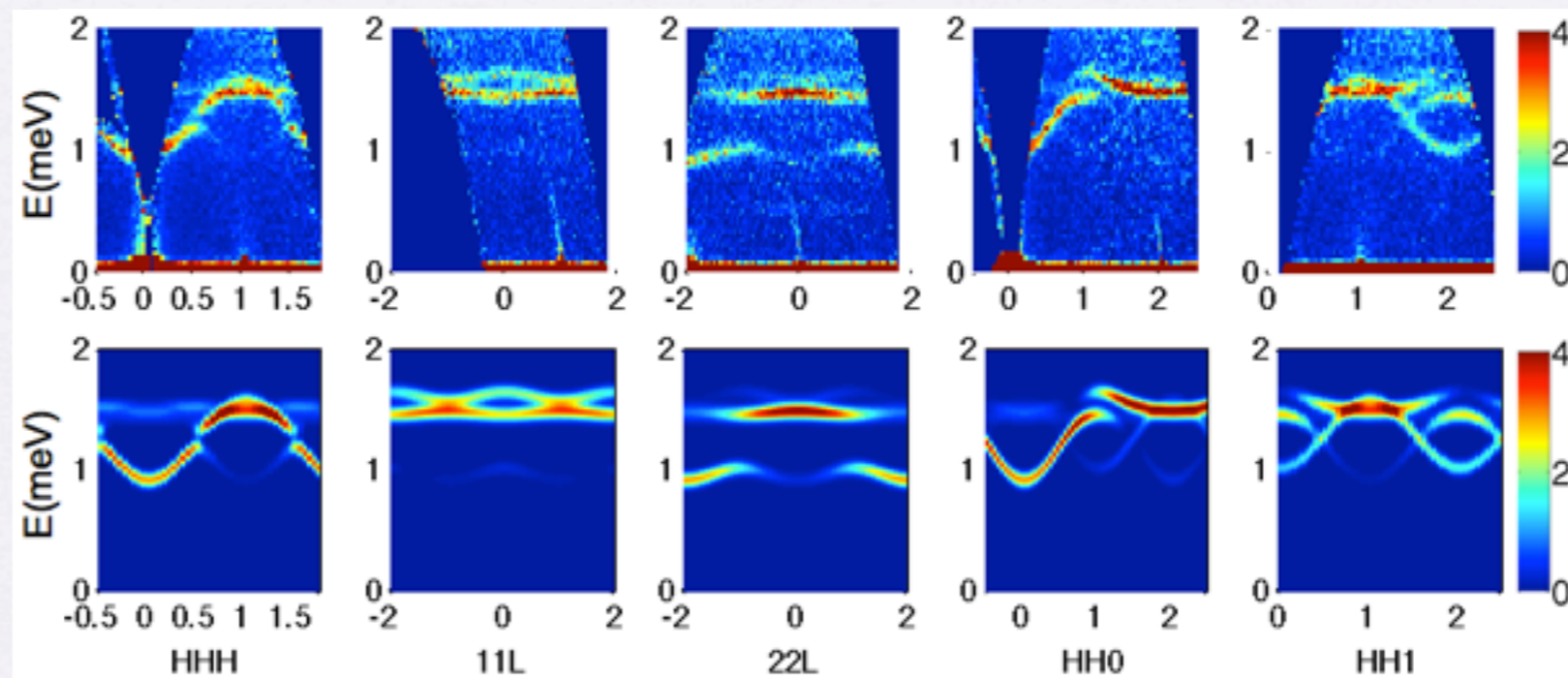
# Yb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>



high field  $H = 5\text{T}$

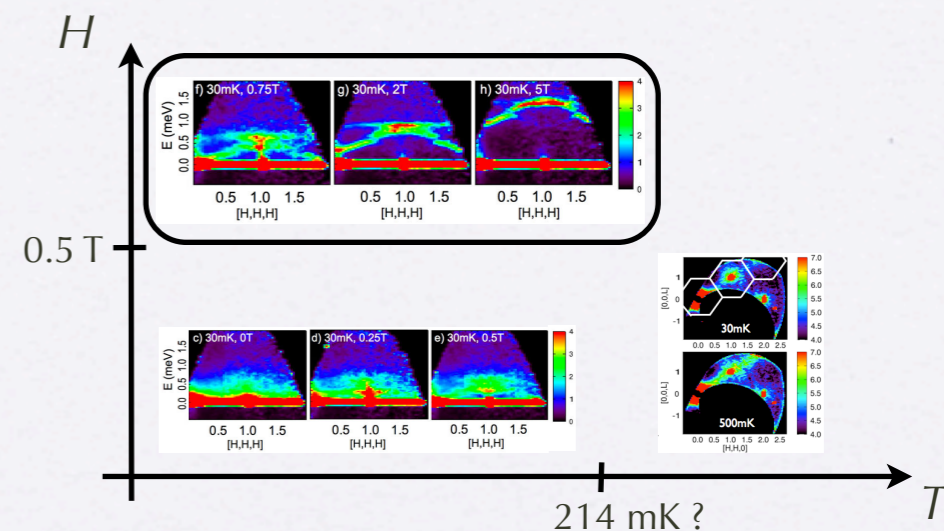
experiment

spin wave theory





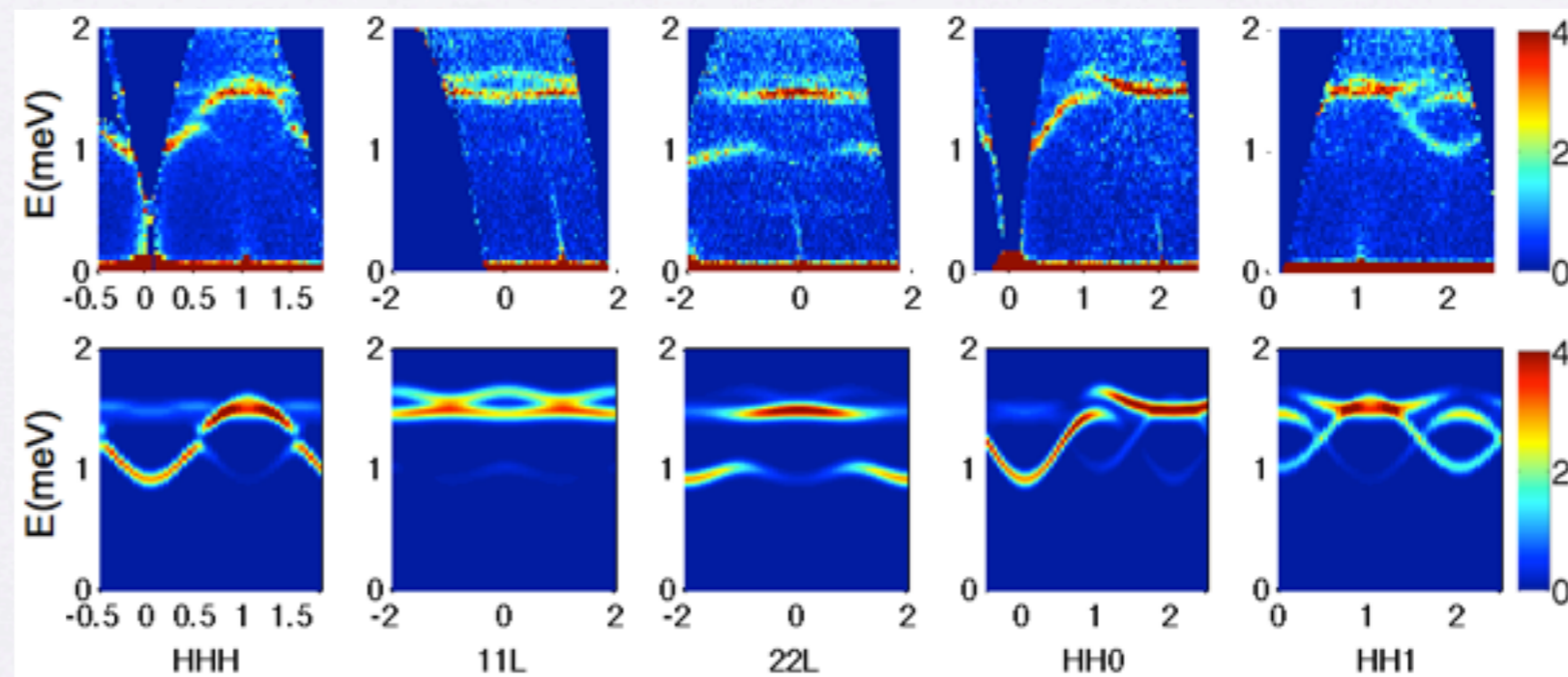
# Yb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>



high field  $H = 5T$

experiment

spin wave theory

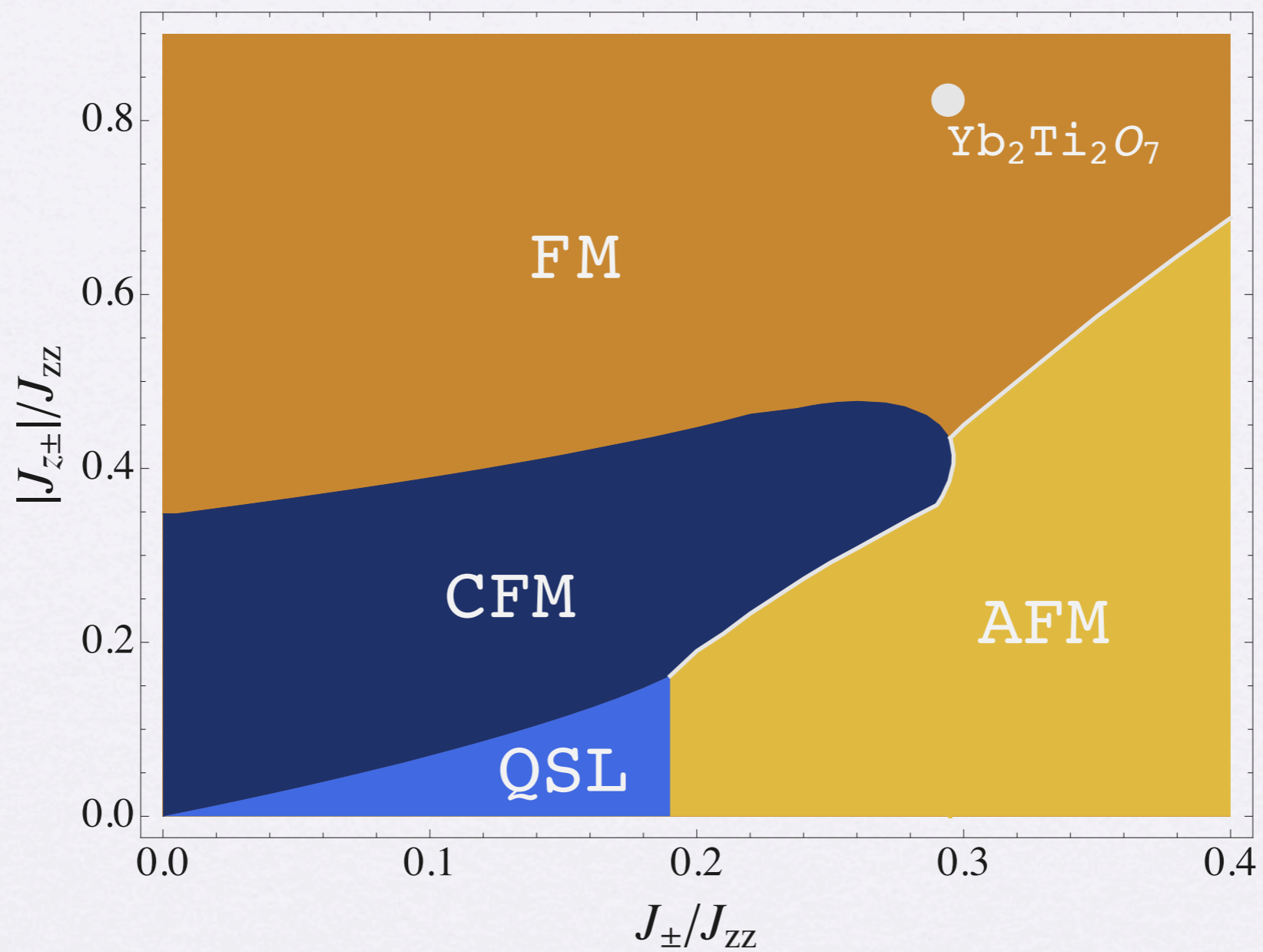


$$J_{zz} = 0.17, \quad J_{\pm} = 0.05, \quad J_{z\pm} = -0.14, \quad J_{\pm\pm} = 0.05 \quad \text{meV}$$



# Yb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>

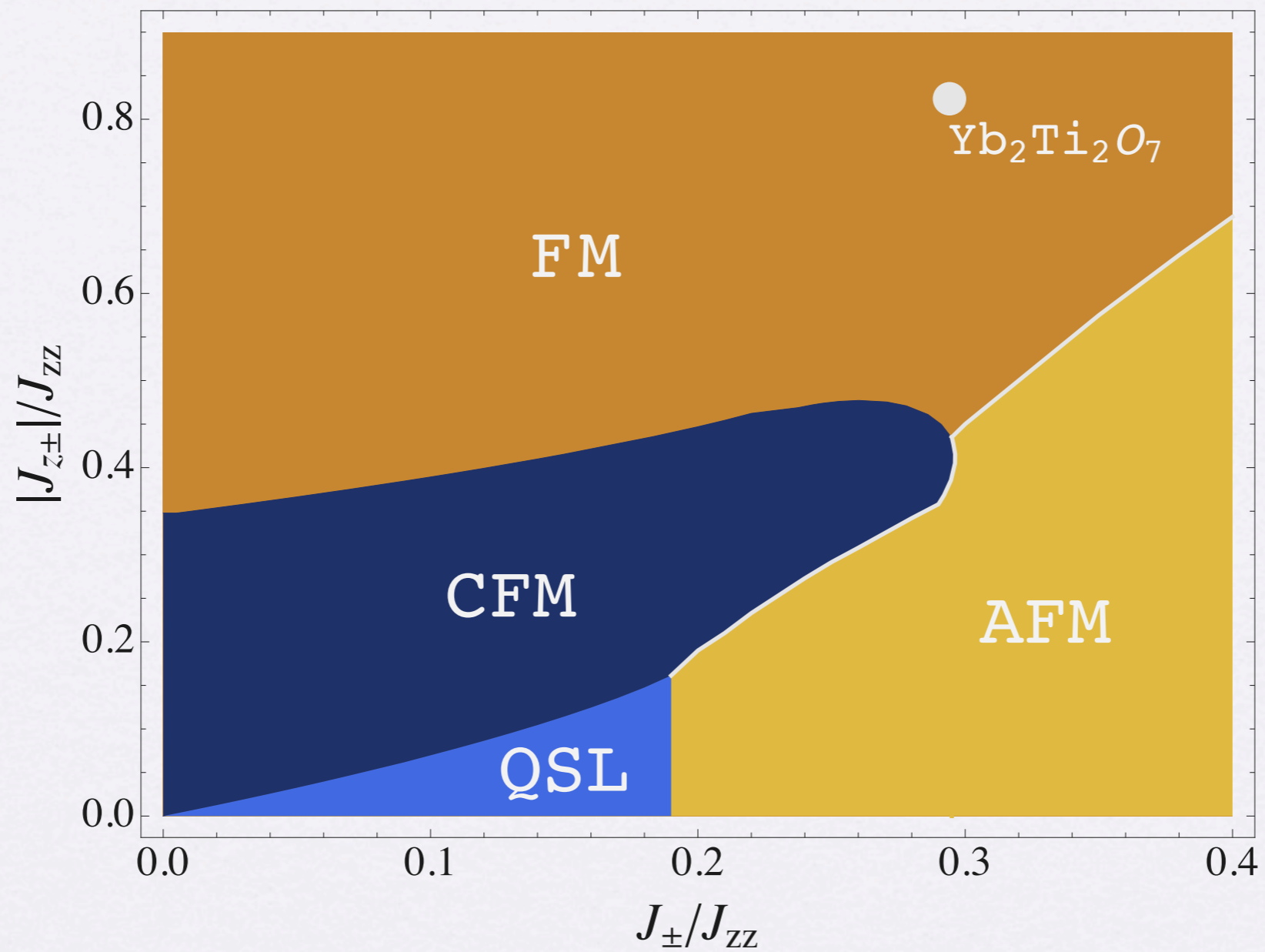
$$J_{zz} = 0.17, \quad J_{\pm} = 0.05, \quad J_{z\pm} = -0.14, \quad J_{\pm\pm} = 0.05 \text{ meV}$$





# Yb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>

$$J_{zz} = 0.17, \quad J_{\pm} = 0.05, \quad J_{z\pm} = -0.14, \quad J_{\pm\pm} = 0.05 \text{ meV}$$

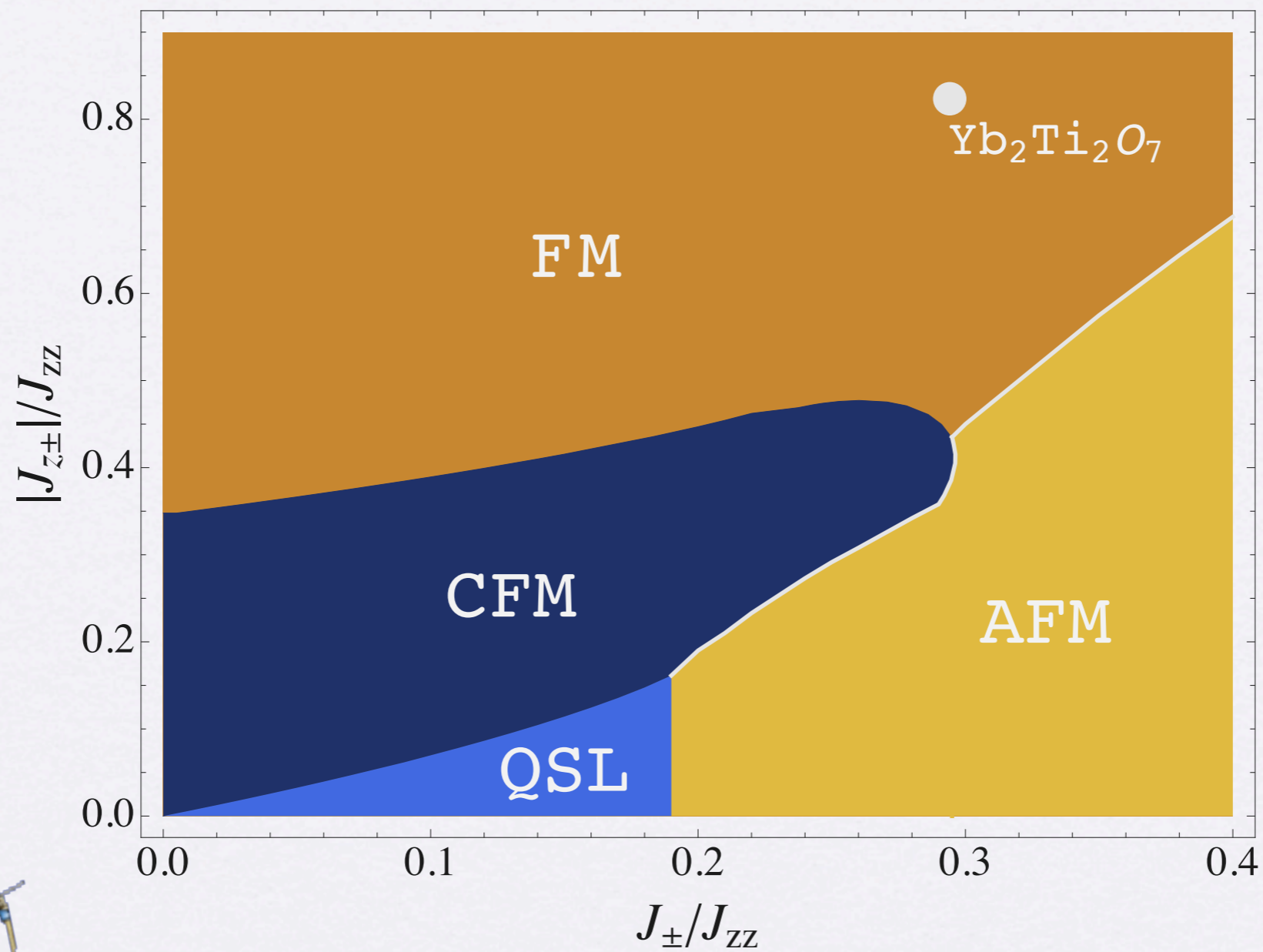


some  
uncertainties



# Yb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>

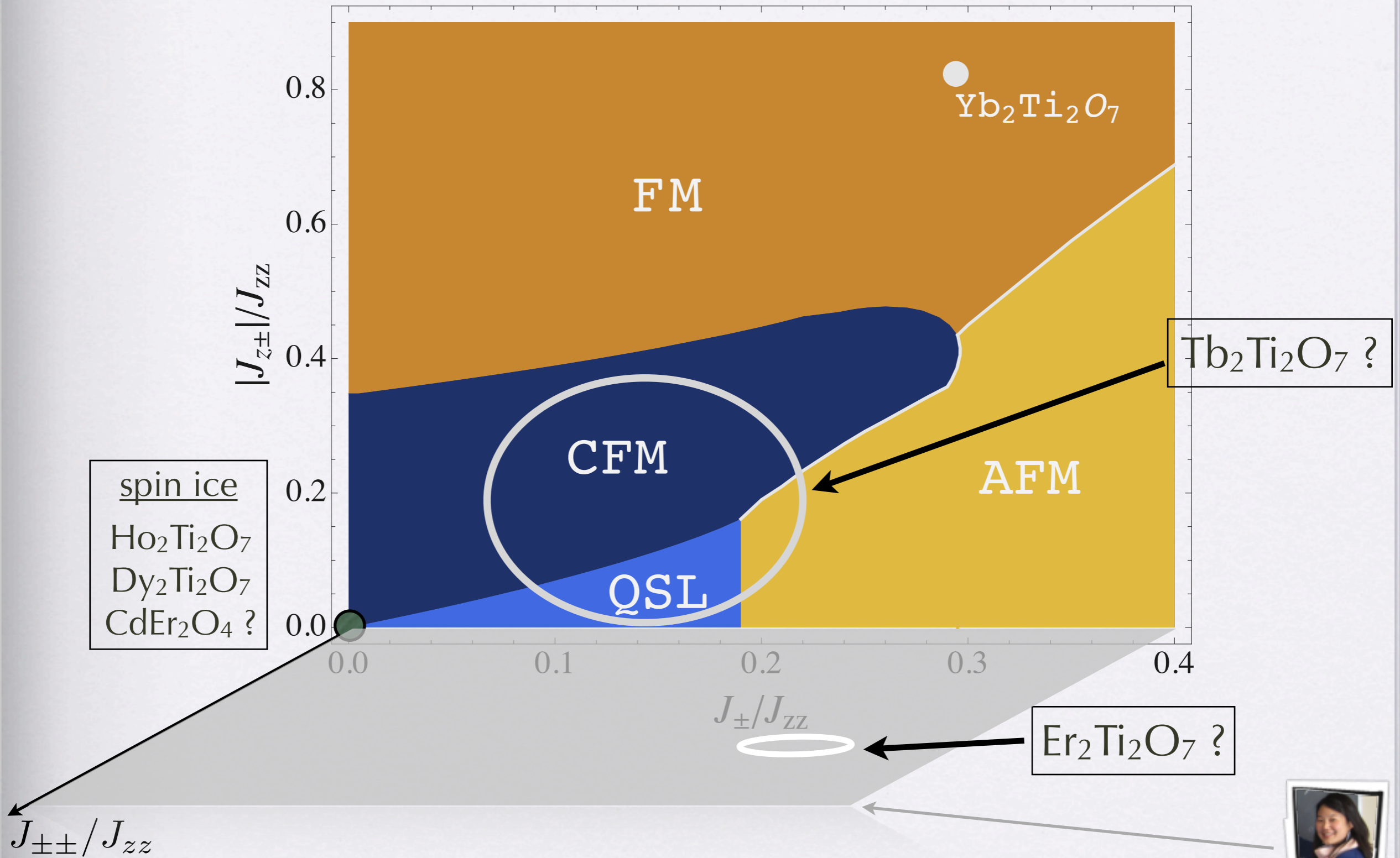
$$J_{zz} = 0.17, \quad J_{\pm} = 0.05, \quad J_{z\pm} = -0.14, \quad J_{\pm\pm} = 0.05 \text{ meV}$$



Tb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> ? Er<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> ? CdEr<sub>2</sub>O<sub>4</sub> ? ...



# Materials



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# Conclusions and perspectives

- Model and phase diagram which should apply to a **wide spectrum of materials**
- Realization of the **U(1) QSL** in a phase diagram for **real materials**
- Existence of a **new phase of matter: the Coulomb FM**
- Need **numerics**
- Need exchange constants of **more materials**
- Need more **low temperature specific heat** data
- Effects of **disorder**
- Effects of **temperature**
- **Longer range** interactions...





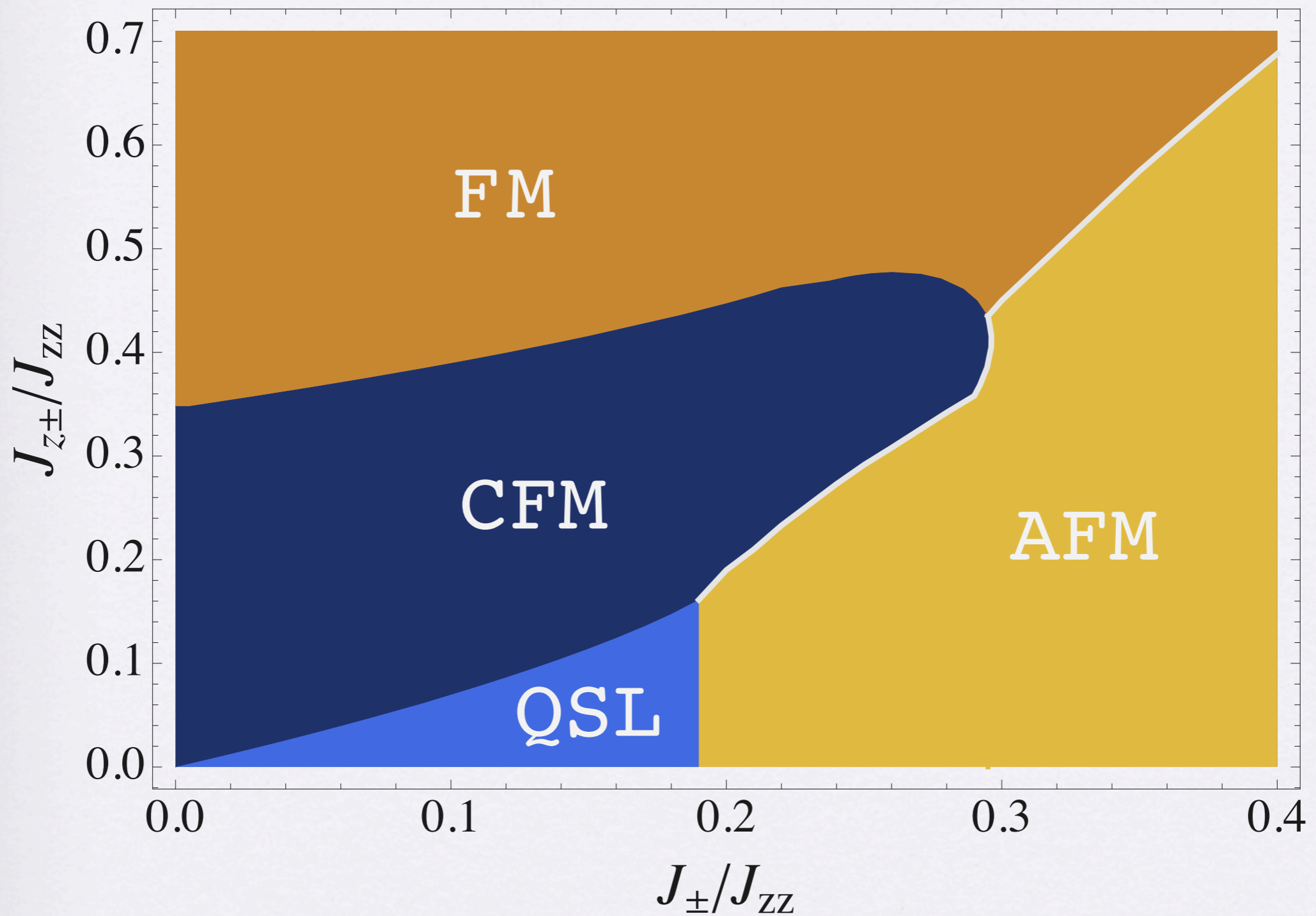
**Thank you for your attention**



extra slides for  
questions



# Phase diagram





# Order parameters

$\langle \Phi \rangle$	$\langle S^z \rangle$	phase
$\neq 0$	$= 0$	AFM
$\neq 0$	$\neq 0$	FM
$= 0$	$= 0$	QSL
$= 0$	$\neq 0$	CFM



# Geometry

$$\begin{cases} \hat{\mathbf{e}}_0 = (1, 1, 1)/\sqrt{3} \\ \hat{\mathbf{e}}_1 = (1, -1, -1)/\sqrt{3} \\ \hat{\mathbf{e}}_2 = (-1, 1, -1)/\sqrt{3} \\ \hat{\mathbf{e}}_3 = (-1, -1, 1)/\sqrt{3}, \end{cases}$$

$$\begin{cases} \hat{\mathbf{a}}_0 = (-2, 1, 1)/\sqrt{6} \\ \hat{\mathbf{a}}_1 = (-2, -1, -1)/\sqrt{6} \\ \hat{\mathbf{a}}_2 = (2, 1, -1)/\sqrt{6} \\ \hat{\mathbf{a}}_3 = (2, -1, 1)/\sqrt{6} \end{cases}$$

$$\hat{\mathbf{b}}_i = \hat{\mathbf{e}}_i \times \hat{\mathbf{a}}_i$$

$$\gamma = \begin{pmatrix} 0 & 1 & w & w^2 \\ 1 & 0 & w^2 & w \\ w & w^2 & 0 & 1 \\ w^2 & w & 1 & 0 \end{pmatrix}$$

$$w = e^{2\pi i/3}$$

$$\zeta = -\gamma^*$$



# Curie-Weiss temperature

$$\Theta_{\text{CW}} = \frac{1}{2k_B(2g_{xy}^2 + g_z^2)} [g_z^2 J_{zz} - 4g_{xy}^2 (J_{\pm} + 2J_{\pm\pm}) - 8\sqrt{2} g_{xy} g_z J_{z\pm}]$$



# parameters

$$J_{zz} = -\frac{1}{3}(2J_1 - J_2 + 2(J_3 + 2J_4))$$

$$J_{\pm} = \frac{1}{6}(2J_1 - J_2 - J_3 - 2J_4)$$

$$J_{z\pm} = \frac{1}{3\sqrt{2}}(J_1 + J_2 + J_3 - J_4)$$

$$J_{\pm\pm} = \frac{1}{6}(J_1 + J_2 - 2J_3 + 2J_4)$$

$$J_1 = \frac{1}{3}(-J_{zz} + 4J_{\pm} + 2\sqrt{2}J_{z\pm} + 2J_{\pm\pm})$$

$$J_3 = \frac{1}{3}(-J_{zz} - 2J_{\pm} + 2\sqrt{2}J_{z\pm} - 4J_{\pm\pm})$$

$$J_2 = \frac{1}{3}(J_{zz} - 4J_{\pm} + 4\sqrt{2}J_{z\pm} + 4J_{\pm\pm})$$

$$J_4 = \frac{1}{3\sqrt{2}}(-\sqrt{2}J_{zz} - 2\sqrt{2}J_{\pm} + 2J_{z\pm} + 2\sqrt{2}J_{\pm\pm})$$

$$\mathbf{J}_{01} = \begin{pmatrix} J_2 & J_4 & J_4 \\ -J_4 & J_1 & J_3 \\ -J_4 & J_3 & J_1 \end{pmatrix}$$



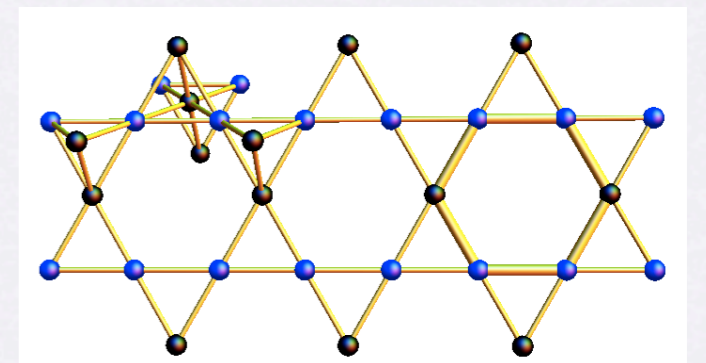
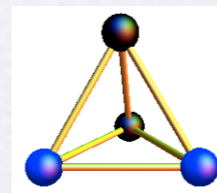
# Perturbation Theory

$$H_{\text{ring}}^{\text{eff}} = -K \sum_{\{i,j,k,l,m,n\}=\text{hexagon}} (S_i^+ S_j^- S_k^+ S_l^- S_m^+ S_n^- + \text{h.c.})$$

$$K = \frac{12J_{\pm}^3}{J_{zz}^2}$$

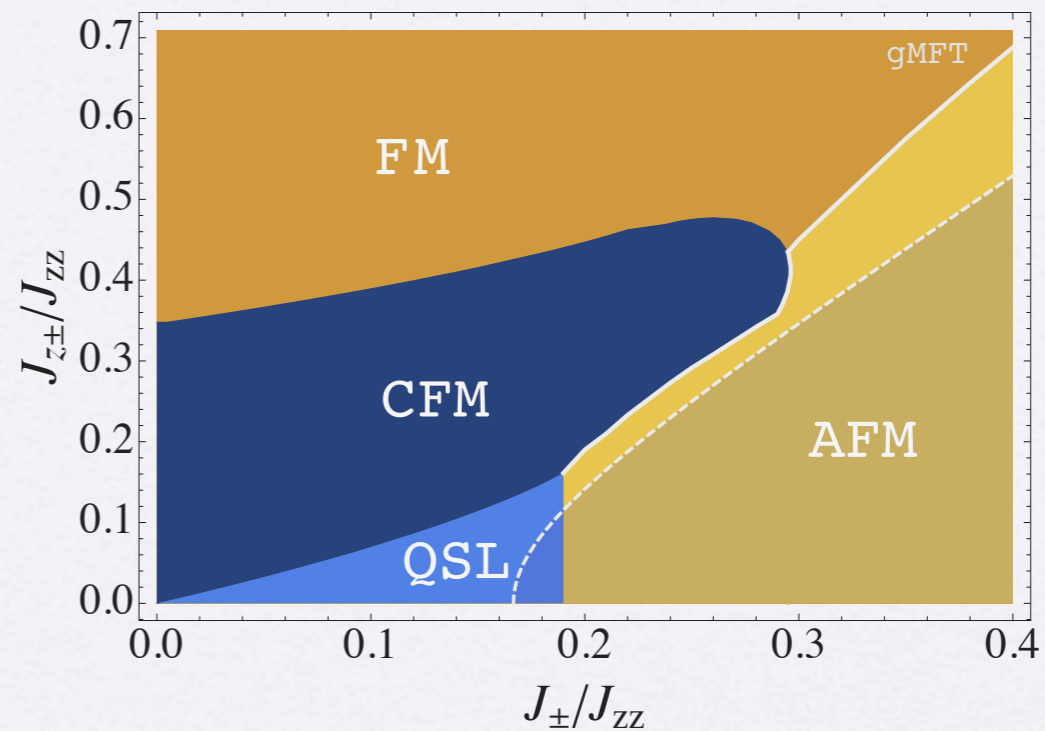
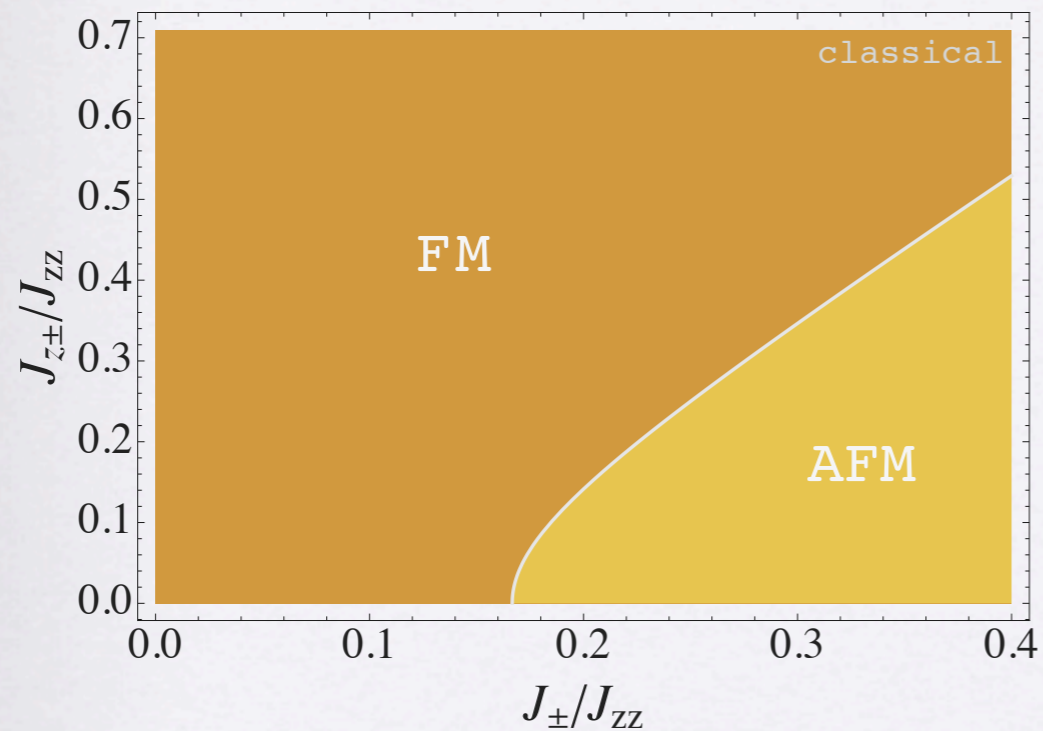
$$H_{\text{3rd Ising}}^{\text{eff}} = -J_{(3)} \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} S_i^z S_j^z$$

$$J_{(3)} = \frac{3J_{z\pm}^2}{J_{zz}}$$

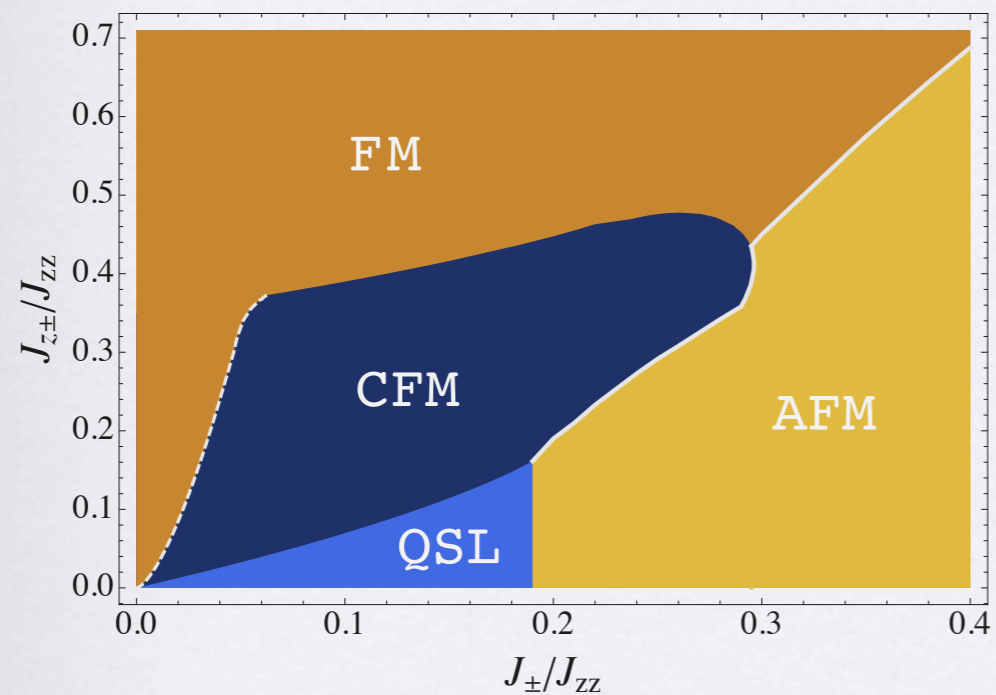




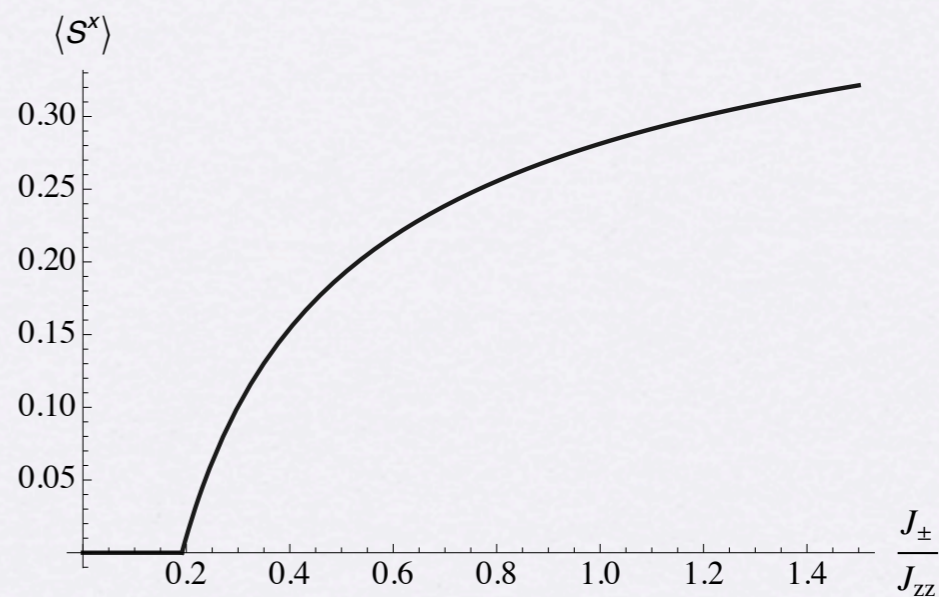
# Other diagrams



corrected gMFT diagram

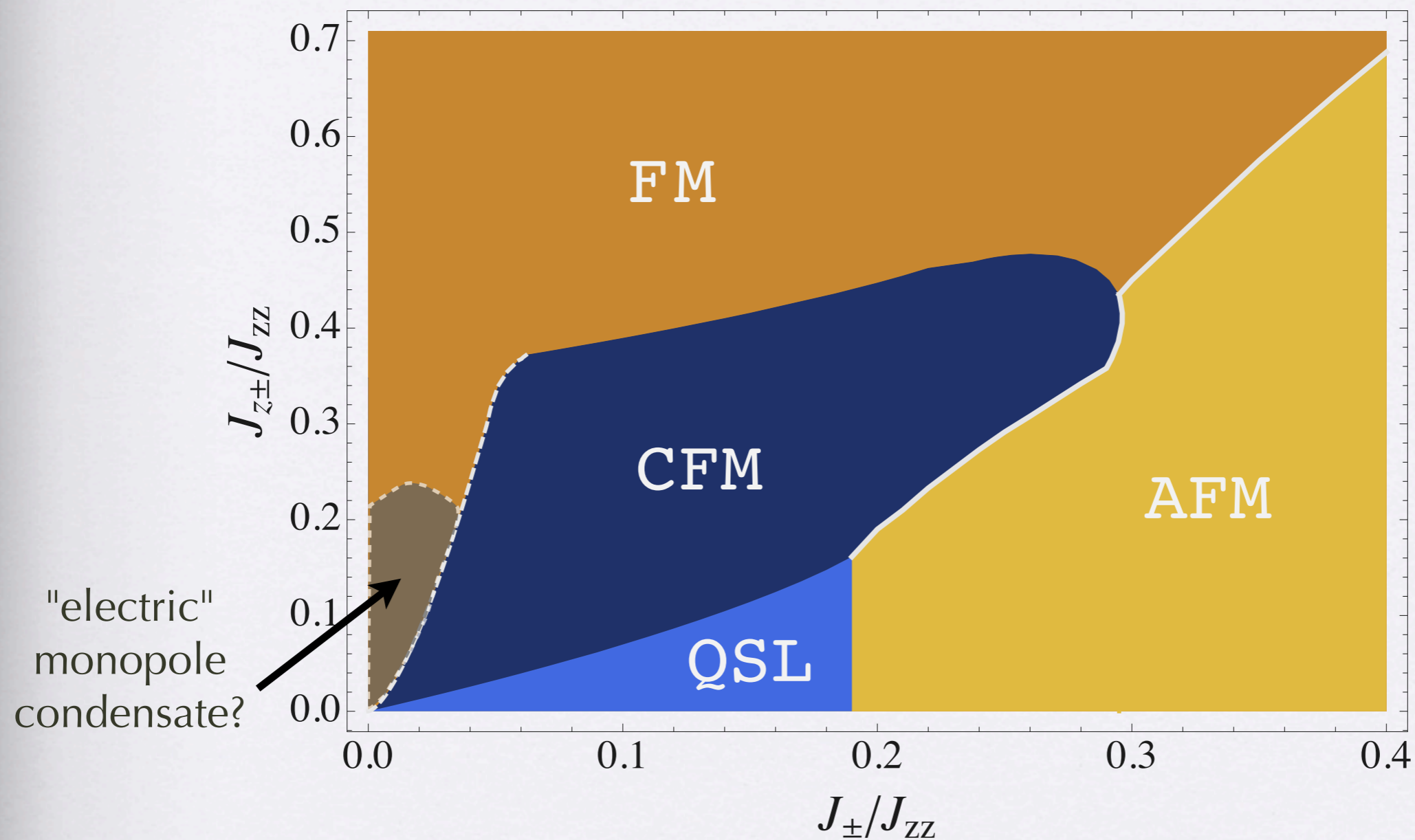


staggered magnetization for  $J_{z\pm} = 0$



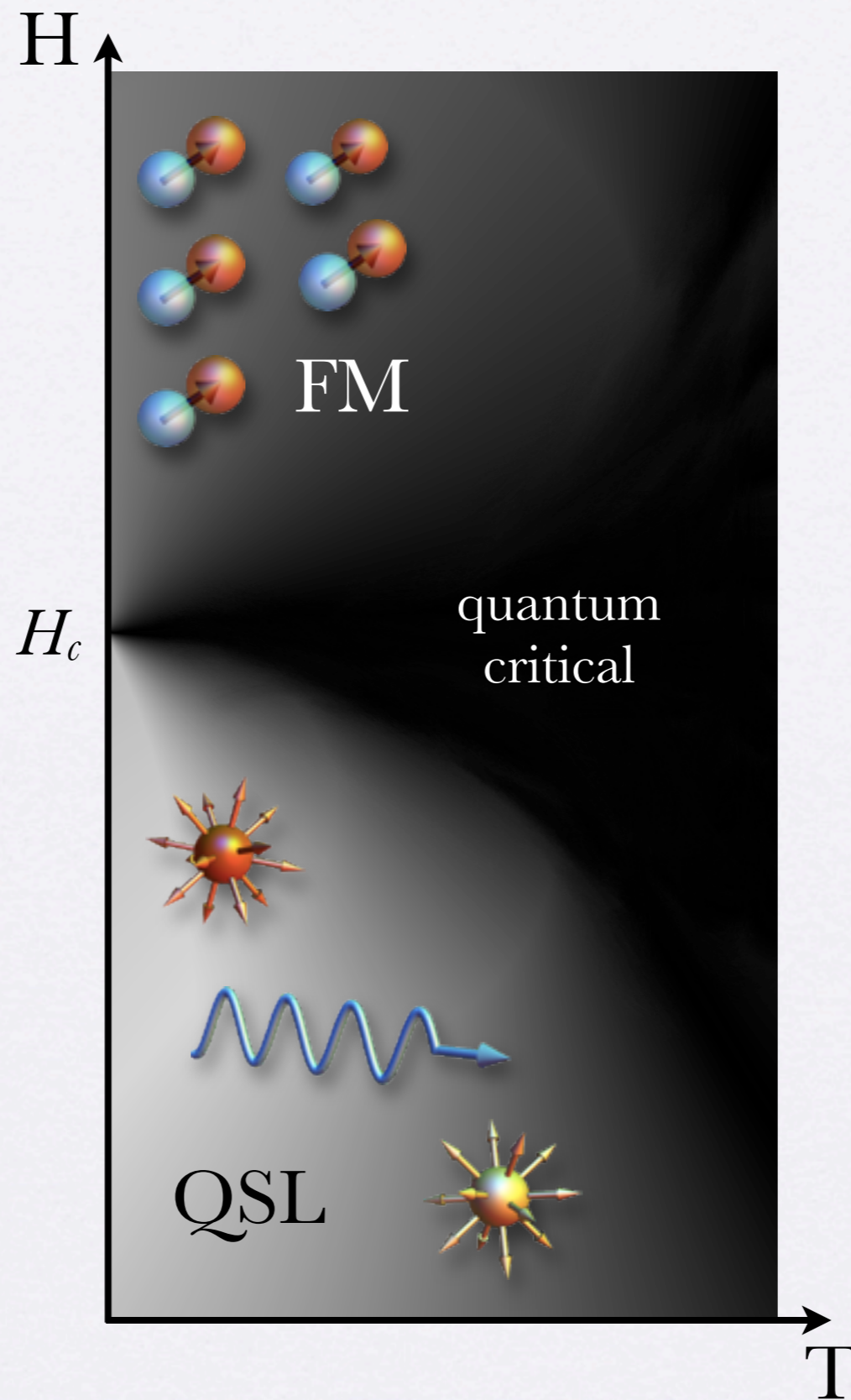


# "Electric" monopole condensate?



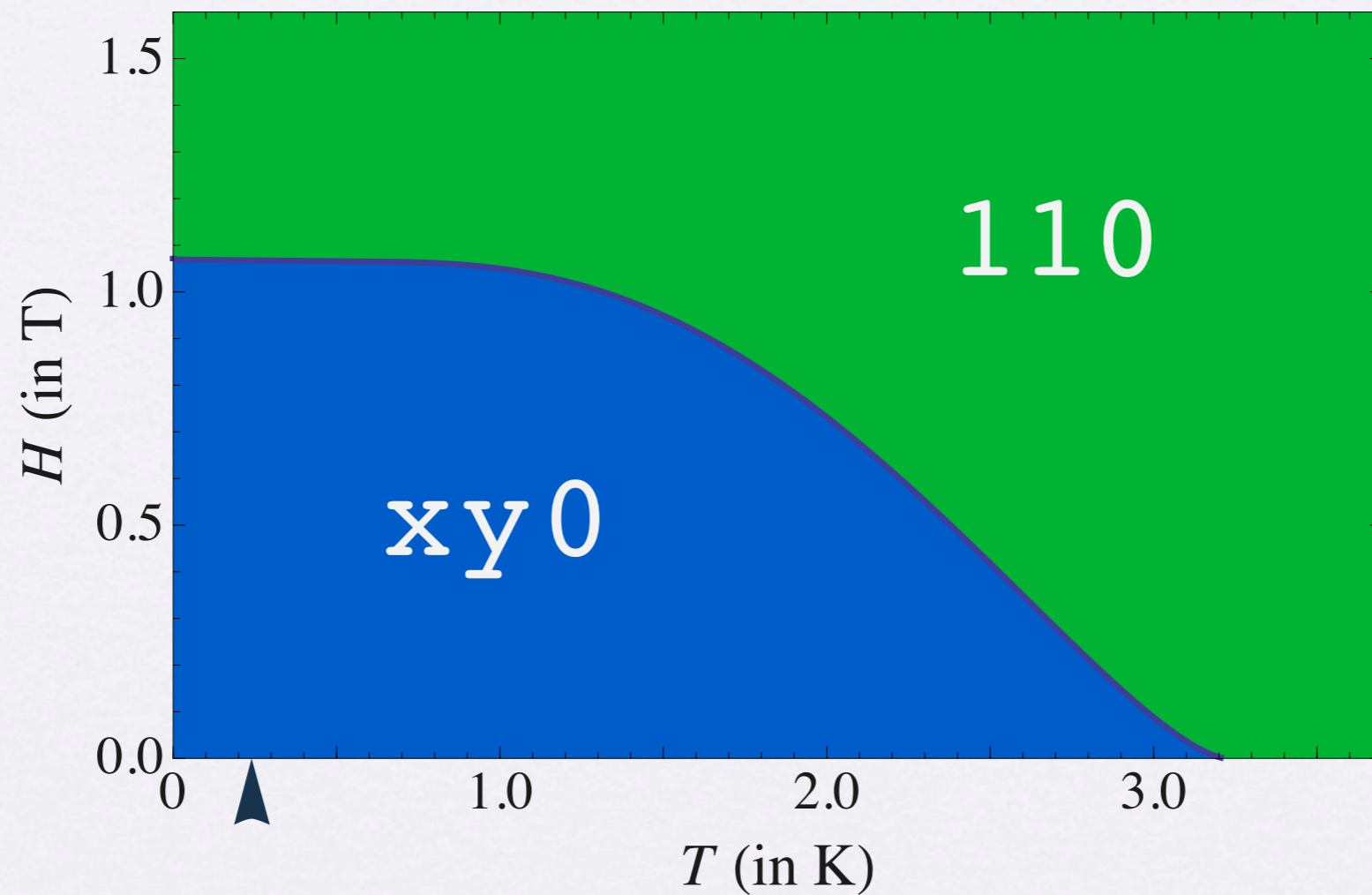


# Field





# Classical $T$ - $H$ MFT diagram for $\text{Yb}_2\text{Ti}_2\text{O}_7$





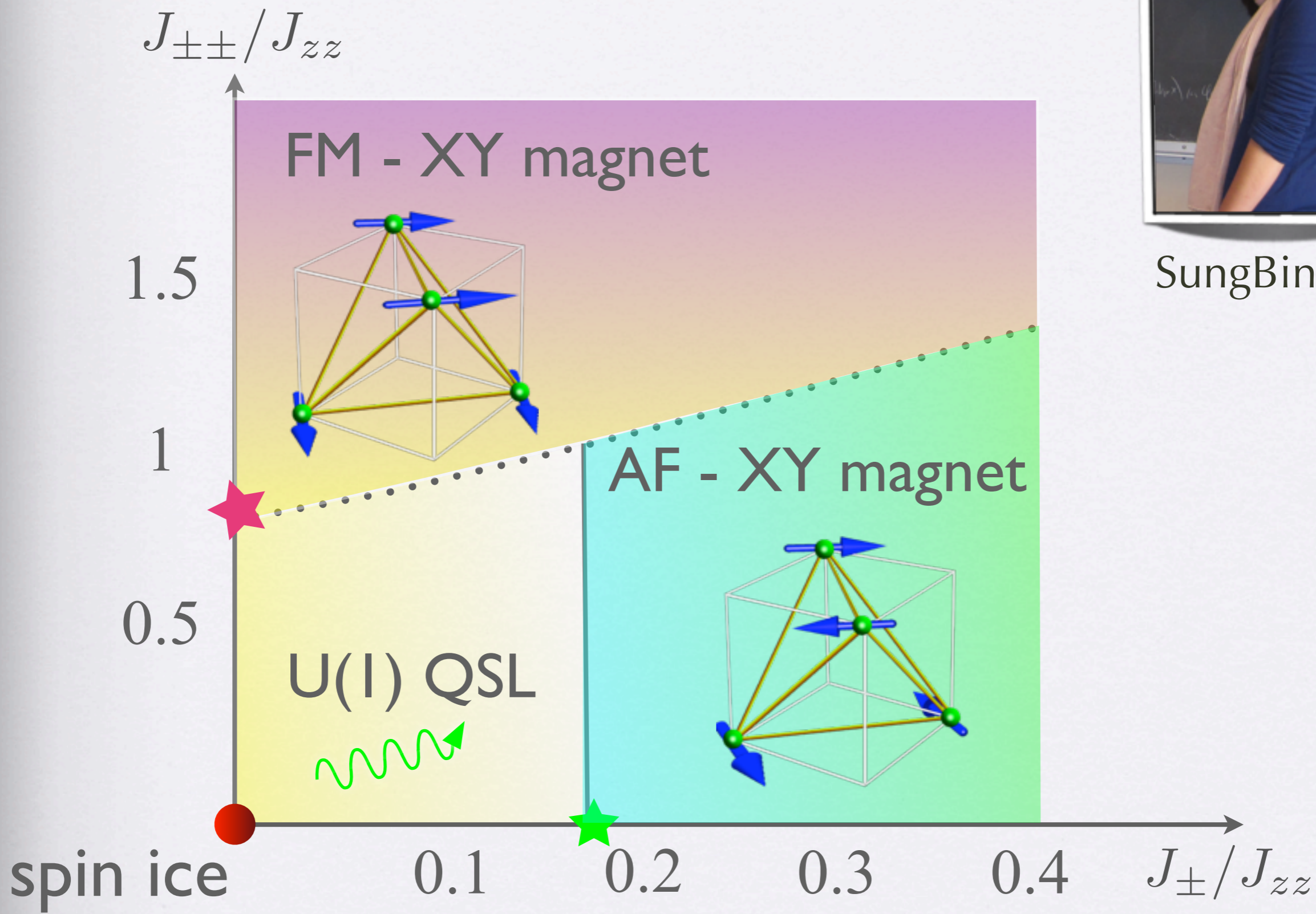
# Rare-earth pyrochlores

Possible A-site elements  
and B site elements

												1 H 1.008											18/VIII 2 He 4.003
														13/III	14/IV	15/V	16/VI	17/VII	18/VIII				
2	3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18					
3	11 Na 22.99	12 Mg 24.30											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95					
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80					
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc 98.91	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3					
6	55 Cs 132.9	56 Ba 137.3	La-Lu	72 Hf 178.5	73 Ta 180.9	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po 210.0	85 At 210.0	86 Rn 222.0					
7	87 Fr 223.0	88 Ra 226.0	Ac-Lr	104 Unq	105 Unp	106 Unh	107 Uns	108 Uno	109 Une	.....													
s block		d block										p block											
		Lanthanides										f block											
		Actinides										f block											
		57 La 138.9	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm 144.9	62 Sm 150.4	63 Eu 152.0	64 Gd 157.2	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0							
		89 Ac 227.0	90 Th 232.0	91 Pa 231.0	92 U 238.0	93 Np 237.0	94 Pu 239.1	95 Am 243.1	96 Cm 247.1	97 Bk 247.1	98 Cf 252.1	99 Es 252.1	100 Fm 257.1	101 Md 256.1	102 No 259.1	103 Lr 260.1							



$$J_{\pm\pm}$$



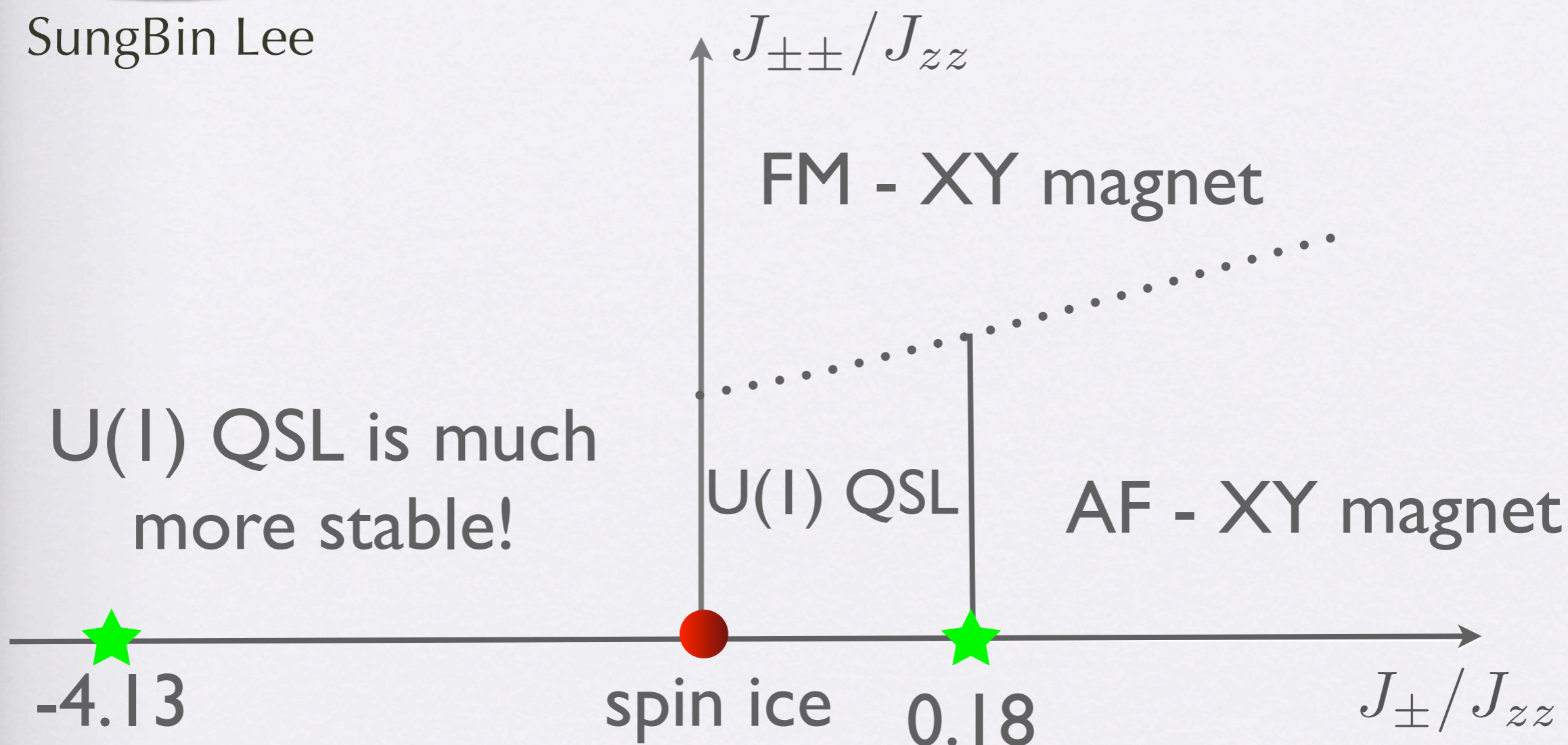
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$$J_{\pm} < 0$$



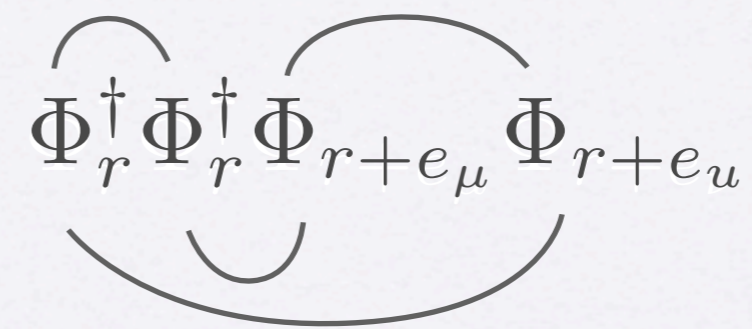


# From U(1) QSL to ???



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quartic spinon hopping



(Q) Which one is energetically favored ?

	$\langle \langle \Phi_r \rangle \rangle$	$\langle \langle \Phi_r \Phi_{r'} \rangle \rangle$	$\langle \langle \Phi_{r_A}^\dagger \Phi_{r_B} \rangle \rangle$	characteristics
XY magnet	$\neq 0$	$\neq 0$	$\neq 0$	ordering on XY
$Z_2$	0	$\neq 0$	0	no ordering gapped excitation
U(1)-XY*	0	0	$\neq 0$	ordering on XY gapless photon
$Z_2$ -XY*	0	$\neq 0$	$\neq 0$	ordering on XY gapped excitation