Title: Theory of Spin Liquids in Integer Spin Pyrochlores

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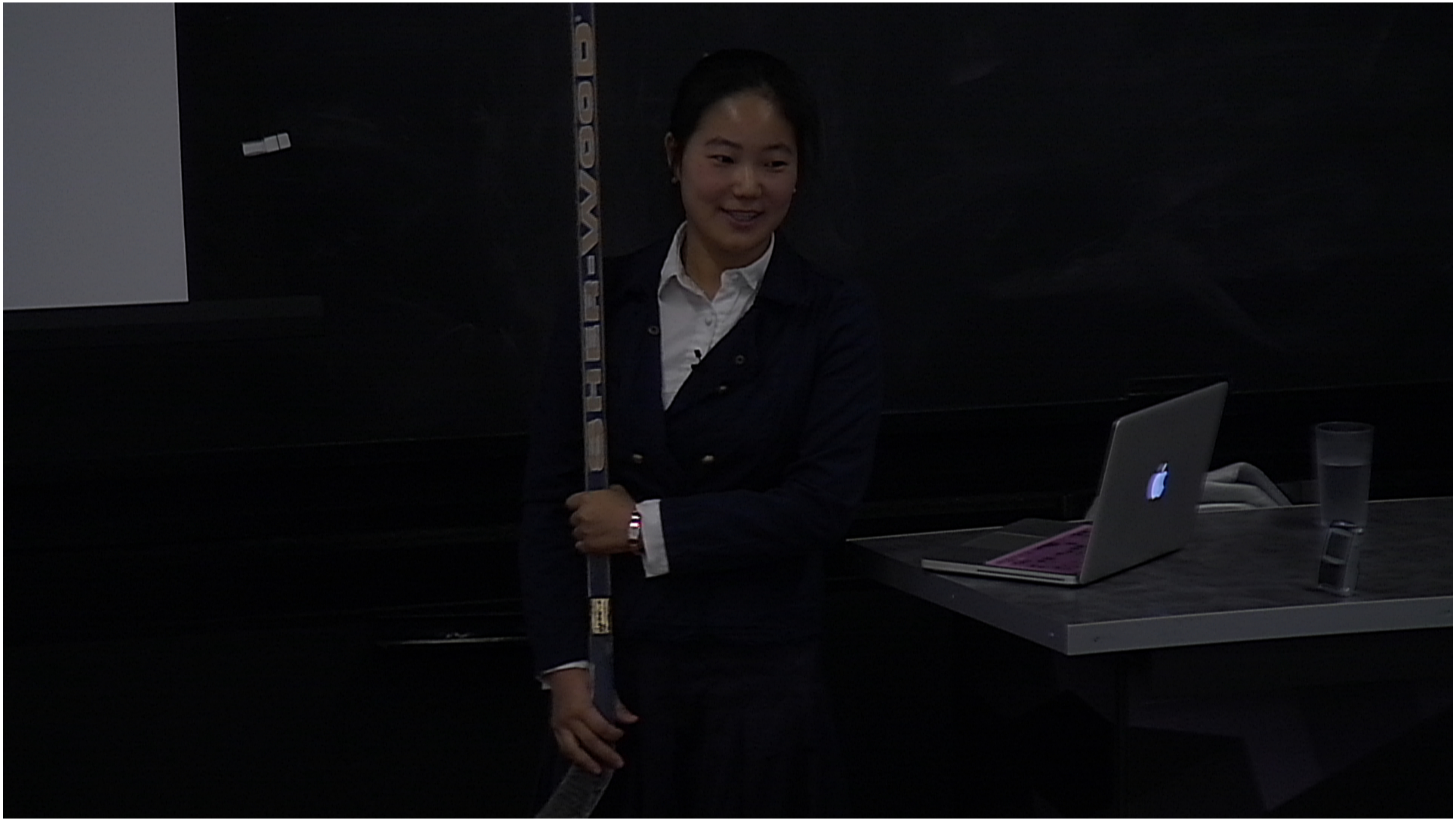
Abstract: Rare earth pyrochlores, with a chemical formula A2B2O7, exhibit many interesting features in A site spin system. Depending on A site rare earth elements, spin ice and magnetically ordered phases are shown in several experiments. Moreover, they have been also focused as possible candidates of U(1) spin liquid. In order to explore such versatile phases, we study the pseudospin-1/2 model, which is quite generic to describe rare earth pyrochlores with integer spins, in the presence of spin-orbit coupling and crystalline electric field. Using a new "gauge mean field theory", we show the possible ground states, corresponding to several phases listed above.


SHER-WOOD

Collaborators

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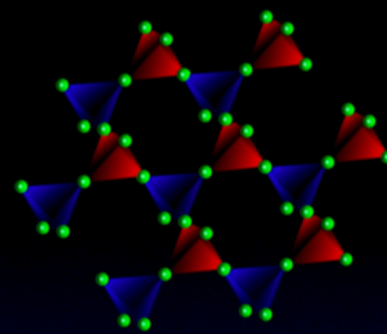
Shigeki Onoda RIKEN, Japan

Leon Balents KITP, UC Santa Barbara

OUTLINE



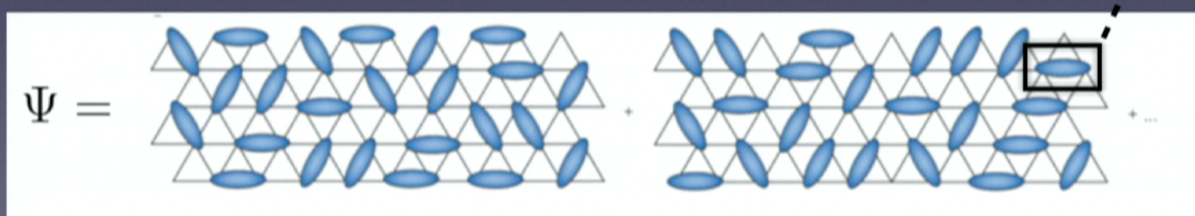
- Motivation
- Pseudospin -1/2 model for rare earth pyrochlores
- Classical limit : spin ice
- Quantum effect : U(1) QSL, magnetic orderings
- Phase diagram using "gauge mean field theory"
- Future work

Quantum Spin Liquids

- interacting local moments without developing any long range order at T=0 due to quantum fluctuations
- long range entanglement

ex) Resonating valence bond : singlet pairs

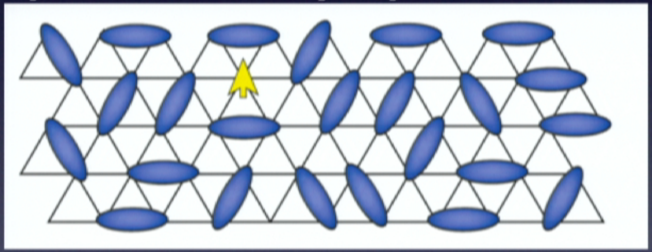
singlets



Why interesting ?

- Emergent gauge structure that supports exotic excitations with fractional quantum numbers

spinons carry spin 1/2

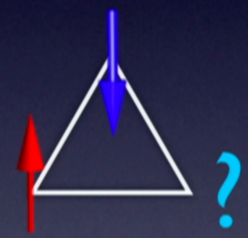


Where do we look for QSLs ?

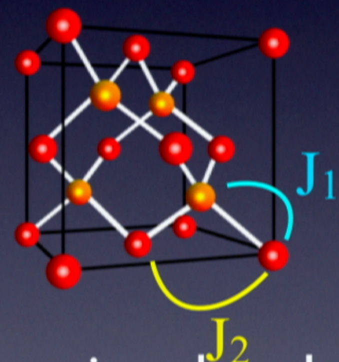
QSLs and Frustration

frustration ? competing interactions cannot be simultaneously minimized

geometrically frustrated

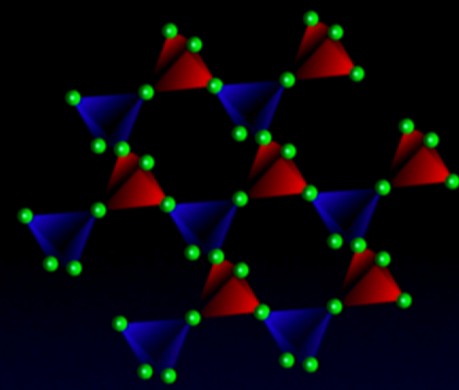


frustrated by further neighbor interaction



- frustration suppresses conventional ordering.
- QSL can be realized when magnetic order is suppressed all the way to zero temperature.

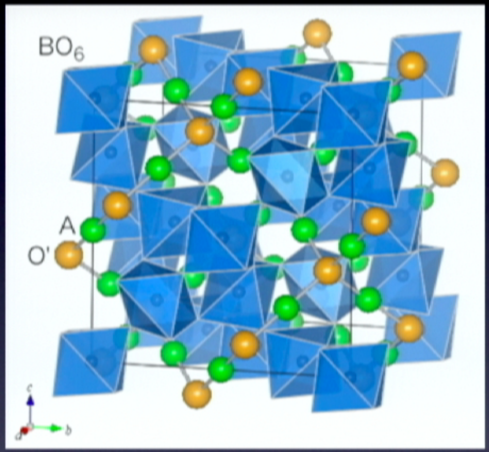
Why pyrochlores?

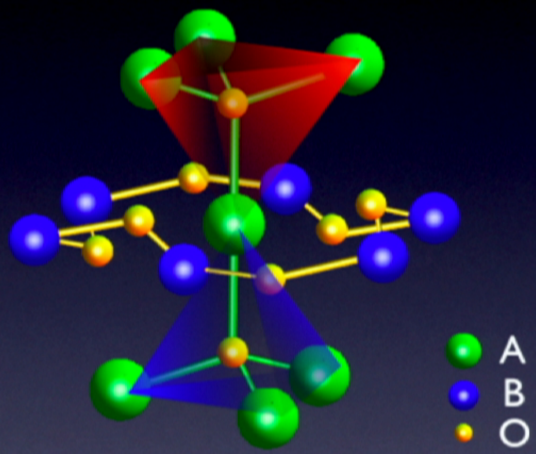


- Most candidates of QSLs are suggested in 2 d lattice (Kagome, triangular) : challenge to find materials
- Several materials exist and actively studied in experiments (spin ice materials)
- Realization of QSL due to geometric frustration

M. Hermele et al (2004)

Rare earth pyrochlores

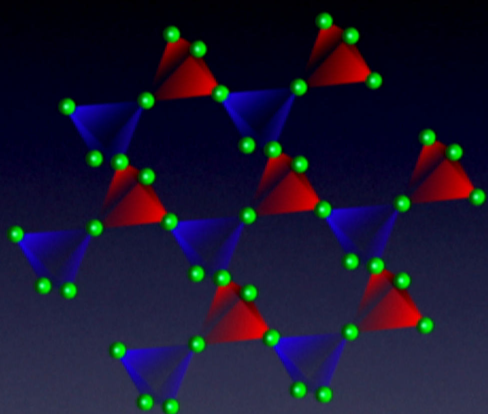




$A_2B_2O_7$

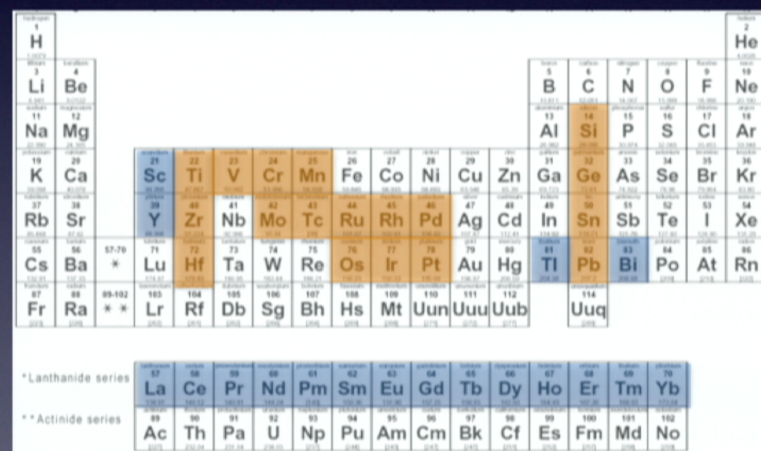
$(A^{3+})_2(B^{4+})_2(O^{2-})_7$

Rare earth pyrochlores



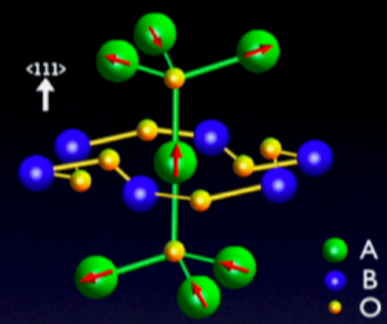
Possible A-site elements

B-site elements



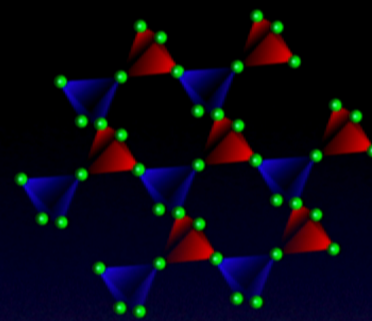
A or B sublattice : pyrochlore lattice

Rare earth pyrochlore materials $A_2B_2O_7$



- $R_2Ti_2O_7$
  - ★ R = Ho, Dy : spin ice
  - ★ R = Yb, Tb : spin liquid ?
  - ★ R = Er : magnetic ordering?
- $Pr_2TM_2O_7$
  - ★ TM = Sn, Zr : spin ice ?
  - ★ TM = Ir : chiral spin liquid?

A site of rare earth pyrochlores



(1) electrons/holes in f orbitals

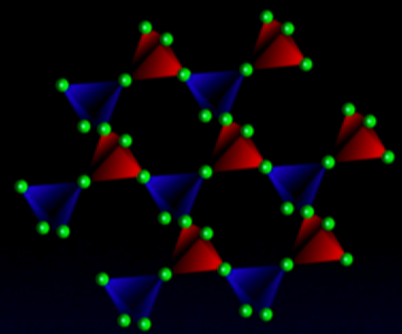
Pr^{3+} $4f^2$
Eu^{3+} $4f^6$ well localized f orbitals
Yb^{3+} $4f^{13}$

(2) rare earth materials : $J = L \pm S$ eigenstates
strong spin-orbit coupling

(3) crystalline electric fields :

→ doublet ground state

OUTLINE



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Hamiltonian

S. Curnoe et al, 2008
S. Onoda et al, 2010

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

classical spin ice

$$-J_{\pm}(S_i^+ S_j^- + S_i^- S_j^+)$$

quantum fluctuations

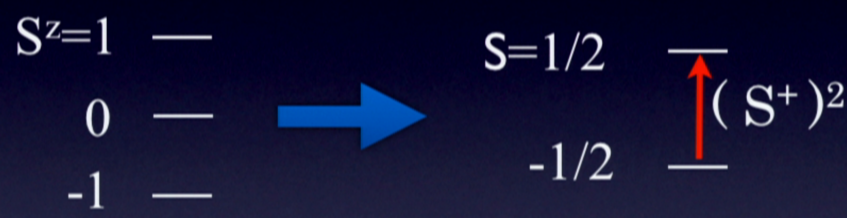
$$+J_{\pm\pm}(S_i^+ S_j^+ \gamma_{ij}^2 + S_i^- S_j^- \gamma_{ij}^{*2})$$

$$+J_{z\pm}(S_i^z(\gamma_{ij} S_j^+ + \gamma_{ij}^* S_j^-) + (i \leftrightarrow j))$$

Non Kramer's doublet

Pseudospin S which describes ground state $S_{eff} = \pm 1/2$

Integer spins only allow even powers of $S^{\pm}$



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

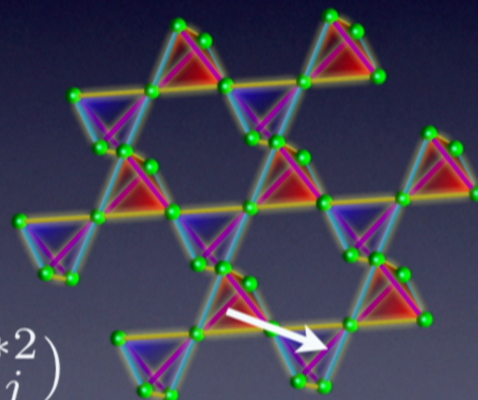
$$+ J_{\pm\pm}(S_i^+ S_j^+ \gamma_{ij}^2 + S_i^- S_j^- \gamma_{ij}^{*2})$$

$$+ J_{z\pm}(S_i^z(\gamma_{ij} S_j^+ + \gamma_{ij}^* S_j^-) + (i \leftrightarrow j))$$

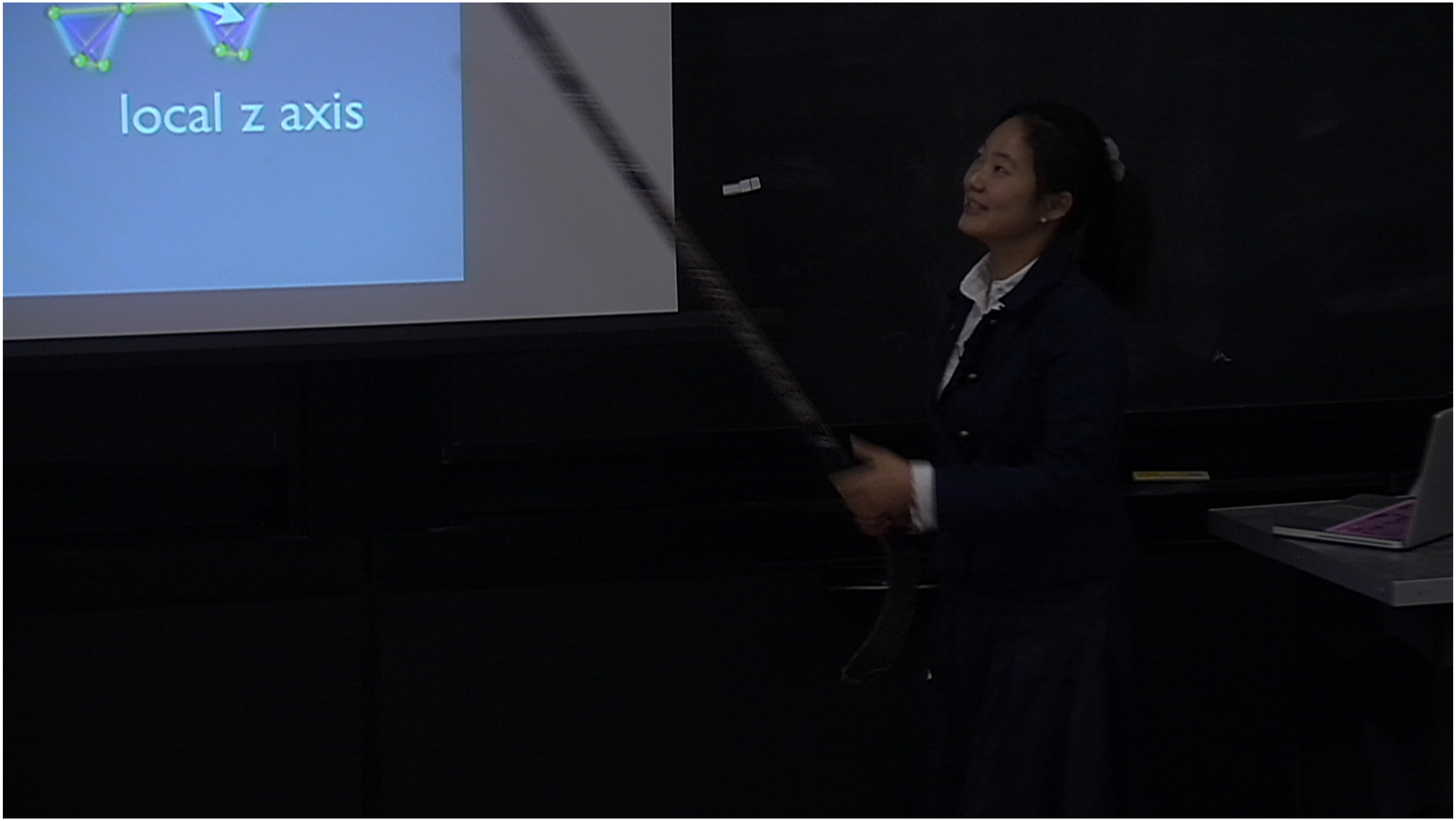
Pseudospin-1/2 model

S. Onoda et al, 2010

$$H = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z$$
$$- J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+)$$
$$+ J_{\pm\pm} (S_i^+ S_j^+ \gamma_{ij}^2 + S_i^- S_j^- \gamma_{ij}^{*2})$$



local z axis


local z axis

Pseudospin-1/2 model

S. Onoda et al, 2010

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classical spin ice

$$- J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+)$$

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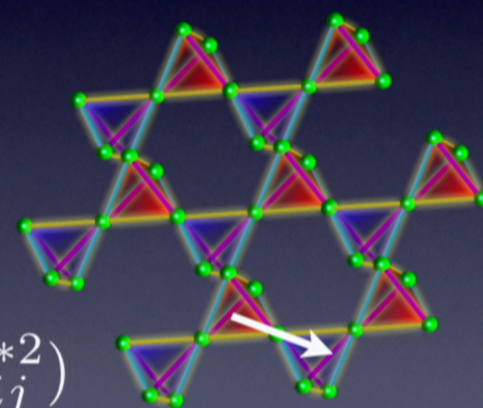
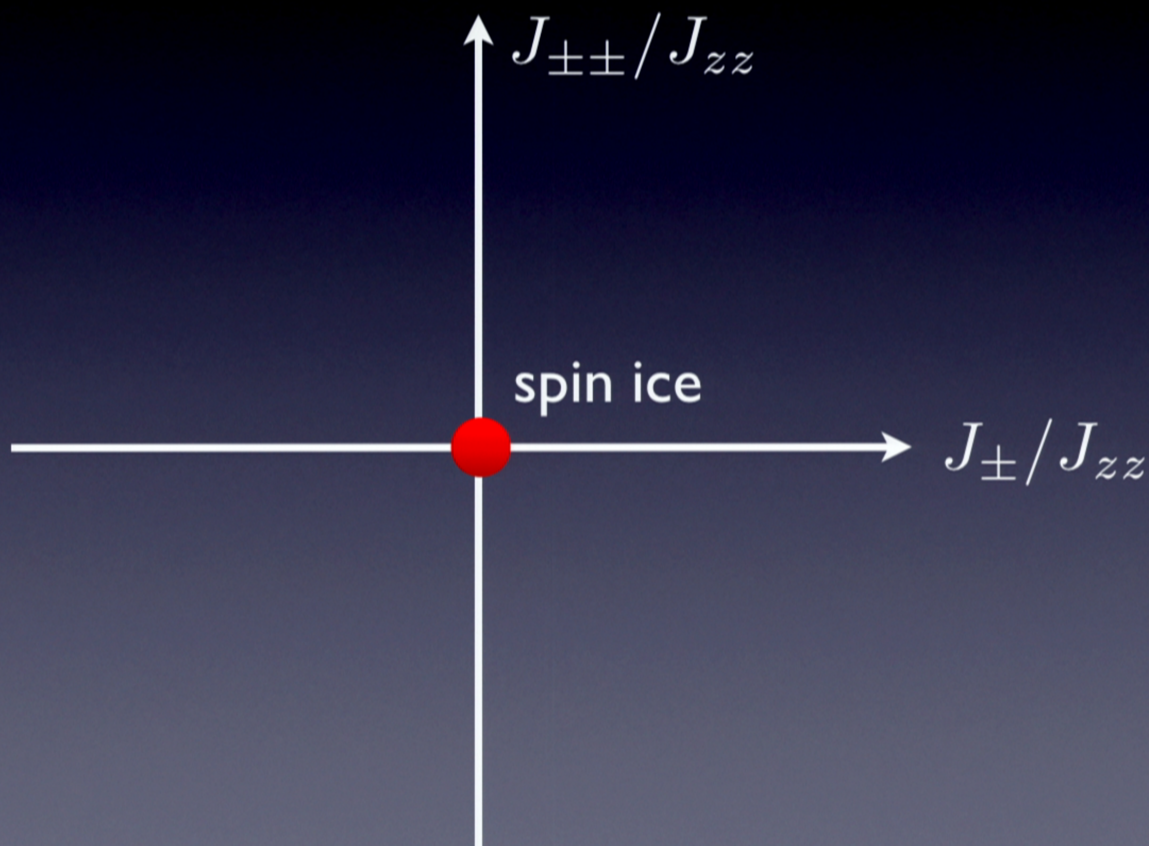


local z axis

T=0 Phase diagram ?

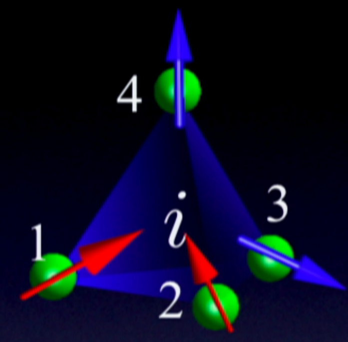


Spin Ice

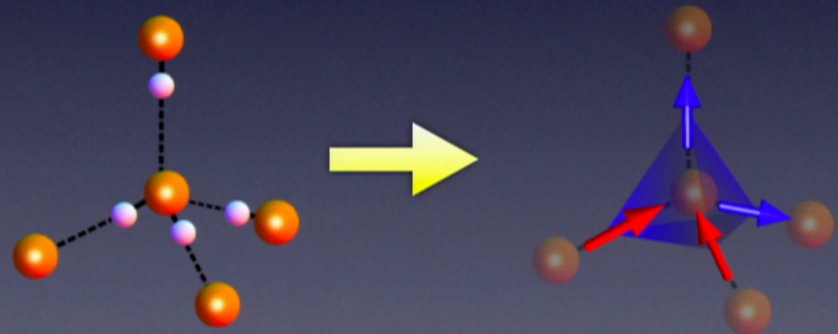
Harris et al, 1997

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

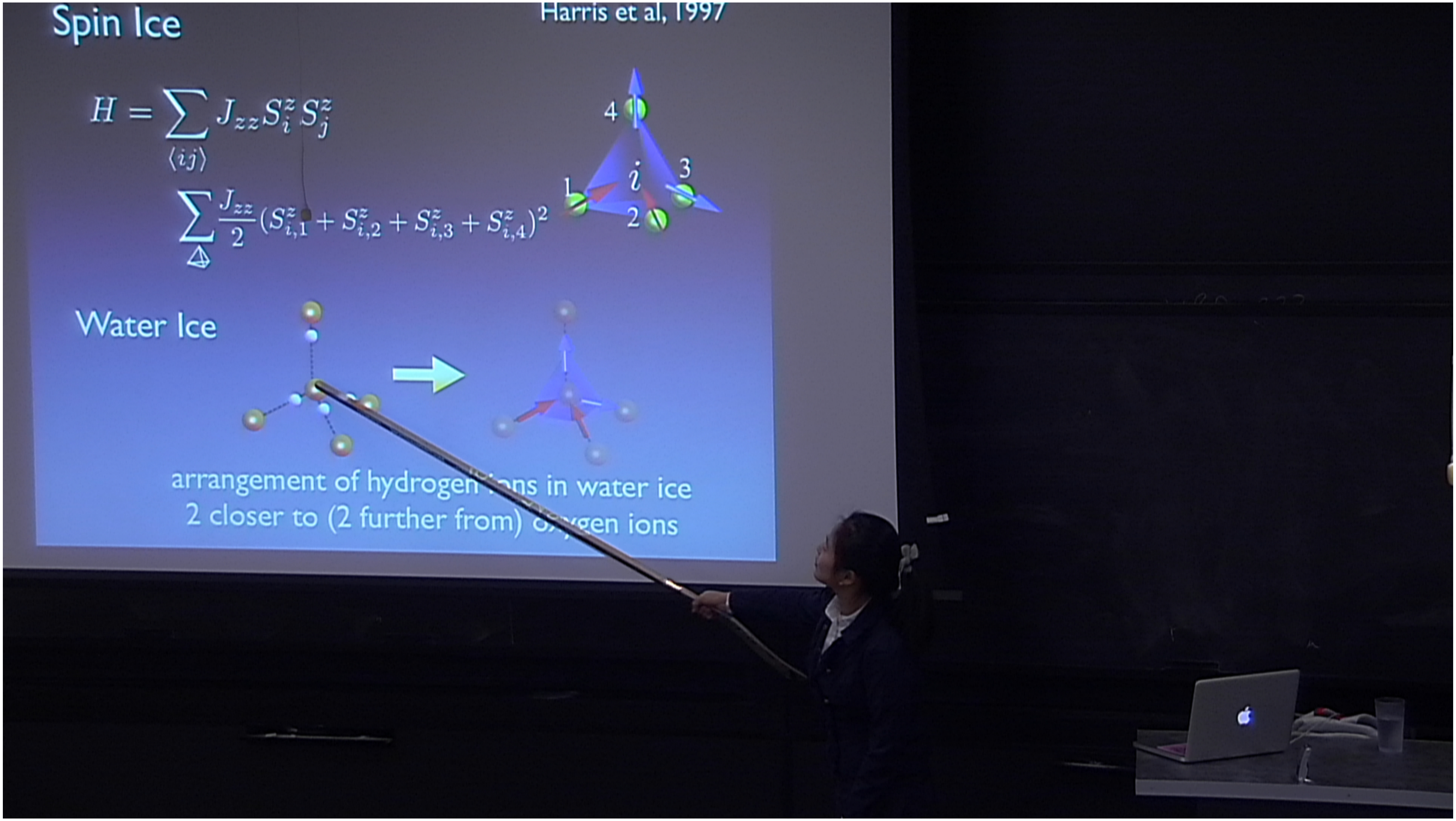
$$\sum_{\triangle} \frac{J_{zz}}{2} (S_{i,1}^z + S_{i,2}^z + S_{i,3}^z + S_{i,4}^z)^2$$



Water Ice



arrangement of hydrogen ions in water ice
2 closer to (2 further from) oxygen ions


Spin Ice
Harris et al, 1997
$H = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z$
$\sum_{\triangle} \frac{J_{zz}}{2} (S_{i,1}^z + S_{i,2}^z + S_{i,3}^z + S_{i,4}^z)^2$
4
3
1
2
i
Water Ice
arrangement of hydrogen ions in water ice
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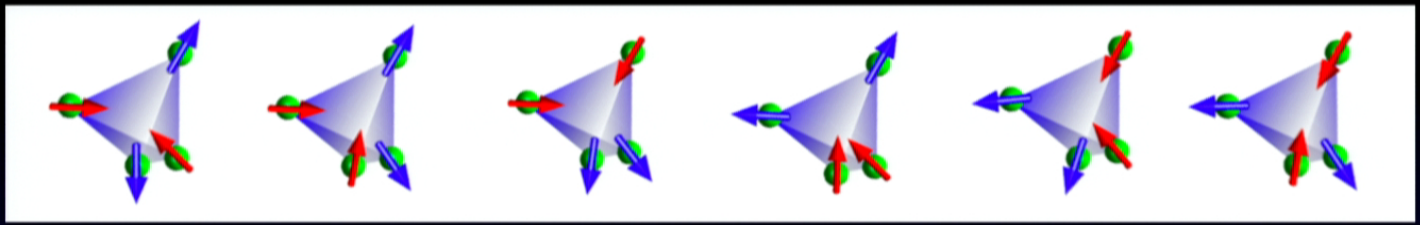
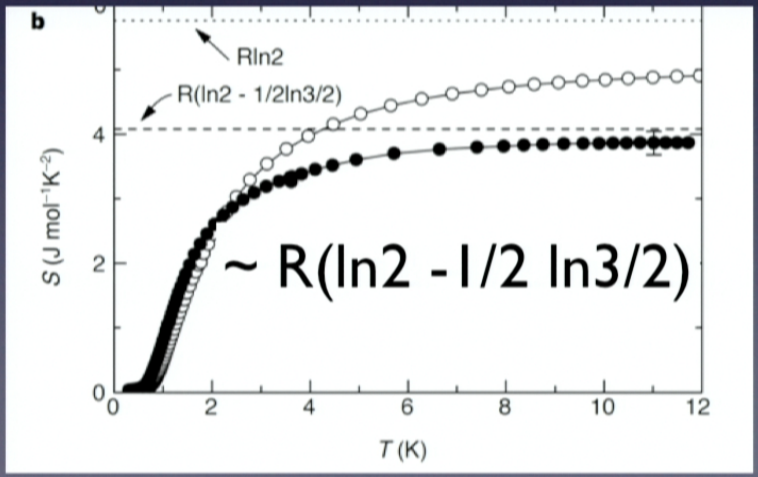
Spin Ice



local constraint : "2-in 2-out" ground state
highly degenerate !



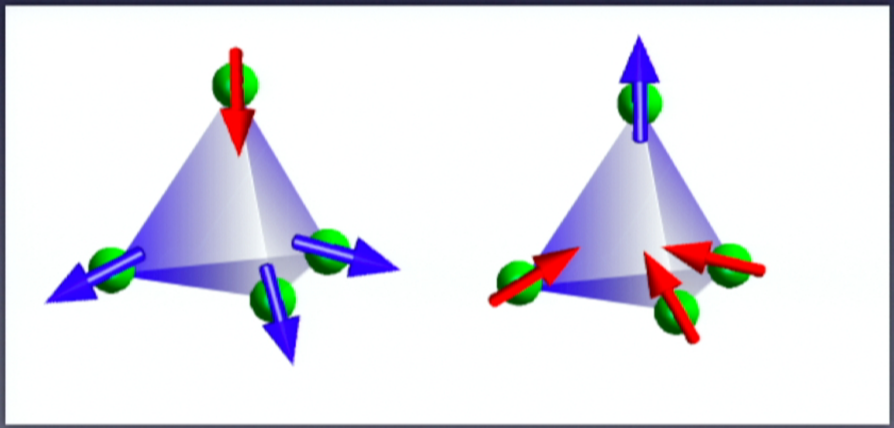
zero point entropy observed in spin ice material $Dy_2Ti_2O_7$

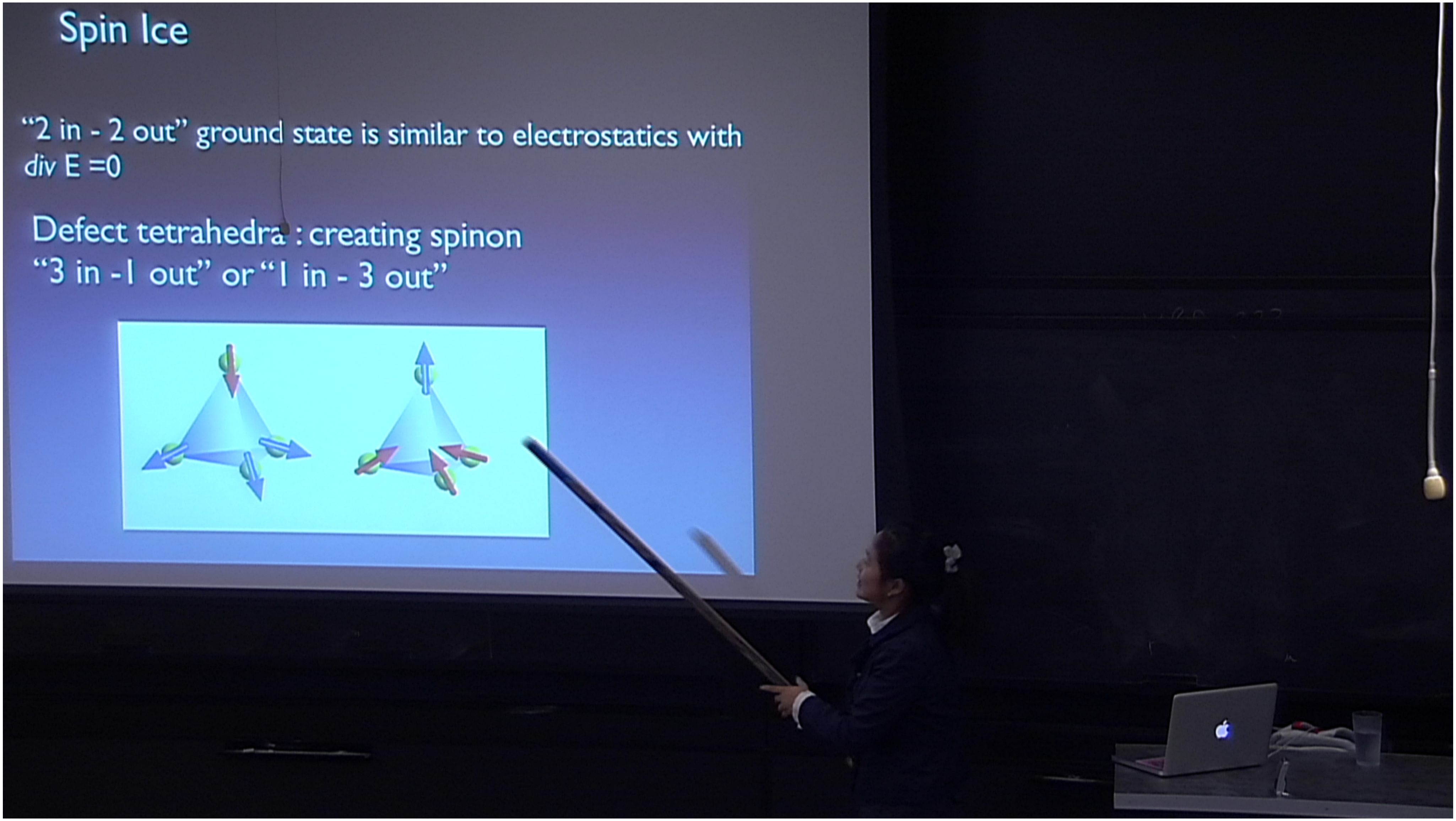
A.P. Ramirez et al, 1999

Spin Ice

"2 in - 2 out" ground state is similar to electrostatics with *div* E =0

Defect tetrahedra : creating spinon
"3 in -1 out" or "1 in - 3 out"




Spin Ice
"2 in - 2 out" ground state is similar to electrostatics with
div E =0
Defect tetrahedra : creating spinon
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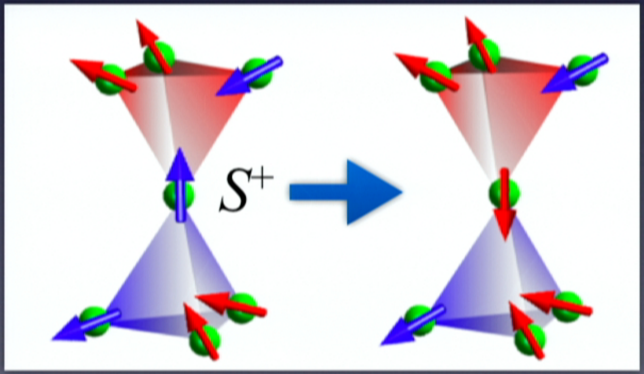
Quantum effects on spin ice ?

$$H = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z$$
$$-J_{\pm}(S_i^+ S_j^- + S_i^- S_j^+)$$
$$+J_{\pm\pm}(S_i^+ S_j^+ \gamma_{ij}^2 + S_i^- S_j^- \gamma_{ij}^{*2})$$

quantum fluctuations

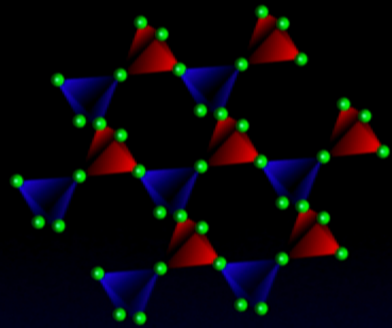
spinon defects



"2 in - 2 out"

"3 in -1 out" / "1 in - 3 out"

OUTLINE



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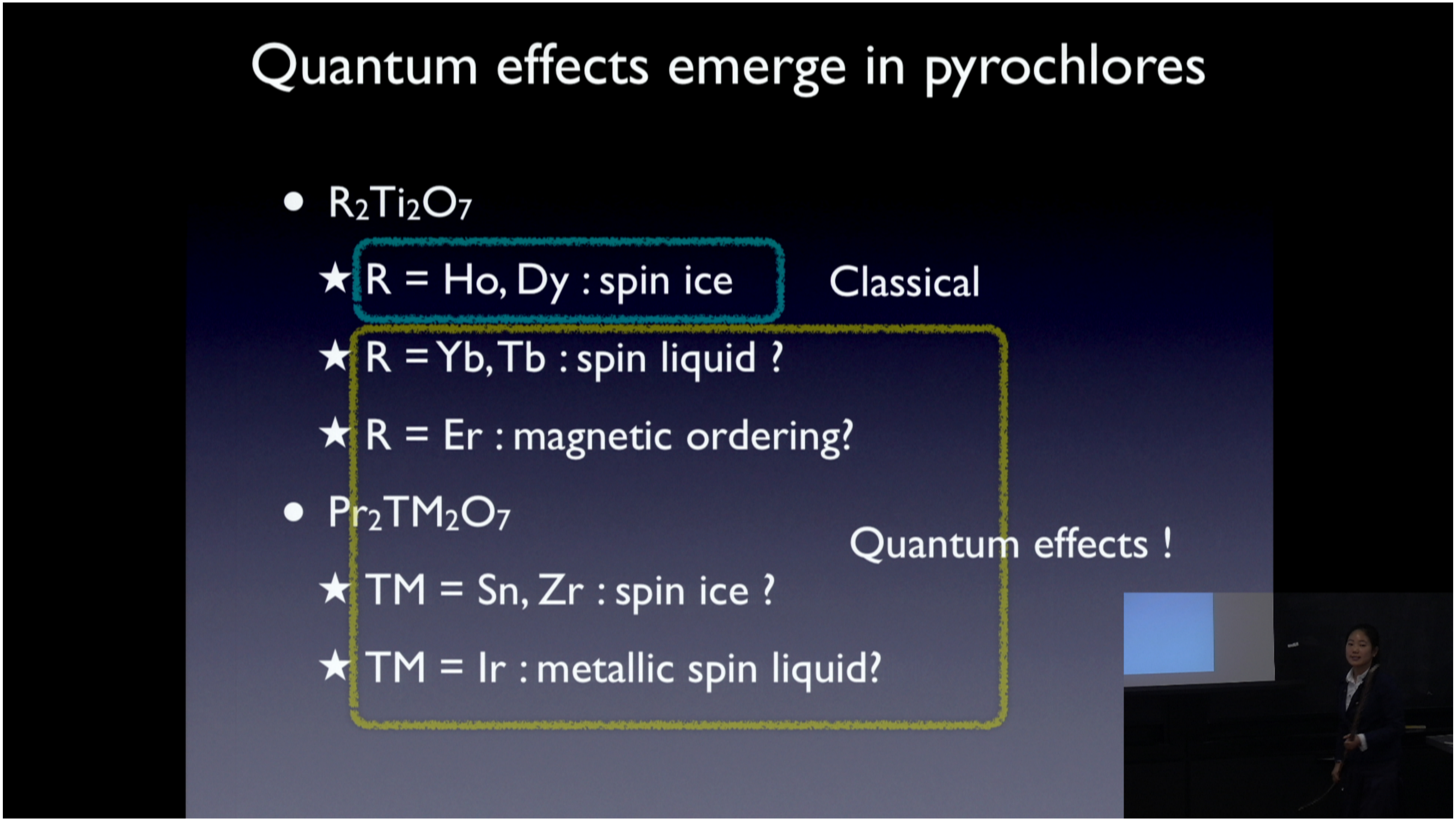
Quantum effects emerge in pyrochlores

- $R_2Ti_2O_7$
  - ★ R = Ho, Dy : spin ice — Classical
  - ★ R = Yb, Tb : spin liquid ?
  - ★ R = Er : magnetic ordering?
- $Pr_2TM_2O_7$
  - ★ TM = Sn, Zr : spin ice ?
  - ★ TM = Ir : metallic spin liquid?

Quantum effects !


Quantum effects emerge in pyrochlores
• $R_2Ti_2O_7$
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Classical
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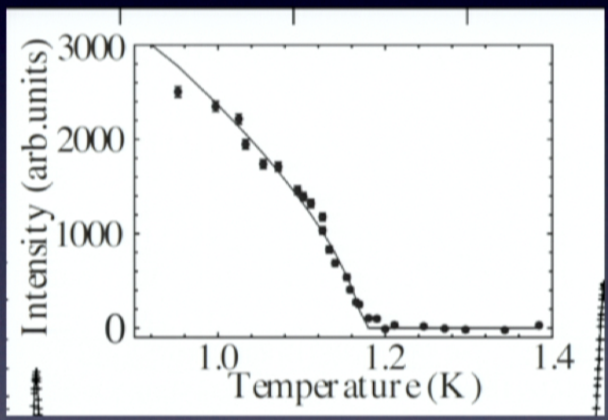
★ R = Er : magnetic ordering?
• $Pr_2TM_2O_7$
Quantum effects !
★ TM = Sn, Zr : spin ice ?
★ TM = Ir : metallic spin liquid?

$Er_2Ti_2O_7$: XY magnet

single crystal Bragg intensity



$$\vec{\mu} = g \cdot \vec{S}$$
$$\mu_z = g_z S^z$$
$$\mu_x = g_x S^x$$

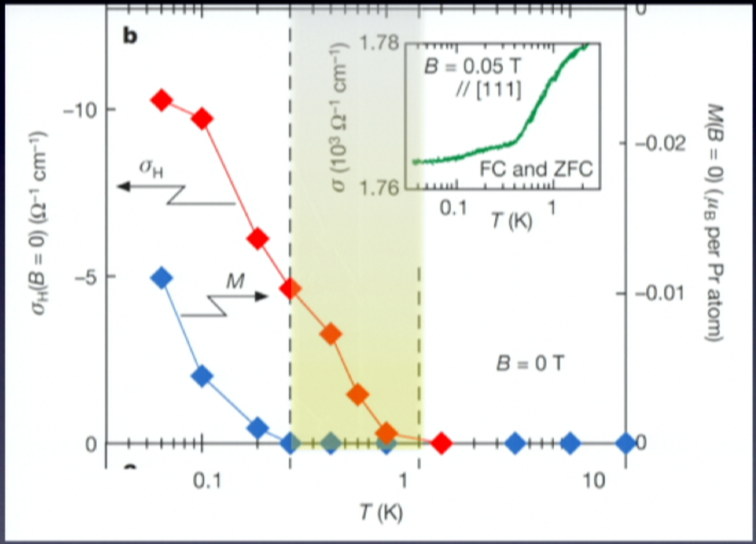
$$g_z << g_x$$

Below 1.2K, magnetic ordering on XY plane

J.D.M Champion et al (2003)
A. Poole et al (2007)

$Pr_2Ir_2O_7$: chiral spin lquid ?

Y. Machida et al (2010)

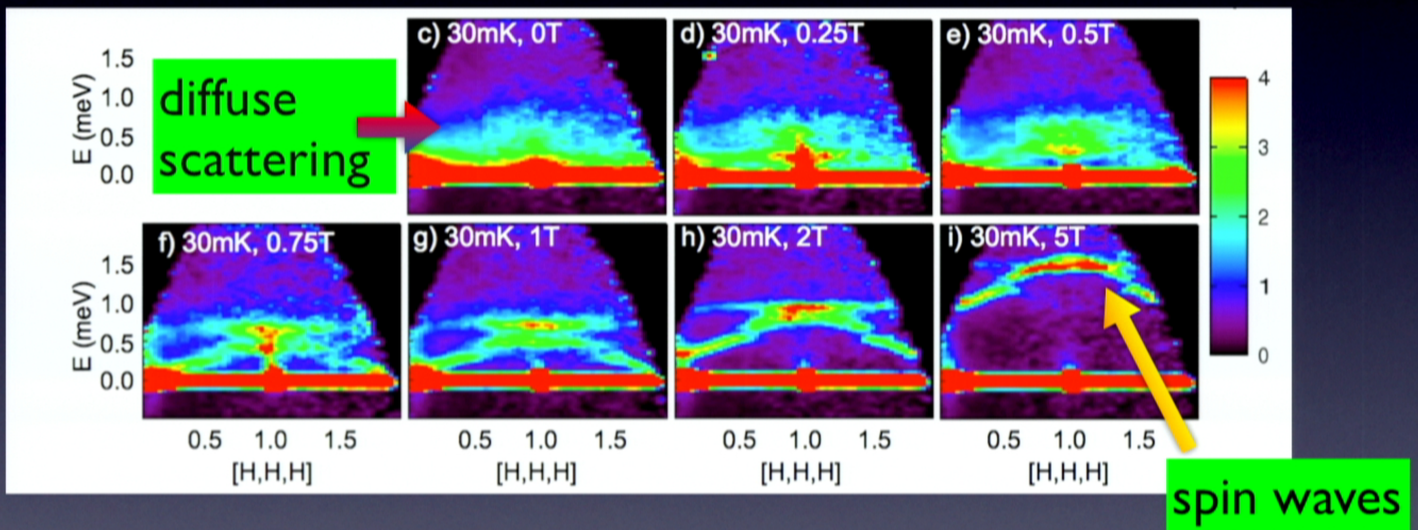


spontaneous TRS breaking

magnetic ordering at $T < 0.3$ K

$Yb_2Ti_2O_7$: quantum spin liquid?

K.A. Ross et al (2009)



Spin waves emerge for B > 0.5T,
but disappear in a low field

Quantum spin liquid state at a low field?

Quantum effects emerge in pyrochlores

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How can we understand quantum effects?

Pseudospin-1/2 model

S. Onoda et al, 2010

classical spin ice

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

$$-J_{\pm}(S_i^+ S_j^- + S_i^- S_j^+)$$

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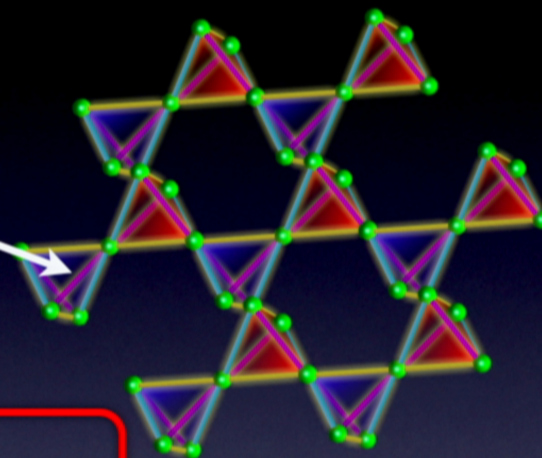
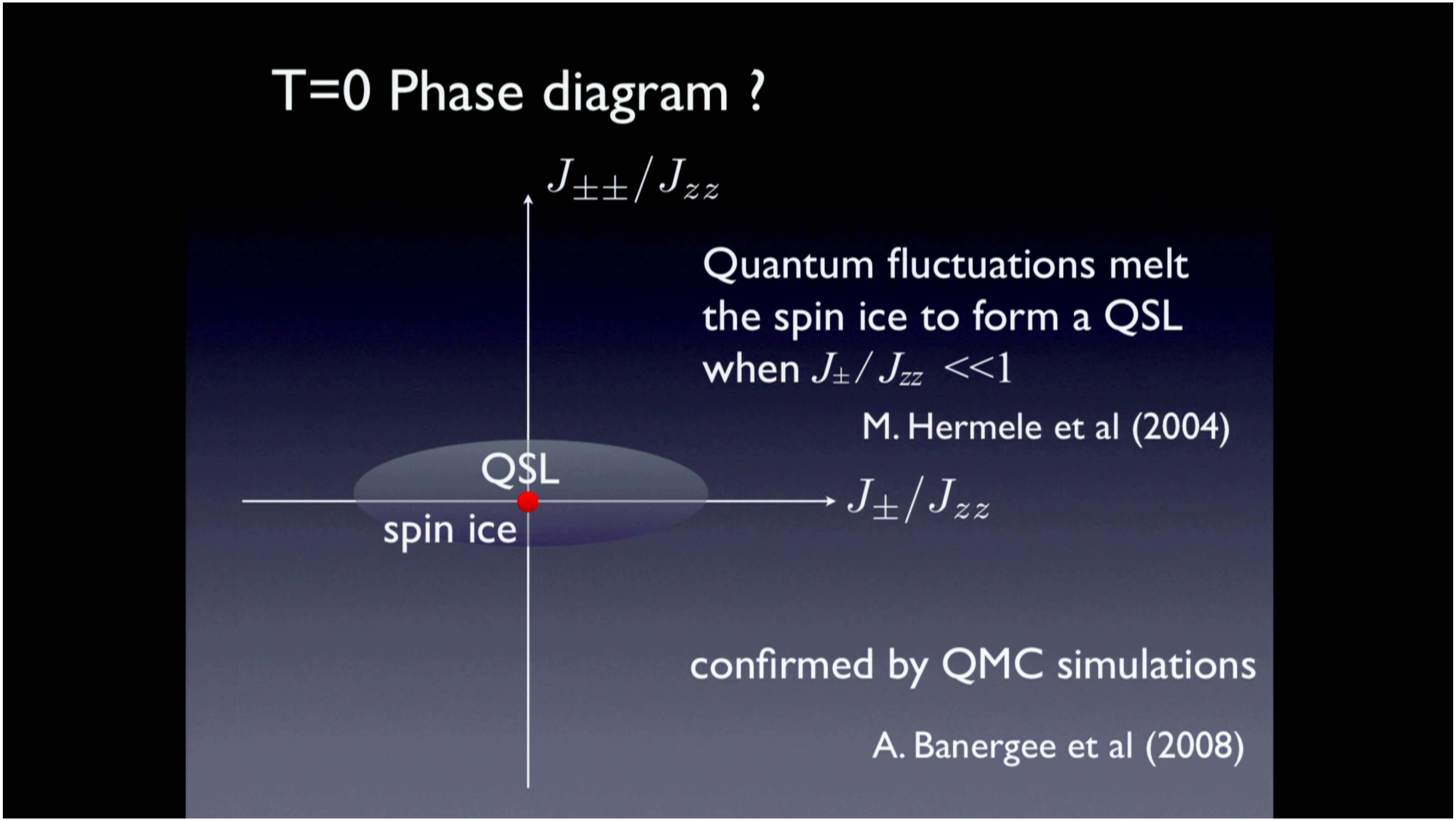


quantum effect



T=0 Phase diagram ?
$J_{\pm\pm}/J_{zz}$
Quantum fluctuations melt the spin ice to form a QSL when $J_{\pm}/J_{zz} <<1$
M. Hermele et al (2004)
QSL
$J_{\pm}/J_{zz}$
spin ice
confirmed by QMC simulations
A. Banergee et al (2008)

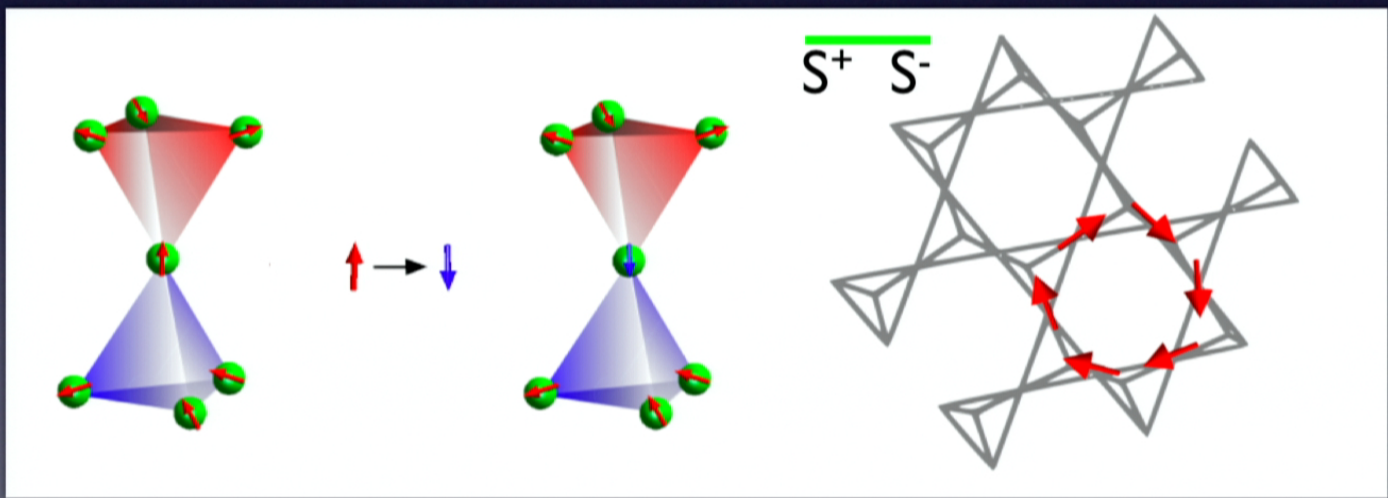
U(1) QSL

M. Hermele et al (2004)

spin fluctuations of "2-in 2-out" state induces ring exchange : described by a U(1) gauge theory

spin ice state "2-in 2-out'

3rd order of DPT of $J_{\pm}$ ring exchange



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M. Hermele et al (2004)

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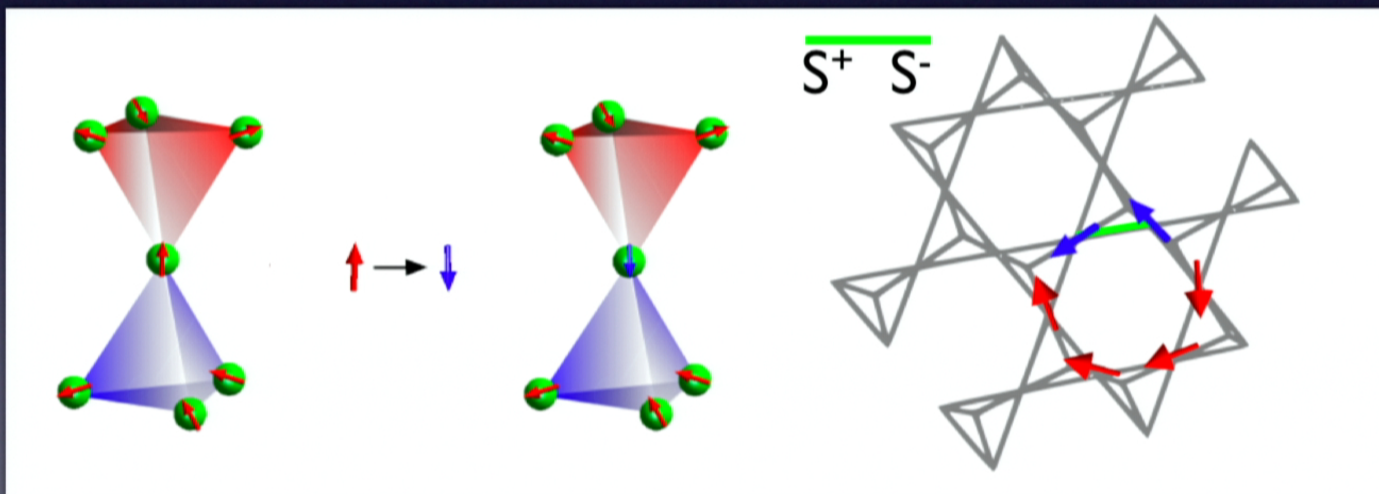


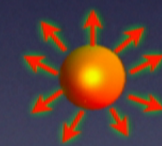
Excitations

M. Hermele et al (2004)

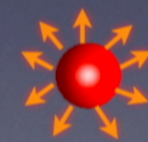
Spin Ice : emergent electrostatics *div* E=0

- a gapped spinon

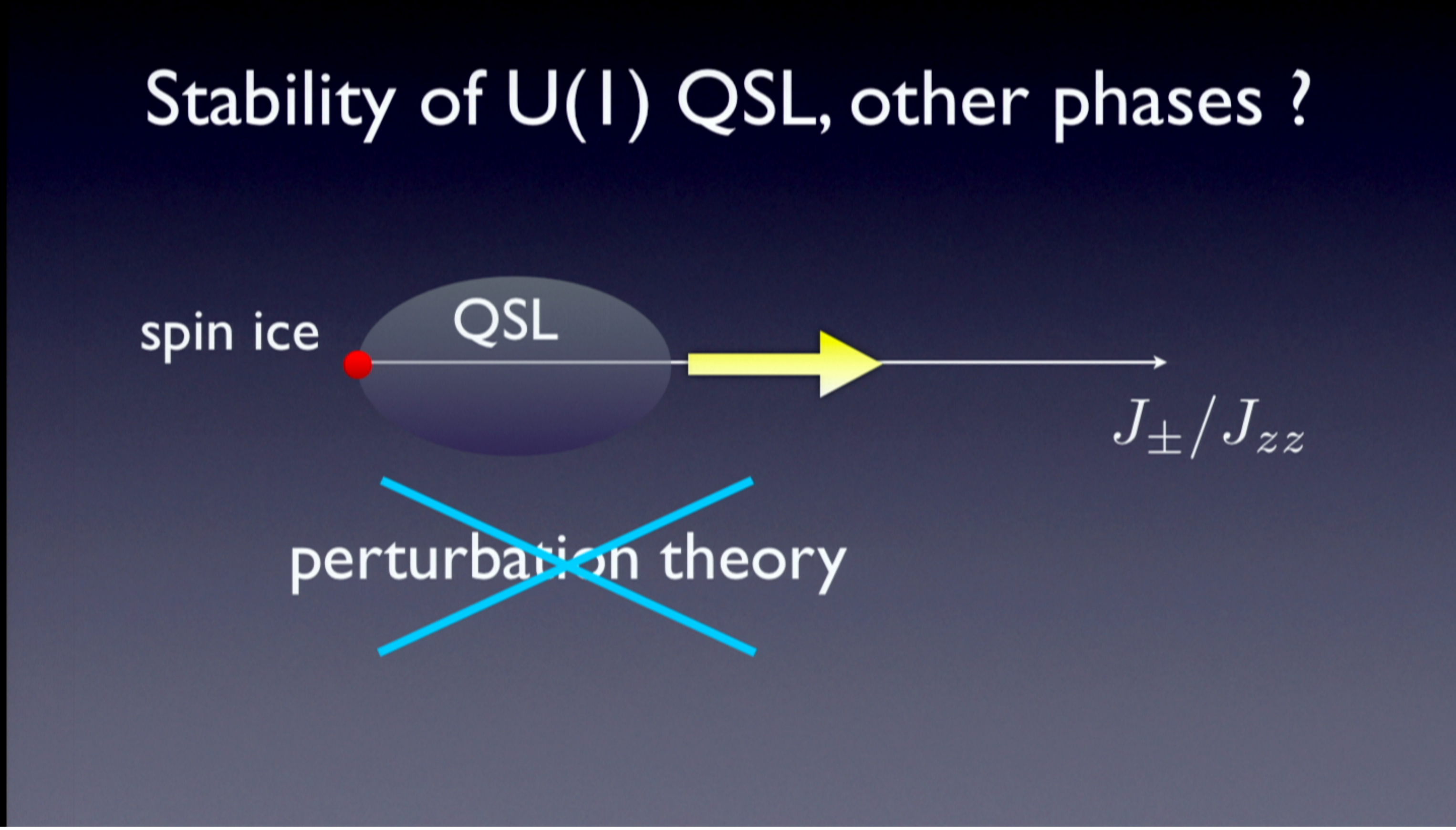
U(1) QSL : emergent compact quantum electrodynamics (QED)



- a gapped spinon : carrying "electric" gauge charge
- a gapped monopole



- artificial gapless photon

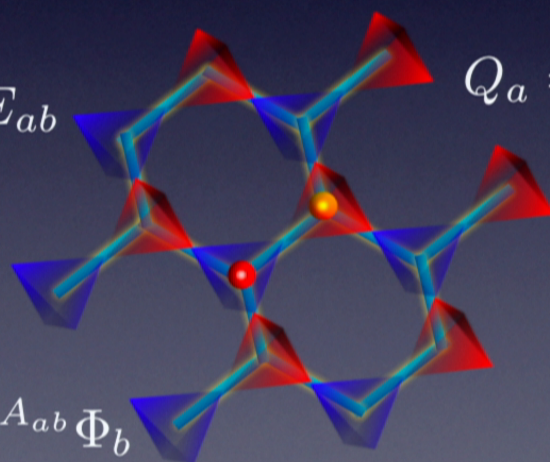

Stability of U(1) QSL, other phases ?
spin ice
QSL
$J_\pm / J_{zz}$
perturbation theory

non perturbative method

U(1) gauge theory

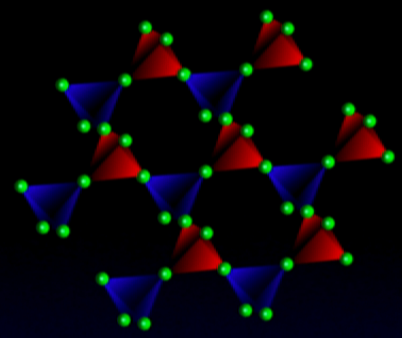
$$S_i^z = E_{ab}$$

$$Q_a = (div E)_a$$



$$S_i^+ = \Phi_a^\dagger e^{iA_{ab}} \Phi_b$$

OUTLINE



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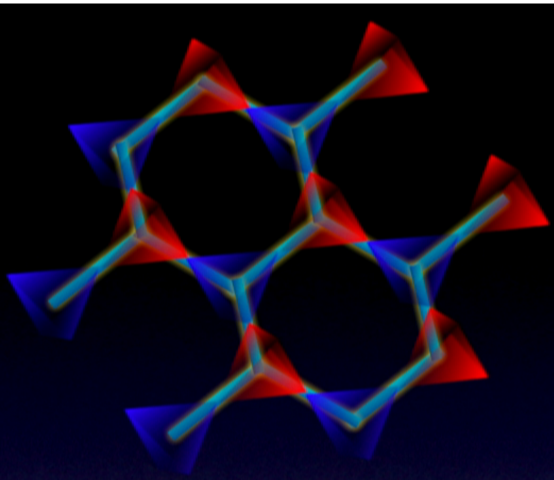
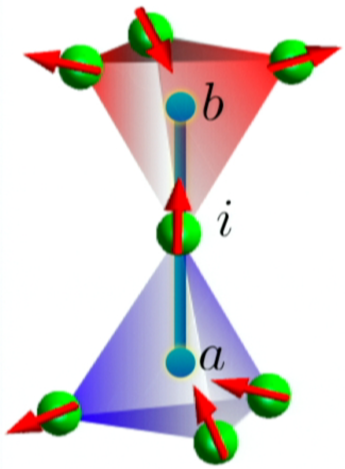
U(1) gauge theory



spinons in a diamond lattice
gauge fields live on its links



$$S_i^z = \eta_a E_{ab}$$

$\eta_a = \pm 1 [a \in A(B)]$

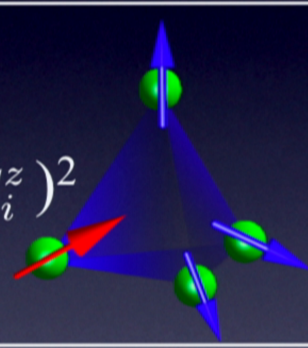
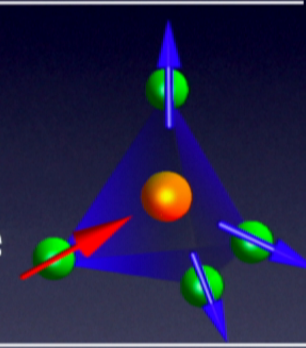
$$S_i^+ = \Phi_a^\dagger e^{iA_{ab}} \Phi_b \qquad \Phi_a = e^{-i\varphi_a}$$

$$Q_a = (divE)_a \qquad \Phi_a^\dagger \Phi_a = 1$$

$$[A_{ab}, E_{ab}] = i$$

$$[\Phi_a, Q_a] = \Phi_a$$

Mapping into U(1) gauge theory

Pseudospin-1/2 model	U(1) gauge theory
$\sum_{\langle ij \rangle} S_i^z S_j^z \to \sum_{\triangle} (S_i^z)^2$ 	$Q = div(E)$ electric charge 
$\sum_{\langle ij \rangle} S_i^+ S_j^-$	$\Phi_r^\dagger e^{iA_{rr'}} \Phi_{r'}$ spinon hopping in the background of fluctuating gauge fields

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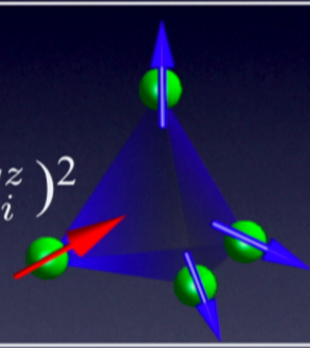
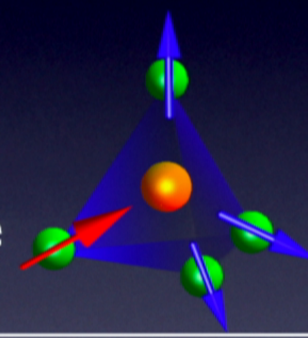
$\sum_{\langle ij \rangle} S_i^z S_j^z \rightarrow \sum_{\triangle} (S_i^z)^2$ 	$Q = div(E)$ electric charge 
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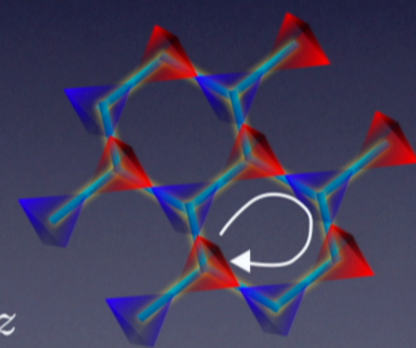
From Spin Ice to U(1) QSL

Projection to the spin ice ground state
3rd order of DPT

$$PH_{QED}P = \frac{J_{zz}}{2}\sum_{r\in A,B} Q_r^2 - \frac{12J_\pm^3}{J_{zz}}\sum_{\hexagon}\cos\left(\nabla\times A\right)$$

U(1) spin liquid ???

spin ice $J_\pm / J_{zz}$



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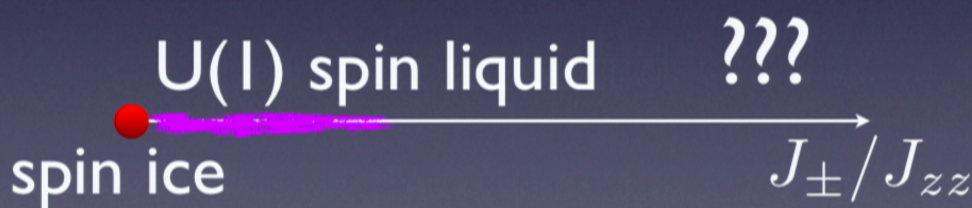
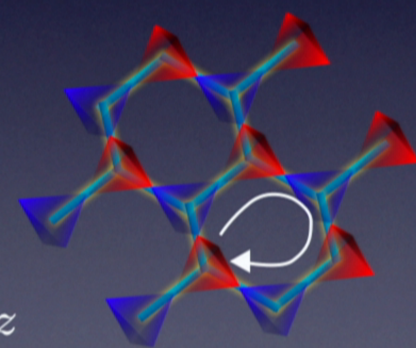
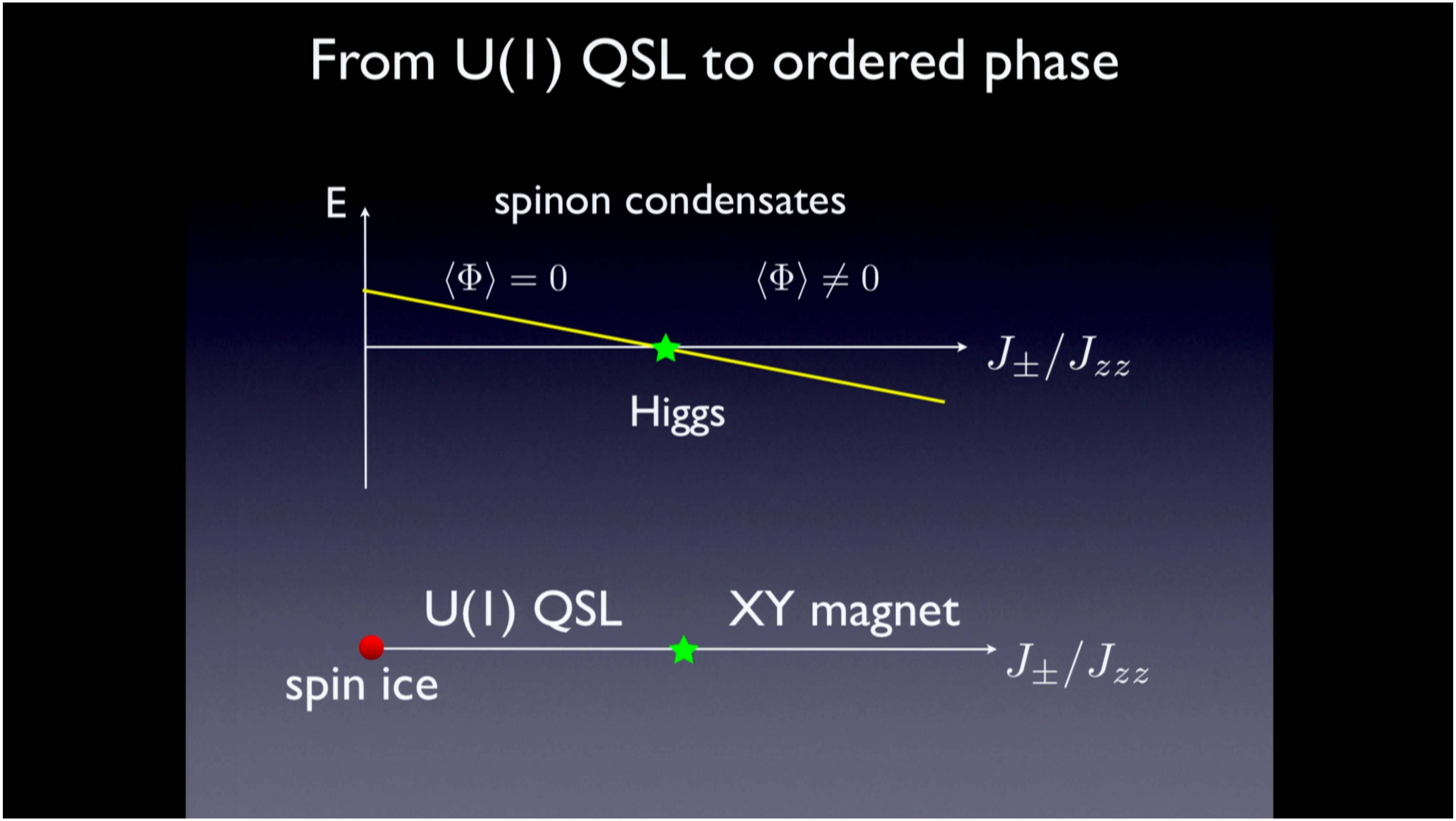





From U(1) QSL to ordered phase
E
spinon condensates
$\langle\Phi\rangle = 0$
$\langle\Phi\rangle \neq 0$
$J_{\pm}/J_{zz}$
Higgs
U(1) QSL
XY magnet
spin ice
$J_{\pm}/J_{zz}$

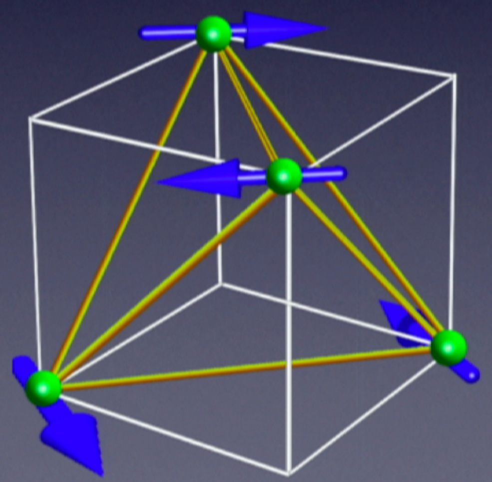
magnetic ordering : XY-AF

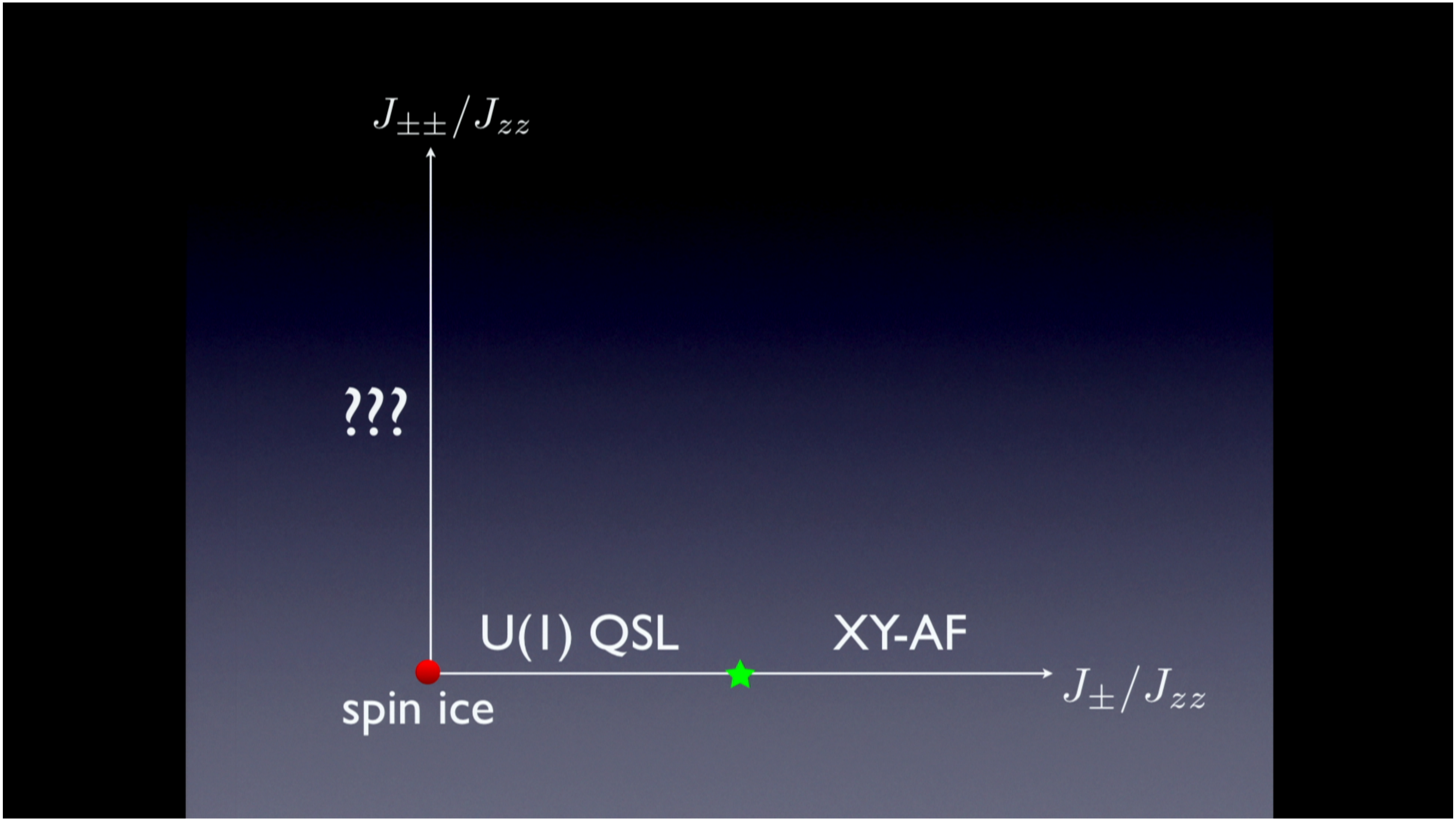
spinon condensates induce magnetic ordering on XY plane

$$\langle S_r^+ \rangle = \langle \Phi_a^\dagger \rangle \langle e^{iA_{ab}} \rangle \langle \Phi_b \rangle \neq 0$$

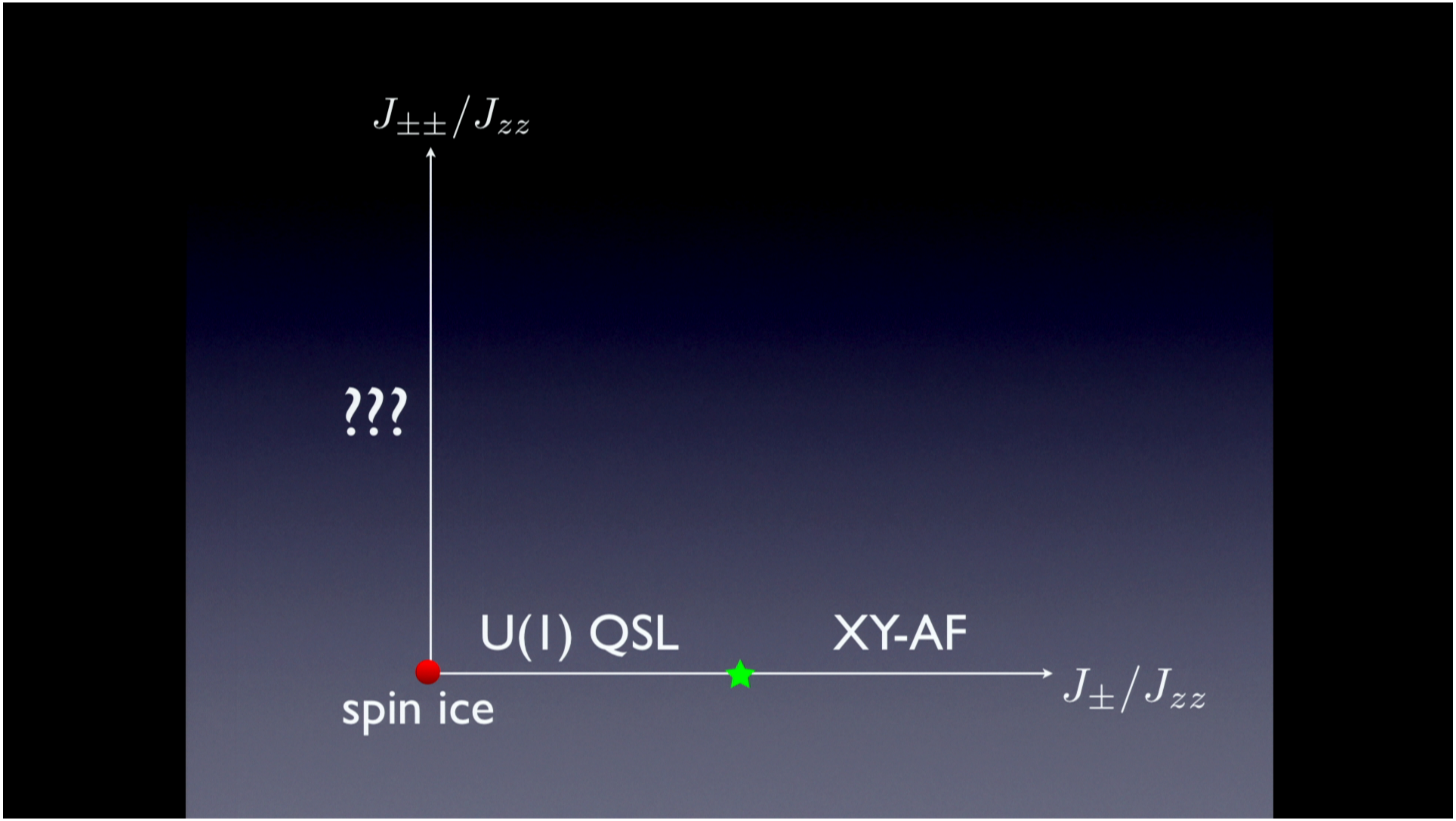
wave vector of spinon condensates $k_s = 0$

4 sublattice XY-AF




$J_{\pm\pm}/J_{zz}$
???
U(1) QSL
XY-AF
spin ice
$J_{\pm}/J_{zz}$


AF
$J_{\pm}/J_{zz}$

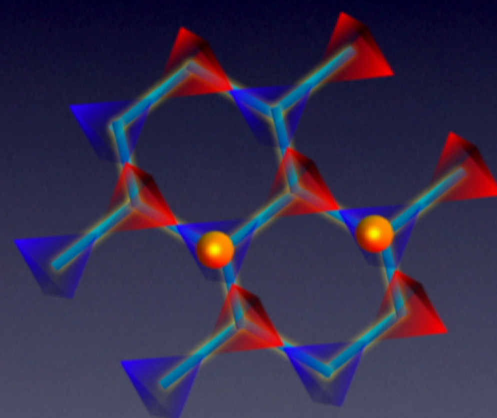


$J_{\pm\pm}/J_{zz}$
???
U(1) QSL
XY-AF
$J_{\pm}/J_{zz}$
spin ice

Mapping into U(1) gauge theory

$$H = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z + J_{\pm\pm}(S_i^+ S_j^+ \gamma_{ij}^2 + S_i^- S_j^- \gamma_{ij}^{*2})$$

quartic spinon hopping



$$H_{QED} = \frac{J_{zz}}{2} \sum_r Q_r^2 + \frac{J_{\pm\pm}}{2} \sum_r \sum_{\mu \neq \nu} \gamma_{\mu\nu}^{-2\eta_r} \Phi_r^\dagger \Phi_r^\dagger \Phi_{r+\eta_r e_\mu} \Phi_{r+\eta_r e_\nu} e^{-i(\eta_r A_{r,\eta_r(e_\mu + e_\nu)})} + h.c$$

Mapping into U(1) gauge theory

$$H = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z + J_{\pm\pm}(S_i^+ S_j^+ \gamma_{ij}^2 + S_i^- S_j^- \gamma_{ij}^{*2})$$

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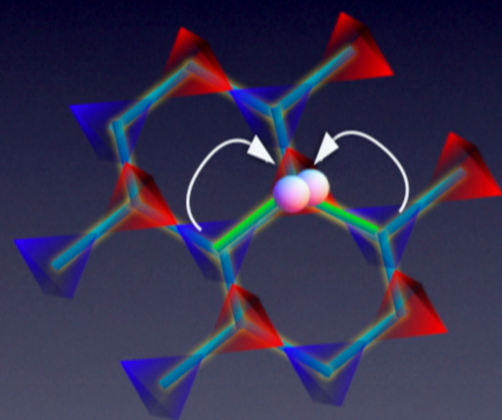

$$H_{QED} = \frac{J_{zz}}{2} \sum_r Q_r^2$$
$$+ \frac{J_{\pm\pm}}{2} \sum_r \sum_{\mu \neq \nu} \gamma_{\mu\nu}^{-2\eta_r} \Phi_r^\dagger \Phi_r^\dagger \Phi_{r+\eta_r e_\mu} \Phi_{r+\eta_r e_\nu} e^{-i(\eta_r A_{r,\eta_r(e_\mu+e_\nu)})} + h.c$$

From U(1) QSL to ???

quartic spinon hopping $\Phi_r^\dagger \Phi_r^\dagger \Phi_{r+e_\mu} \Phi_{r+e_\nu}$

(Q) Which one is energetically favored ?

	$\langle \Phi_r \rangle$	$\langle \Phi_r \Phi_{r'} \rangle$	$\langle \Phi_{r_A}^\dagger \Phi_{r_B} \rangle$	characteristics
XY magnet	$\neq 0$	$\neq 0$	$\neq 0$	ordering on XY
Z_2	0	$\neq 0$	0	no local ordering charge 2 condensates
U(1)-XY*	0	0	$\neq 0$	ordering on XY gapless photon
Z_2-XY*	0	$\neq 0$	$\neq 0$	ordering on XY charge 2 condensates

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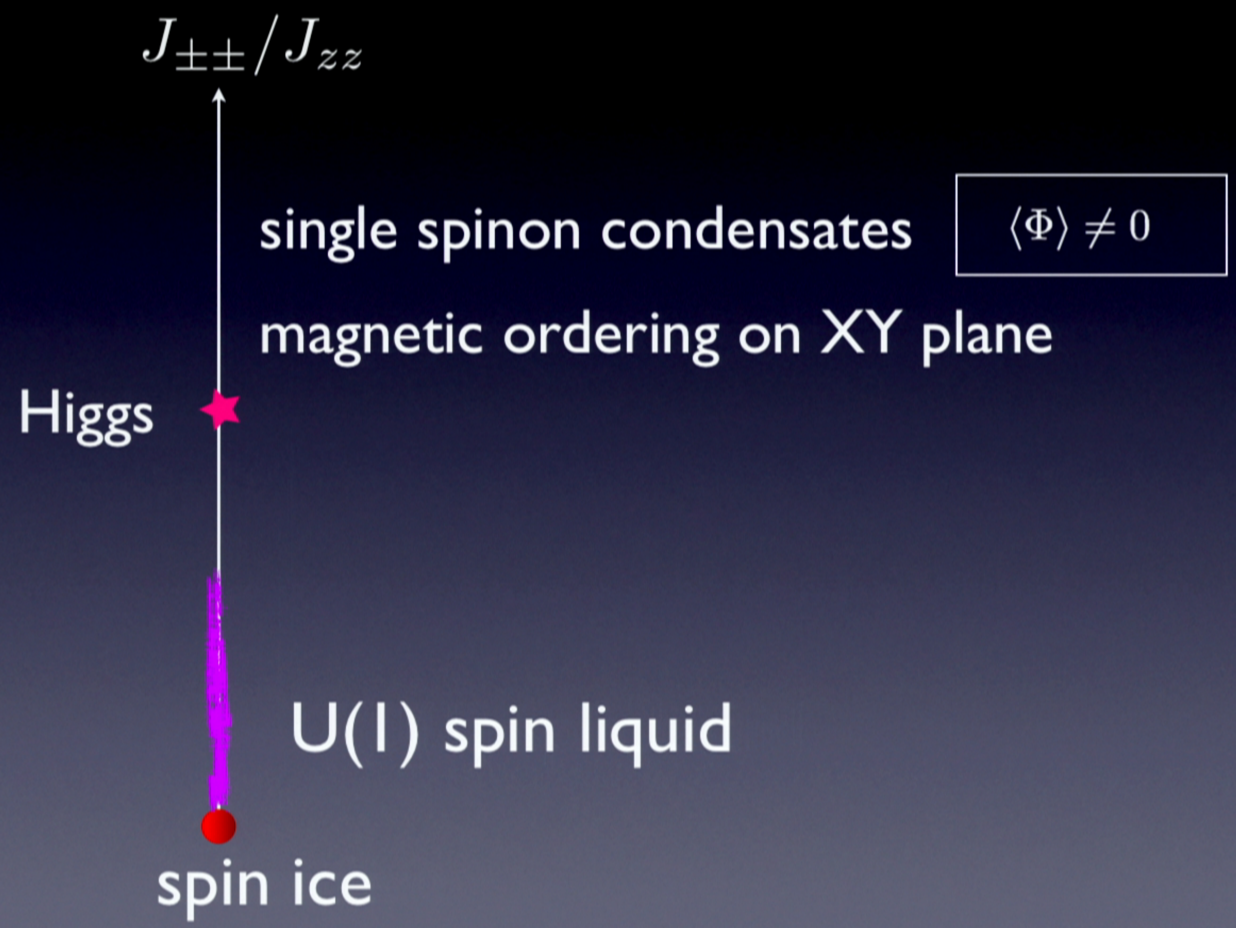
From U(1) QSL to XY-FM



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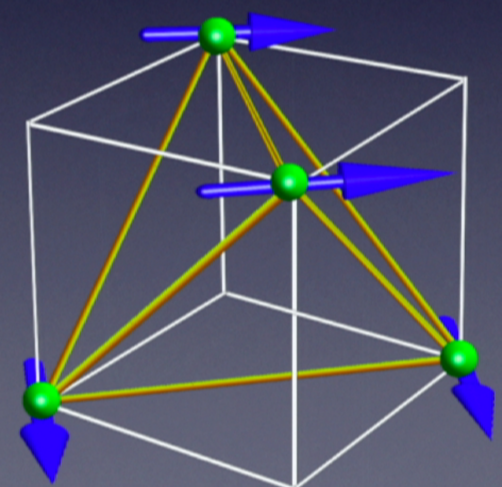
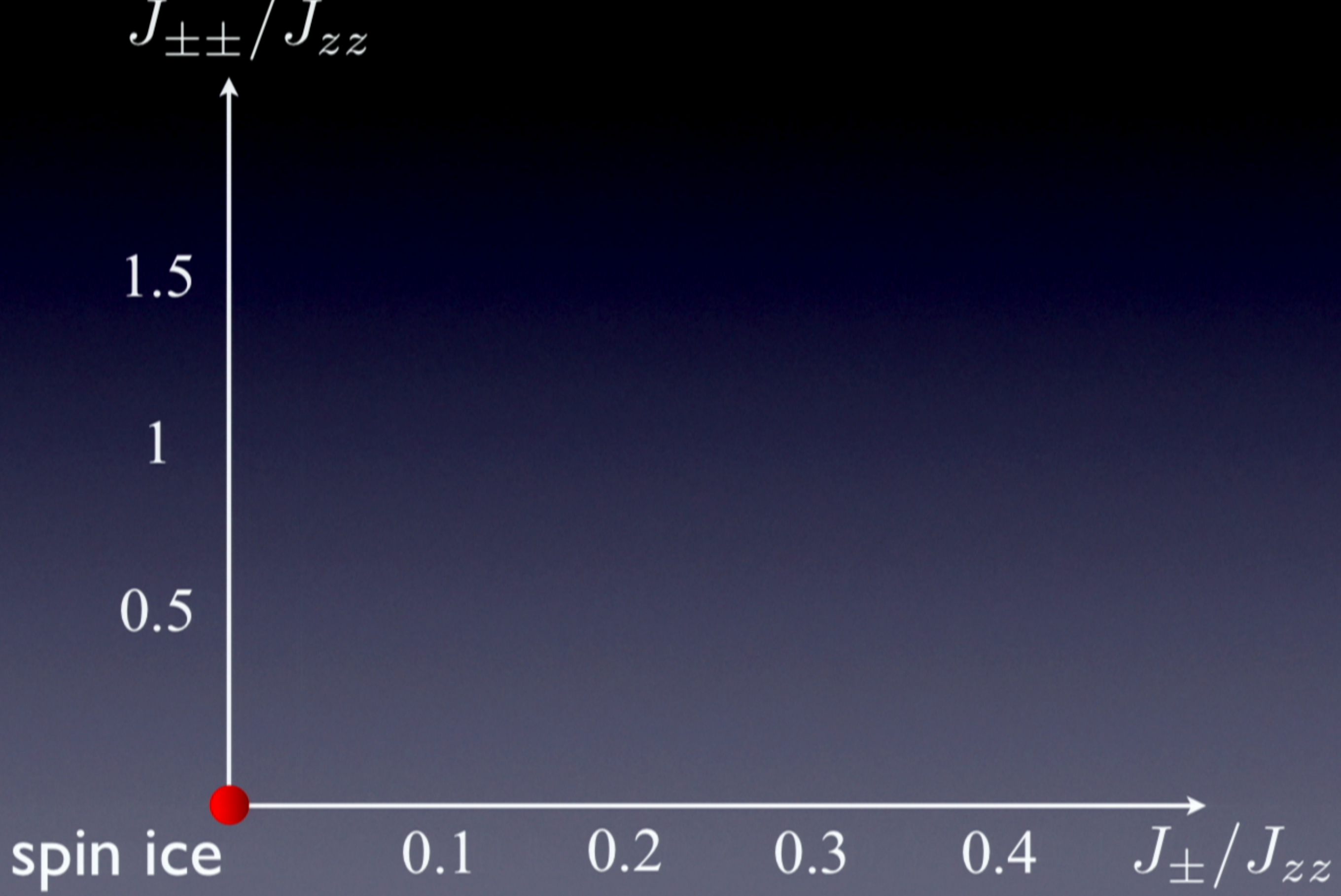
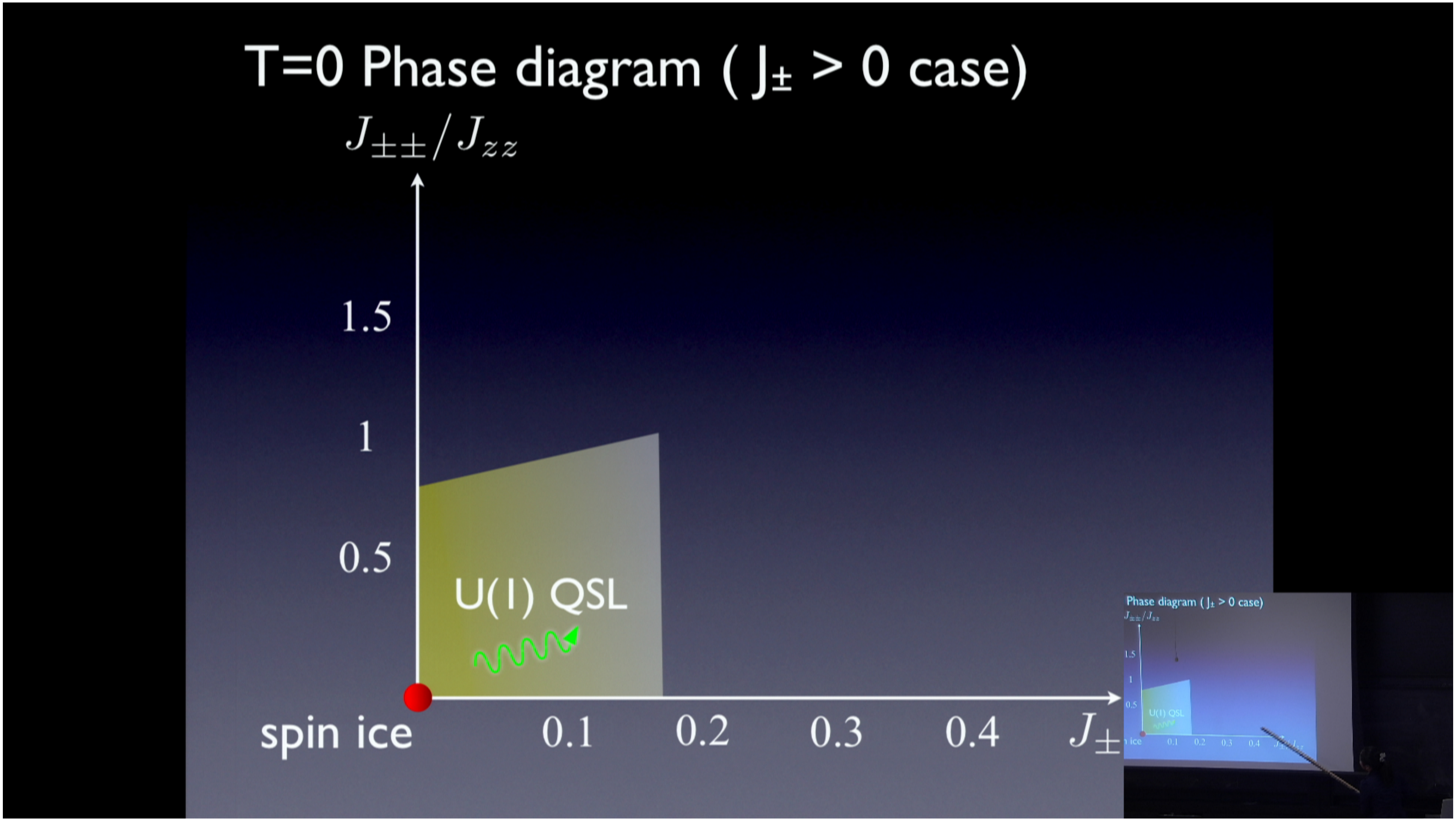
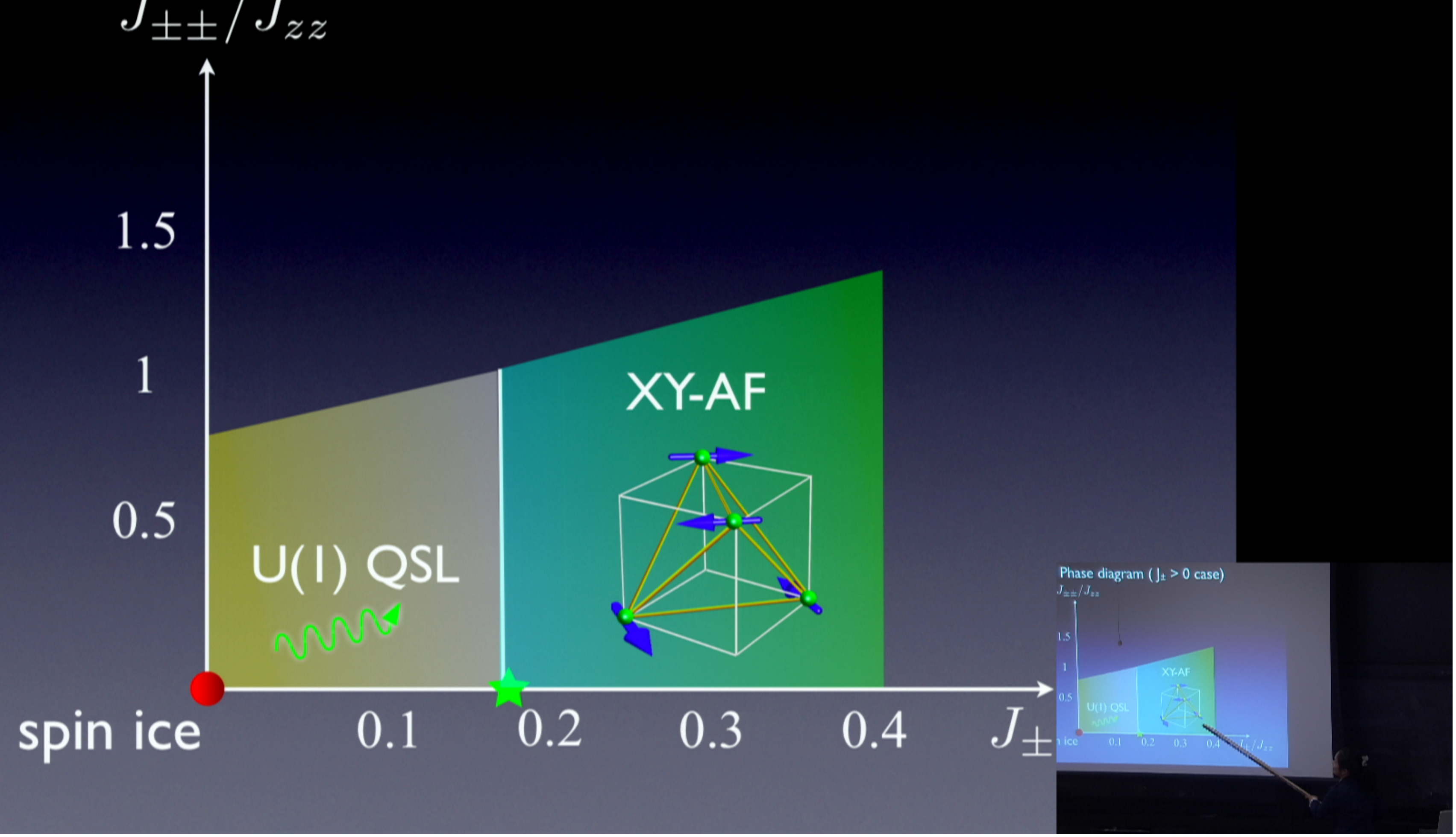


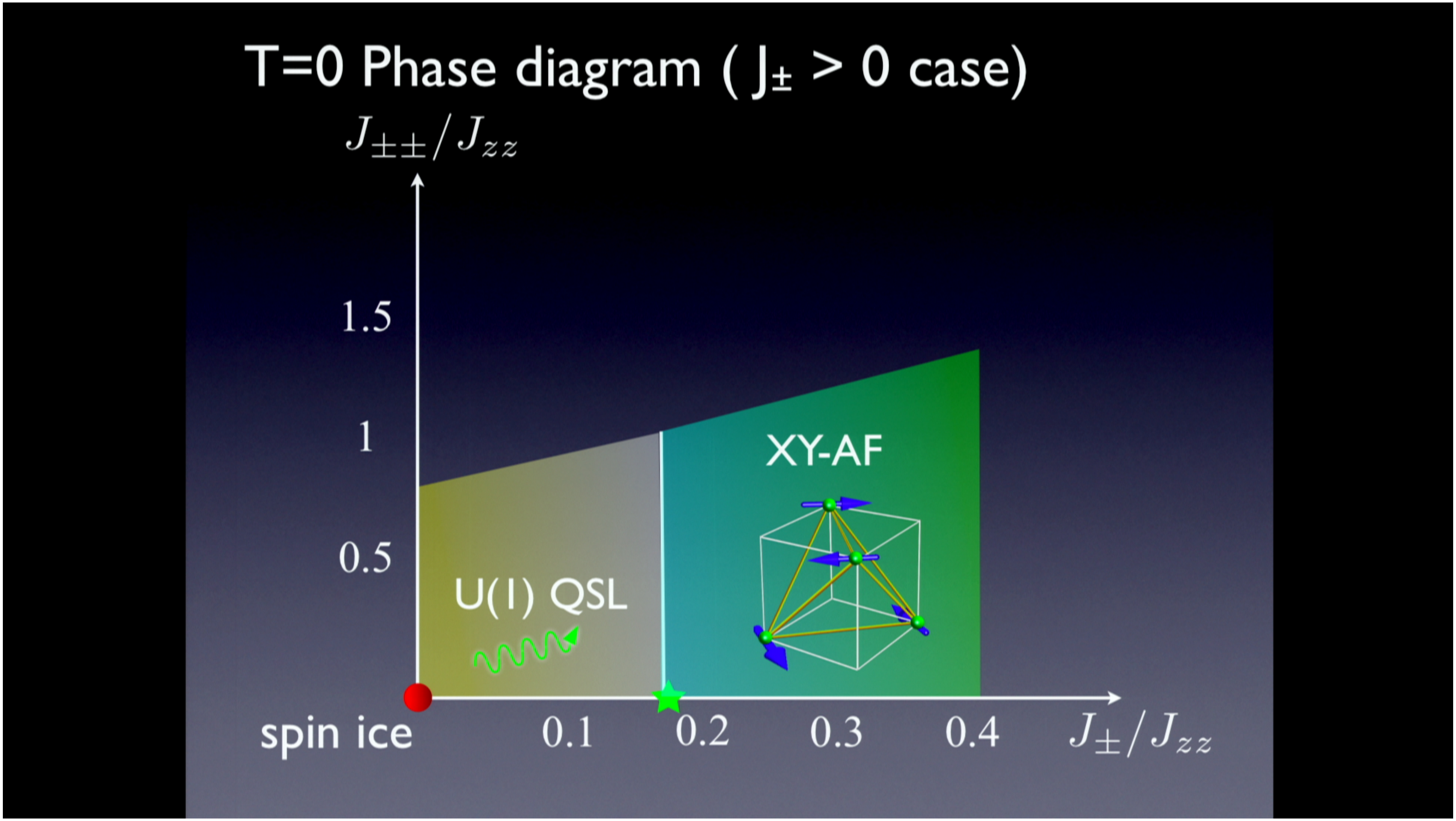
T=0 Phase diagram ($J_\pm > 0$ case)




T=0 Phase diagram (J± > 0 case)
$J_{\pm\pm}/J_{zz}$
1.5
1
0.5
U(1) QSL
spin ice
0.1
0.2
0.3
0.4
$J_\pm$
Phase diagram (J± > 0 case)

T=0 Phase diagram ($J_\pm > 0$ case)

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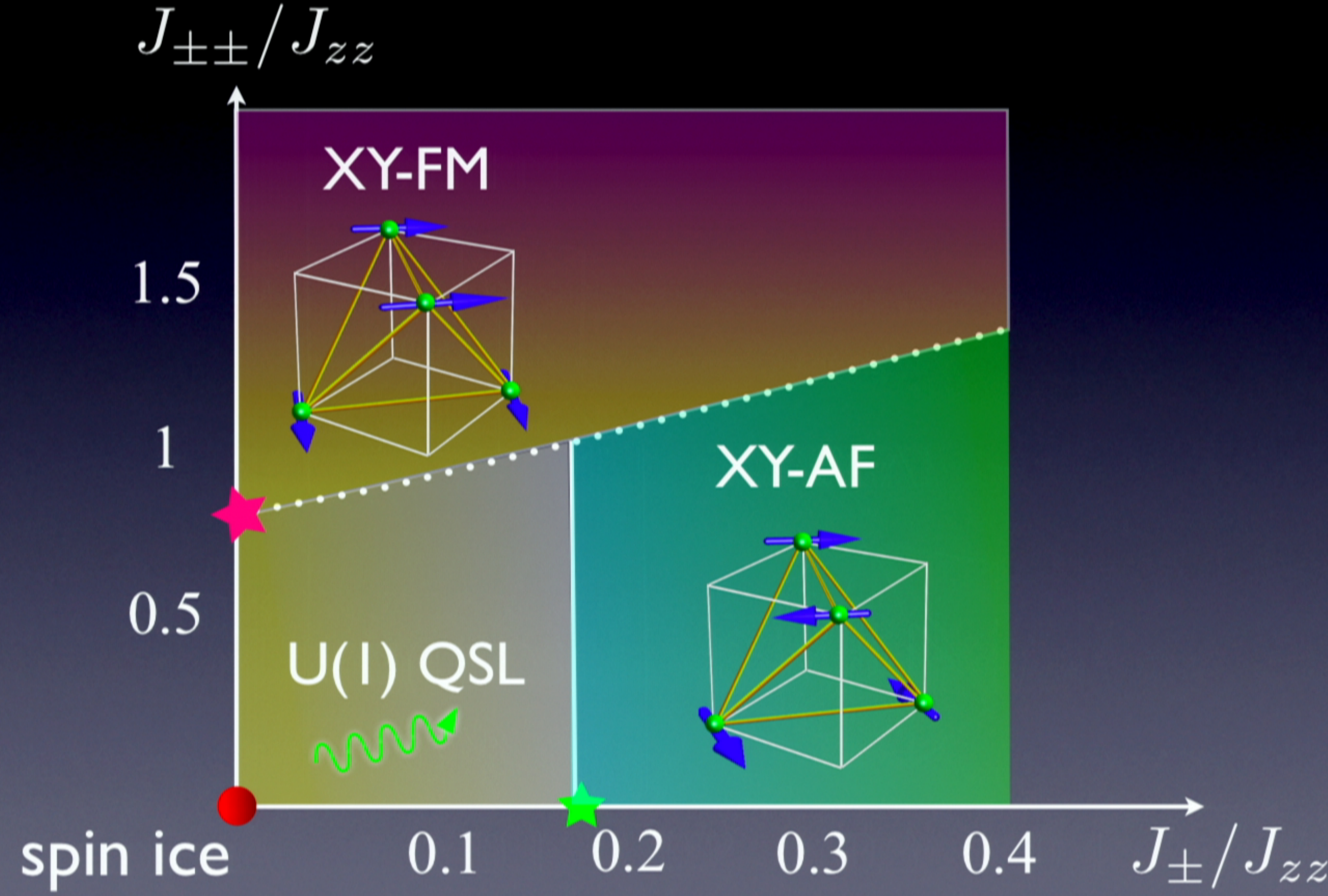
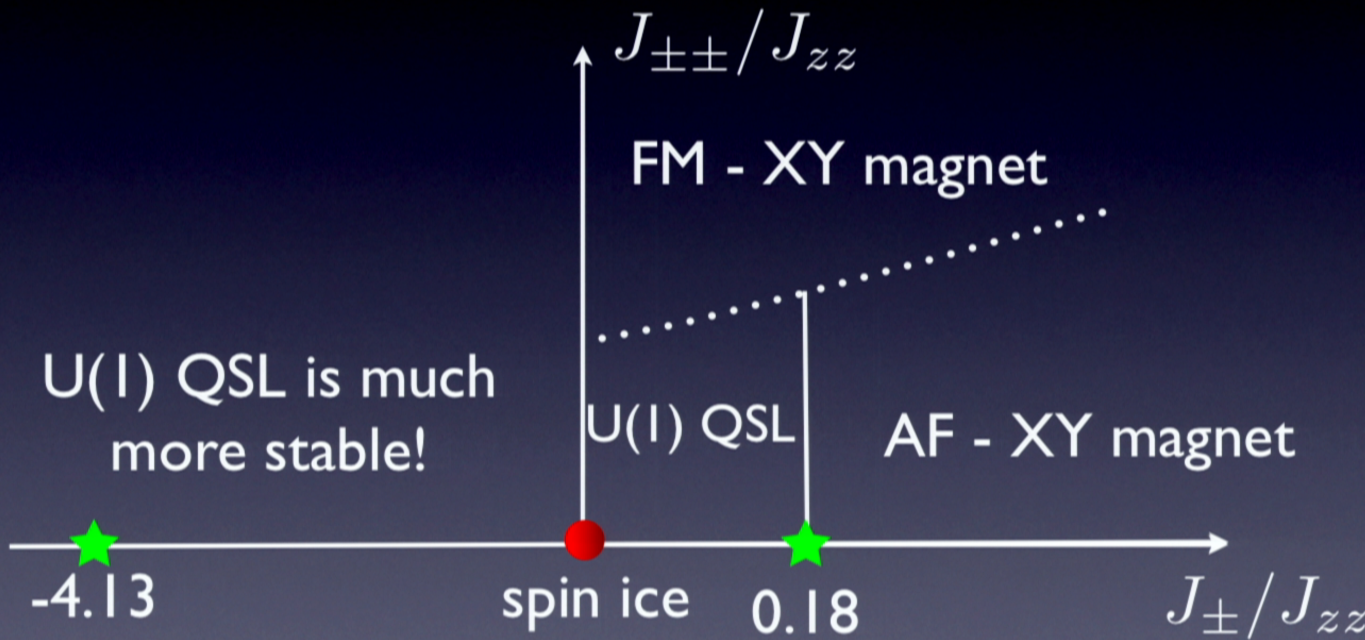
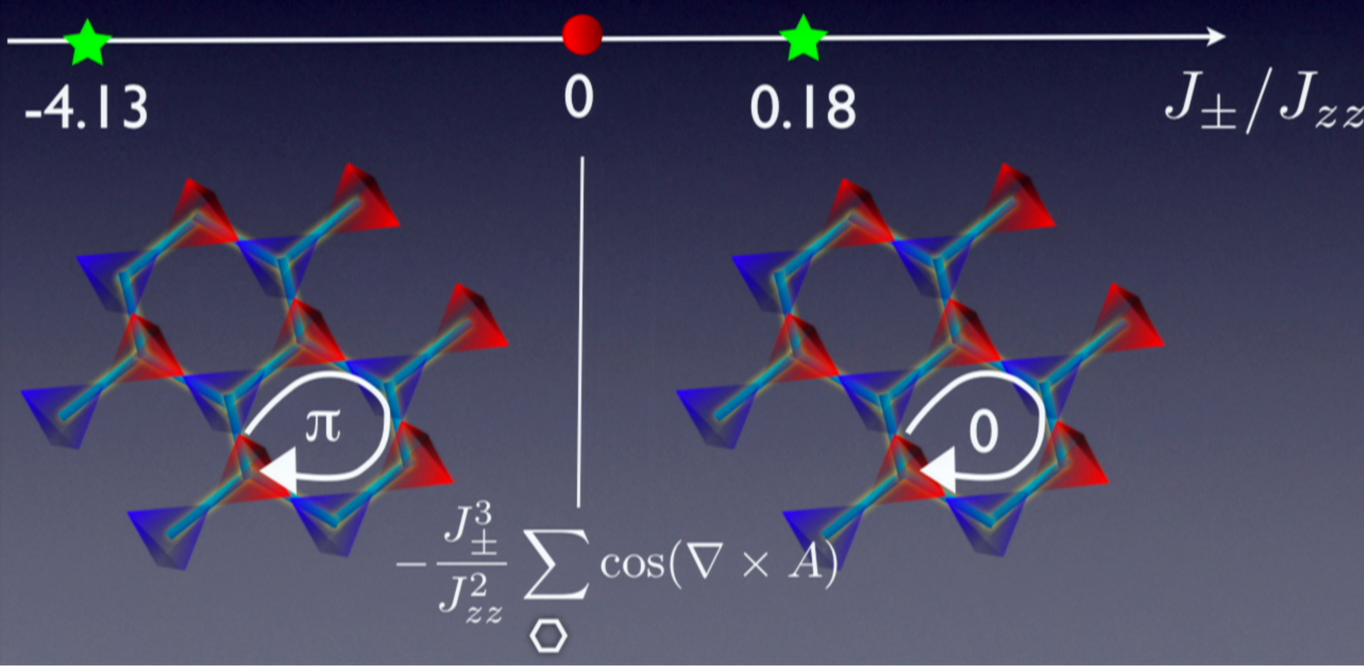


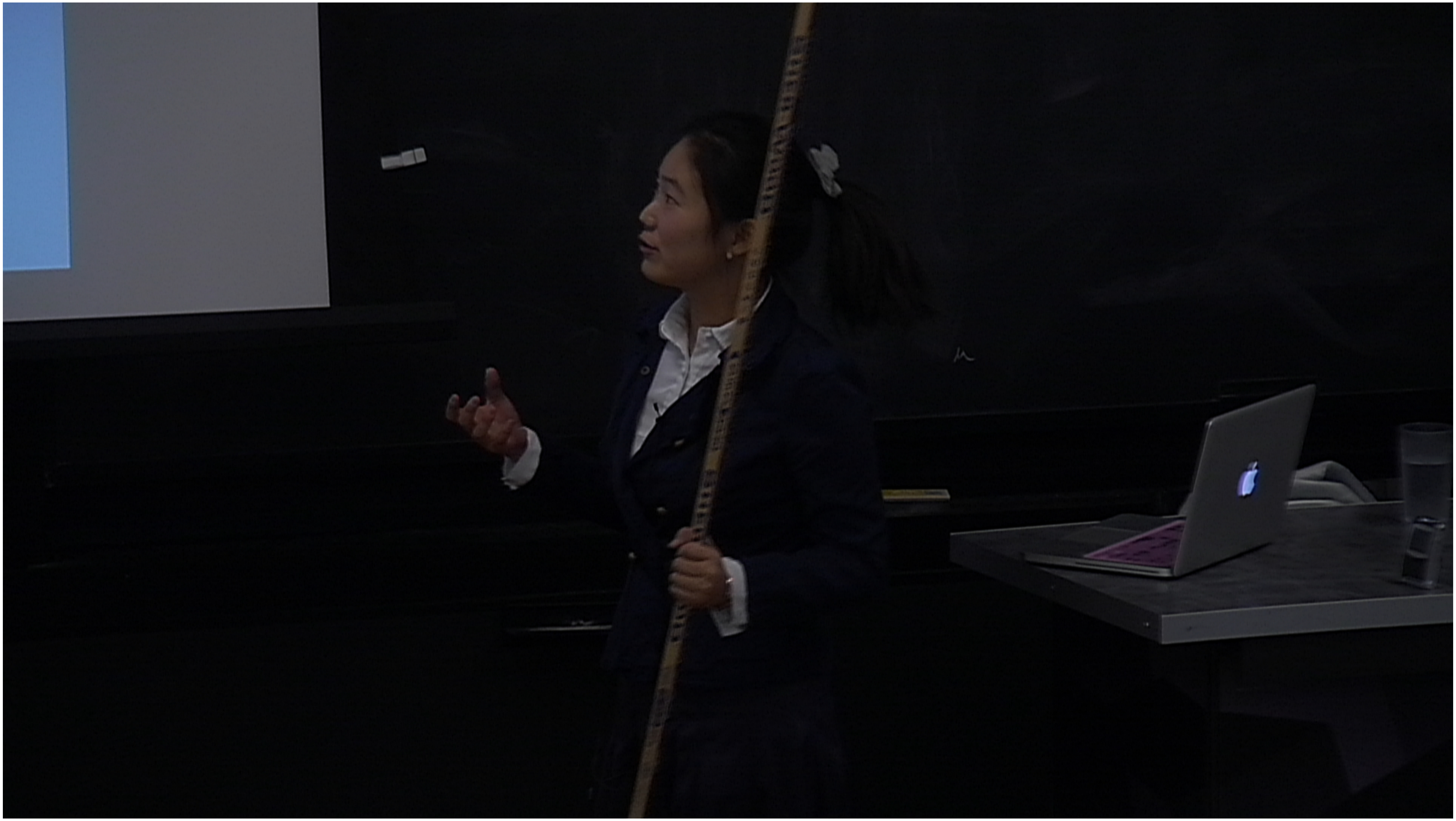
AF $J_\pm$ case ($J_\pm < 0$)

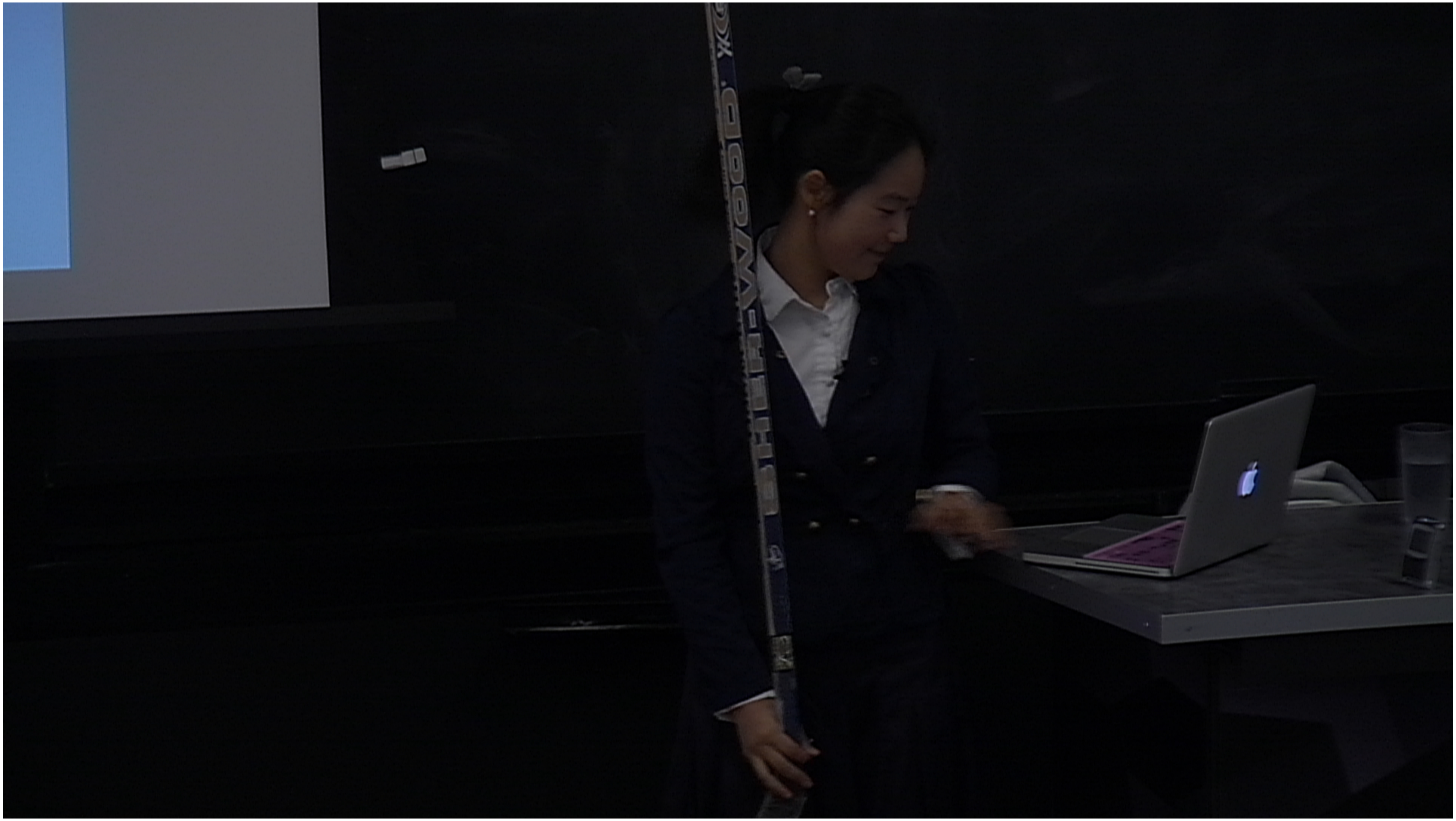


AF $J_\pm$ case ($J_\pm$ < 0)

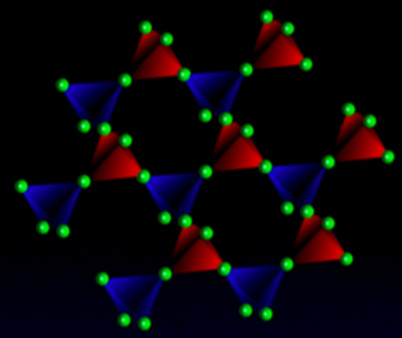
Stability of U(1) QSL is induced by "emergent" line degeneracy of spinon condensation wave vector due to π flux






SHER-WOOD

OUTLINE



- Motivation
- Pseudospin -1/2 model for rare earth pyrochlores
- Classical limit : spin ice
- Quantum effect : U(1) QSL , magnetic orderings
- Phase diagram using "gauge mean field theory"
- Future work

Other Projects

Frustrated Magnet

"Classical" Spin Liquids in a diamond lattice
SBL and Leon Balents
Phys. Rev. B 78,144417(2008)

Geometric frustrations vs Quantum Criticality
SBL, Ribhu K. Kaul and Leon Balents
Nat. Phys 6, 702-706 (2010)

"Quantum" Spin Liquids in rare earth pyrochlores

Mott transition in nickelates

Optical conductivity of $LaNiO_3$
Daniel G. Ouellette, SBL et al
Phys. Rev. B 82,165112 (2010)

Charge and spin ordering in Nickelates
SBL, Ru Chen and Leon Balents
Phys. Rev. Lett 106,016405 (2011)

Metal-Insulator Transition in perovskite nickelates
SBL, Ru Chen and Leon Balents
Phys. Rev. B 84,165119 (2011)


Thank you!


SHER-WOOD