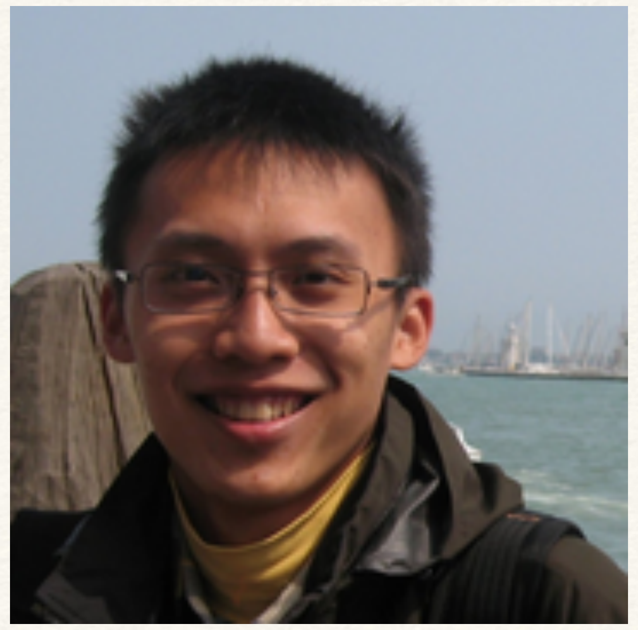

Kai-Hsin Wu (NTU)

Yi-Ping Huang (MPIPKS)

Tunneling-induced restoration of classical degeneracy in quantum kagome ice

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National Taiwan University

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2nd Asia-Pacific Workshop on Quantum Magnetism

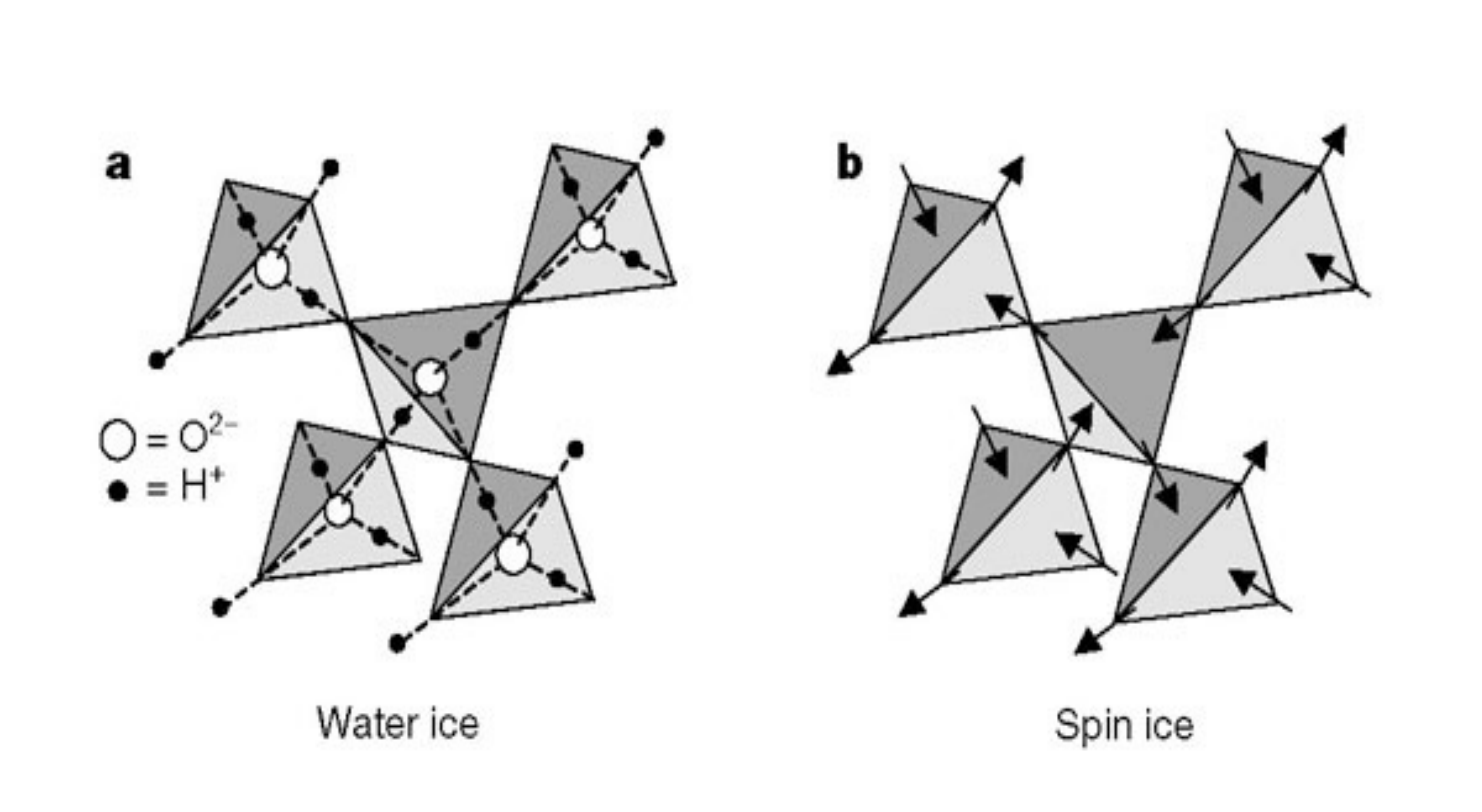
ICTS, Bangaluru, India, 11/29-12/6, 2018

arXiv:1806.08145

Outline

- Introduction to Spin Ice and Kagome Ice
- QMC: Topological Entanglement Entropy / Thermal Entropy
- Degenerate Perturbation Theory: Competing Quantum Processes
- Conclusions

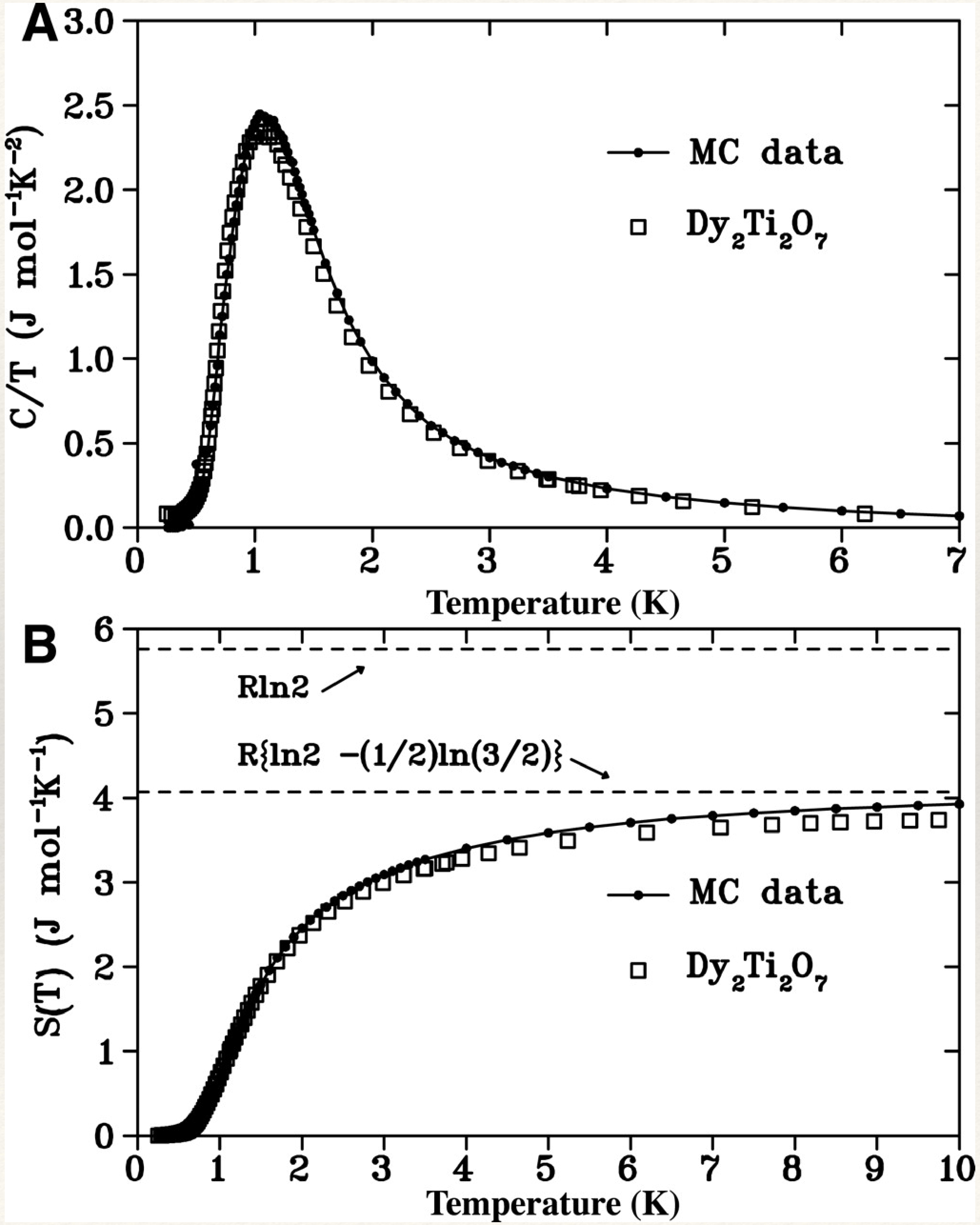
Spin Ice

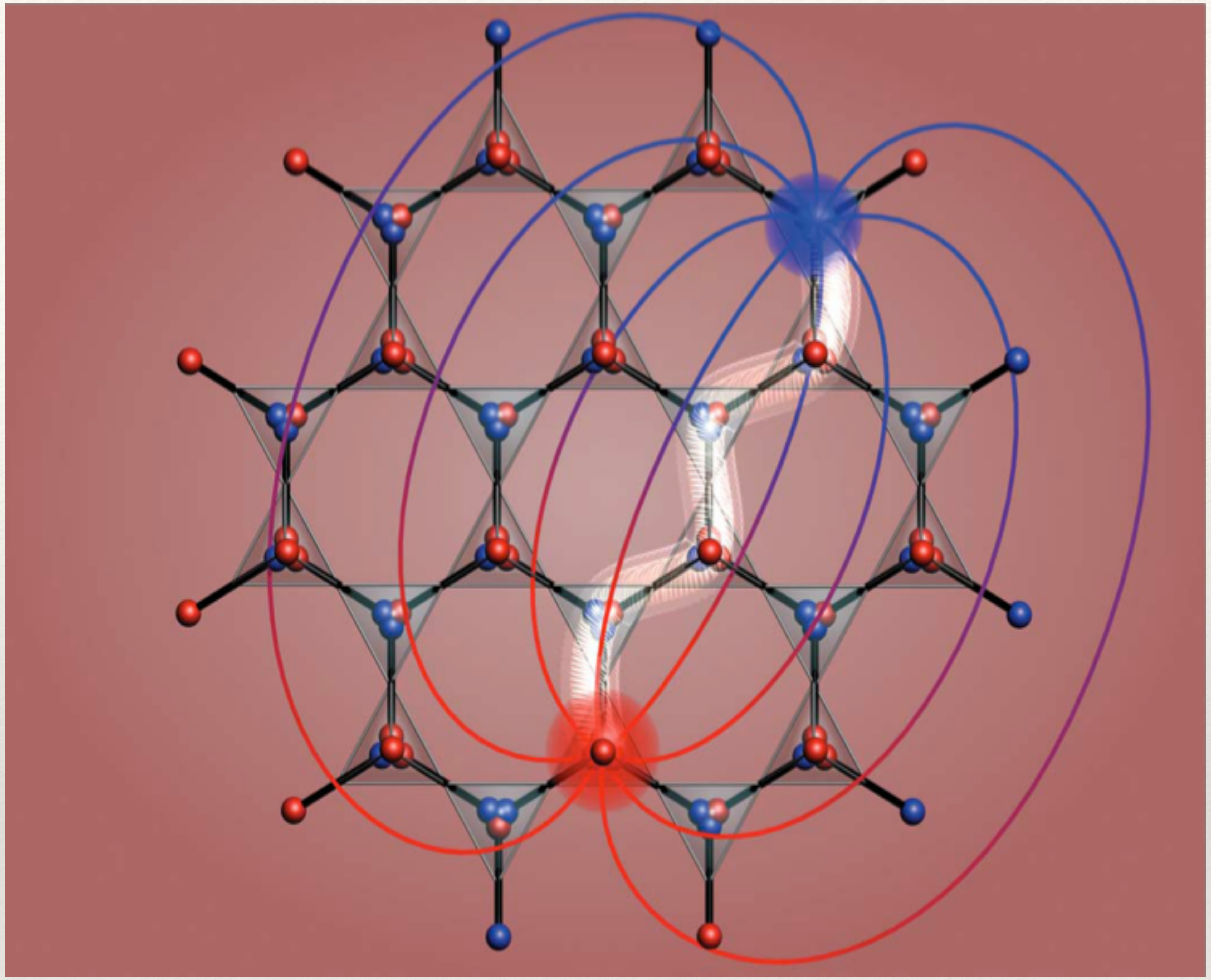


- Ice rule: 2-in, 2-out
- Extensive ground state degeneracy

Residual Entropy (Pauling) $$\frac{S}{N} = \frac{1}{2}\ln\left(\frac{3}{2}\right)$$

Nature 413, 48-51 (2001)





A.P. Ramirez et al., Nature 399, 333 (1999)
B.C. den Hertog et al., PRL 84, 3430 (2000)
C. Castelnovo et al. Nature 451, 42–45 (2008)

Quantum Spin Ice

Dipolar Kramers doublet (Yb^{3+})

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

Sign problem in QMC

Kate A. Ross, Lucile Savary, Bruce D. Gaulin, and Leon Balents Phys. Rev. X 1, 021002 (2011)

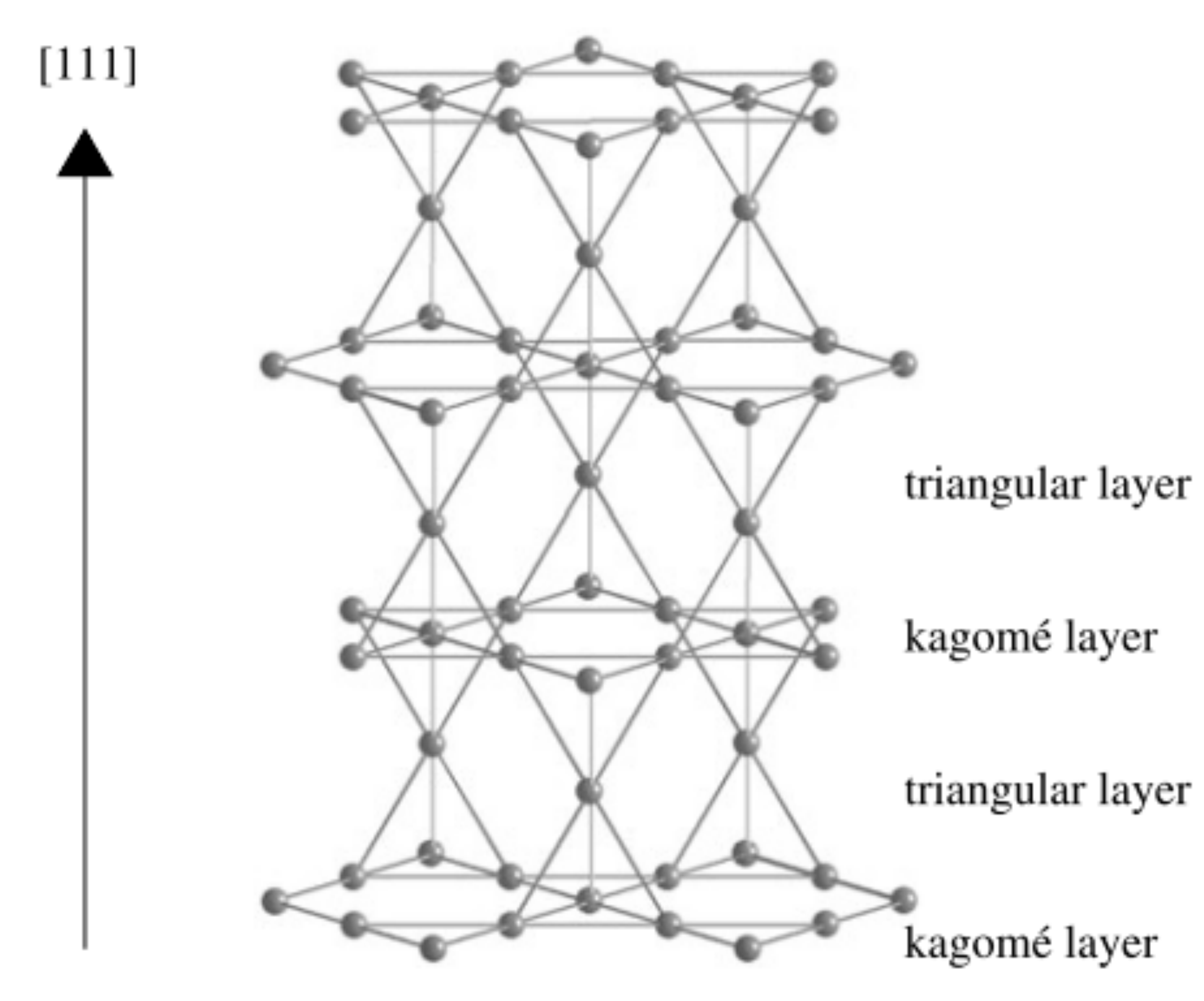
Dipolar-Octupolar Kramers doublet (Nd^{3+},Dy^{3+})

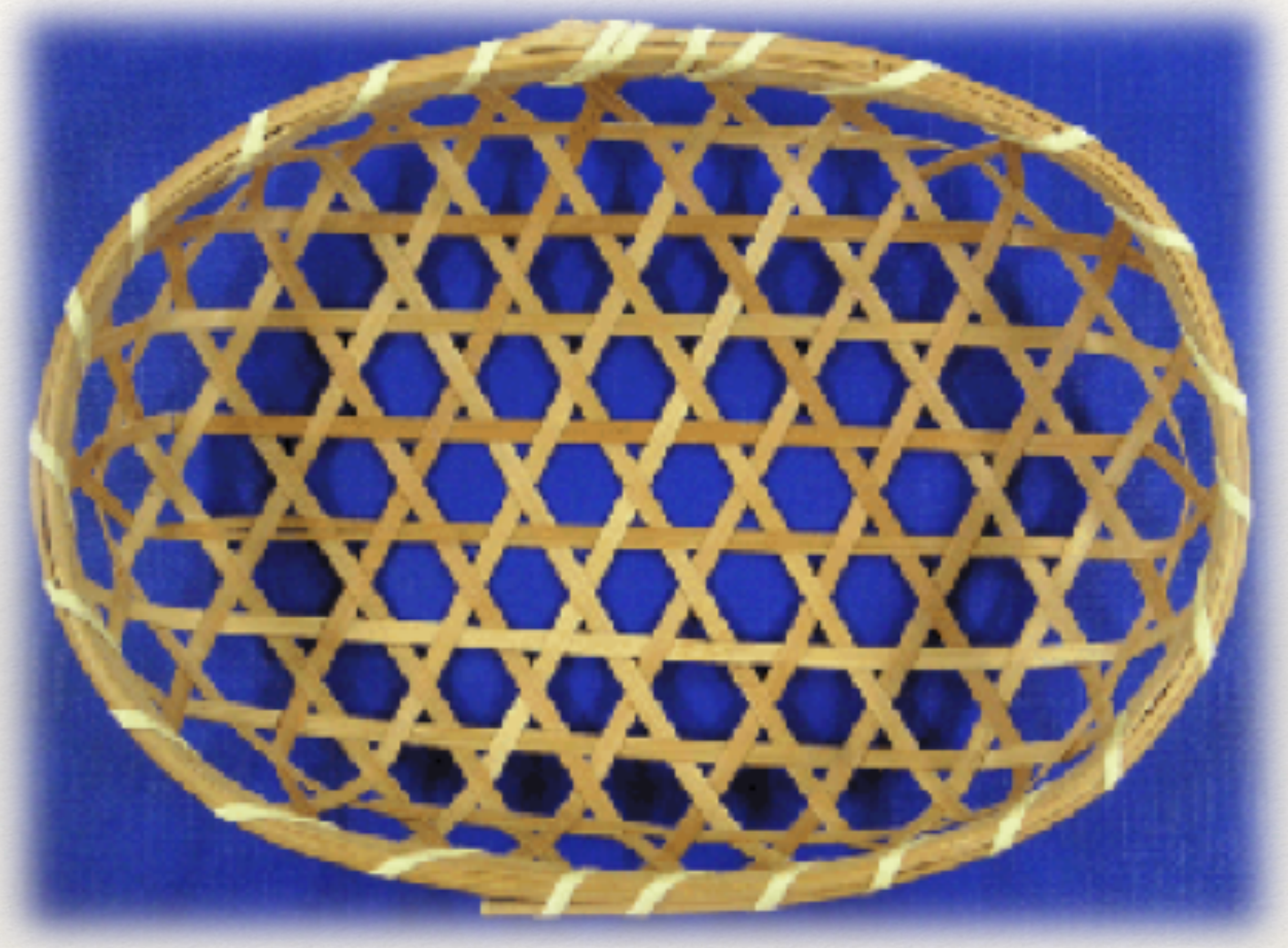
$$H_{\mathrm{XYZ}} = \sum_{\langle \boldsymbol{r}\boldsymbol{r}' \rangle} J_x S_{\boldsymbol{r}}^x S_{\boldsymbol{r}'}^x + J_y S_{\boldsymbol{r}}^y S_{\boldsymbol{r}'}^y + J_z S_{\boldsymbol{r}}^z S_{\boldsymbol{r}'}^z$$

Sign problem free

Yi-Ping Huang, Gang Chen, Michael Hermele, Phys. Rev. Lett. 112, 167203 (2014)

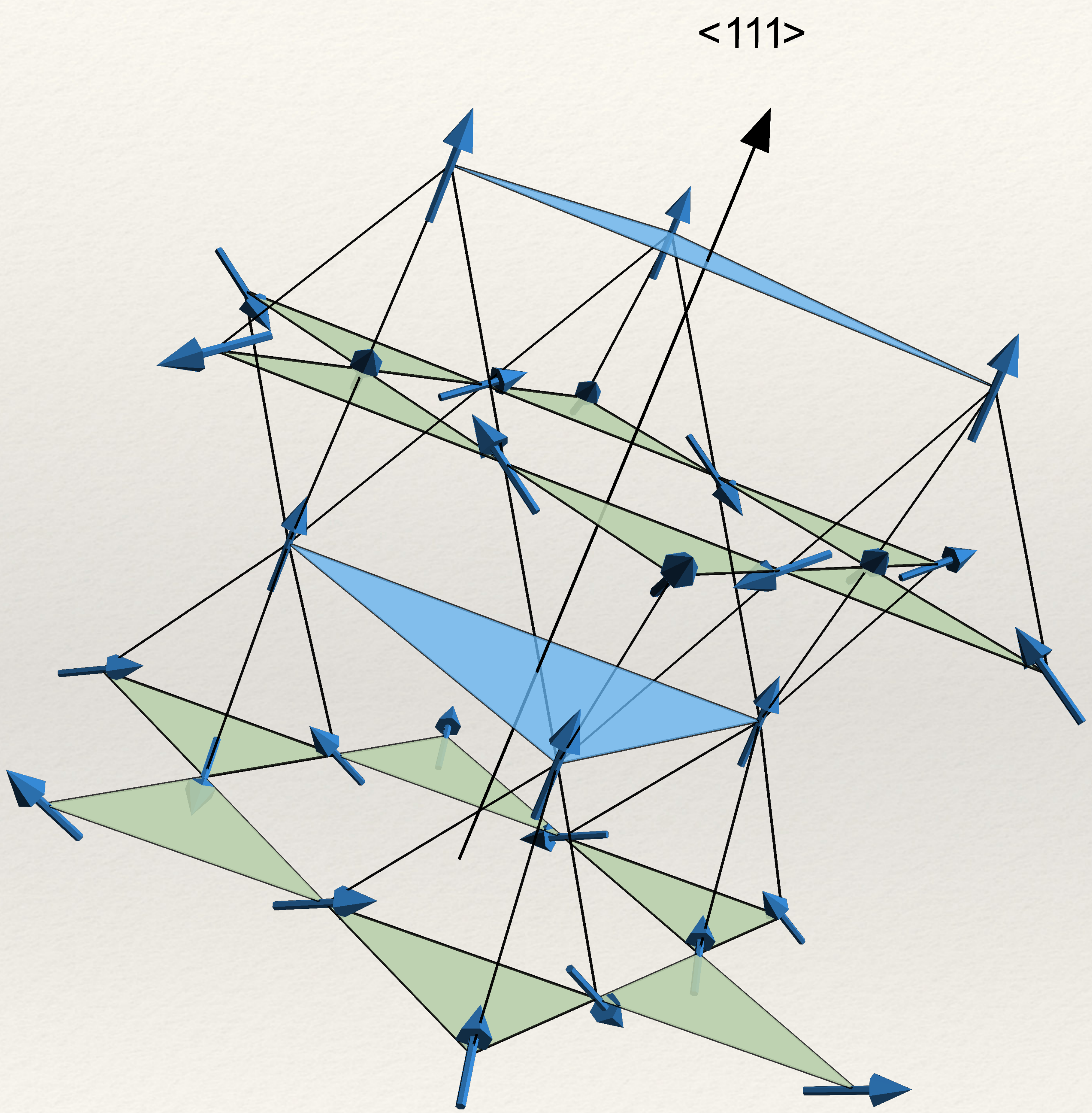
Kagome Ice



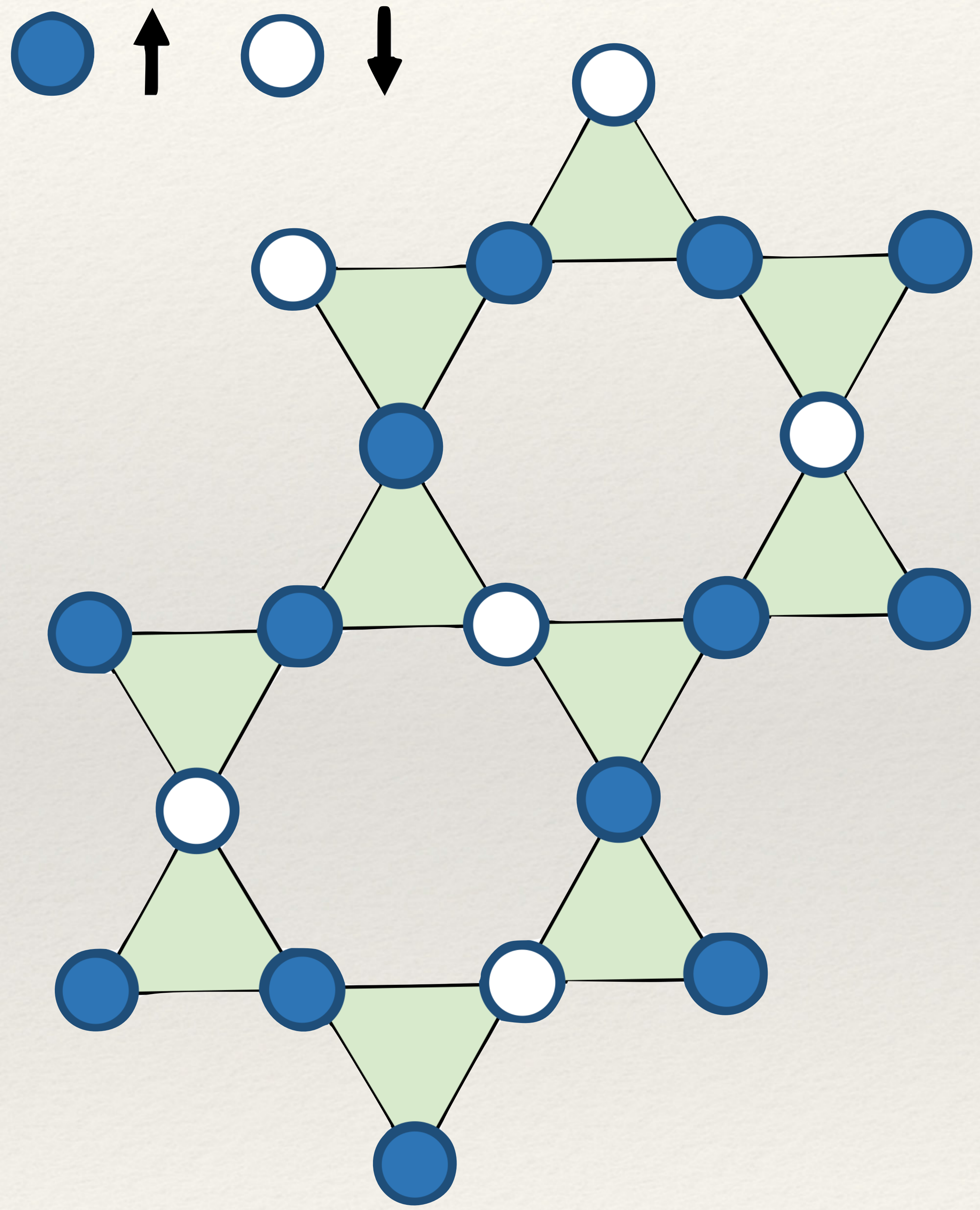


kagome 籠目

Kagome Ice



Ice rule: 2-in, 1-out or 2-in, 1-out



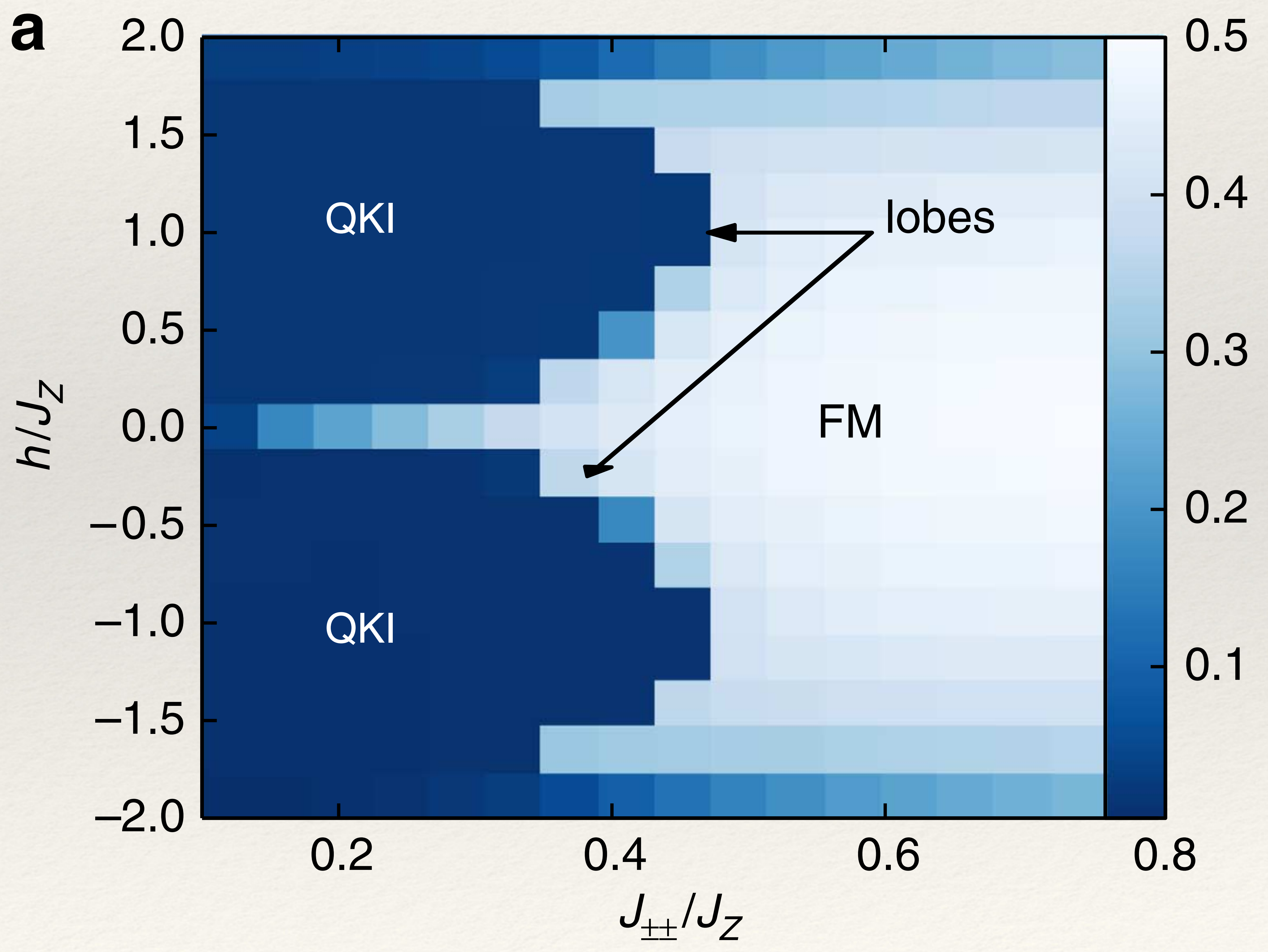
Residual Entropy (Pauling)

$$\frac{S}{N} = \frac{1}{2}\ln\left(\frac{4}{3}\right)$$

Quantum Kagome Ice

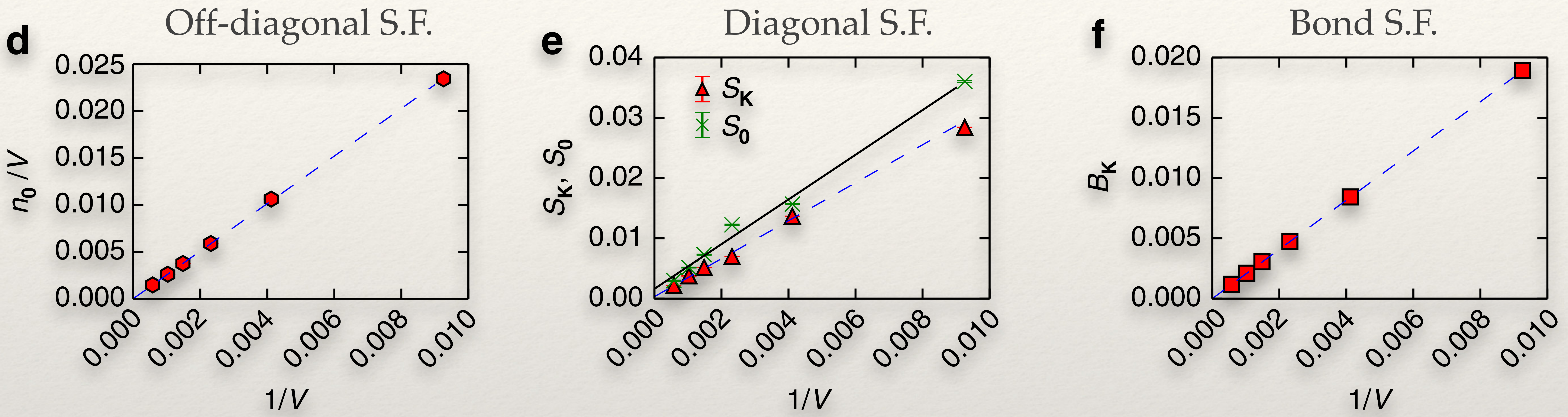
$$H_{\mathrm{XYZ}} = \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} J_z S^z_{\mathbf{r}} S^z_{\mathbf{r}'} \cancel{- \frac{J_\pm}{2} \left(S^+_{\mathbf{r}} S^-_{\mathbf{r}'} + S^-_{\mathbf{r}} S^+_{\mathbf{r}'} \right)} + \frac{J_{\pm\pm}}{2} \left(S^+_{\mathbf{r}} S^+_{\mathbf{r}'} + S^-_{\mathbf{r}} S^-_{\mathbf{r}'} \right) - h \sum_{\mathbf{r}} S^z_{\mathbf{r}}$$

- No sign problem; large-scale QMC simulations possible
- Two lobes of **QKI** states
- No long-range magnetic order inside lobe

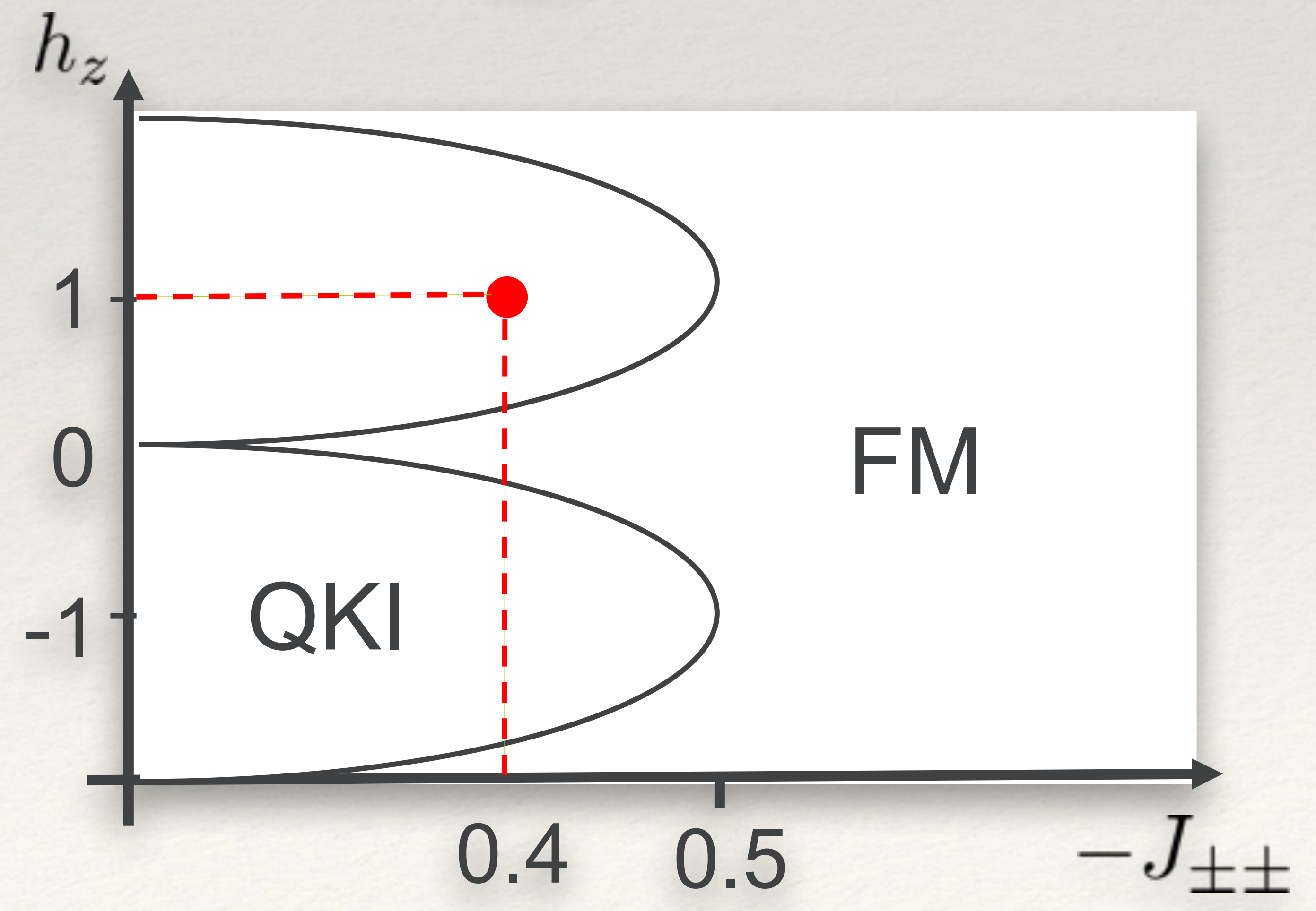


Y. P. Huang, G. Chen and M. Hermele , Phys. Rev. Lett. 112, 167203 (2014)
J. Carrasquilla, Z. Hao and R. G. Melko, Nat. Comm. 6, 7421 (2015)
Y. P. Huang and M. Hermele, Phys. Rev. B 95, 075130 (2017)

Z_2 Spin Liquid?



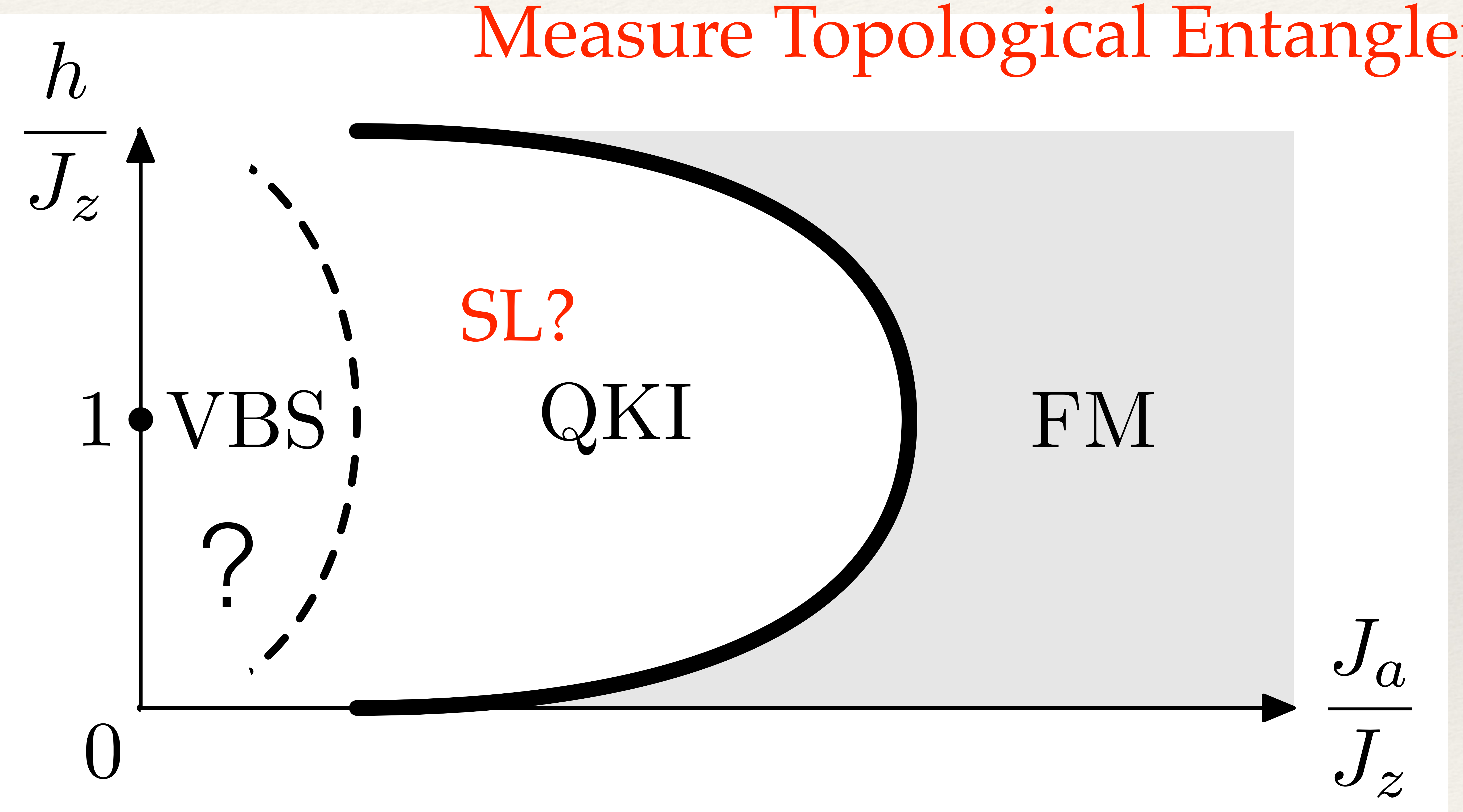
- Inside the lobe:
  - Gapped ground state
  - No long-range order
  - Z_2 quantum spin liquid?



J. Carrasquilla, Z. Hao and R. G. Melko, Nat. Comm. 6, 7421 (2015)

$$H_{\mathrm{XYZh}} = \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} J_z S^z_{\mathbf{r}} S^z_{\mathbf{r}'} - h \sum_{\mathbf{r}} S^z_{\mathbf{r}} - \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} + \frac{J_{\pm\pm}}{2} \left(S^+_{\mathbf{r}} S^+_{\mathbf{r}'} + S^-_{\mathbf{r}} S^-_{\mathbf{r}'} \right)$$

Measure Topological Entanglement Entropy



Y.-P. Huang and M. Hermele, Phys. Rev. B 95, 075130 (2017).

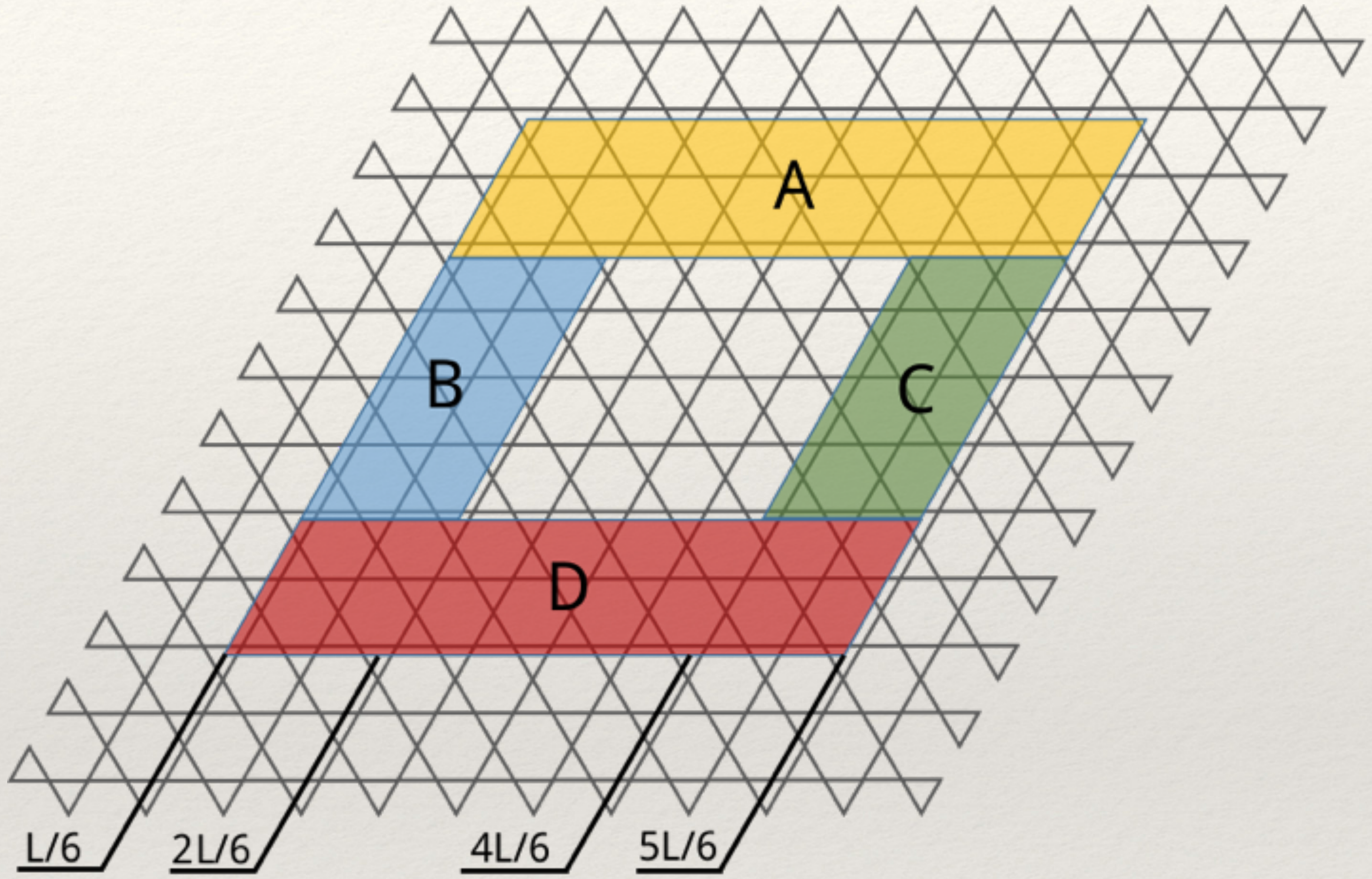
Topological Entanglement Entropy

$$S_A = \boxed{\kappa l} - \alpha\boxed{\gamma} + O(L^{-1})$$

Area law

TEE

$$R_{LC} = A \cap B \cap D$$
$$R_{RC} = A \cap C \cap D$$
$$R_{2T} = A \cap D$$
$$R_O = A \cap B \cap C \cap D$$

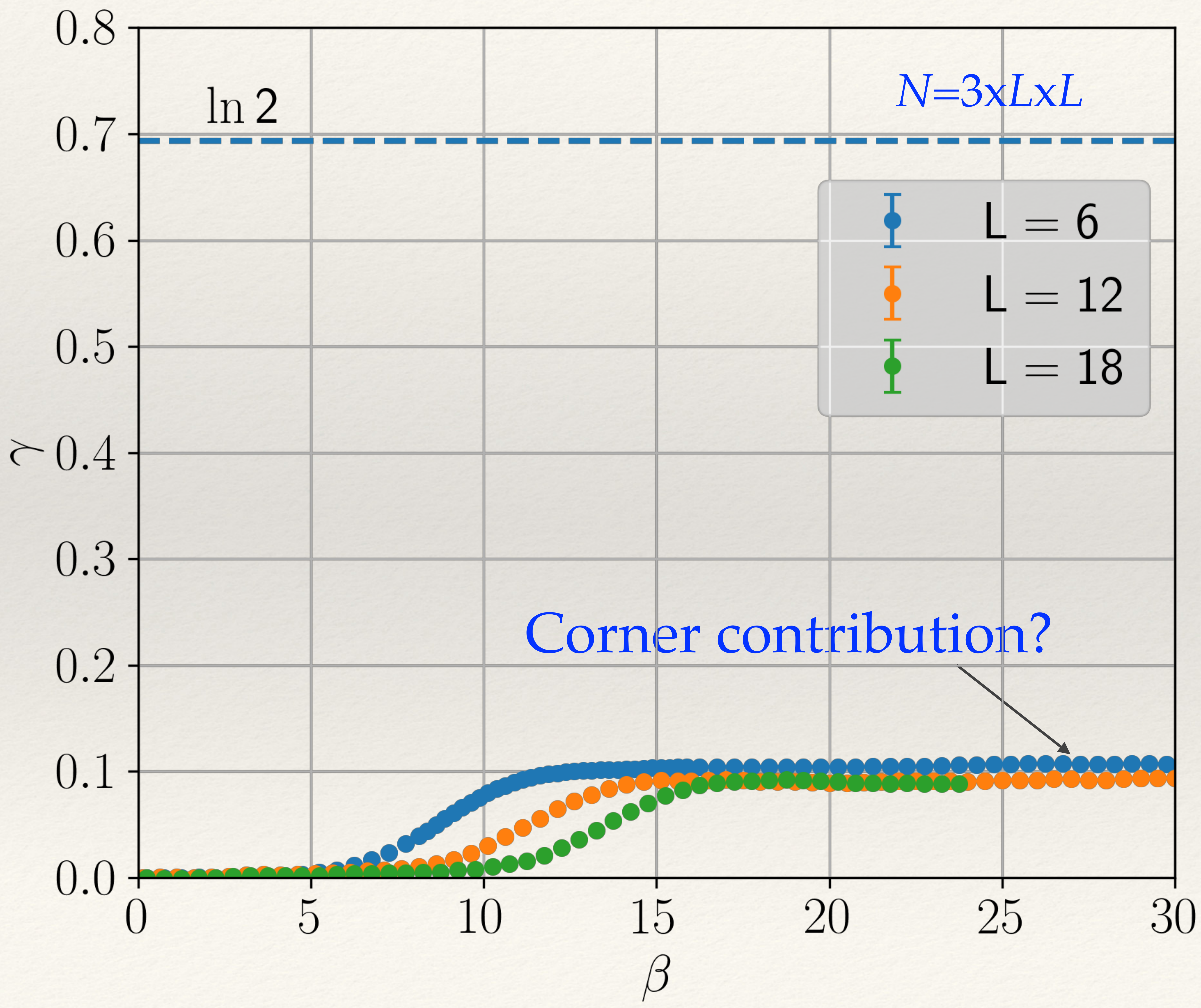


$$2\gamma = -S_2(R_{LC}) - S_2(R_{RC}) + S_2(R_{2T}) + S_2(R_O) \text{ + corner contribution}$$

$$\gamma = \ln(2) \quad \text{for } Z_2 \text{ QSL}$$

M. Levin and X. G. Wen, Phys. Rev. Lett 96, 110405 (2006)
A. Kitaev and J. Preskill, Phys. Rev. Lett. 96, 110404 (2006)
S. V. Isakov, M. B. Hastings and R. G. Melko, Nat. Phys. 7, 772 (2016)

Topological Entanglement Entropy



- Renyi Entropy (n=2)

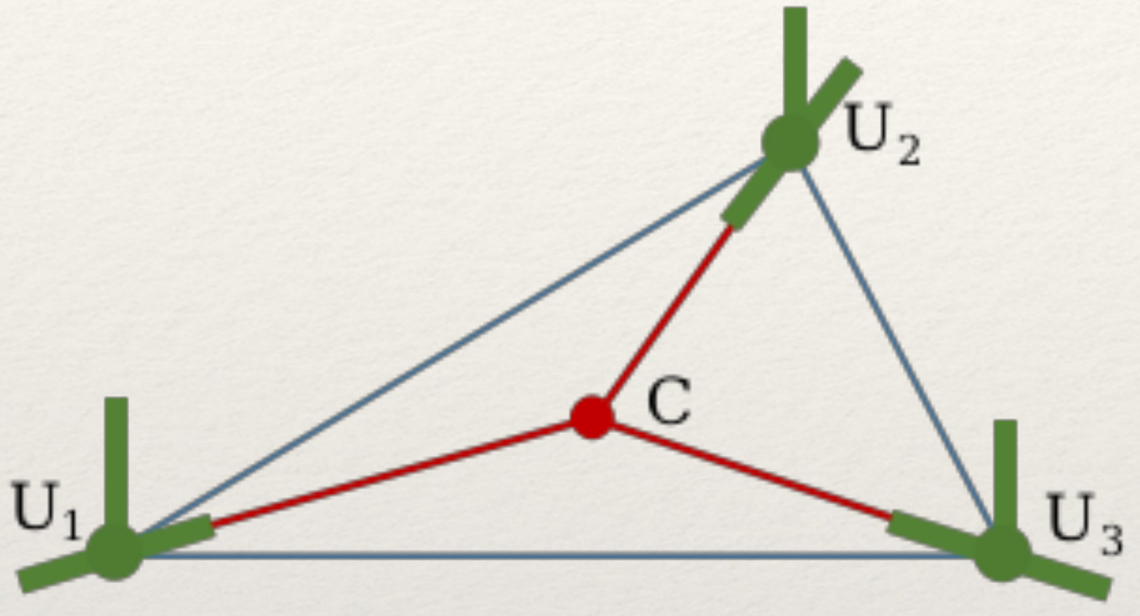
$$S_n(\rho) = \frac{1}{1-n} \ln\left[\mathrm{Tr}(\rho^n)\right]$$

- SSE + replica trick
- TEE is far below expected value for Z_2 topological order
- Not a Z_2 QSL !

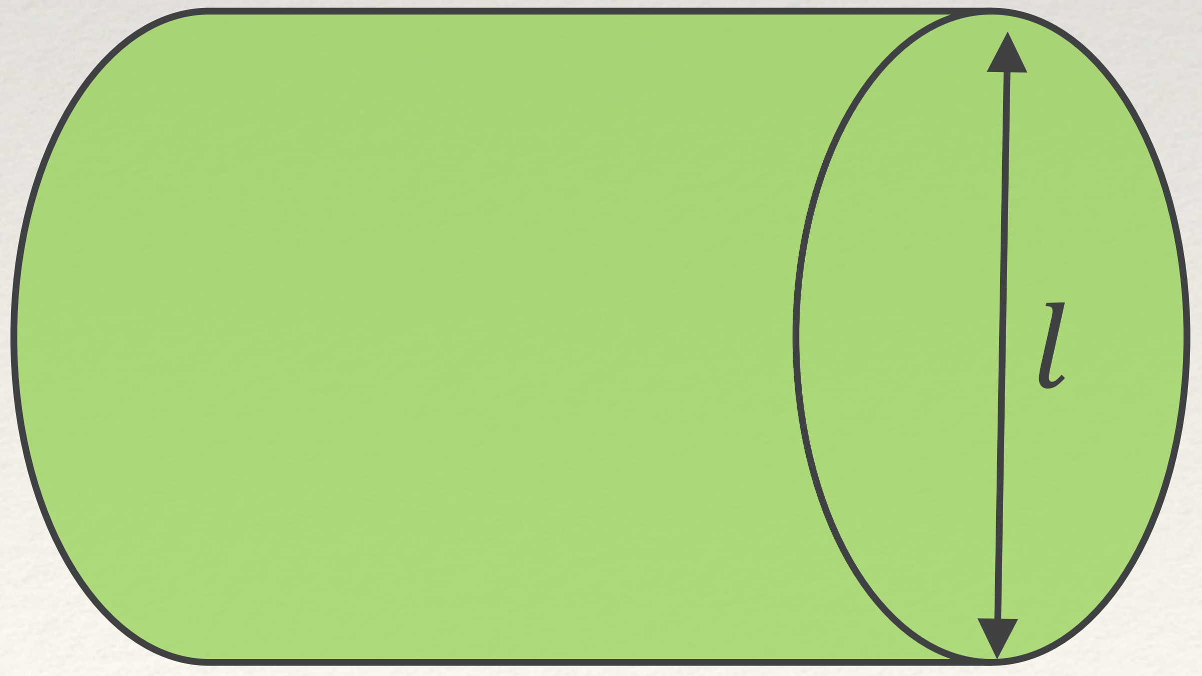
arXiv:1806.08145

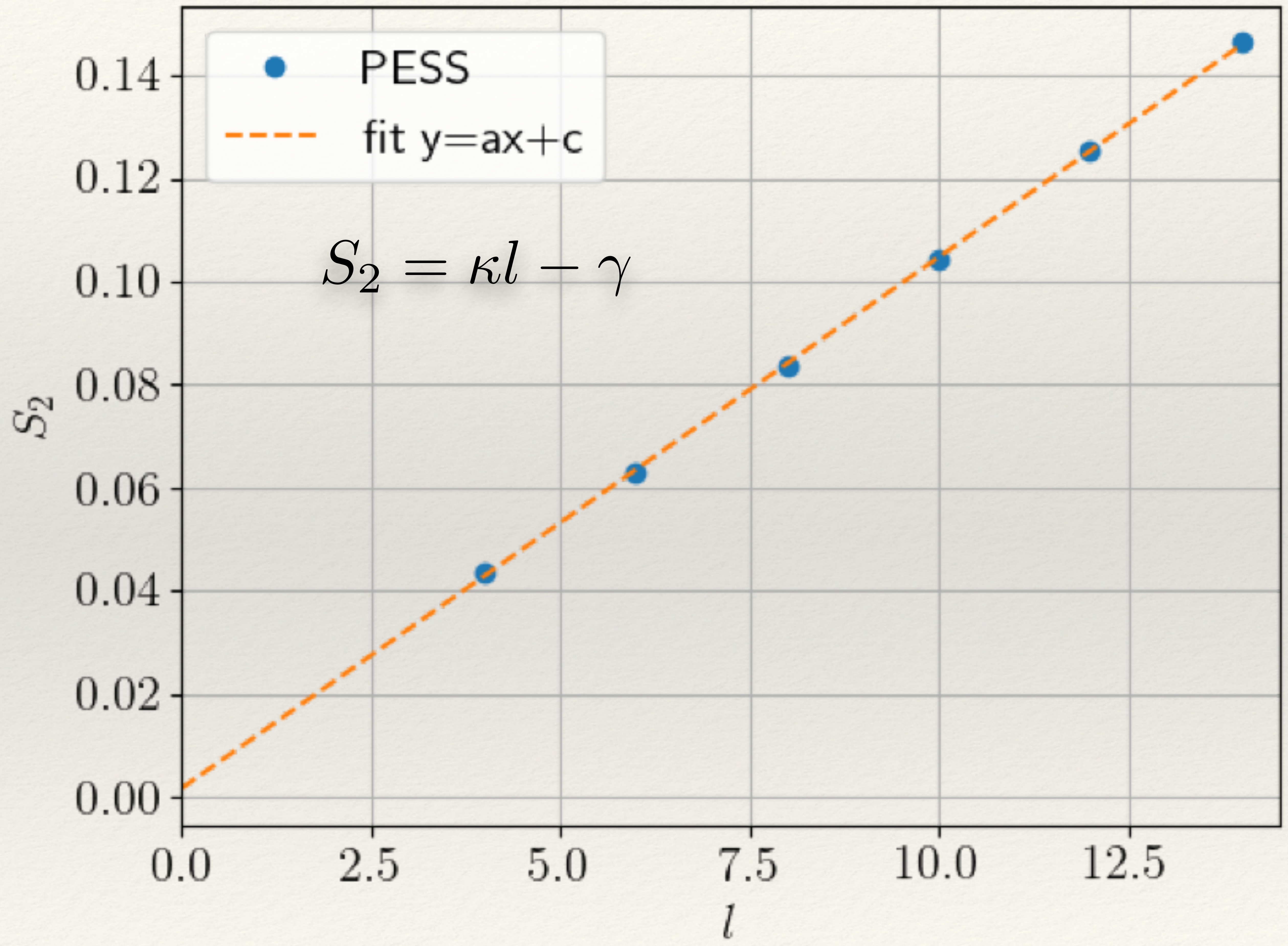
TEE: PESS

Projected entangled-simplex state: 3PESS



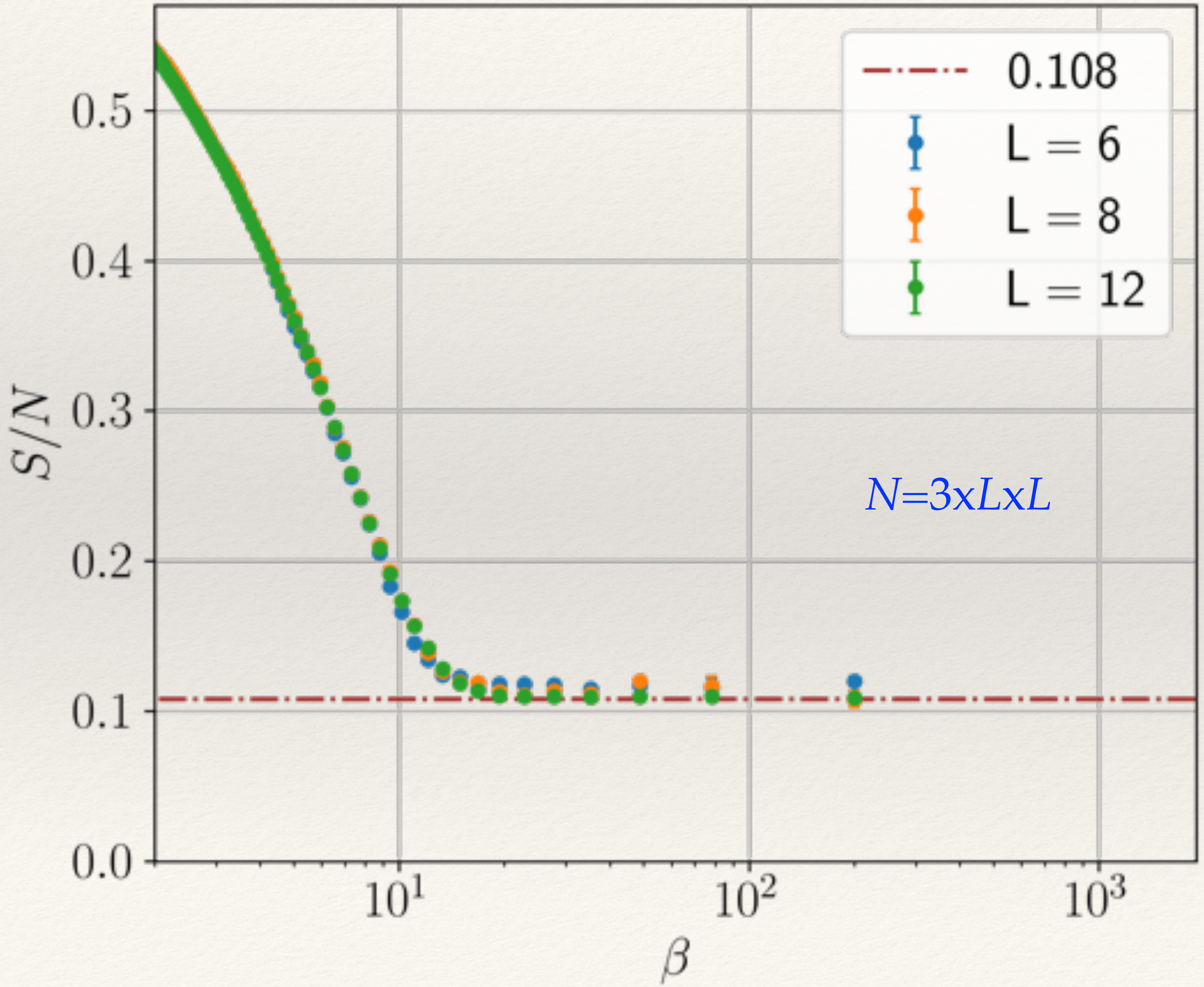
Boundary matrix product state





http://uni10.gitlab.io

Thermal Entropy



- SSE + Wang-Landau method
- Down to β ~ 200
- Need high accuracy data; thus smaller sizes
- Plateau corresponds to the residual entropy of a classical kagome ice with 2-up 1-down in up triangles

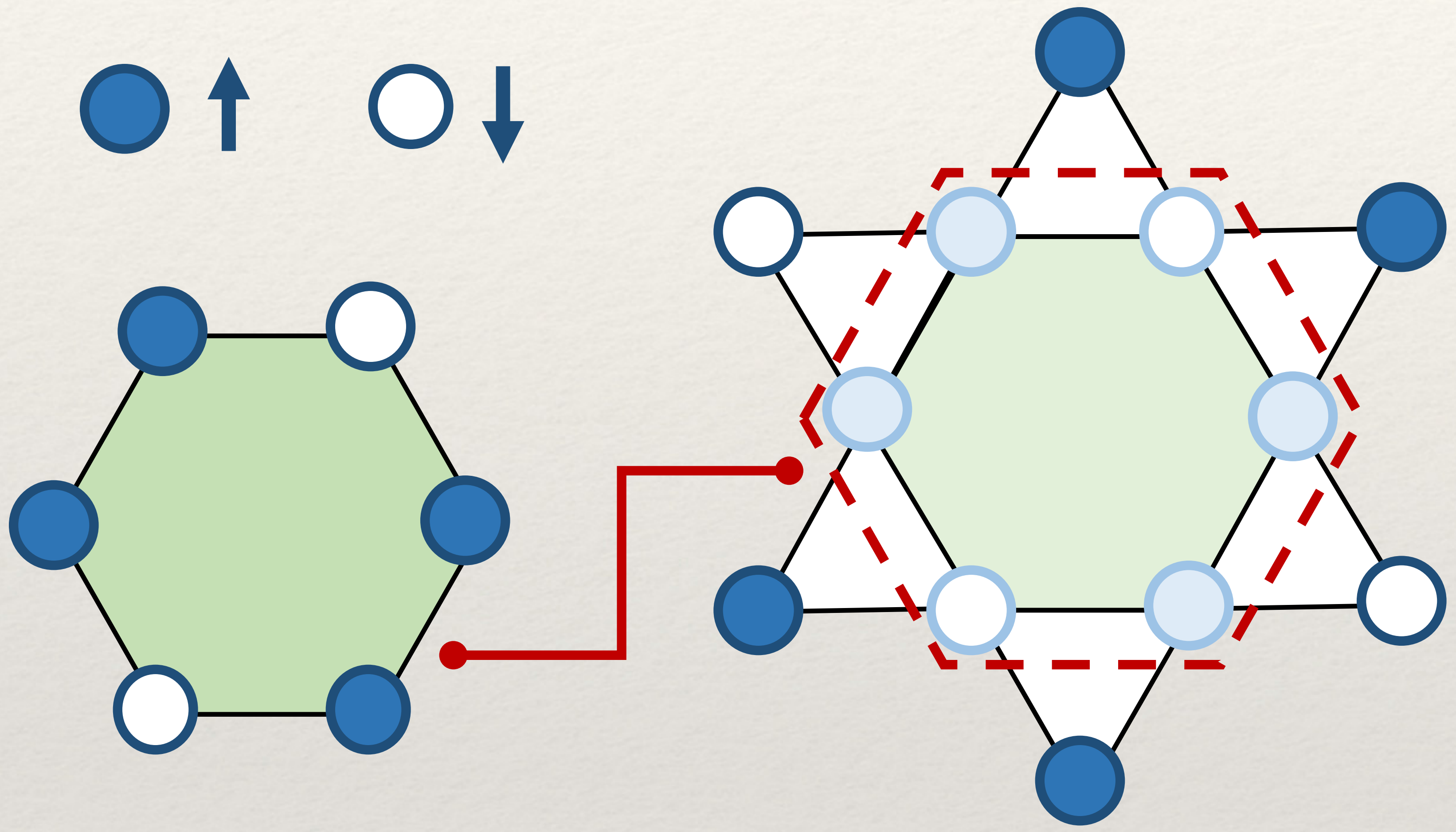
arXiv:1806.08145

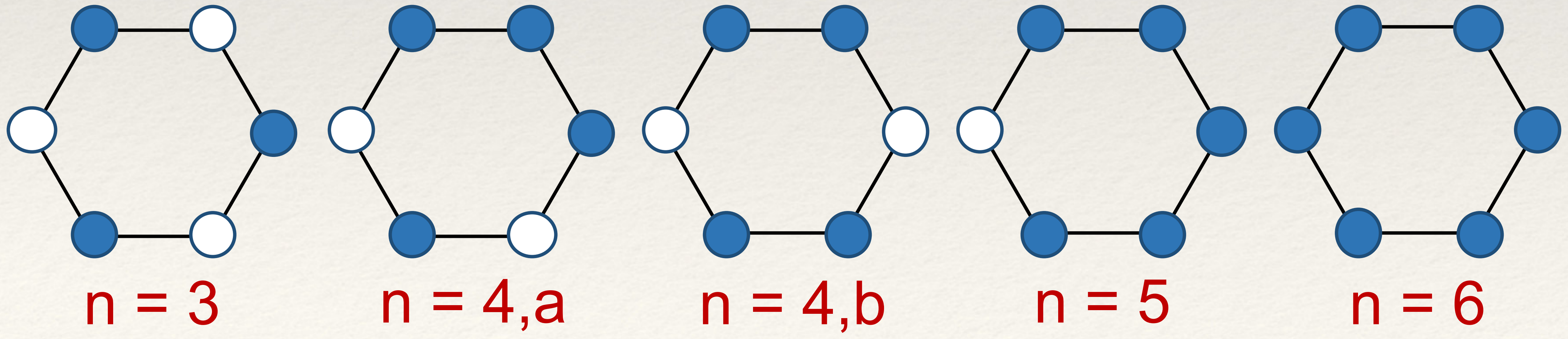
Degenerate Perturbation Theory

$$H = \sum_{\langle i,j\rangle} S_z^i S_z^j - h\sum_i S_z^i + V \qquad V = \begin{cases} +\sum_{\langle ij\rangle} J_{\pm\pm}\left(S_i^+ S_j^+ + \text{h.c}\right) \\ -\sum_{\langle ij\rangle} J_{\pm}\left(S_i^+ S_j^- + \text{h.c}\right) \end{cases}$$

- Quantum term V as a perturbation acting on the classical ice-manifold
- Non-zero Zeeman field
- Find the lowest non-trivial order that lift the classical degeneracy
- Possible emergent quantum phases

Classical Ice Manifold

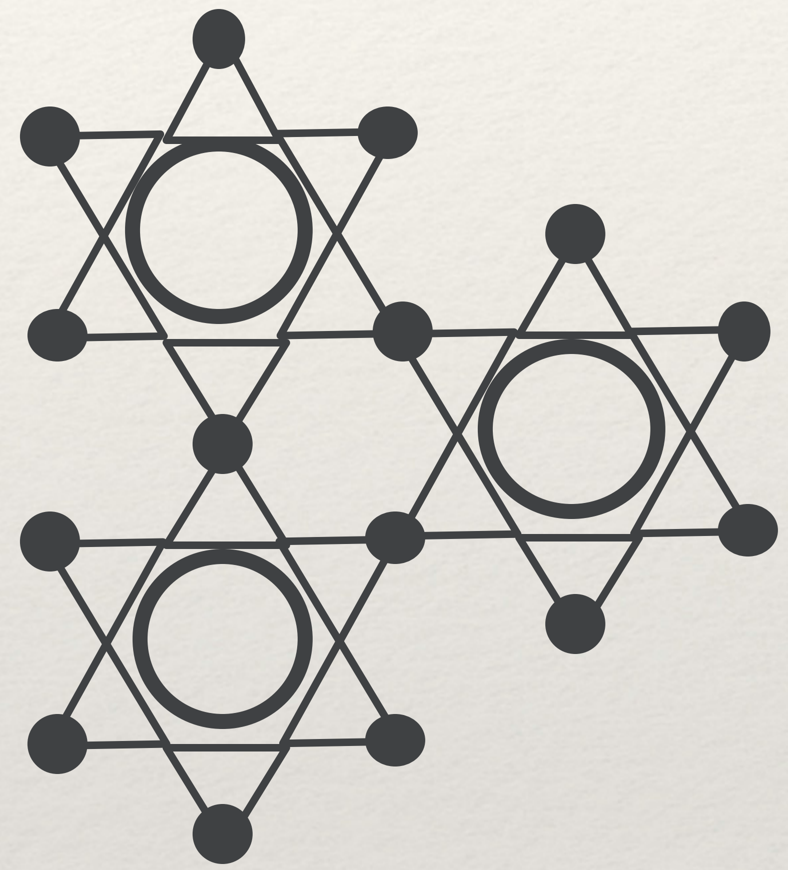




- Finite Zeeman field: only 2-up 1-down configuration is allowed on up triangles
- Hexagon as a basic unit
- Five possible hexagon configurations

Non-trivial Processes

$$H = \sum_{\langle ij \rangle} S_i^z S_j^z - h \sum_i S_i^z + \sum_{\langle ij \rangle} J_{\pm\pm} \left(S_i^+ S_j^+ + \mathrm{h.c} \right)$$



Lowest non-trivial order: **sixth** order perturbation

Non-trivial diagonal processes

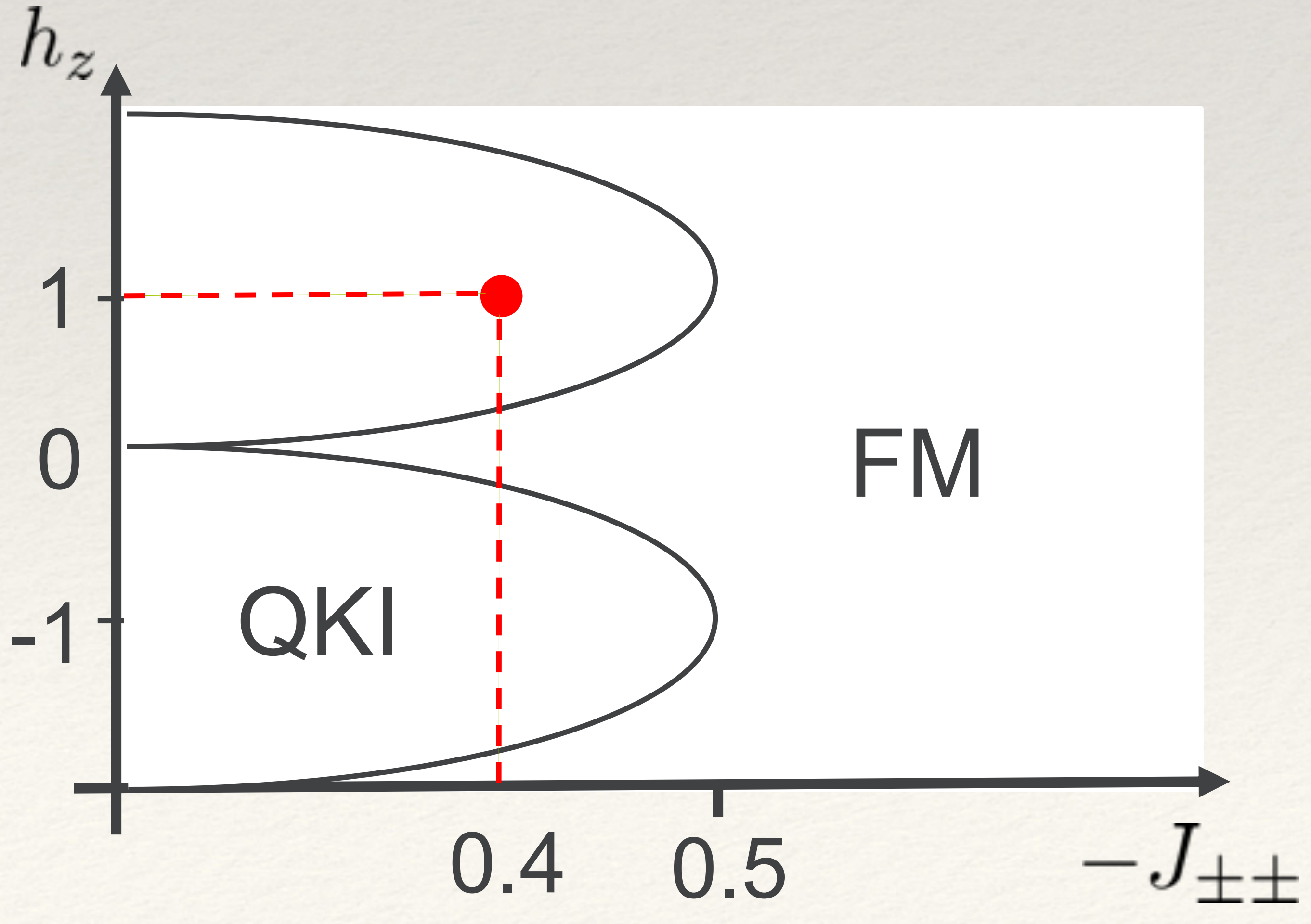
$$\hat{P}_6 = \underbrace{\boxed{D_{4,a} \sum_{\forall \hexagon n=4,a} H_{\hexagon, n=4,a} + D_{4,b} \sum_{\forall \hexagon n=4,b} H_{\hexagon, n=4,b} + D_5 \sum_{\forall \hexagon n=5} H_{\hexagon, n=5} + D_6 \sum_{\forall \hexagon n=6} H_{\hexagon, n=6}}}_{H_d} + \underbrace{\boxed{K_{pp} \sum_{\forall \hexagon n=3} H_{\hexagon}}}_{H_o}$$

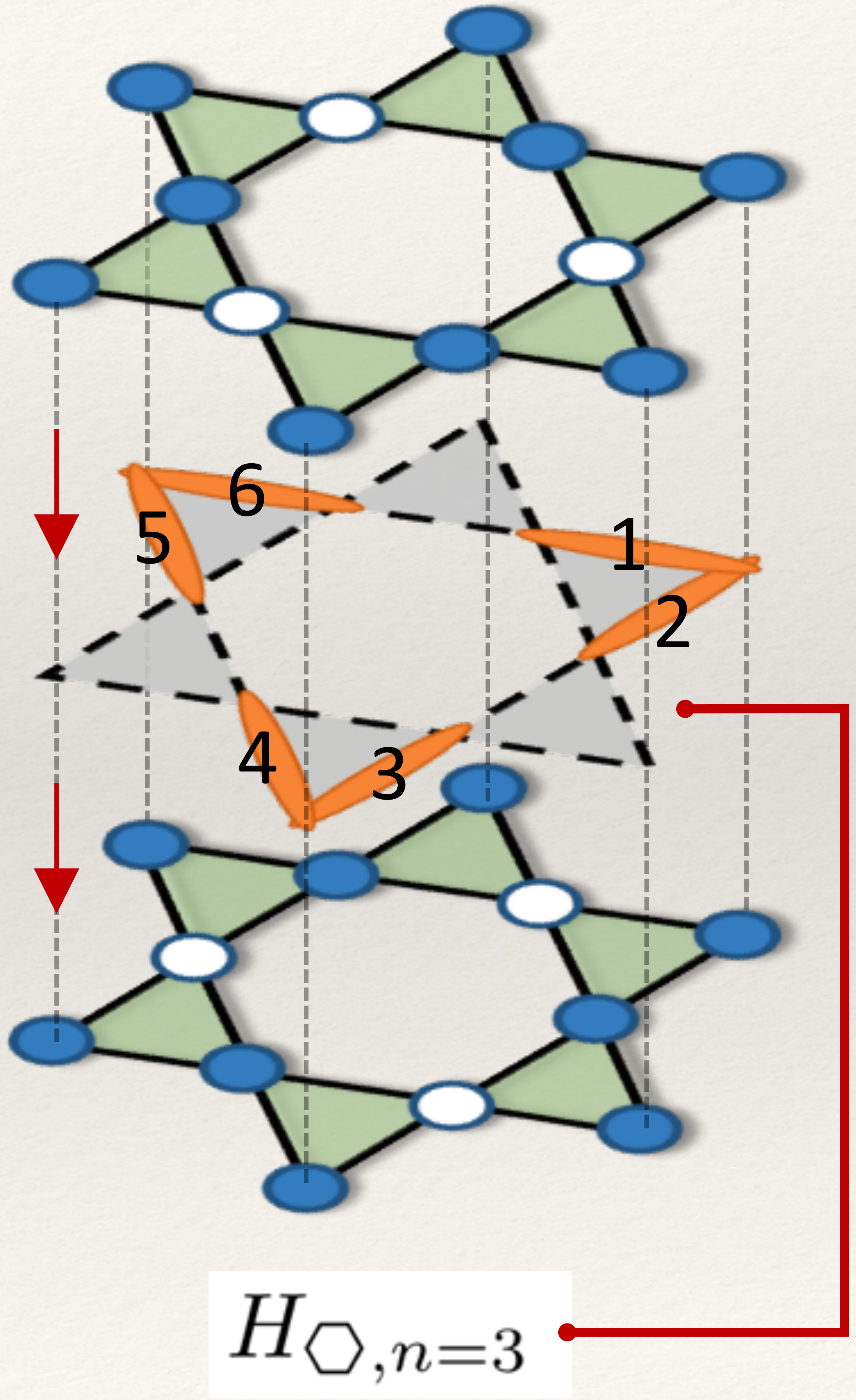
Off-diagonal Process

$$K_{pp} \sum_{\forall \hexagon n=3} H_{\hexagon, n=3}$$

$$K_{pp} = -\frac{6J_{\pm\pm}^6}{J_z^2(2h+J_z)^5}\left[7J_z^2 + 14J_z h + 8h^2\right]$$

$$= -\frac{58}{81}\frac{J_{\pm\pm}^6}{J_z^5} \text{ for } h = J_z$$





Diagonal Processes

$$D_{4,a} \sum_{\forall \hexagon n=4,a} H_{\hexagon,n=4,a} + D_{4,b} \sum_{\forall \hexagon n=4,b} H_{\hexagon,n=4,b} + D_5 \sum_{\forall \hexagon n=5} H_{\hexagon,n=5} + D_6 \sum_{\forall \hexagon n=6} H_{\hexagon,n=6}$$

For $h = J_z$

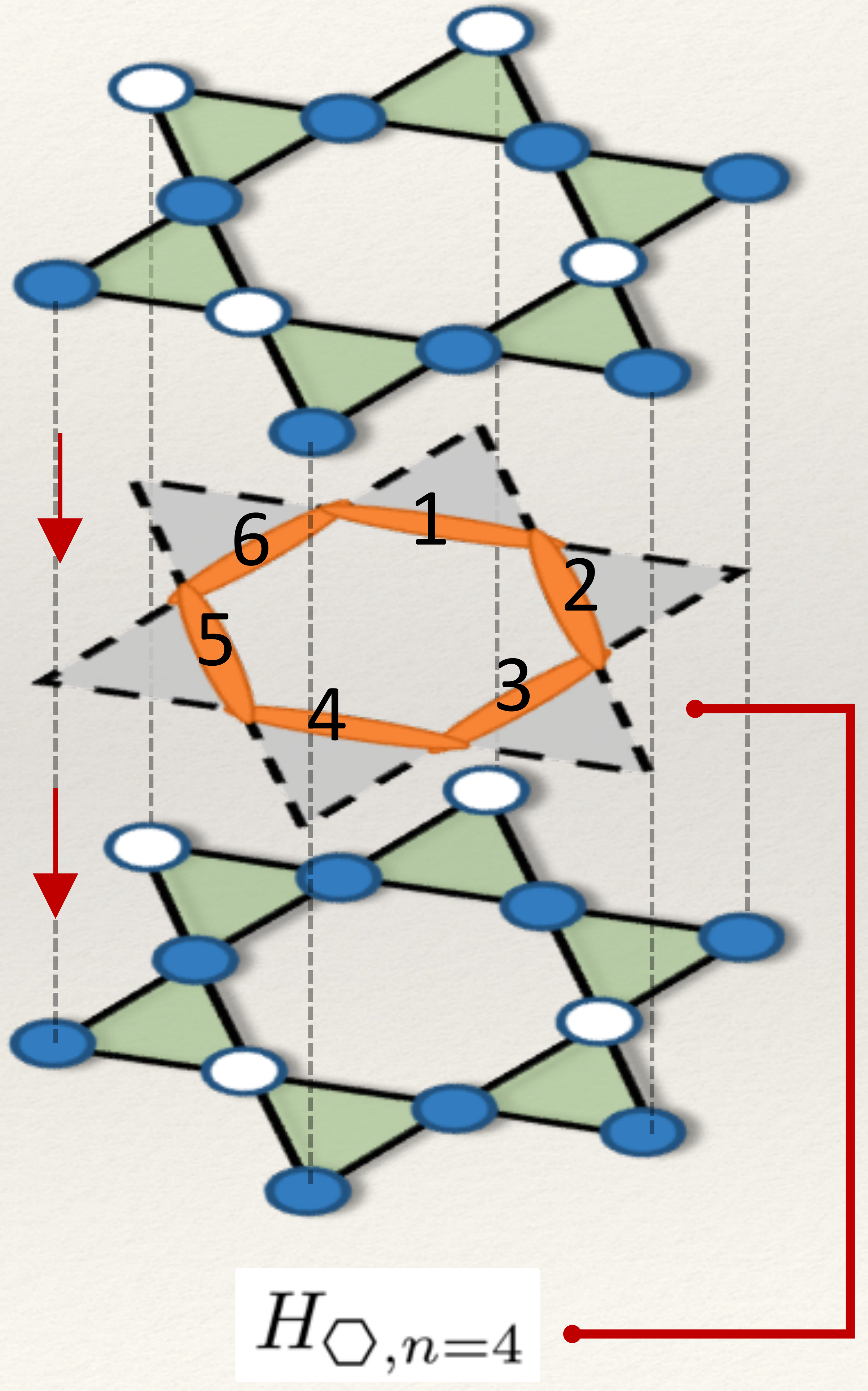
$$K_{pp} = -\frac{58}{81}\frac{J_{\pm\pm}^6}{J_z^5}$$ favors **n=3** hexagons

$$D_{4,a} = -\frac{1}{36}\frac{J_{\pm\pm}^6}{J_z^5}$$ **n=4**

$$D_{4,b} = -\frac{1}{6}\frac{J_{\pm\pm}^6}{J_z^5}$$

$$D_5 = -\frac{289}{5292}\frac{J_{\pm\pm}^6}{J_z^5}$$ **n=5**

$$D_6 = -\frac{2}{49}\frac{J_{\pm\pm}^6}{J_z^5}$$ **n=6**



On the other hand

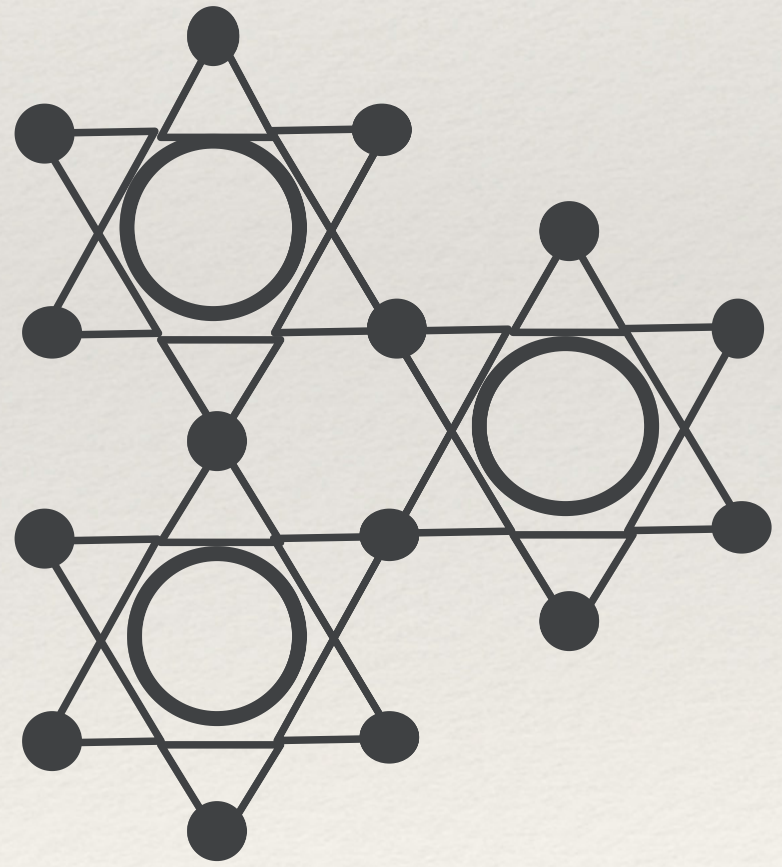
$$H = \sum_{\langle ij \rangle} S_i^z S_j^z - h \sum_i S_i^z - \sum_{\langle ij \rangle} J_{\pm} \left(S_i^+ S_j^- + \mathrm{h.c} \right)$$

Lowest non-trivial order: **third** order perturbation

$$\hat{P}_3 = K_{np} \sum_{\forall \hexagon n=3} H_{\hexagon, n=3} + c$$

Non-trivial diagonal processes are higher order

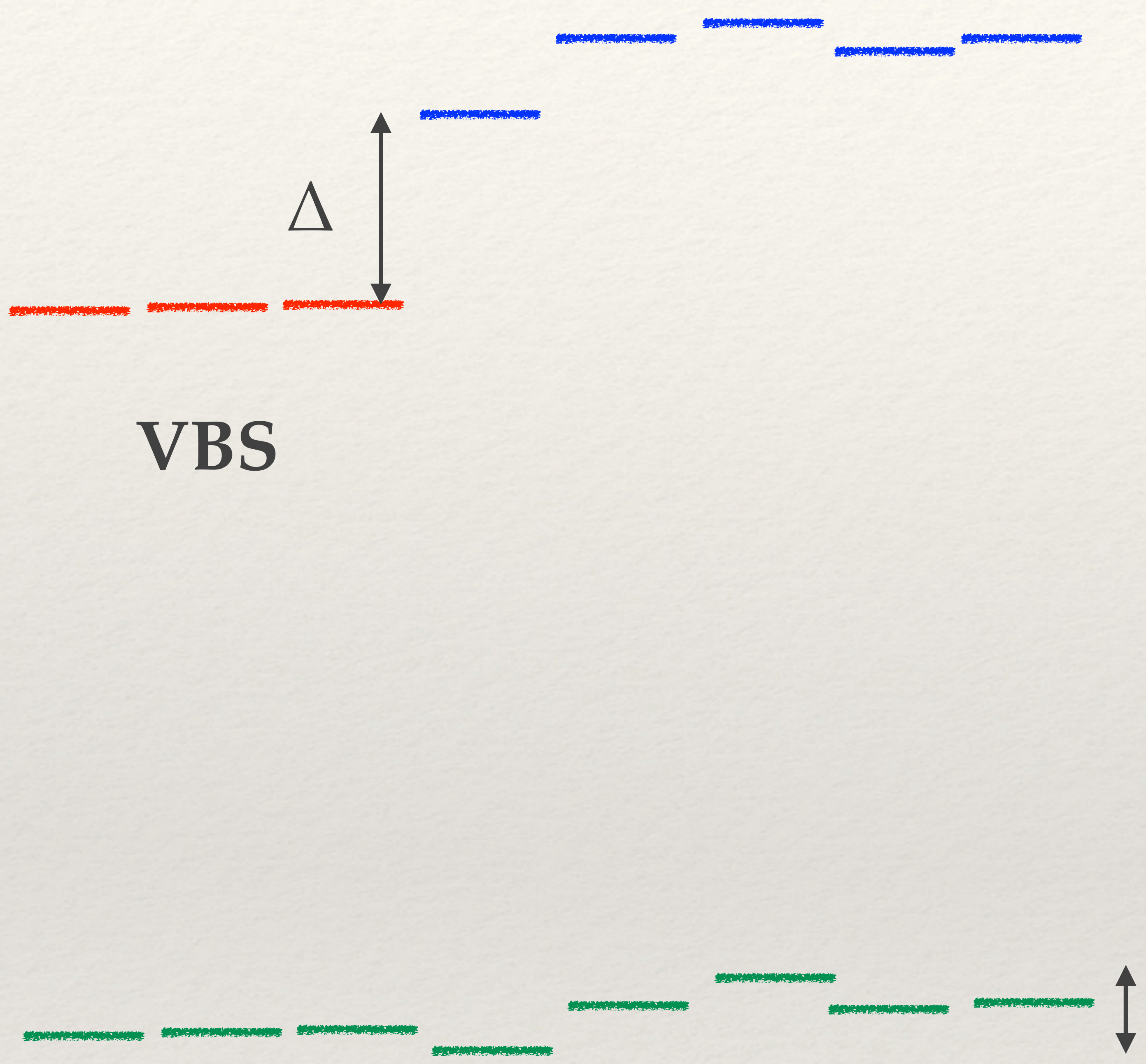
$$K_{np} = -12 \frac{J_{\pm}^3}{J_z^2}$$



VBS

S. V. Isakov, et al., Phys. Rev. Lett. 97, 147202 (2006).

Classical kagome ice manifold



Add $\quad K_{pp} \sum_{\forall \hexagon n=3} H_{\hexagon, n=3} \quad$ or $\quad K_{np} \sum_{\forall \hexagon n=3} H_{\hexagon, n=3}$

Add $$D_{4,a} \sum_{\forall \hexagon n=4,a} H_{\hexagon, n=4,a} + D_{4,b} \sum_{\forall \hexagon n=4,b} H_{\hexagon, n=4,b} + D_5 \sum_{\forall \hexagon n=5} H_{\hexagon, n=5} + D_6 \sum_{\forall \hexagon n=6} H_{\hexagon, n=6}$$

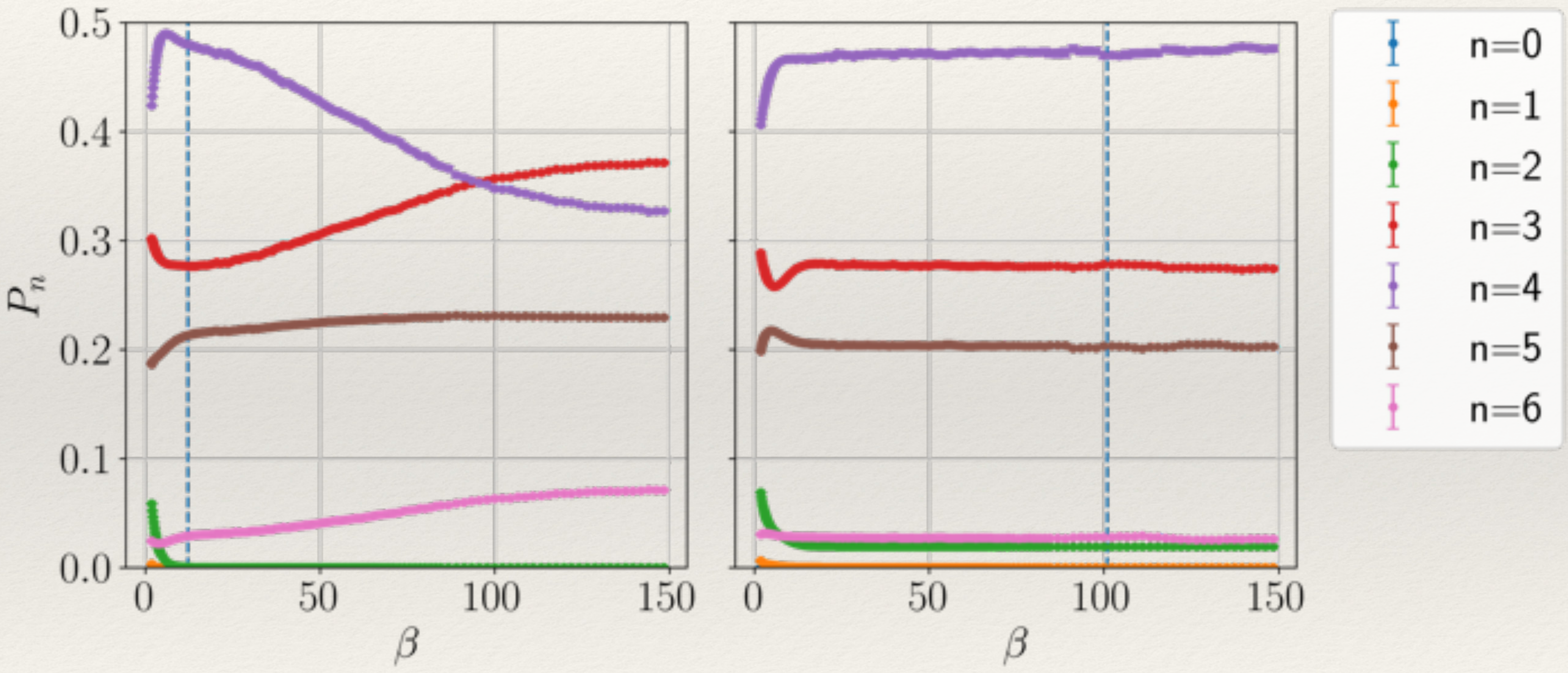
Quasi-degenerate spectrum

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

Hexagon Fractions

- $P_{\mathbf{n}}$: fraction of hexagons with n up spins

VBS $J_{\pm\pm} = 0$ **QKI** $J_{\pm} = 0$



$$H_{\mathrm{XYZ}} = \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} J_z S^z_{\mathbf{r}} S^z_{\mathbf{r}'} - \frac{J_\pm}{2}\left(S^+_{\mathbf{r}} S^-_{\mathbf{r}'} + S^-_{\mathbf{r}} S^+_{\mathbf{r}'}\right) + \frac{J_{\pm\pm}}{2}\left(S^+_{\mathbf{r}} S^+_{\mathbf{r}'} + S^-_{\mathbf{r}} S^-_{\mathbf{r}'}\right) - h \sum_{\mathbf{r}} S^z_{\mathbf{r}}$$

arXiv:1806.08145

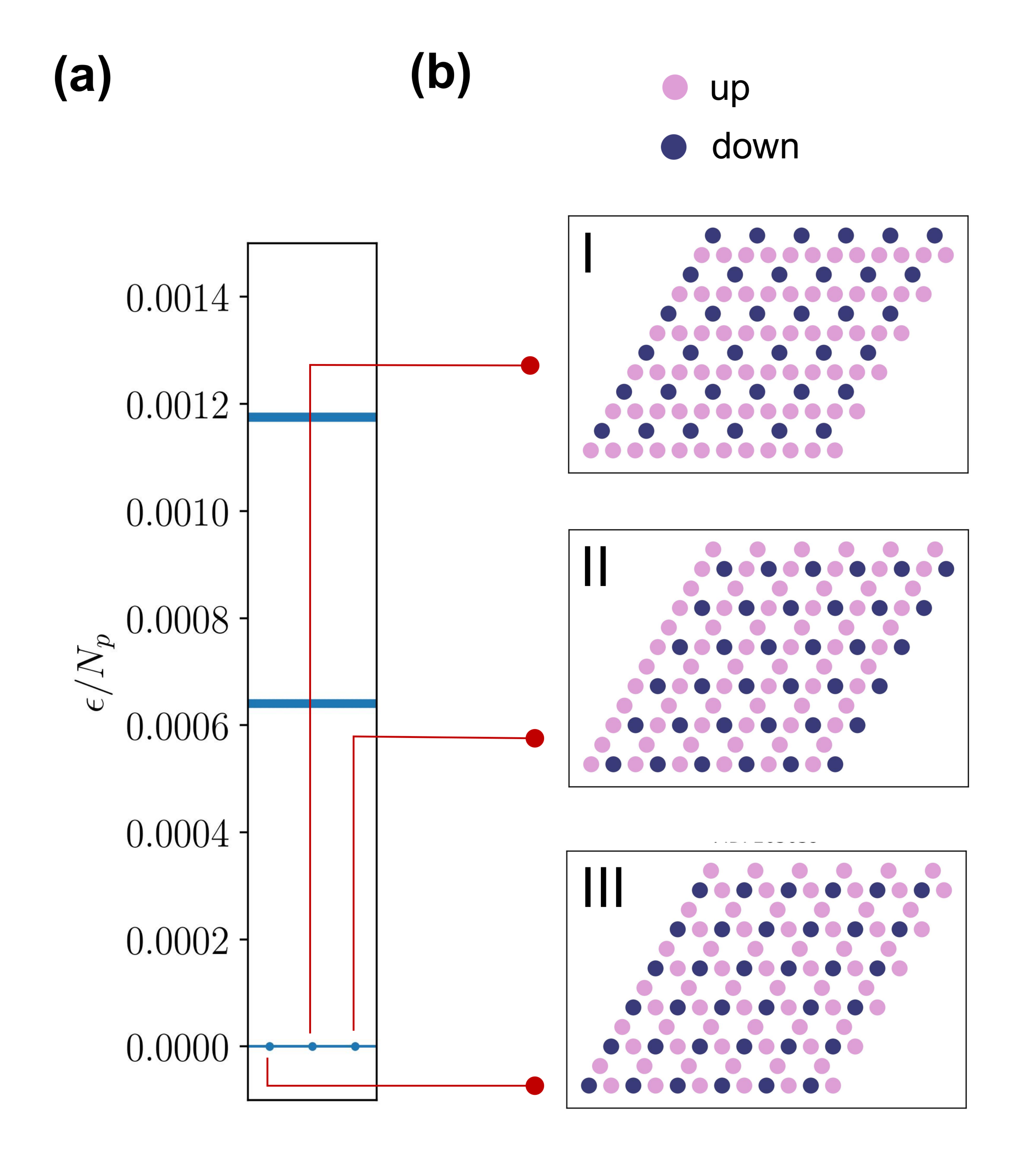
Effective Hamiltonian

$$\hat{P}_6 = H_d + H_o \quad \longrightarrow \quad \hat{P}'_6(\alpha) = H_o + \alpha H_d$$

- Effect is non-perturbative as shown in the QMC results
- Study the spectrum of the effective Hamiltonian, derived from degenerate perturbation theory, tuning the relative weights of diagonal and off-diagonal processes.
- Should see the states piling toward the ground state at some α

$$\hat{P}'_6(\alpha \to \infty) \to H_d$$

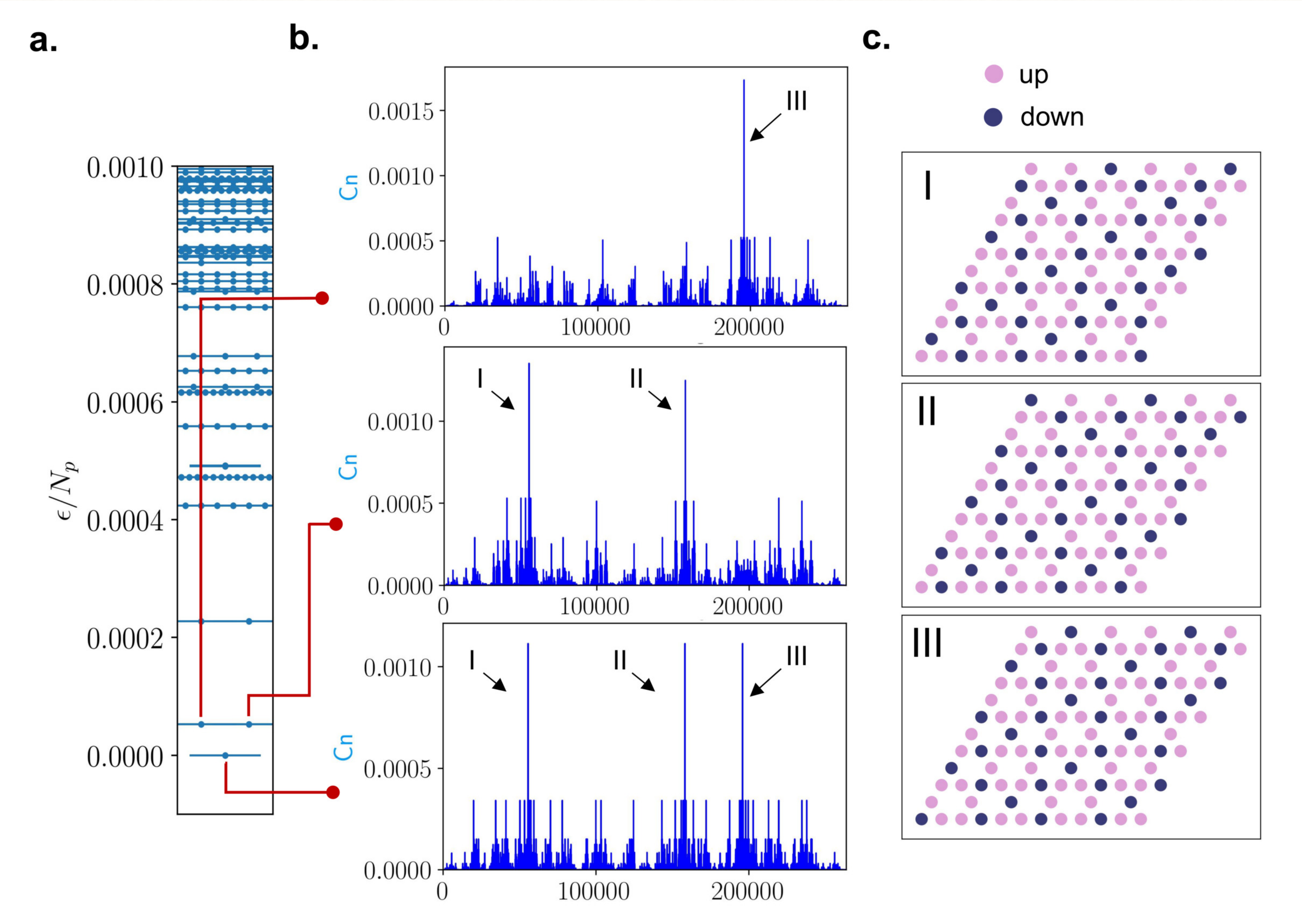
- Classical potential energy
- Three-fold degenerate charge-ordered states with n=4 hexagons in classical kagome ice



$$\hat{P}'_6(\alpha = 0) = H_o$$

- Three-fold degenerate VBS ground state in thermodynamic limit (Finite-size gap)

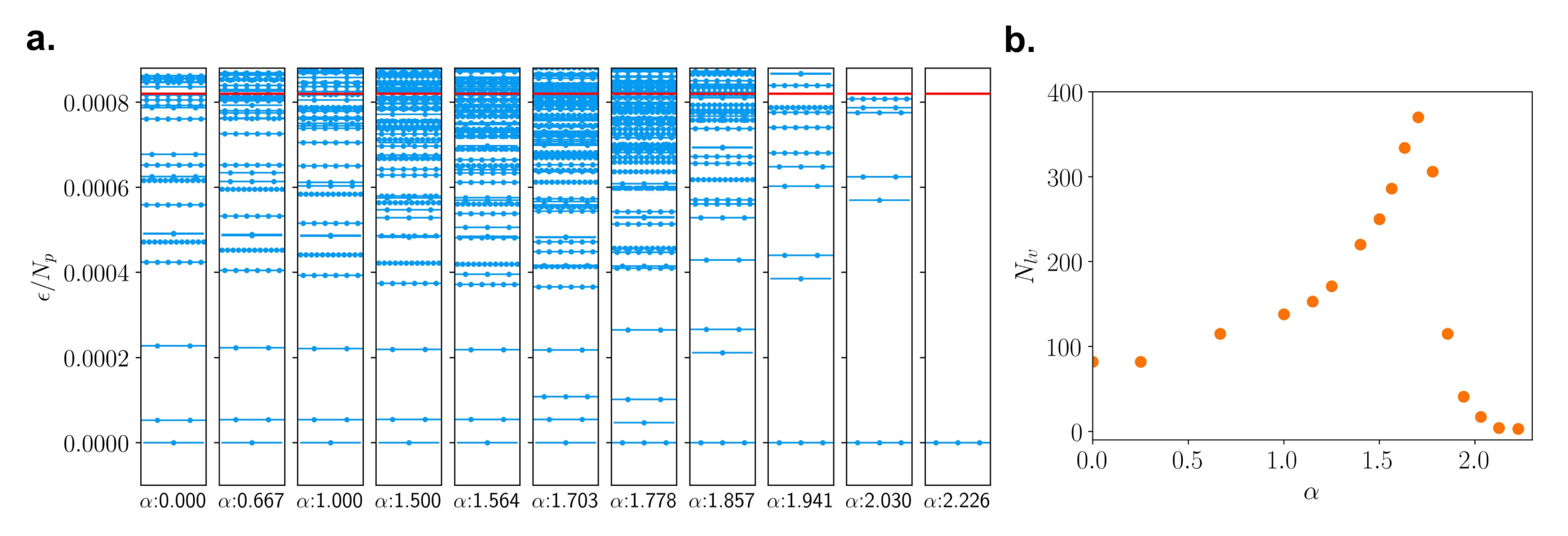
- Admixing of states with n=3 hexagons with the dominant component from classical $\sqrt{3}\times\sqrt{3}$ ordered states



ED of effective Hamiltonian

$$\hat{P}_6 = H_d + H_o \quad \Rightarrow \quad \hat{P}'_6(\alpha) = H_o + \alpha H_d$$

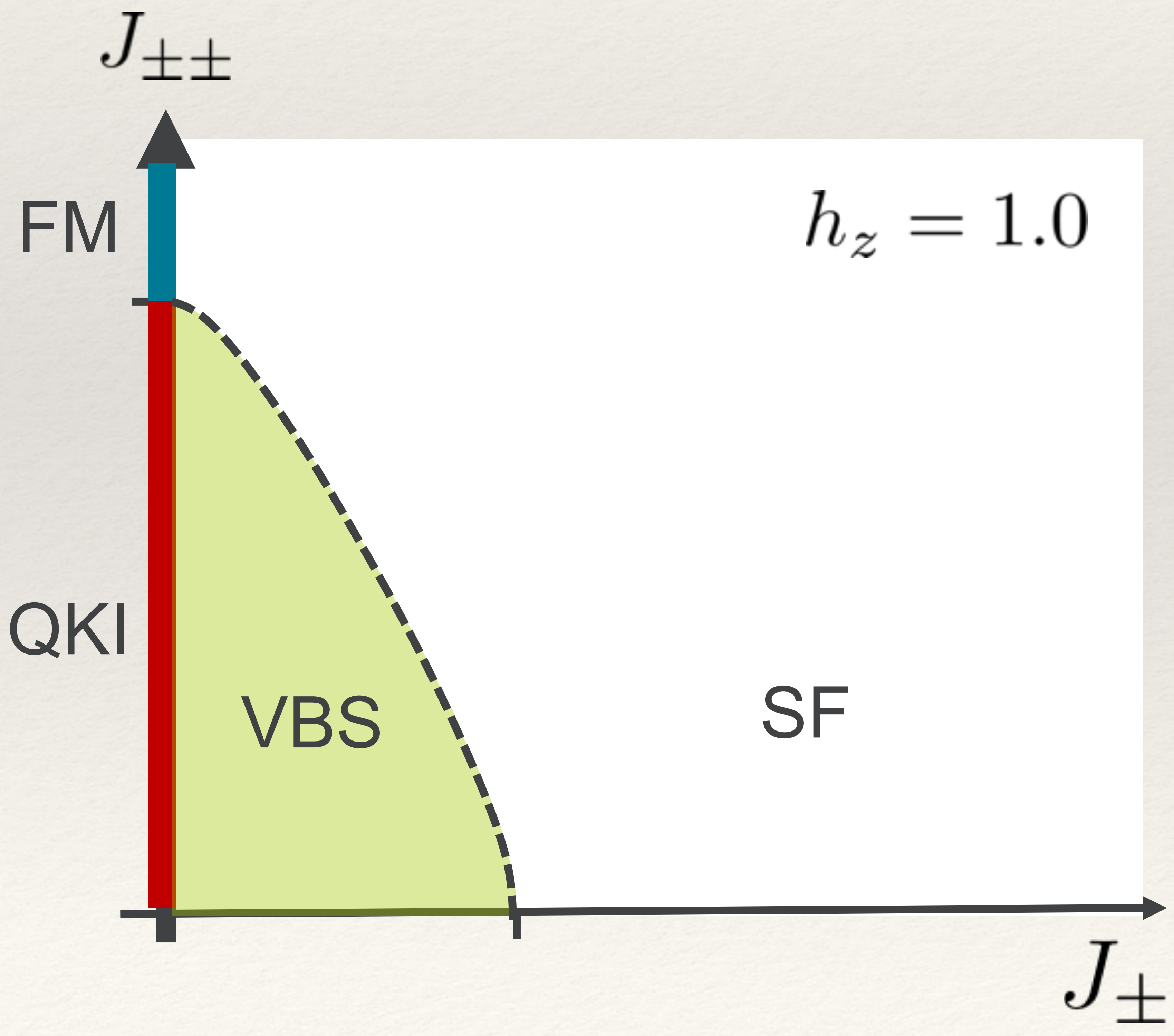
N=3x6x6



Valence Bond Solid

$$H_{\text{XYZ}} = \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} J_z S^z_{\mathbf{r}} S^z_{\mathbf{r}'} - \frac{J_\pm}{2} \left(S^+_{\mathbf{r}} S^-_{\mathbf{r}'} + S^-_{\mathbf{r}} S^+_{\mathbf{r}'} \right) + \frac{J_{\pm\pm}}{2} \left(S^+_{\mathbf{r}} S^+_{\mathbf{r}'} + S^-_{\mathbf{r}} S^-_{\mathbf{r}'} \right) - h \sum_{\mathbf{r}} S^z_{\mathbf{r}}$$

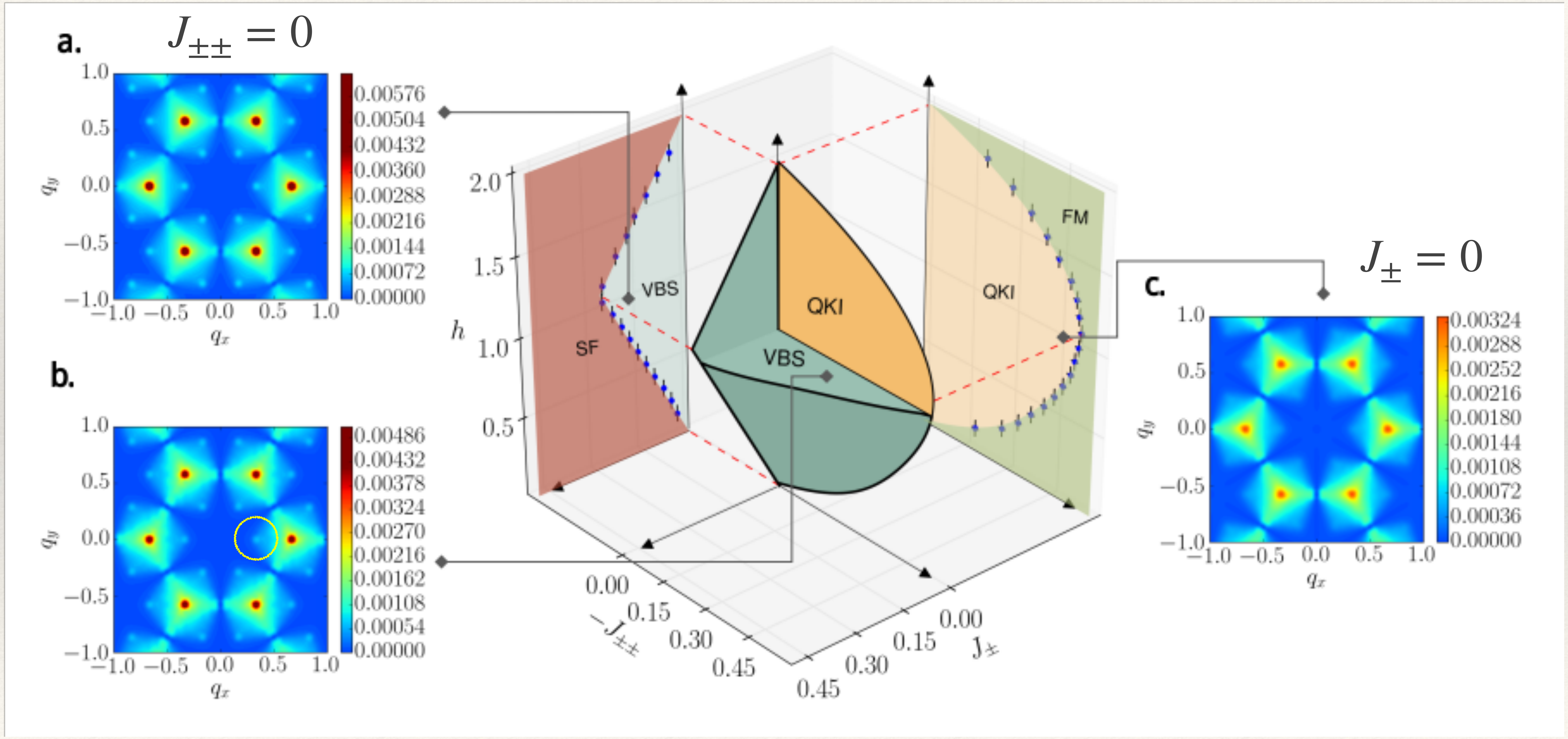
Add hopping term $J_\pm > 0$



- VBS order emerges when $J_\pm$ is added.
- VBS to superfuild transition.

S. V. Isakov, et al., Phys. Rev. Lett. 97, 147202 (2006)

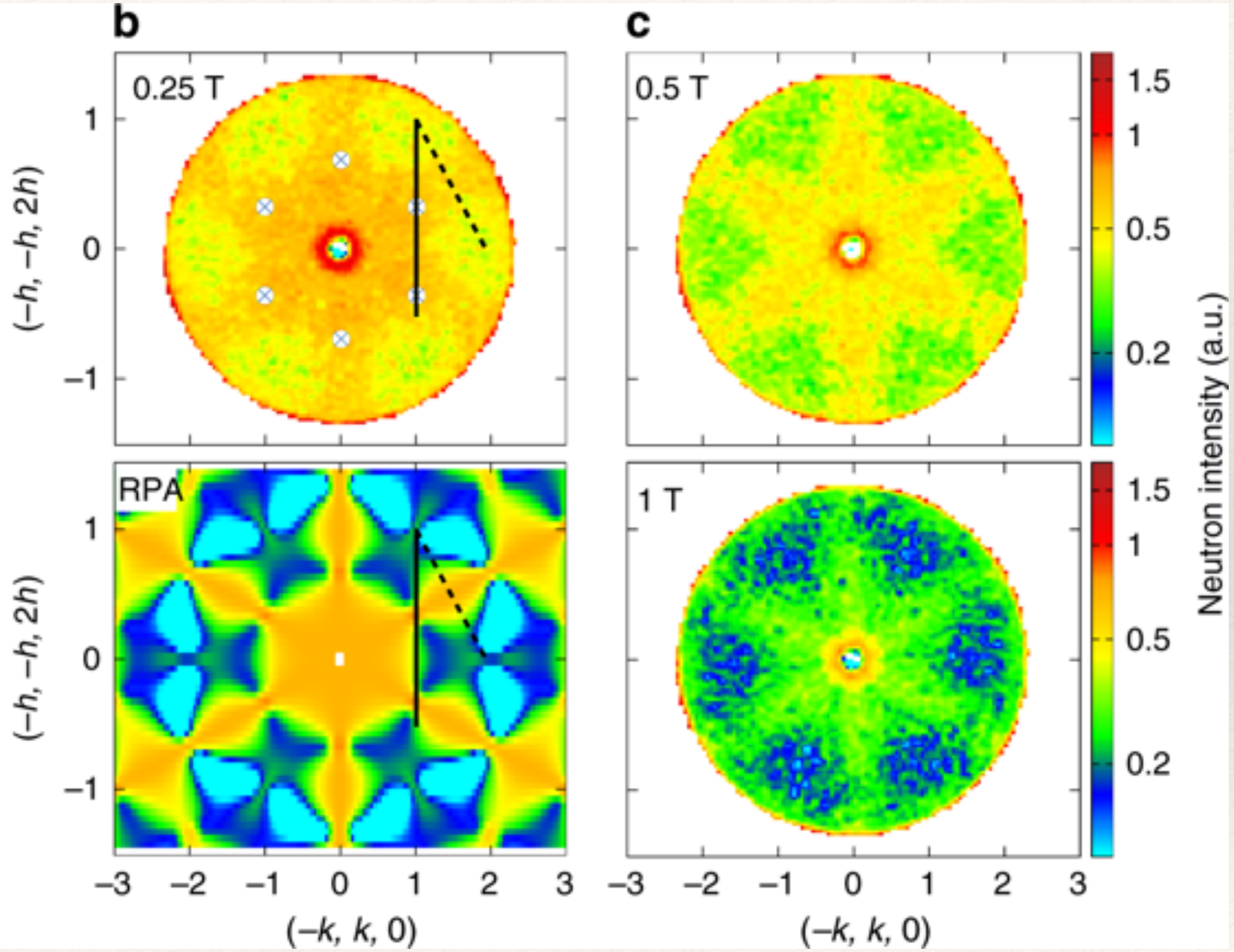
$$H_{\mathrm{XYZ}} = \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} J_z S^z_{\mathbf{r}} S^z_{\mathbf{r}'} - \frac{J_{\pm}}{2}\left(S^+_{\mathbf{r}} S^-_{\mathbf{r}'} + S^-_{\mathbf{r}} S^+_{\mathbf{r}'}\right) + \frac{J_{\pm\pm}}{2}\left(S^+_{\mathbf{r}} S^+_{\mathbf{r}'} + S^-_{\mathbf{r}} S^-_{\mathbf{r}'}\right) - h\sum_{\mathbf{r}} S^z_{\mathbf{r}}$$



arXiv:1806.08145

Dynamic Kagome Ice in $Nd_2Zr_2O_7$

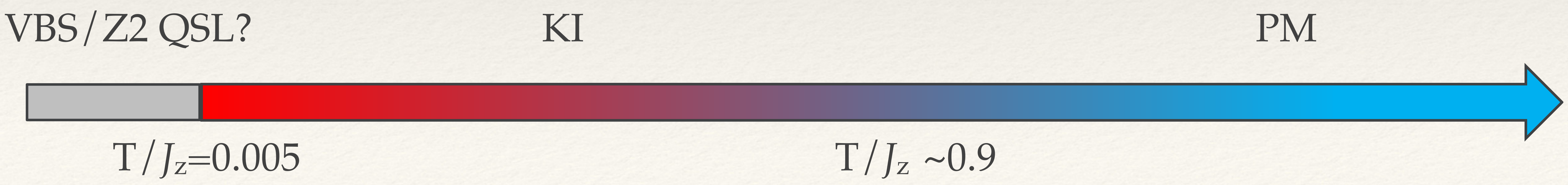
- Dynamic kagome ice state seen in inelastic neutron scattering in [111] field.
- Inelastic intensity averaged around E = (50 ± 5) μeV
- Expected pinch points blurred.



E. Lhotel, et al. Nat

Conclusions

- QKI state is not a Z_2 QSL.
- System remains classical due to diagonal processes at the same order.
- Rare case for a quantum model to stay classical down to very low *T*.
- Semi-classical model reproduces correlations.
- Quasi-degeneracy at low *T* due to competition two processes.
- What is the true ground state? Difficult to probe numerically or experimentally.
- Dynamic Kagome ice in $Nd_2Zr_2O_7$?



arXiv:1806.08145