Quantum phase transition between spin liquid and spin nematics in spin-1 Kitaev honeycomb model

（スピン-1ハニカム格子模型における キタエフスピン液体-スピンネマティック秩序相転移）

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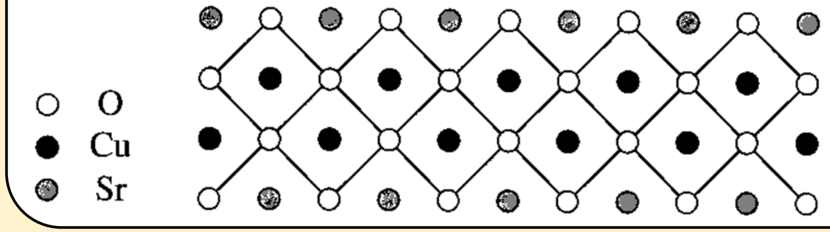
T. Mashiko and T. Okubo, Phys. Rev. Res. 6, 033110 (2024).

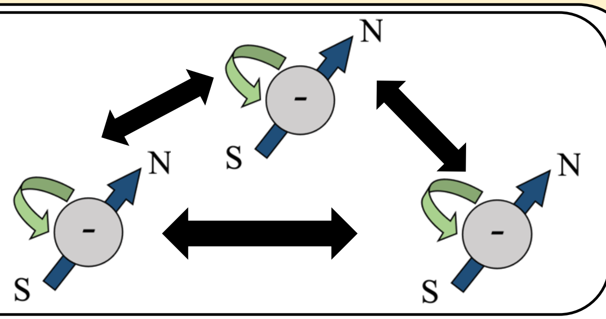
1. Intro: Quantum spin system

Quantum spin system

Many body system composed of quantum spins

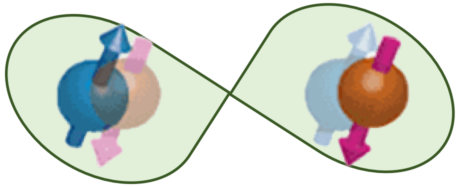
Cryogenic magnets （Sr_2CuO_3 etc）



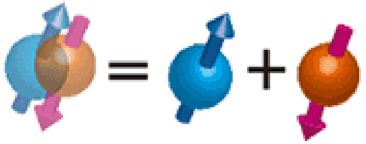


Quantum spin liquid：Quantum state of solid matters, in which electronic spins fluctuate without showing any long-range order even at zero temperature

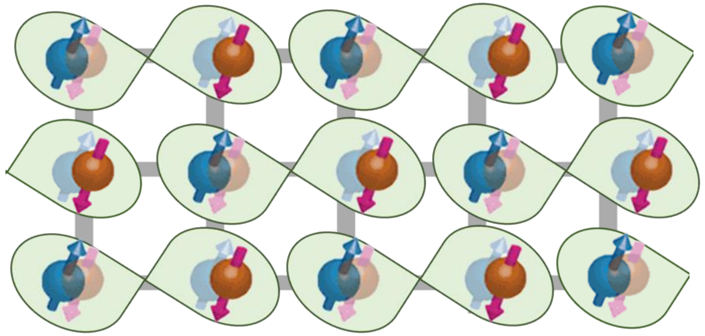
Entanglement



Composition



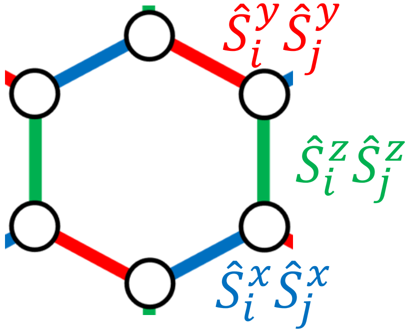
Quantum computation ?



1. Intro: Kitaev model

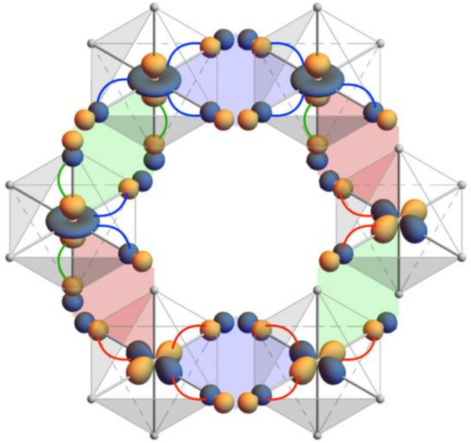
- **Kitaev model** Kitaev, Ann. Phys. (NY) **321**, 2 (2006).

$$\hat{H}_{\mathrm{Kitaev}} \equiv K \sum_{\gamma=x,y,z} \sum_{\langle i,j\rangle_\gamma} \hat{S}_i^\gamma \hat{S}_j^\gamma + \text{other terms (in magnets)}$$



- S = 1/2 (exactly solvable)
  - ① Ground state is Quantum spin liquid (Kitaev spin liquid; KSL)
  - ② Candidate materials: Li_2IrO_3 , α-$RuCl_3$, etc.

    Jackeli & Khaliullin PRL (2009), Burch et al., PRB (2014) etc.

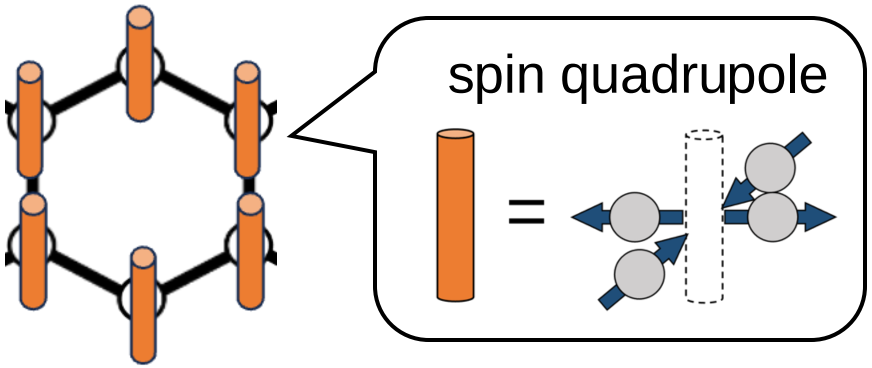


- ***S* > 1/2** (not exactly solvable)
  - ① Numerical and analytical works supporting the existence of KSL Oitmaa et al., PRB (2018) etc.
  - ② Candidate materials: $Li_3Ni_2SbO_6$ etc. (S = 1) Stavropoulos et al., PRL (2019).

    $CrSiTe_3$ etc. (S = 3/2) Xu et al., PRL (2020).

1. Intro: Interplay between KSL and spin nematics

・Spin quadrupole (nematic) state



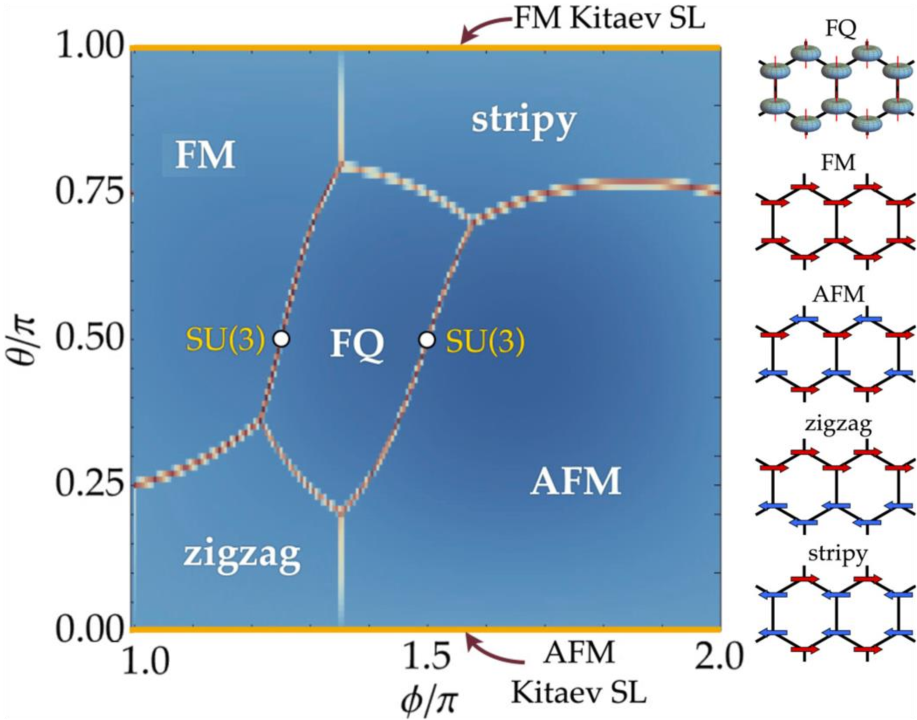
・Multiferroic materials（caused by electric field）?

・Magnets with strong spin-phonon coupling (SPC) ?

・New ground-state & dynamical properties in the spin liquid caused by quadrupole (or multipole)

・$S = 1$ BBQ-K model R. Pohle et al., PRB, **107**, L140403 (2023).

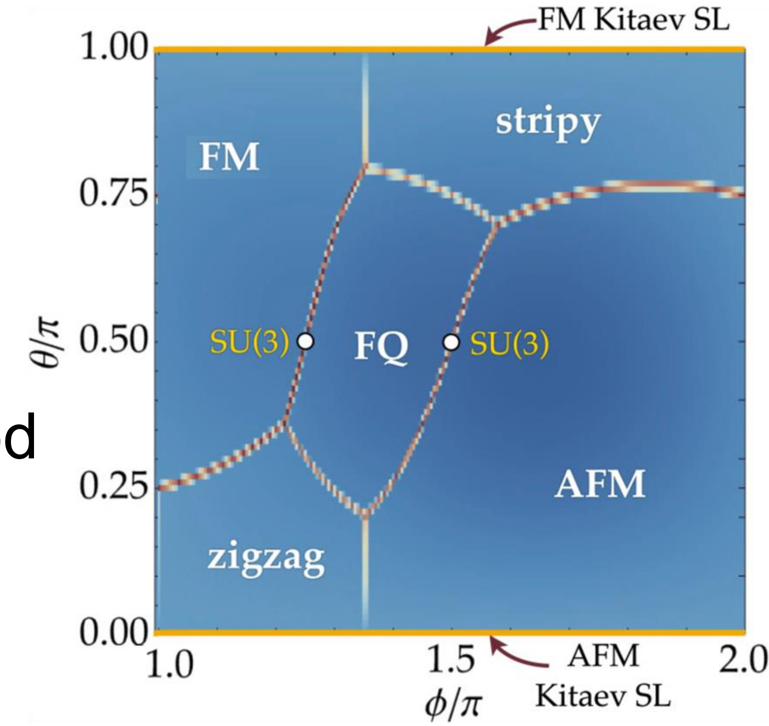
$$\hat{H} = \cos\theta \sum_{\gamma=x,y,z} \sum_{\langle i,j\rangle_\gamma} \hat{S}_i^\gamma \hat{S}_j^\gamma + \sin\theta \sum_{\langle i,j\rangle} \left[\cos\phi \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j + \sin\phi \left(\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j \right)^2 \right]$$



1. Intro: Challenge, Objective

- **Challenge**

In the previous work (Pohle et al., PRB (2023)),
they solved the BBQ–K model with “semi-classical” method
(neglecting quantum entanglements between local spins)



⬇

Objective

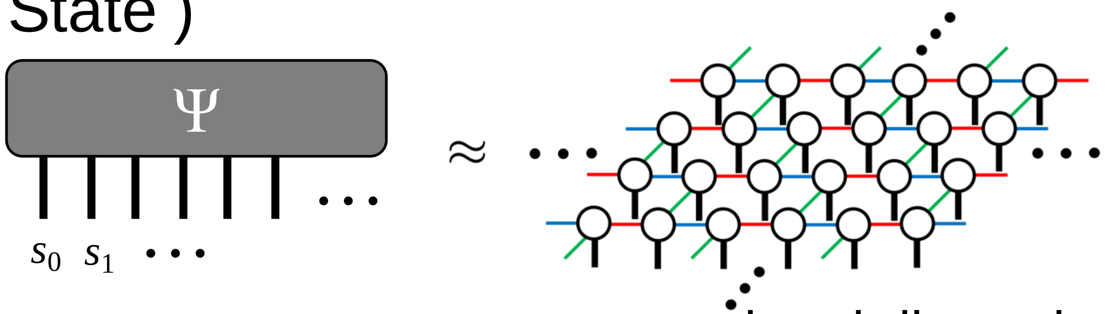
We introduce quantum entanglements between spins utilizing tensor network method (2D iPEPS) to probe quantum phase transitions in the parameter regions where Kitaev term becomes dominant.
(by calculating order parameters characterizing ground states)

2. Method: 2D iPEPS

- 2D iPEPS (infinite Projected Entangled Pair State)

$$|\Psi\rangle \equiv \sum_{\{s_i=0,\pm1\}} \Psi^{s_0,s_1\cdots} |s_0\rangle \otimes |s_1\rangle \otimes \cdots$$

$\Psi^{s_0,s_1\cdots} =$



bond-dimension: D

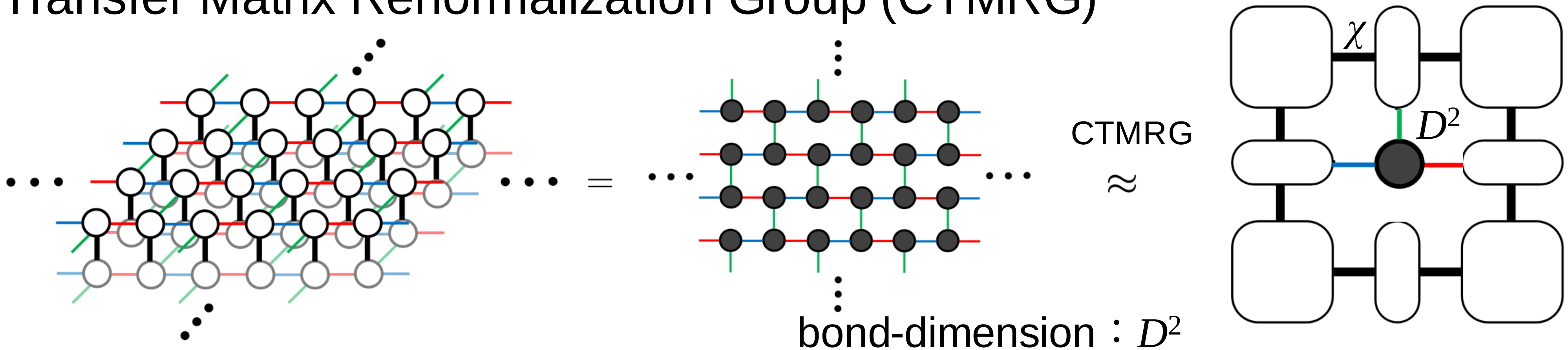
- Optimization：Imaginary Time Evolution (ITE), Suzuki-Trotter decomposition

$$|\Psi\rangle = e^{-T\hat{H}} |\Psi_0\rangle = \left[\left(\prod_{\langle i,j \rangle} e^{-\tau \hat{H}_{ij}} \right)^{N_\tau} + O(\tau) \right] |\Psi_0\rangle$$

$|\Psi_0\rangle$： initial state

- Corner Transfer Matrix Renormalization Group (CTMRG)

$\langle\Psi|\Psi\rangle =$

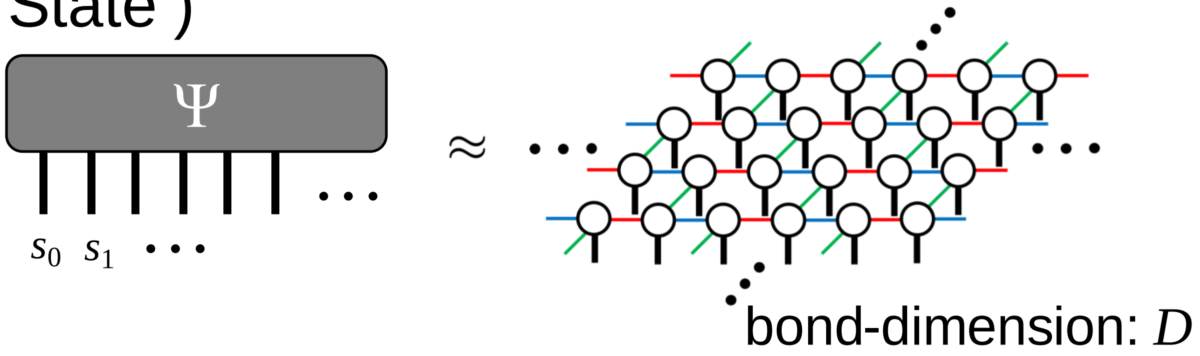


bond-dimension：D^2

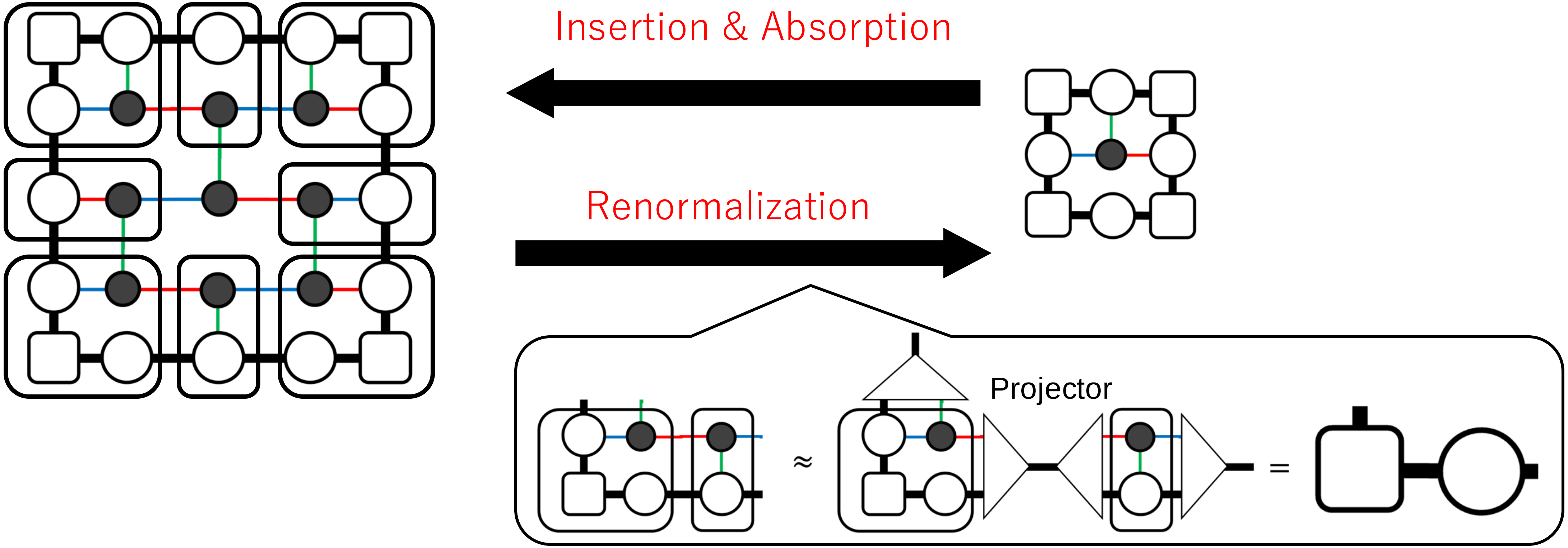
2. Method: 2D iPEPS

- 2D iPEPS (infinite Projected Entangled Pair State)

$$|\Psi\rangle \equiv \sum_{\{s_i=0,\pm1\}} \Psi^{s_0,s_1\cdots} |s_0\rangle \otimes |s_1\rangle \otimes \cdots \qquad \Psi^{s_0,s_1\cdots} =$$

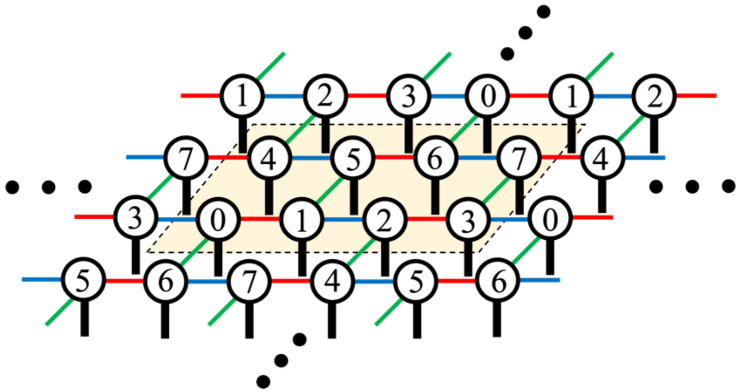


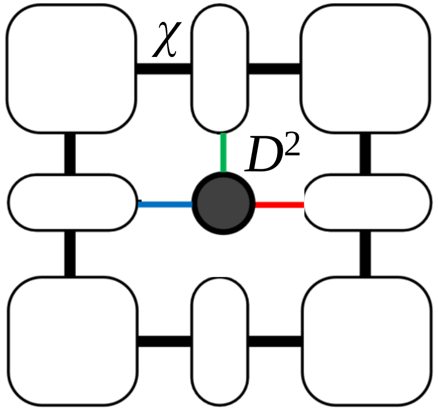
Corner Transfer Matrix Renormalization Group (CTMRG)



2. Method: Settings

- iPEPS: (D, χ) = (8, 64) or (8, 128)





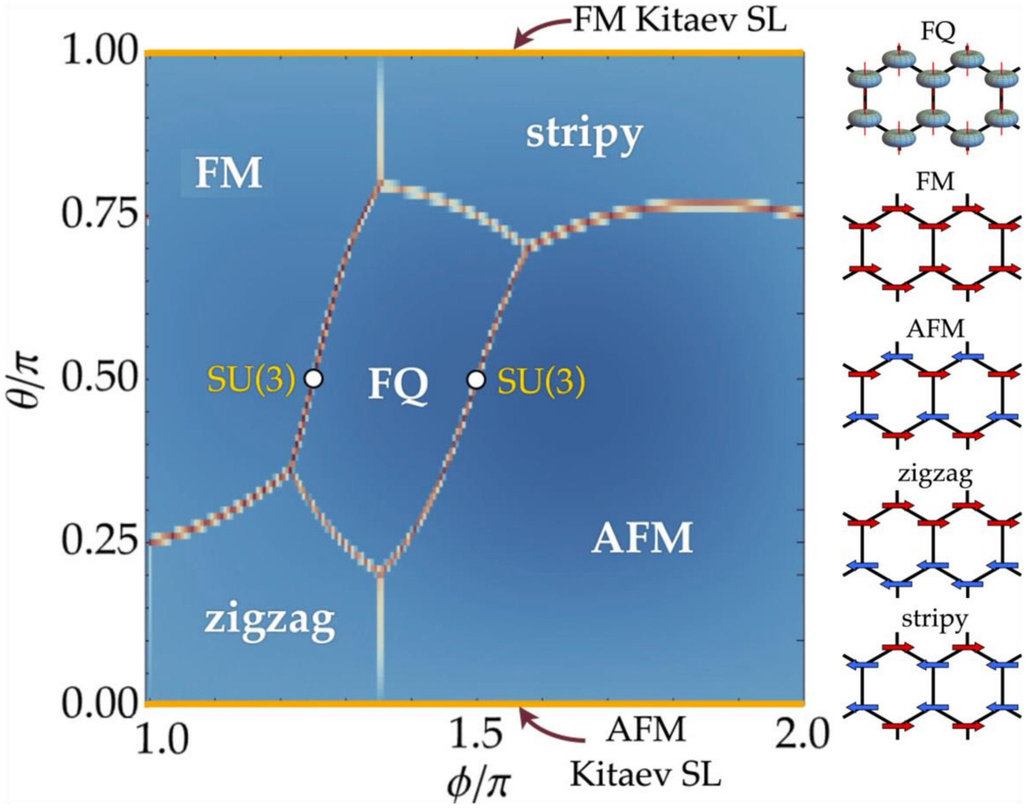
- 7 initial states for ITE
  - ① AFM, FM, FQ, zigzag, stripy, anitferro loop gas state (LGS), ferro LGS Lee et al., PRR (2020).
  - ② For each model parameter, we adopt an initial state where the energy becomes the lowest

- The number of steps
  - ① ITE: 10000 steps, (τ = 0.01)
  - ② CTMRG: 100 steps

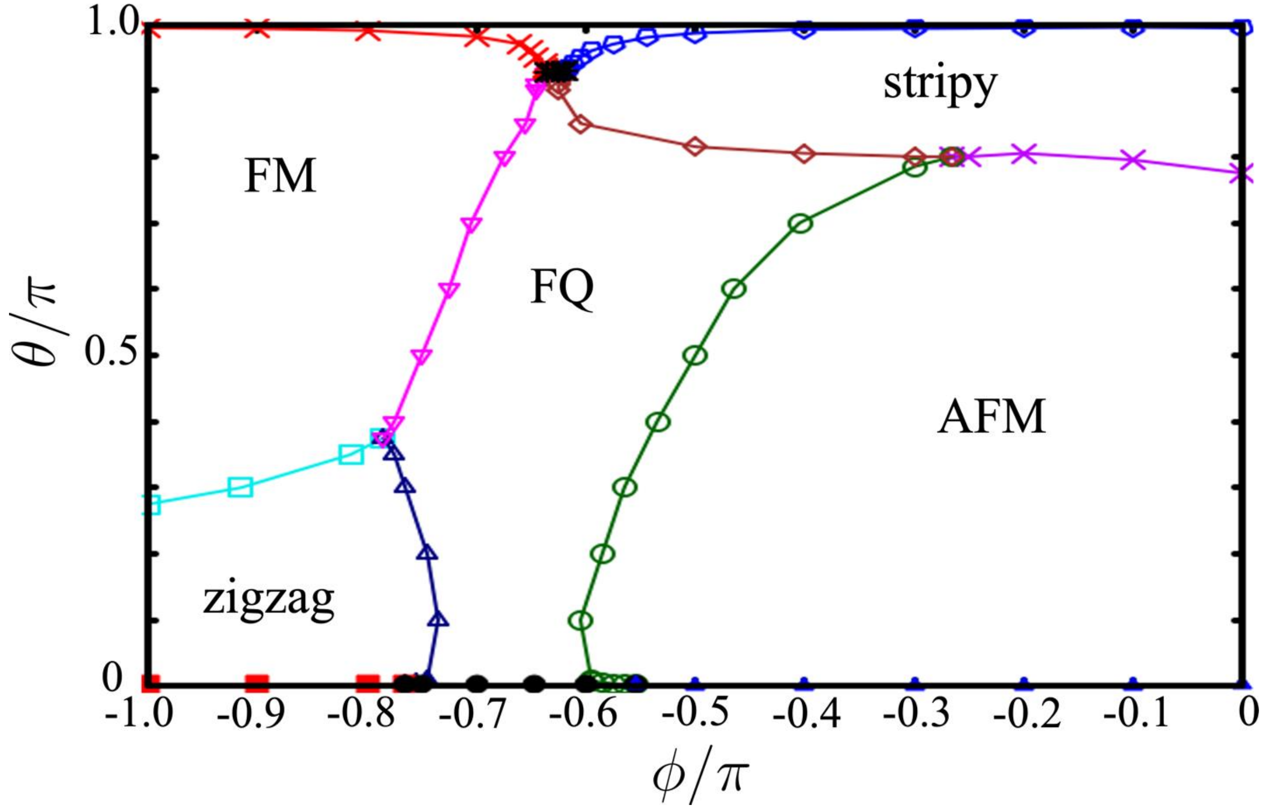
3. Results: Phase diagrams

$$\hat{H}_{\mathrm{BBQ-K}} \equiv \sin\theta \sum_{\langle i,j\rangle} \left[\cos\phi \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j + \sin\phi \left(\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j\right)^2\right] + \cos\theta \sum_{\gamma=x,y,z} \sum_{\langle i,j\rangle_\gamma} \hat{S}_i^\gamma \hat{S}_j^\gamma$$

R. Pohle et al., PRB (2023)



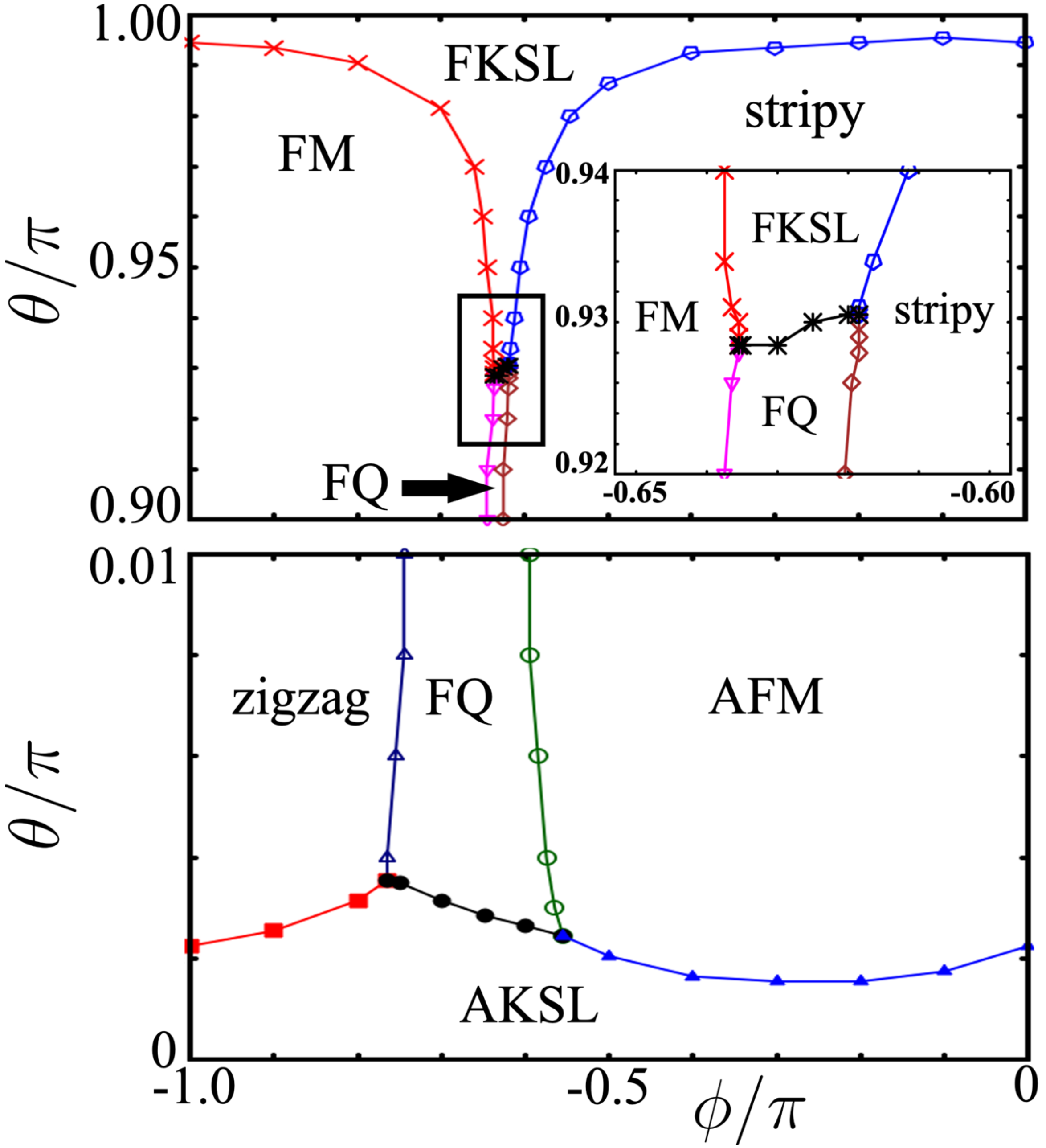
Our result



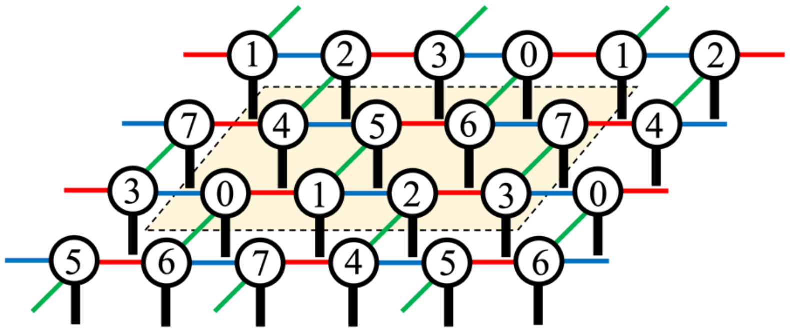
・Extension of FQ phase in the vicinity of the antiferro–Kitaev limit ($\theta/\pi = 0.0$)

3. Results: Phase diagrams

- Extended KSL phases
- Direct phase transitions between KSL phase and FQ phase
- Extension of ferro–KSL (FKSL) phase (when quadrupolar term prevails over Heisenberg term)



3. Results: FQ-FKSL transition

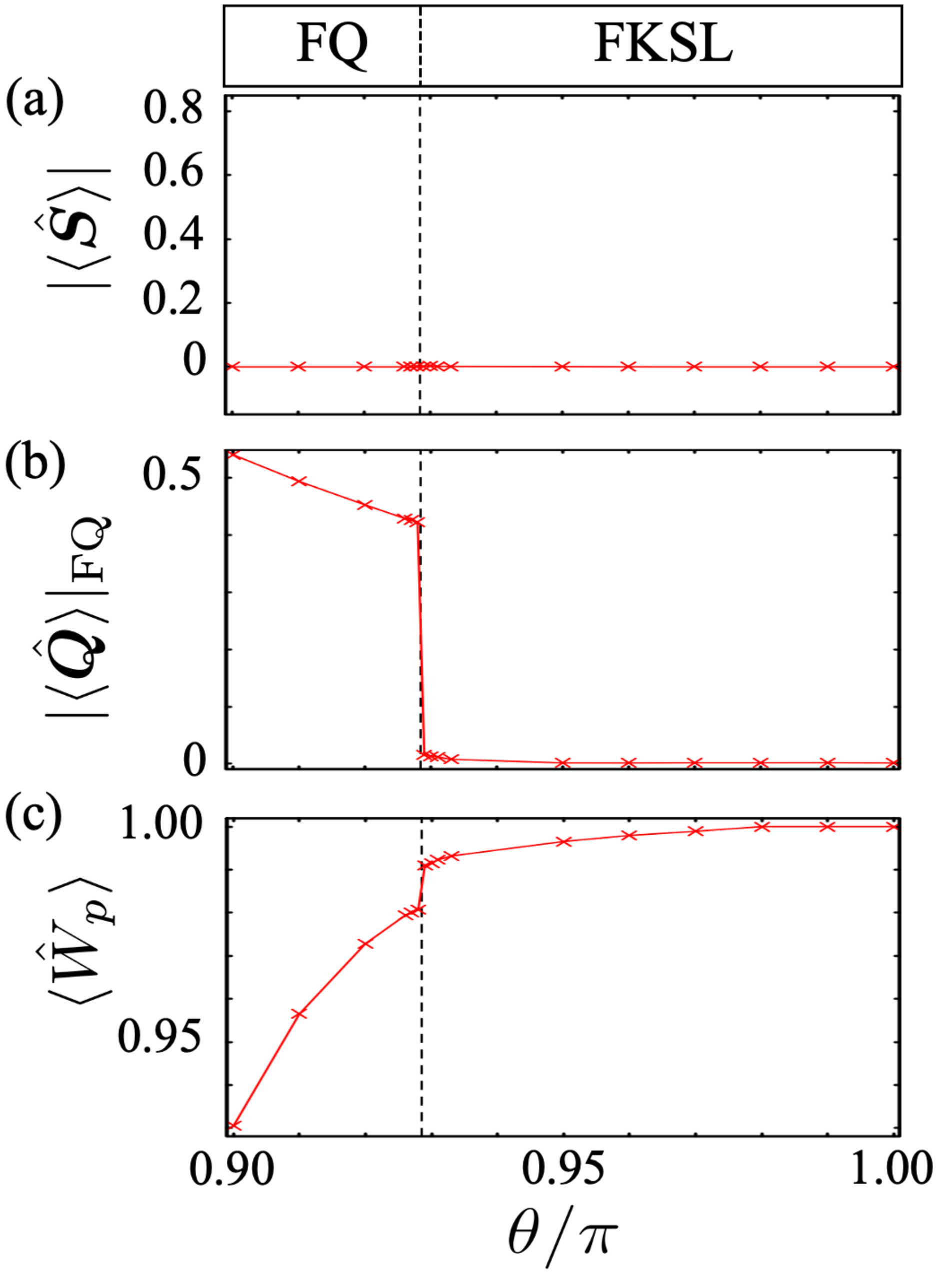


- $|\langle \hat{\boldsymbol{S}} \rangle| \equiv \frac{1}{8} \sum_{i \in \{0,\cdots,7\}} \sqrt{\langle \hat{S}_i^x \rangle^2 + \langle \hat{S}_i^y \rangle^2 + \langle \hat{S}_i^z \rangle^2}$
- $|\langle \hat{\boldsymbol{Q}} \rangle|_{\mathrm{FQ}} \equiv \sqrt{\sum_{\gamma=1}^{5} \left(\frac{1}{8} \sum_{i \in \{0,\cdots,7\}} \langle \hat{Q}_i^\gamma \rangle \right)^2}$
- $\langle \hat{W}_p \rangle \equiv \frac{1}{4} \sum_{j=1}^{4} \langle \hat{W}_{p_j} \rangle$

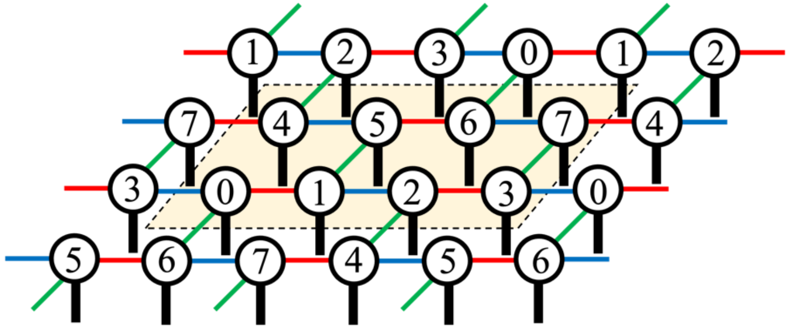
$$\hat{W}_{p_1} \equiv \hat{U}_0^z \hat{U}_1^y \hat{U}_5^x \hat{U}_4^z \hat{U}_7^y \hat{U}_3^x, \quad \hat{W}_{p_2} \equiv \hat{U}_2^z \hat{U}_3^y \hat{U}_7^x \hat{U}_6^z \hat{U}_5^y \hat{U}_1^x$$

$$\hat{W}_{p_3} \equiv \hat{U}_5^z \hat{U}_6^y \hat{U}_0^x \hat{U}_3^z \hat{U}_2^y \hat{U}_4^x, \quad \hat{W}_{p_4} \equiv \hat{U}_7^z \hat{U}_4^y \hat{U}_2^x \hat{U}_1^z \hat{U}_0^y \hat{U}_6^x$$

$$\hat{U}_i^\gamma \equiv \exp(i\pi \hat{S}_i^\gamma) \qquad \gamma = x, y, z$$



3. Results: FM-FQ-stripy transition



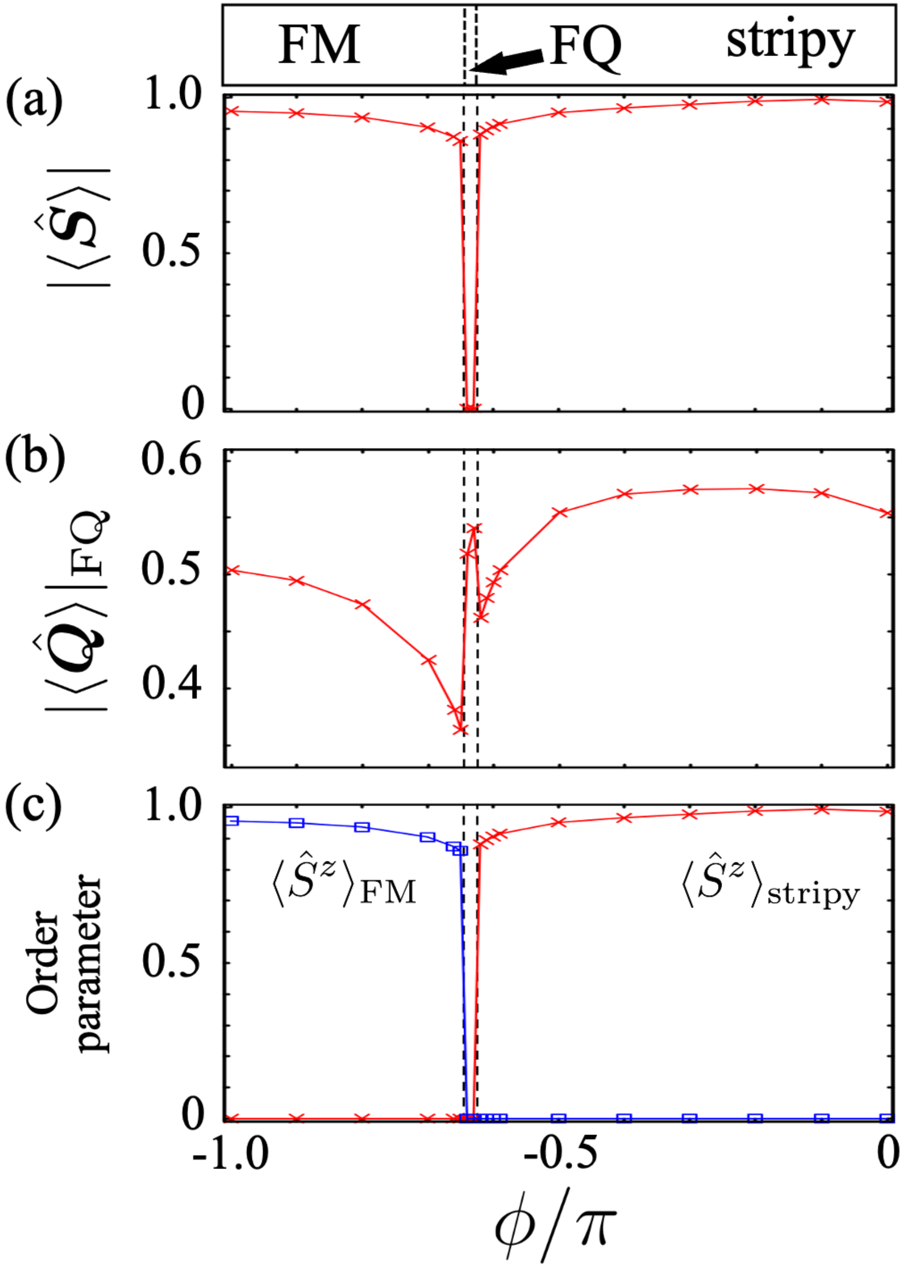
- $\langle \hat{S}^z \rangle_{\mathrm{FM}} \equiv \frac{1}{8} \left| \sum_{i \in \{0,\cdots,7\}} \langle \hat{S}^z_i \rangle \right|$
- $\langle \hat{S}^z \rangle_{\mathrm{stripy}} \equiv \max \left\{ \langle \hat{S}^z \rangle_{\mathrm{stripy1}}, \langle \hat{S}^z \rangle_{\mathrm{stripy2}}, \langle \hat{S}^z \rangle_{\mathrm{stripy3}} \right\}$

$$\langle \hat{S}^z \rangle_{\mathrm{stripy}a} \equiv \frac{1}{8} \left| \left(\sum_{i \in A_a} - \sum_{i \in B_a} \right) \langle \hat{S}^z_i \rangle \right|$$

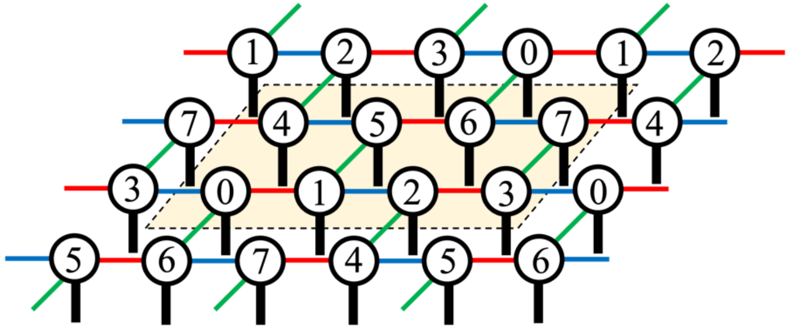
$$A_1 = \{0, 2, 4, 6\} \quad B_1 = \{1, 3, 5, 7\}$$

$$A_2 = \{0, 1, 4, 7\} \quad B_2 = \{2, 3, 5, 6\}$$

$$A_3 = \{0, 3, 4, 5\} \quad B_3 = \{1, 2, 6, 7\}$$



3. Results: AKSL-FQ transition



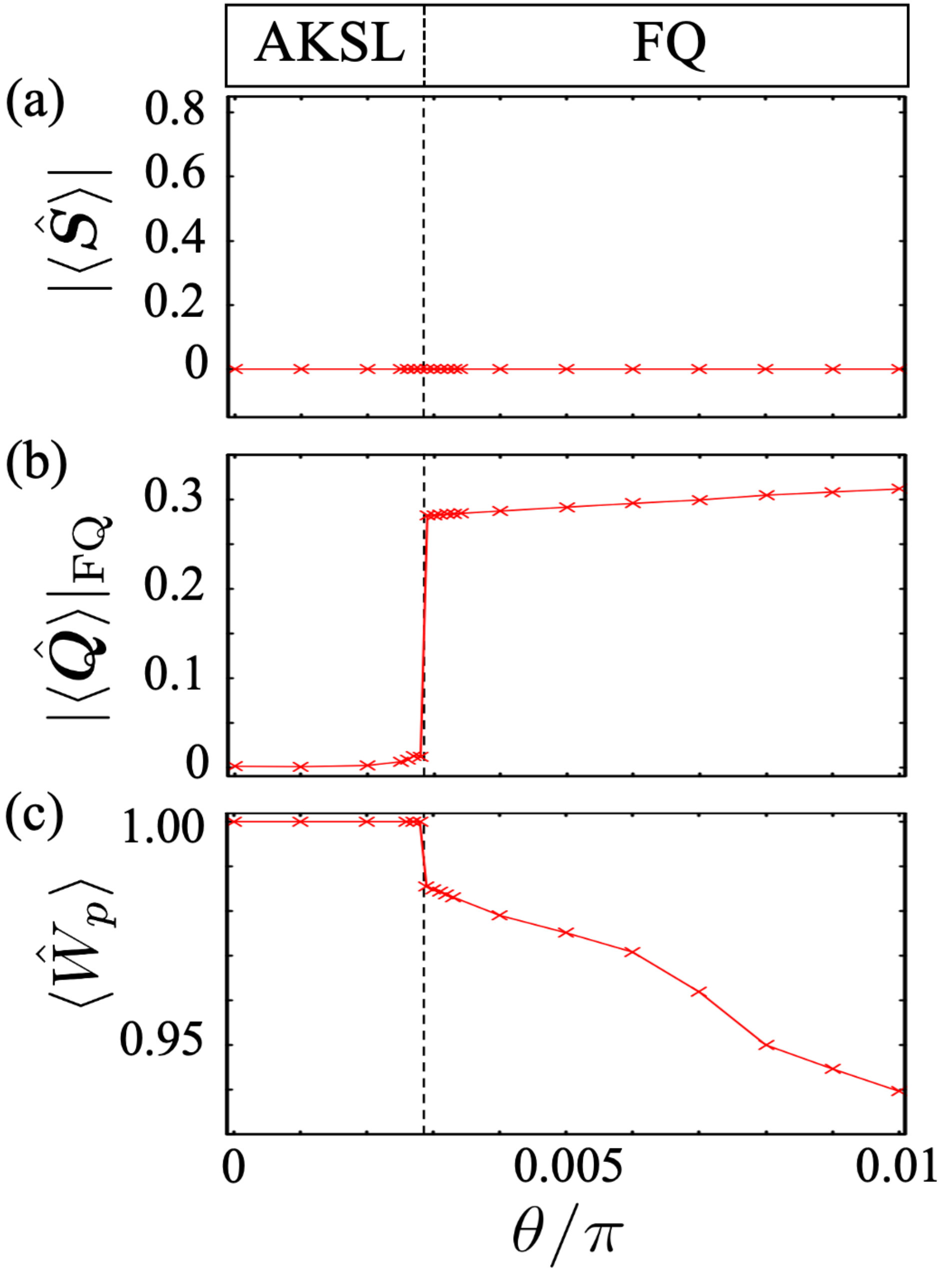
- $|\langle \hat{\boldsymbol{S}} \rangle| \equiv \frac{1}{8} \sum_{i \in \{0,\cdots,7\}} \sqrt{\langle \hat{S}_i^x \rangle^2 + \langle \hat{S}_i^y \rangle^2 + \langle \hat{S}_i^z \rangle^2}$

- $|\langle \hat{\boldsymbol{Q}} \rangle|_{\mathrm{FQ}} \equiv \sqrt{\sum_{\gamma=1}^{5} \left(\frac{1}{8} \sum_{i \in \{0,\cdots,7\}} \langle \hat{Q}_i^\gamma \rangle \right)^2}$

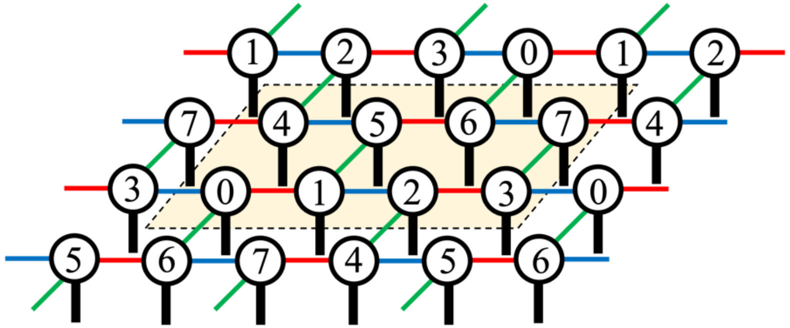
- $\langle \hat{W}_p \rangle \equiv \frac{1}{4} \sum_{j=1}^{4} \langle \hat{W}_{p_j} \rangle$

$$\hat{W}_{p_1} \equiv \hat{U}_0^z \hat{U}_1^y \hat{U}_5^x \hat{U}_4^z \hat{U}_7^y \hat{U}_3^x, \quad \hat{W}_{p_2} \equiv \hat{U}_2^z \hat{U}_3^y \hat{U}_7^x \hat{U}_6^z \hat{U}_5^y \hat{U}_1^x$$
$$\hat{W}_{p_3} \equiv \hat{U}_5^z \hat{U}_6^y \hat{U}_0^x \hat{U}_3^z \hat{U}_2^y \hat{U}_4^x, \quad \hat{W}_{p_4} \equiv \hat{U}_7^z \hat{U}_4^y \hat{U}_2^x \hat{U}_1^z \hat{U}_0^y \hat{U}_6^x$$

$$\hat{U}_i^\gamma \equiv \exp(i\pi \hat{S}_i^\gamma) \qquad \gamma = x, y, z$$



3. Results: zigzag-FQ-AFM transition



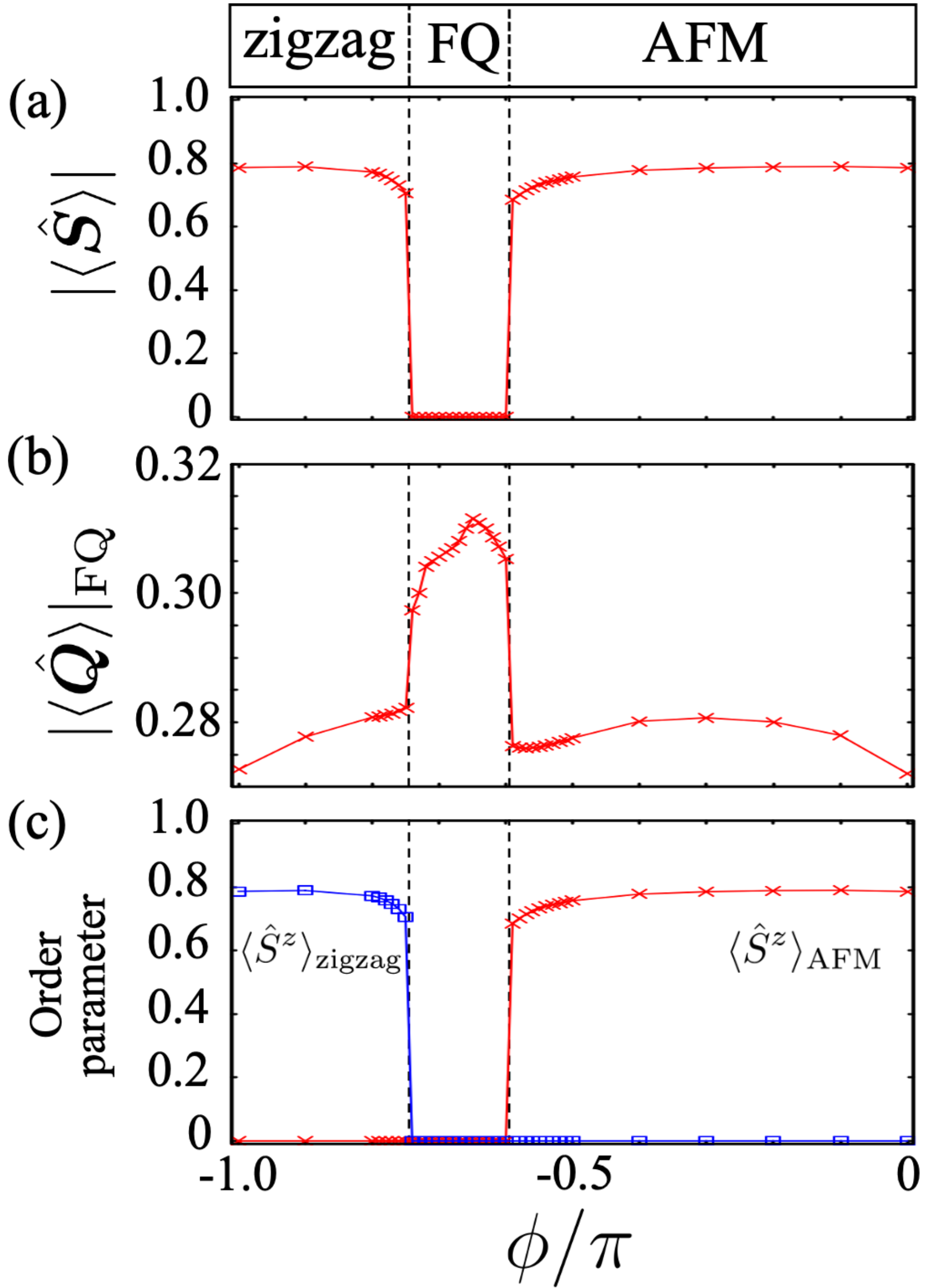
- $\langle \hat{S}^z \rangle_{\mathrm{AFM}} \equiv \frac{1}{8} \left| \left(\sum_{i \in \{0,2,5,7\}} - \sum_{i \in \{1,3,4,6\}} \right) \langle \hat{S}_i^z \rangle \right|$
- $\langle \hat{S}^z \rangle_{\mathrm{zigzag}} \equiv \max \left\{ \langle \hat{S}^z \rangle_{\mathrm{zigzag1}}, \langle \hat{S}^z \rangle_{\mathrm{zigzag2}}, \langle \hat{S}^z \rangle_{\mathrm{zigzag3}} \right\}$

$$\langle \hat{S}^z \rangle_{\mathrm{zigzag}a} \equiv \frac{1}{8} \left| \left(\sum_{i \in C_a} - \sum_{i \in D_a} \right) \langle \hat{S}_i^z \rangle \right|$$

$$C_1 = \{0, 1, 2, 3\} \qquad D_1 = \{4, 5, 6, 7\}$$

$$C_2 = \{0, 3, 6, 7\} \qquad D_2 = \{1, 2, 4, 5\}$$

$$C_3 = \{0, 1, 5, 6\} \qquad D_3 = \{2, 3, 4, 7\}$$



Summary etc

1. We investigated quantum phase transition of $S = 1$ BBQ−K model with iPEPS
2. Several quantum properties in the vicinity of Kitaev limits ($\theta/\pi = 0.0$ or 1.0)
3. Robustness of the FKSL phase against the spin-quadrupolar interaction

- Future perspectives
  1. Possible application to materials which stabilize the spin liquid state?
  2. Analysis of low-energy excitation, or dynamical properties (→ application to inelastic neutron scattering experiments?)