Tensor network study of honeycomb lattice Kitaev model

Department of Physics, The University of Tokyo, **Tsuyoshi Okubo**

Main collaborators: *Korea Univ.* H.-Y. Lee,
Kinki Univ. R. Kaneko
ISSP N. Kawashima,

Ref:

- T.O. *et al,* Phys. Rev. B **96**, 054434 (2017).
- H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019), PRB 101, 035140 (2020).

Contents

Contents

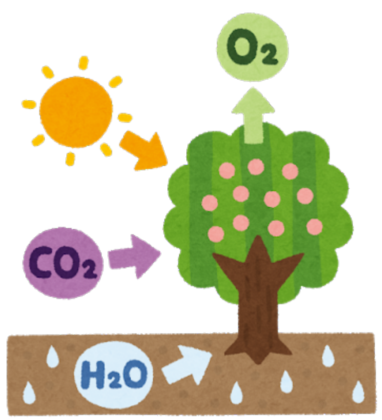
- Introduction
  - Tensor network representation for quantum states
  - Honeycomb lattice Kitaev model
- Compact tensor network representation for the gapless Kitaev spin liquid
- Finite temperature simulation (on going)
- Summary

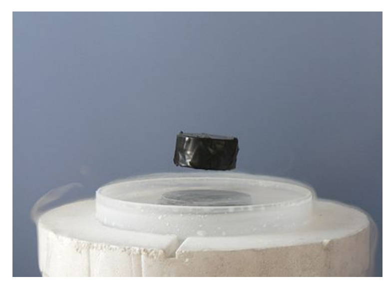
Quantum many-body problems

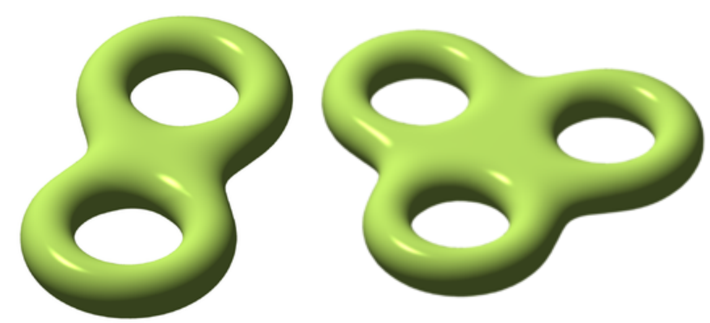
A variety of phenomena in condensed matter physics

- Chemical reaction
- Superconductivity
- Topological states
- ...

→ **Quantum many-body problems**







Cited from wikipedia: "Meisner effect", "Torus"

(Time independent) Schrödinger equation = Eigen value problem

$$\mathcal{H}|\Psi\rangle = E|\Psi\rangle$$

- Dimension of the vector space increases exponentially as # of particles increases
- Quantum many-body problem ~ Eigenvalue problem of huge matrices

→ **To solve the problem numerically by (classical) computer, we need huge memory and huge computation time.**

Numerical approach for quantum (spin) systems

- **Numerical diagonalization**

  Exact and applicable for any systems, but system size is limited.

  S=1/2 spin models ~ 50 sites ➡ We need careful extrapolation.

- **Quantum Monte Carlo (QMC)**

  Within statistical error, solving problem "exactly"!
  Easy calculation for very large system.

  But, frustrated interactions are usually suffered from the sign problem!

- **Variational method**

  Assuming a wave-function ansatz

  - Variational Monte Carlo: larger systems than ED
  - **Tensor network method:** Very large system size (infinite)

Information compression by tensor networks

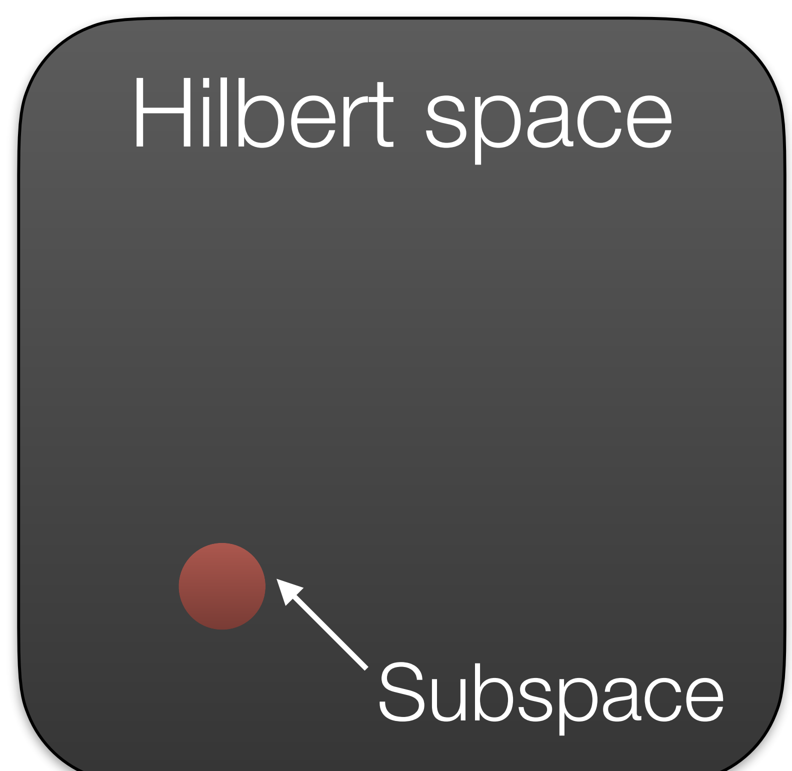
We can not treat entire data in the present computers.

→ Try to reduce the "effective" dimension of (Hilbert) space

By considering proper subspace of the Hilbert space, we can represent a quantum state efficiently.

↓

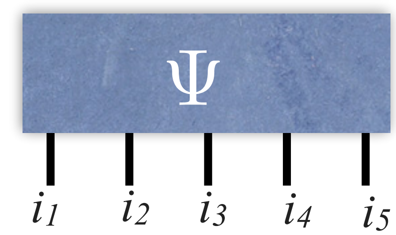
Tensor network quantum states!



Tensor network states (TNS)

G.S. wave function: $|\Psi\rangle = \sum_{\{i_1,i_2,\ldots i_N\}} \Psi_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$

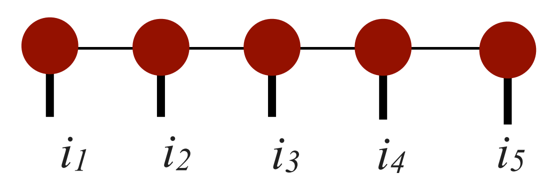
Vector (or N-rank tensor): $\Psi_{i_1 i_2 \ldots i_N}$ =



# of Elements $= a^N$

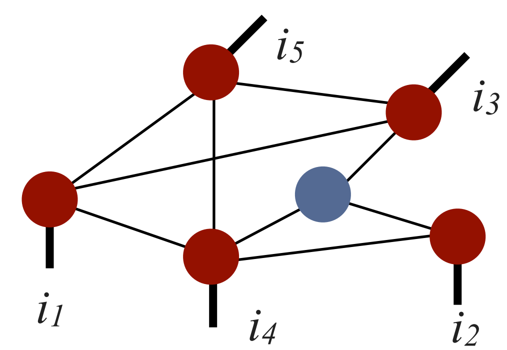
"Tensor network" decomposition

- Matrix Product State (MPS) $A_1[i_1]A_2[i_2]\cdots A_N[i_N]$ =



$A[m]$: Matrix for state m

- General network $\mathrm{Tr} X_1[i_1] X_2[i_2] X_3[i_3] X_4[i_4] X_5[i_5] Y$



X,Y : Tensors

Tr : Tensor network contraction

By choosing a "good" network, we can express G.S. wave function efficiently.

ex. MPS: # of elements $= 2ND^2$ D: dimension of the matrix A

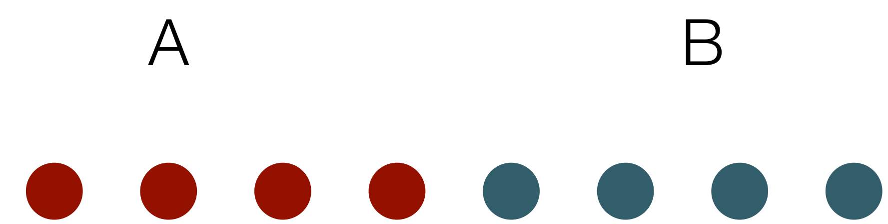
Exponential → Linear   *If D does not depend on N…

Area law of the entanglement entropy

Entanglement entropy:

Reduced density matrix of a sub system (sub space):

$$\rho_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi|$$



Entanglement entropy = von Neumann entropy of ρ_A

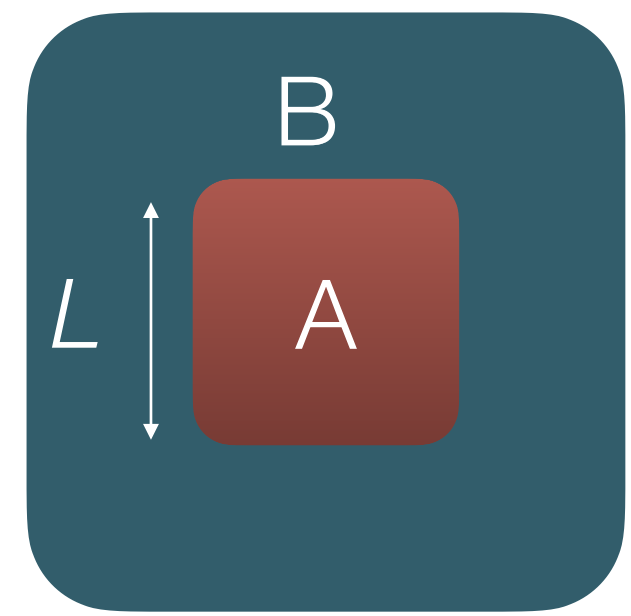
$$S = -\mathrm{Tr}\,(\rho_A \log \rho_A)$$

General wave functions:

EE is proportional to its **volume (# of spins)**.

$$S = -\mathrm{Tr}\,(\rho_A \log \rho_A) \propto L^d$$

(c.f. random vector)



Ground state wave functions:

For a lot of ground states, EE is proportional to its area.

J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys, 277, **82** (2010)

$$S = -\mathrm{Tr}\,(\rho_A \log \rho_A) \propto L^{d-1}$$

Ground state are in a small part of the huge Hilbert space!

Tensor Product States (TPS)

TPS (Tensor Product State) (AKLT, T. Nishino, K. Okunishi, …)

PEPS (Projected Entangled-Pair State)

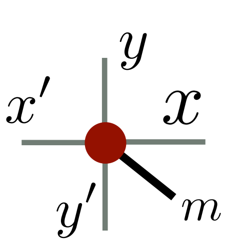
(F. Verstraete and J. Cirac, arXiv:cond-mat/0407066)

> d-dimensional tensor network representation
> for the wave function of a d-dimensional quantum system

$$|\Psi\rangle = \sum_{\{m_i=1,2,\cdots,m\}} \mathrm{Tr}\ A_1[m_1]A_2[m_2]\cdots A_N[m_N]|m_1 m_2\cdots m_N\rangle$$

Tr: tensor network "contraction"

$A_{x_i x_i' y_i y_i'}[m_i]$: Rank 4+1 tensor

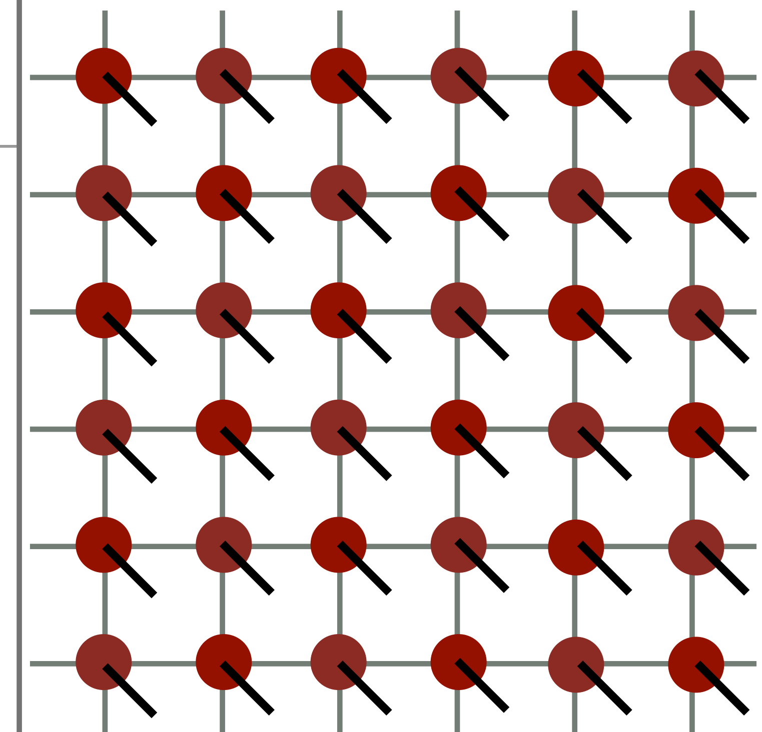


$x, y, x', y' = 1, 2, \ldots D$ D = "bond dimension"

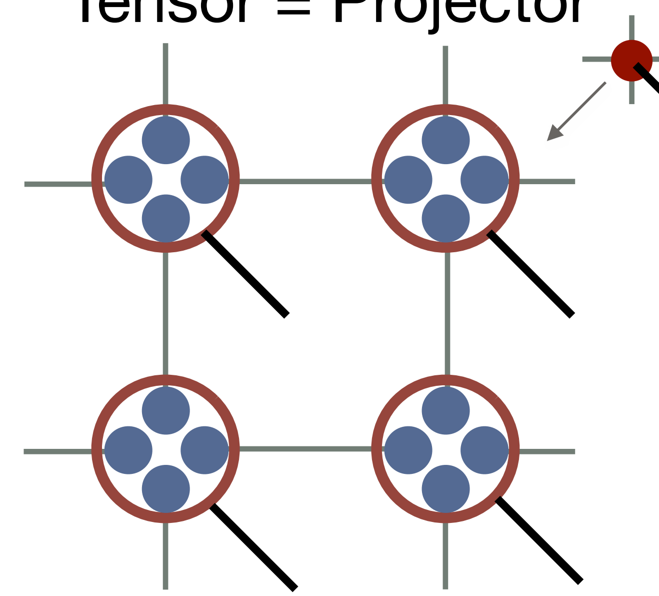
$m_i = 1, 2, \ldots m$ m = dimension of the local Hilbert space

**D* can be larger than m. "Virtual state "

TPS on square lattice

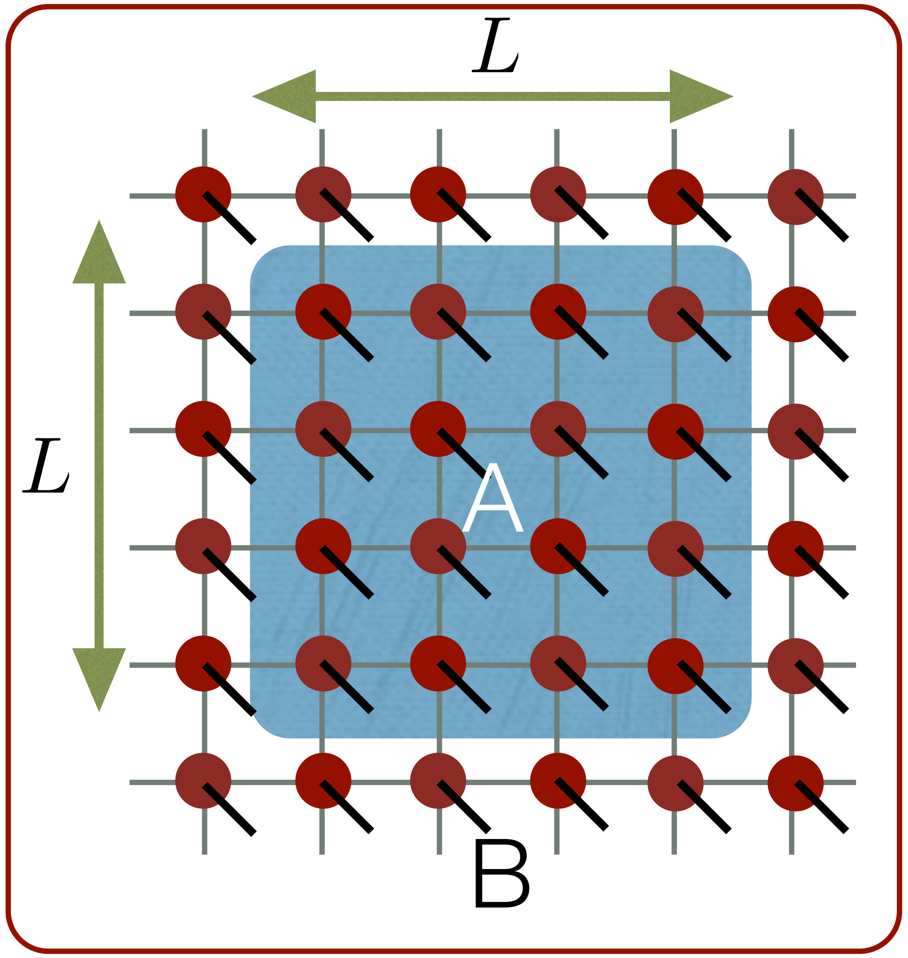


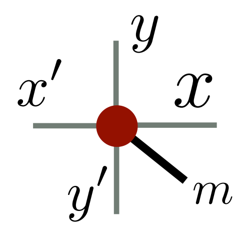
Tensor = Projector



Maximally entangled state between D-state spins

Entanglement entropy of TPS (PEPS)





Bond dimension = D

# of bonds connecting regions A and B

$N_c(L) = 4L$ (square lattice)

$N_c(L) = 2dL^{d-1}$ (d-dimensional hyper cubic lattice)

$$\mathrm{rank}\ \rho_A \leq D^{N_c(L)} \sim D^{2dL^{d-1}}$$

$$S_A = -\mathrm{Tr}\ \rho_A \log \rho_A \leq 2dL^{d-1} \log D$$

TPS can satisfies the area law even for d >1.

We can efficiently approximate vectors in higher dimensional space by TPS.

* It indicates that TPS could approximate **infinite system** with a finite D.

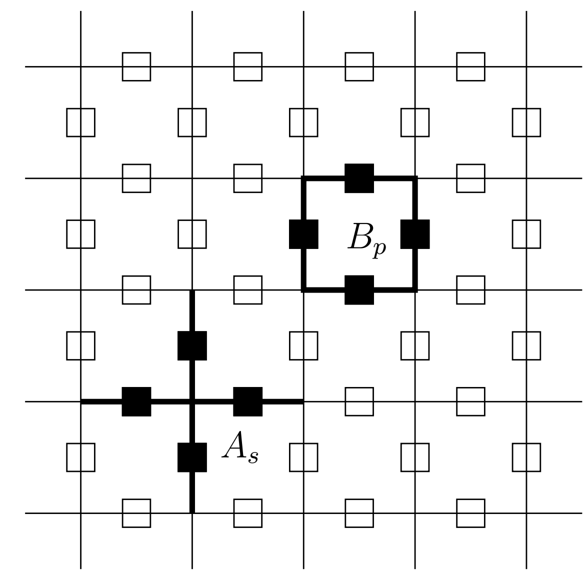
Example: Ground state represented by TPS

Toric code model

(A. Kitaev, Ann. Phys. **303**, 2 (2003).)

$$\mathcal{H} = -\sum_s A_s - \sum_p B_p$$

$$A_s = \prod_{j \in \mathrm{star}(s)} \sigma_j^x \qquad B_p = \prod_{j \in \partial p} \sigma_j^z.$$



Its ground state is so called Z_2 spin liquid state.

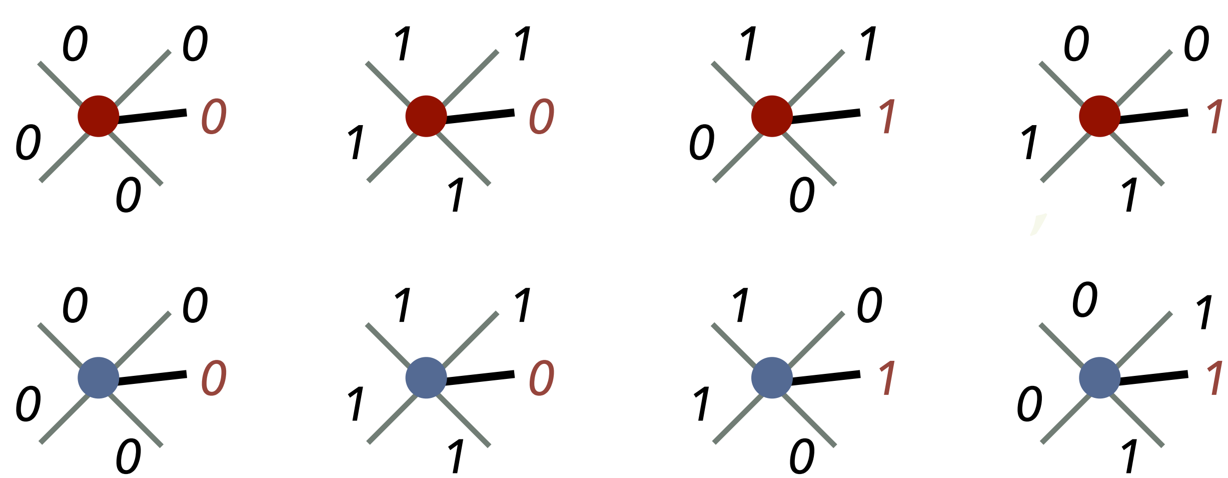
"Spin liquid" is a novel phase different from conventional magnetic orders.

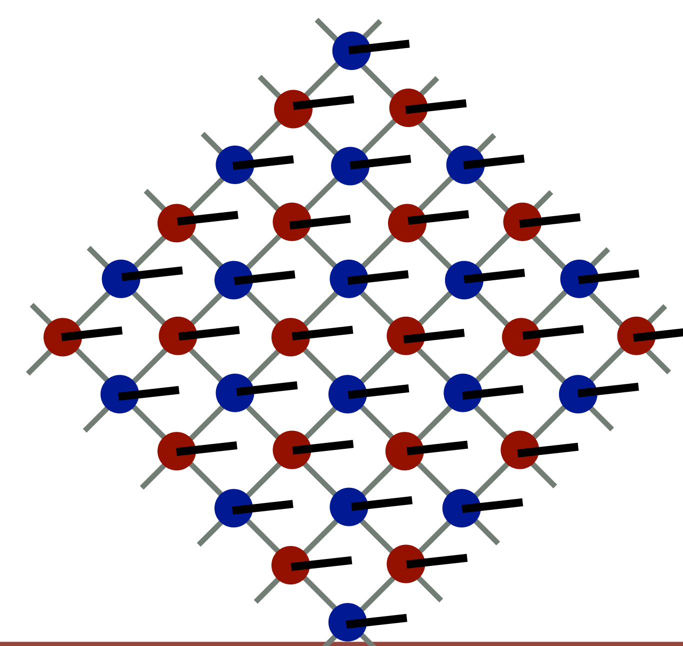
It can be represented by D=2 TPS.

(F. Verstraete, et al, Phys. Rev. Lett. **96**, 220601 (2006).)

0,1: eigenstate of σ_x

(Non-zero elements of tensor)





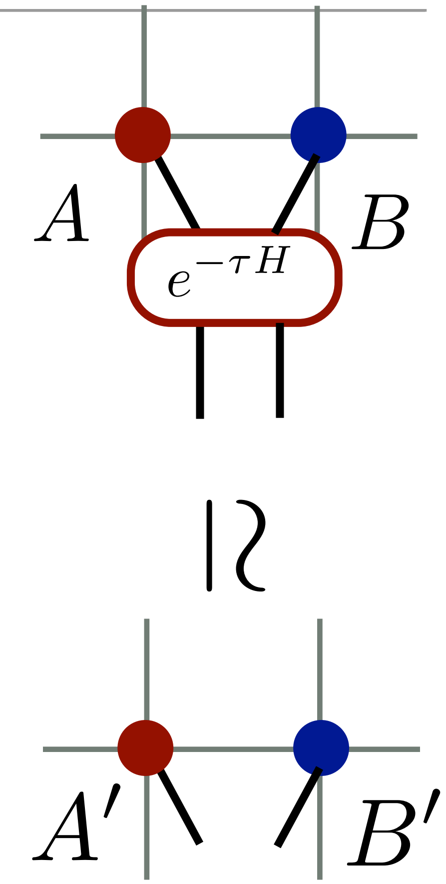
Variational calculation using iTPS

Optimization: **Imaginary time evolution**

$$\lim_{M\to\infty}\left(e^{-\tau\mathcal{H}}\right)^M|\psi\rangle = \text{ground state}$$

Approximatin	Cost	information	Accuracy
Simple update	**$O(D^5)$**	local	bad
Full update	**$O(D^{10})$**	global	better

We repeat updates about 10^3~ 10^5 steps



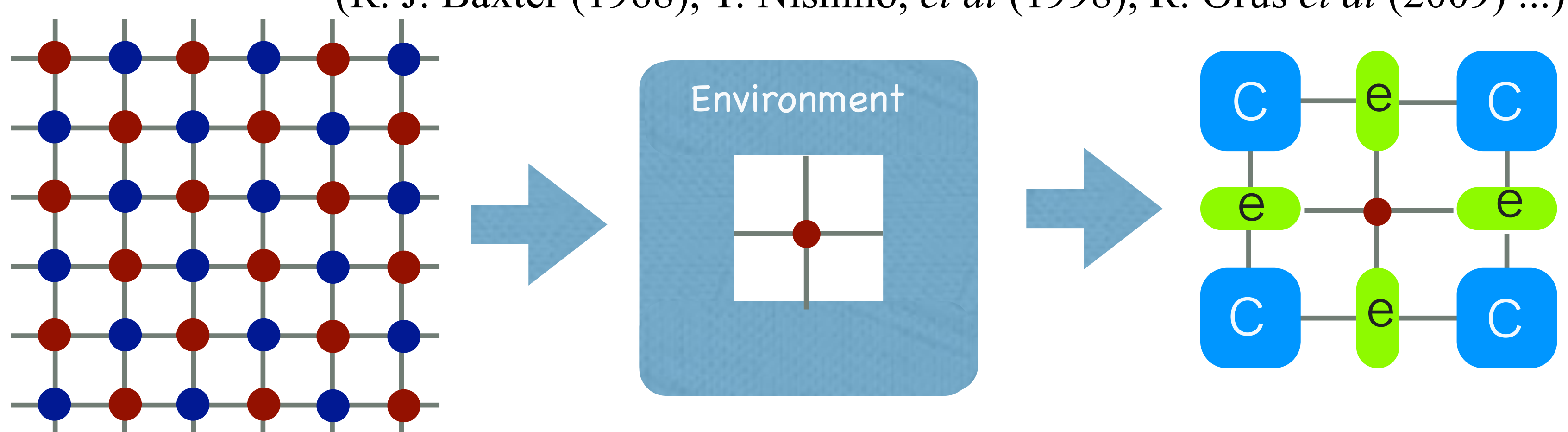
Evaluation: **Contraction of the whole network**

We use the **corner transfer matrix** method.

(R. J. Baxter (1968), T. Nishino, *et al* (1998), R. Orus *et al* (2009) ...)

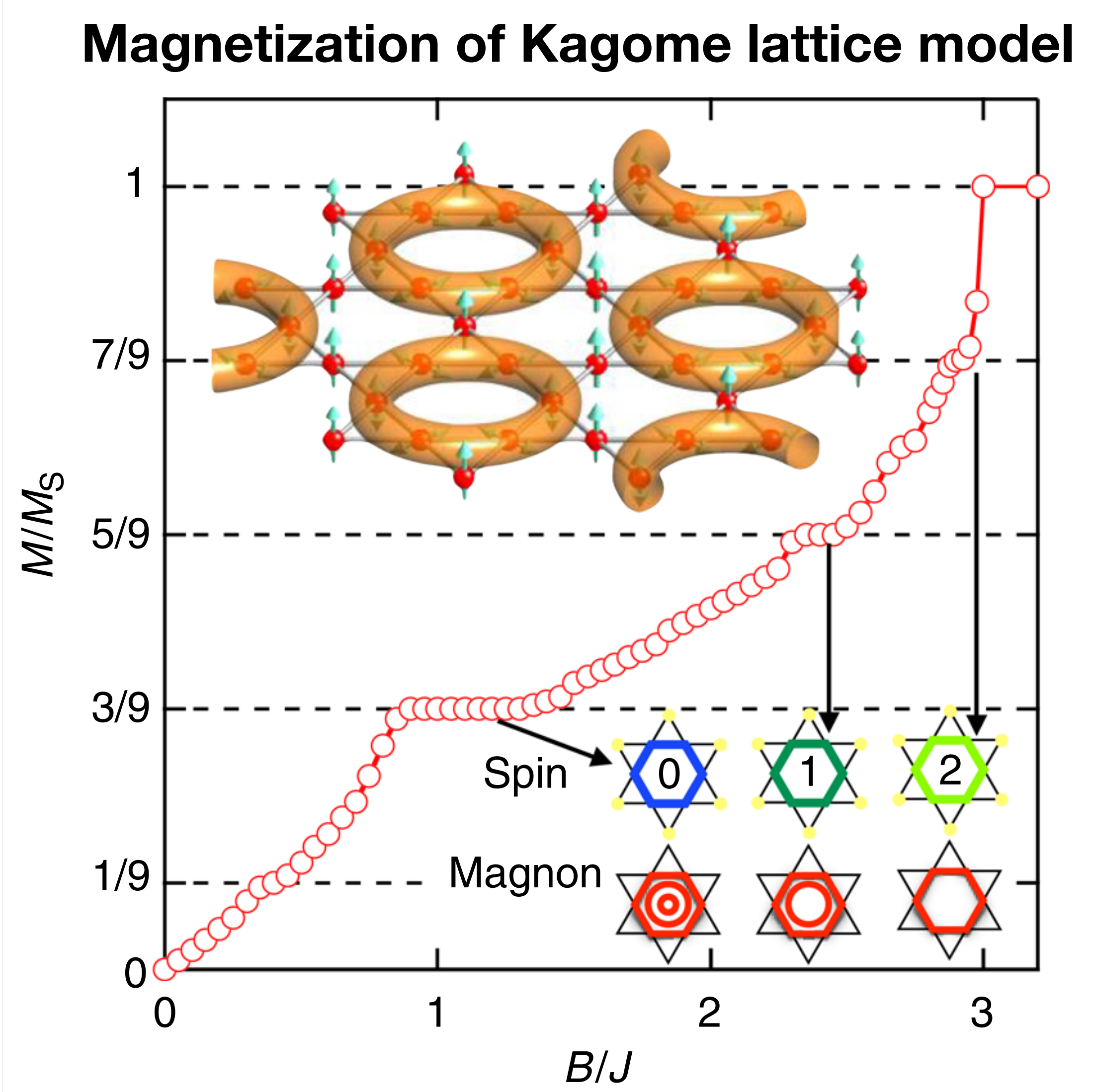
Cost ~ $O(D^{10})$

Only a few calculations

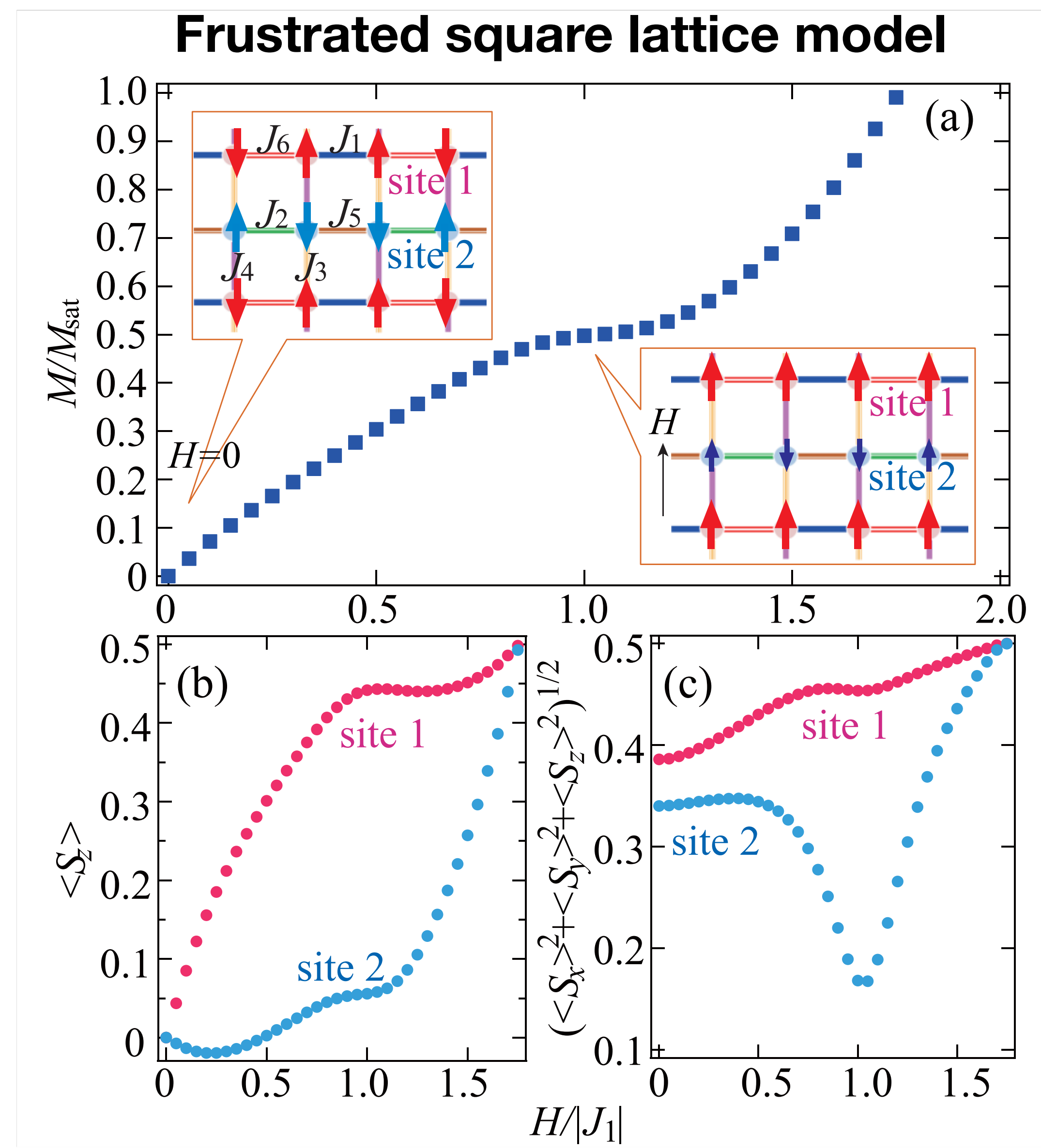


Application to quantum many-body systems

Examples: Frustrated spin systems (We can not apply QMC due to the sing problem.)



R. Okuma, D. Nakamura, T. Okubo et al, Nat. Commun. **10**, 1229 (2019).

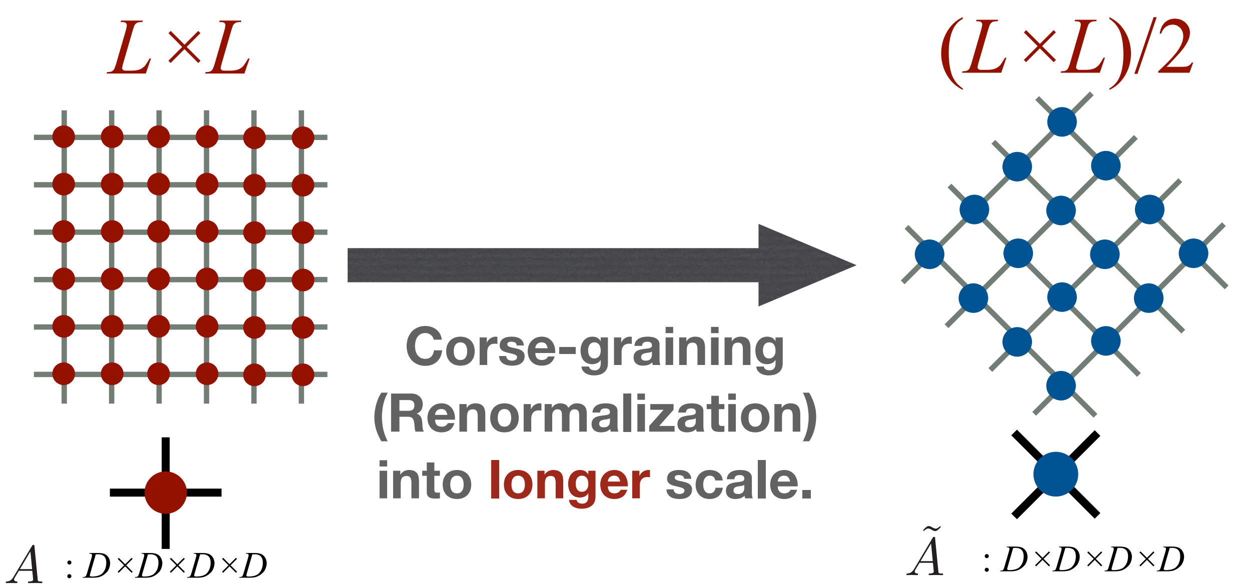


H. Yamaguchi, Y. Sasaki, T. Okubo, Phys. Rev. B **98**, 094402 (2018).

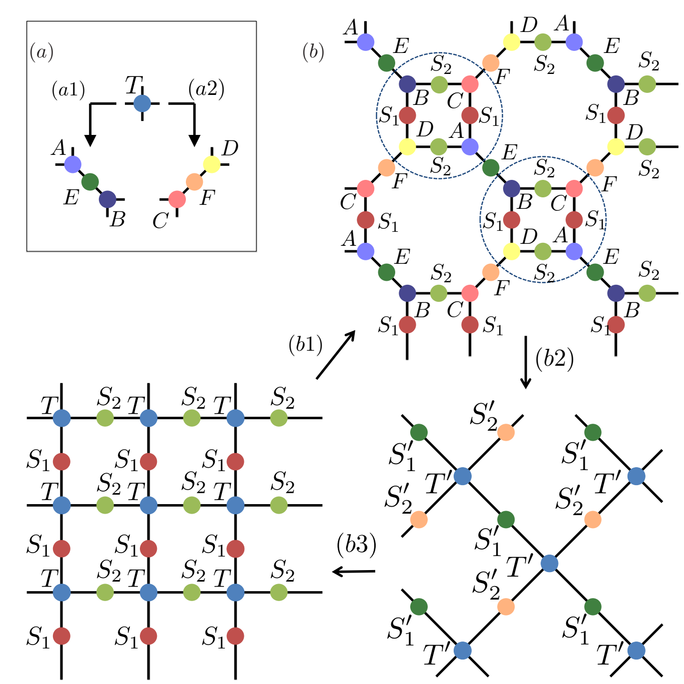
Comment: Tensor network renormalization

Tensor renormalization group (TRG) cf. M. Levin and C. P. Nave, Phys. Rev. Lett. **99**, 120601 (2007)

Approximate contraction of tensor network by using "coarse-graining" of the network



- It reduces the exponentially large contraction cost to polynomial.



- TRG type approaches are also used to solve quantum many-body problems through the path integral formulation.
- It is deeply related to TNS.
  - Importance of short-range entanglement removing.
  - Connection to MERA.
- I have been contributed to TRG by developing new algorithms.
  - D. Adachi, T.O. and S. Todo, PRB **102** 054432 (2020); arXiv:2011.01679.

Contents

- Introduction
  - Tensor network representation for quantum states
  - Honeycomb lattice Kitaev model
- Compact tensor network representation for the gapless Kitaev spin liquid
- Finite temperature simulation (on going)
- Summary

Honeycomb lattice Kitaev Model

A. Kitaev, Annals of Physics **321**, 2 (2006)

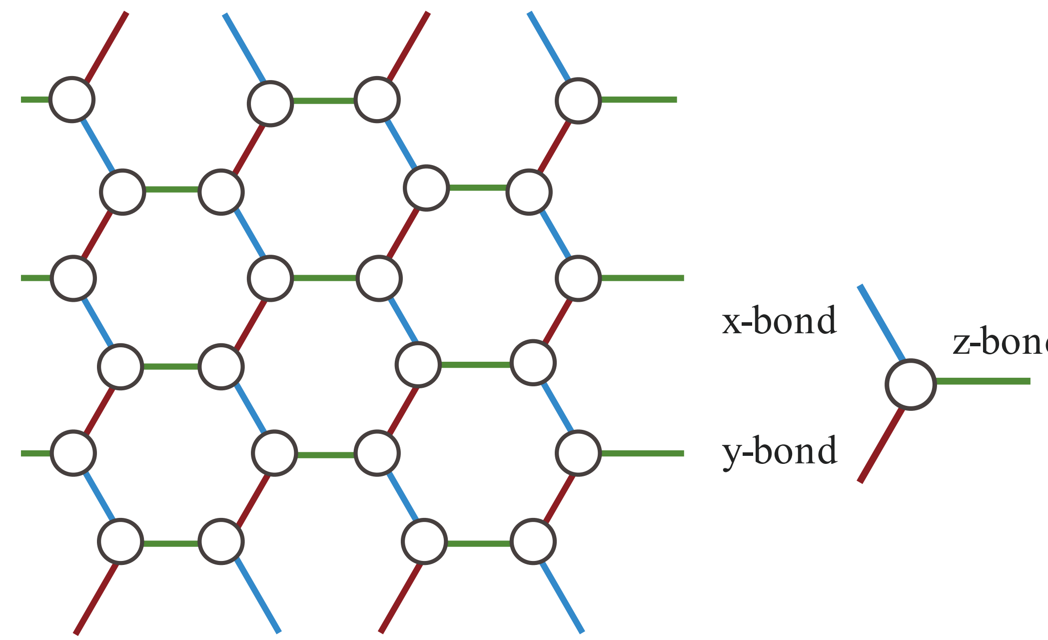
Kitaev model

$$\mathcal{H} = -\sum_{\gamma,\langle i,j\rangle_\gamma} J_\gamma S_i^\gamma S_j^\gamma$$

γ:bond direction

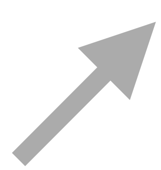
Depending on the bond direction, only specific spin components interact.

Honeycomb lattice



This model is exactly solvable, by introducing Majorana fermions.

Spin

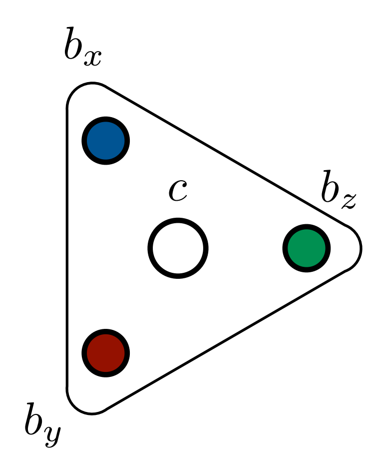


$\vec{S} = (S_x, S_y, S_z)$

$2S^\gamma = \sigma^\gamma = ib^\gamma c$

Majorana fermions: $(b^\gamma)^\dagger = b^\gamma$, $c^\dagger = c$

Four Majorana fermions

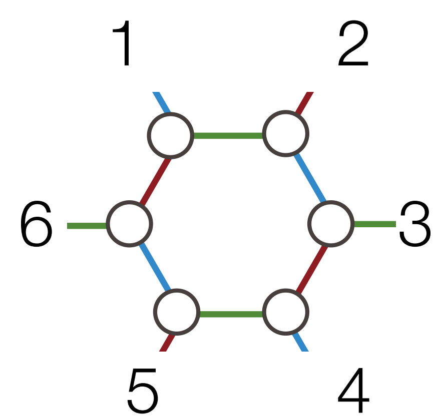


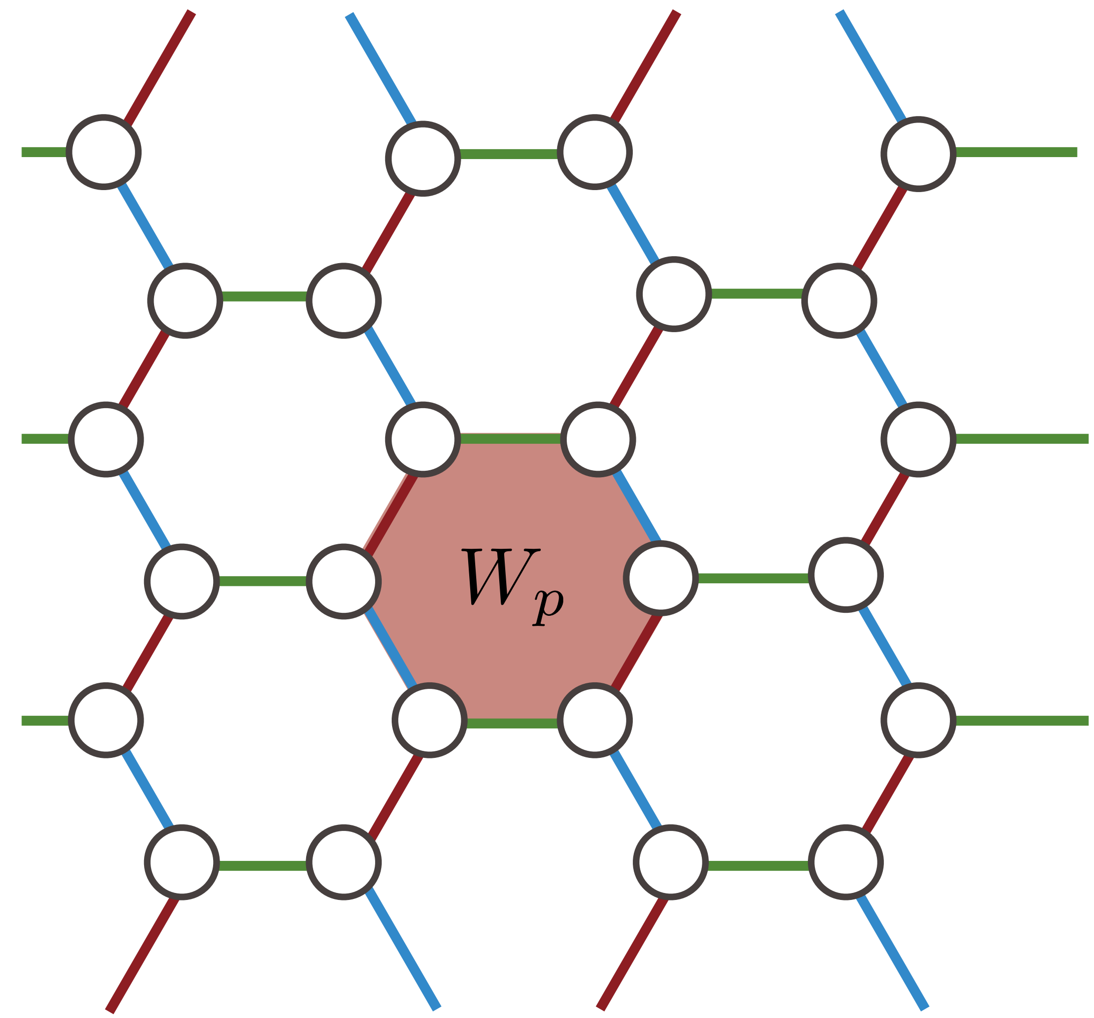
Conserved quantity: Flux

Flux operator

$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

$$[\mathcal{H}, W_p] = 0, [W_p, W_{p'}] = 0$$





Ground state is in the sector with

$$^\forall p, W_p = 1$$

(Vortex free condition)

GS phase diagram

Ground states are spin liquids

$$\mathcal{H} = -\sum_{\gamma,\langle i,j\rangle_\gamma} J_\gamma S_i^\gamma S_j^\gamma$$

Anisotropic region (A) : gapped spin liquid

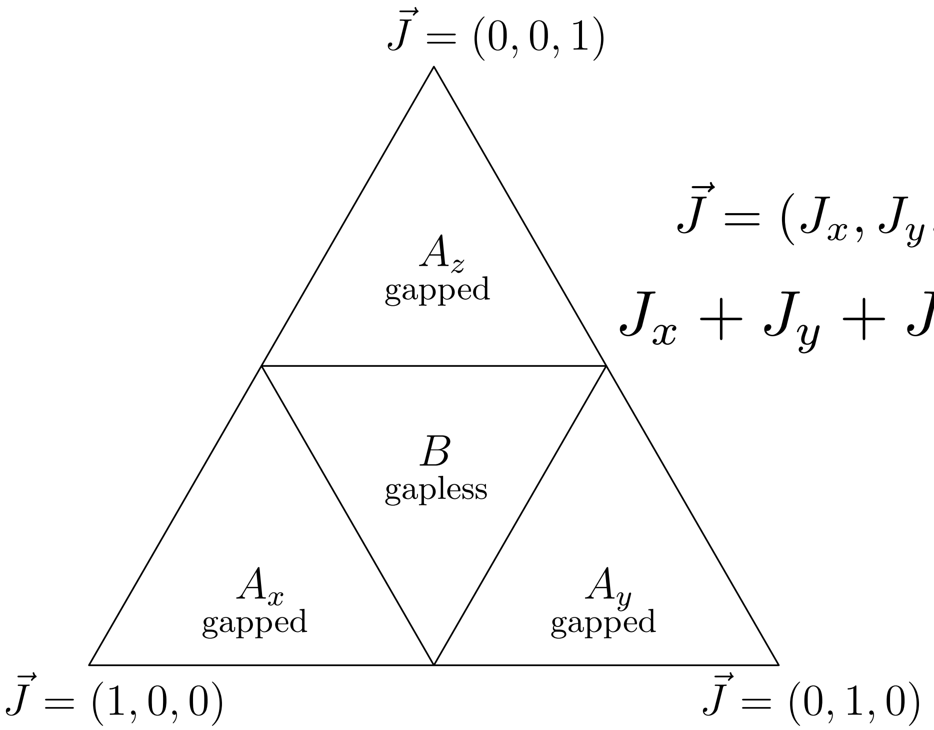
- Excitations of Majorana fermions has finite gap.
- It is adiabatically connected to the toric code.

(In some sense, it is understood well.)

Isotropic region (B) : gapless spin liquid

- Majorana fermions shows gapless excitation.
- The flux excitations is gapped.

G.S. Phase diagram



$\vec{J} = (J_x, J_y, J_z)$

$J_x + J_y + J_z = 1$

Ground state calculation of a Kitaev material

T. Okubo, K. Shinjo, Y. Yamaji et al, Phys. Rev. B **96**, 054434 (2017).

Strong spin-orbit interaction → Kitaev interaction in real compound

G.Jackeli, et al., PRL 102, 017205 (2009)

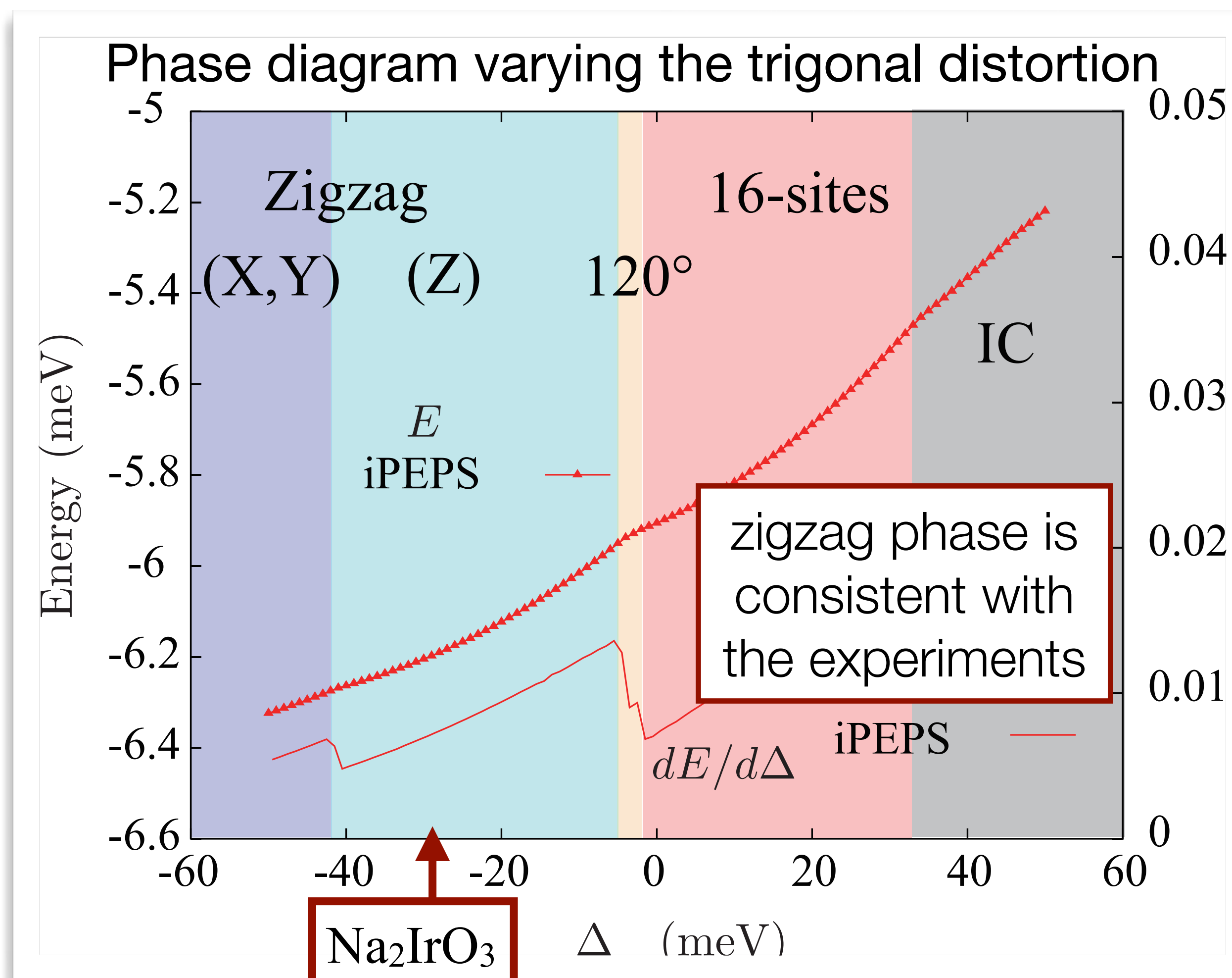
ab initio spin Hamiltonian for Na_2IrO_3

(Y. Yamaji et al. Phys. Rev. Lett. **113**, 107201(2014))

Kitaev + Heisenberg + Off-diagonal interactions
+
2nd and 3rd nearest neighbor interactions

→ Ground state of infinite system calculated by using iTPS

- Due to additional interactions, GS is a magnetically ordered state, instead of the spin liquid.
- In this case, iTPS calculation correctly captured such magnetically ordered GS of the *ab initio* Hamiltonian.

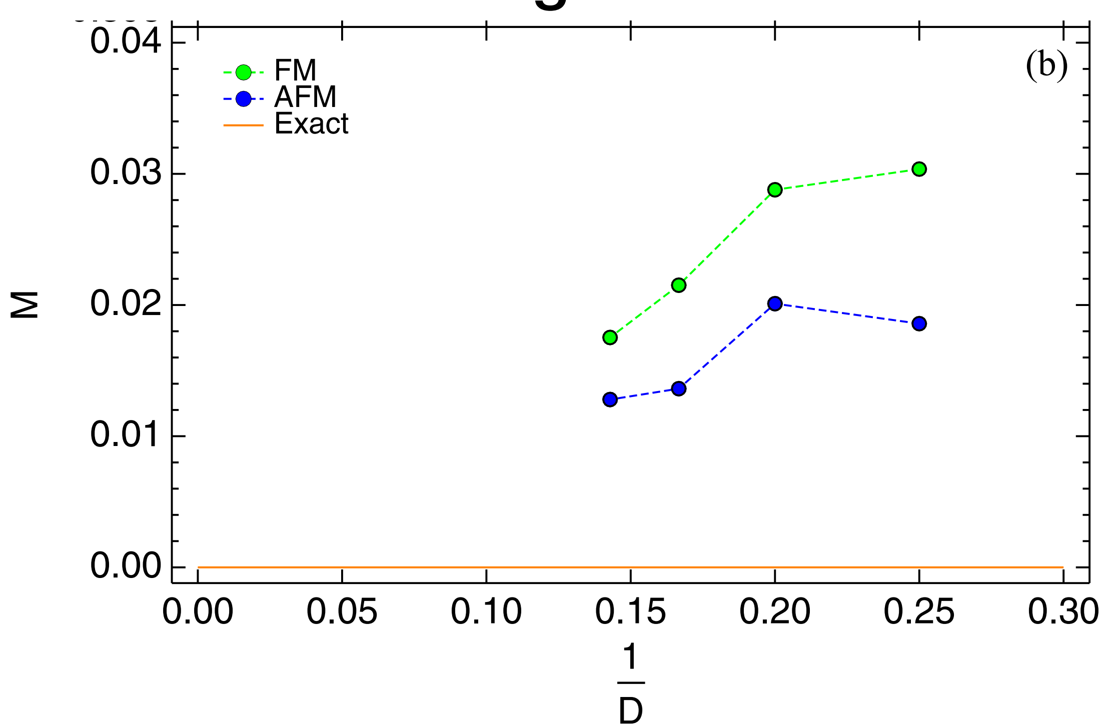


Problems in a standard approach for spin liquid

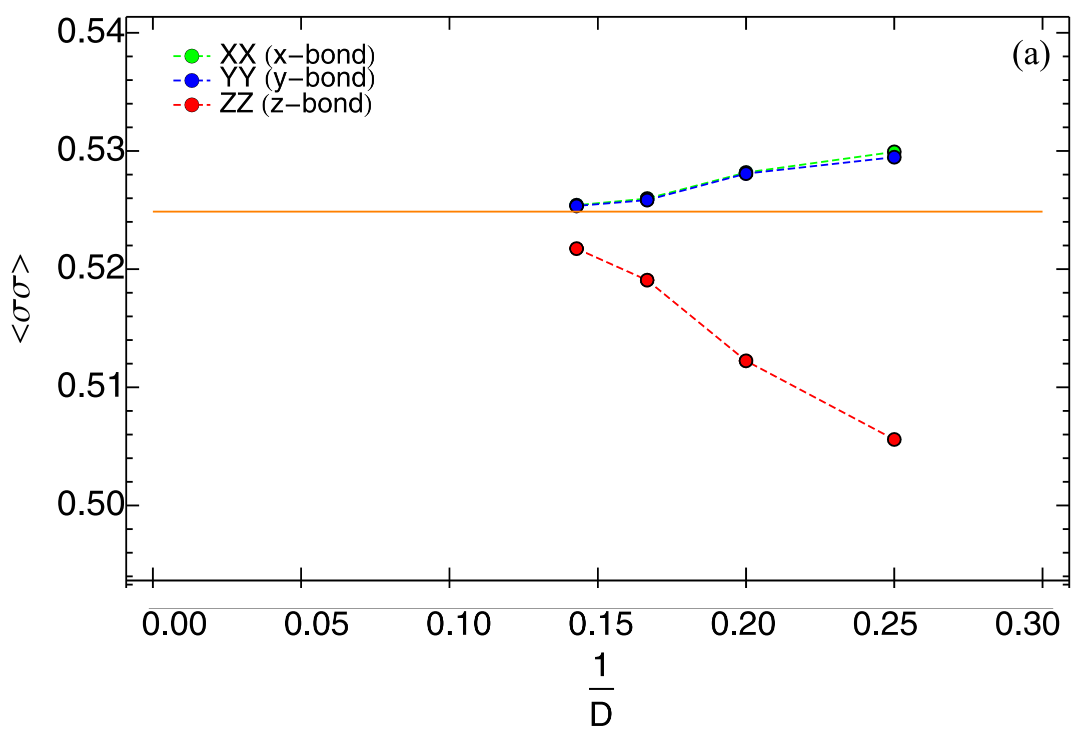
When we use iTPS as a variational wave function, standard optimization scheme (imaginary time evolution) gives a biased result depending on the initial states.

J.O. Iregui, P. Corboz, and M. Troyer, PRB 90, 195102 (2014)

Magnetization



Spin correlation on NN bonds



It is important to find

- A good initial state for the Kitaev spin liquid
- Better optimization methods

in order to investigate models in the vicinity of pure Kitaev model.

Compact TN representation of the spin liquids

Kitaev spin liquids:

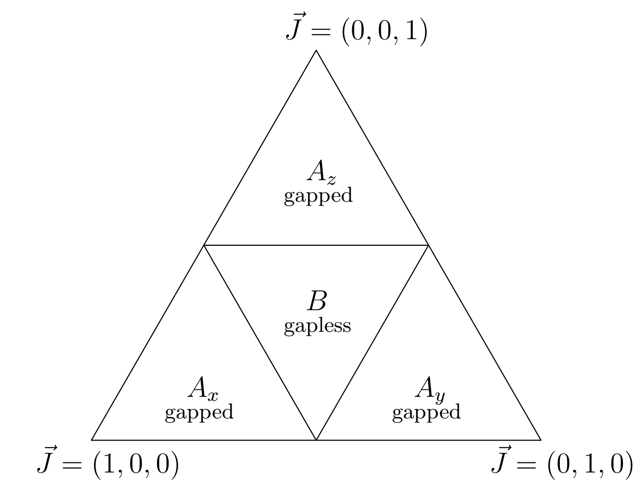
- Gapped spin liquid is adiabatically connected to the toric code
  - The toric code state is represented by D=2 iTPS.

- Gapless spin liquid has no simple tensor network representation.
  - By using Majorana fermions, we can construct a complicated TNS.

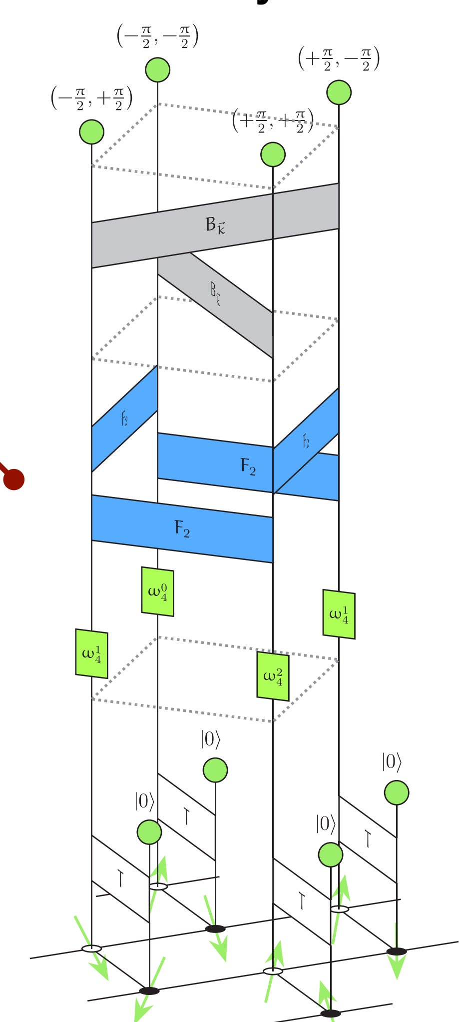
P. Schmoll and R. Orús, Phys. Rev. B, **95** 045112 (2017).

Can we construct simpler TNS for the gapless Kitaev spin liquid?

GS phase diagram



GS for 8 sites honeycomb lattice



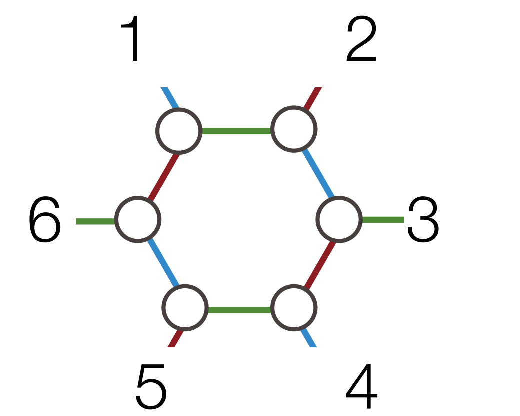
Contents

- Introduction
  - Tensor network representation for quantum states
  - Honeycomb lattice Kitaev model
- Compact tensor network representation for the gapless Kitaev spin liquid
- Finite temperature simulation (on going)
- Summary

Projector onto vortex free sector

The Kitaev spin liquid is in the vortex free sector.

Let us consider the projector onto this sector.



$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

Exercise:

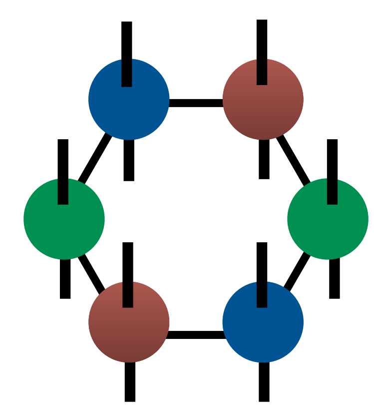
Projector on to $W_i = 1$:

$$P_{i,+} = \frac{I + W_i}{2}$$

It can be represented by D=2 tensor network.

$$P_{i,+} = \mathrm{Tr}\ \left(O_1^x O_2^y O_3^z O_4^x O_5^y O_6^z\right)$$

$$O_i^\alpha = \frac{1}{2^{1/6}} \begin{pmatrix} I & 0 \\ 0 & \sigma_i^\alpha \end{pmatrix}$$



Projector onto vortex free sector

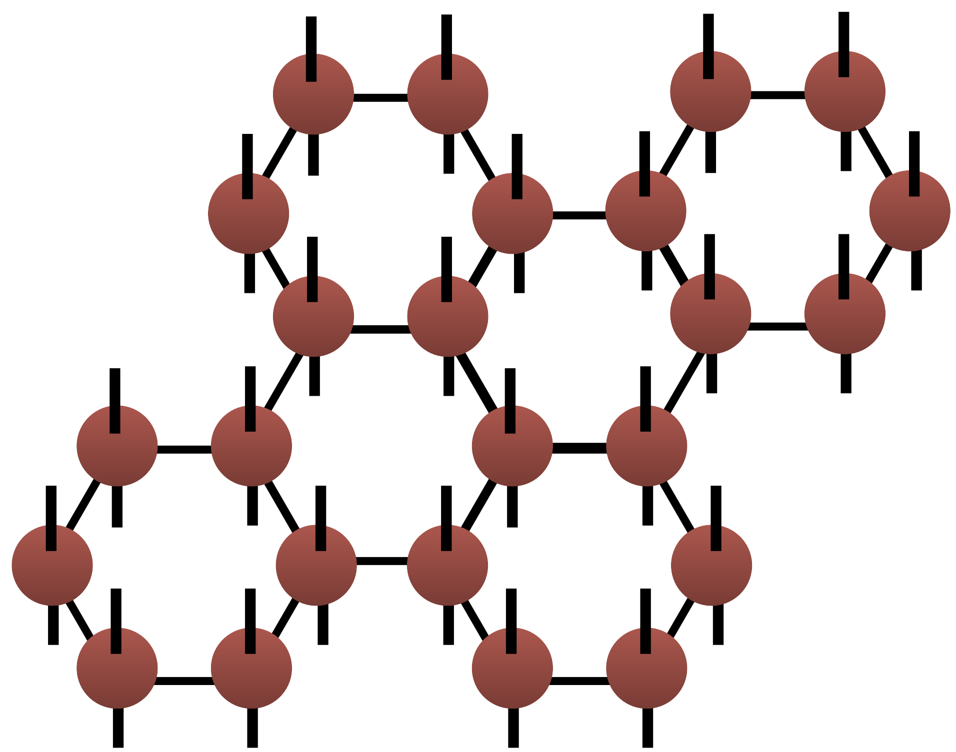
H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

What is a tensor network representation for the vortex free projector?

$$P = \prod_p \frac{I + W_p}{2}$$

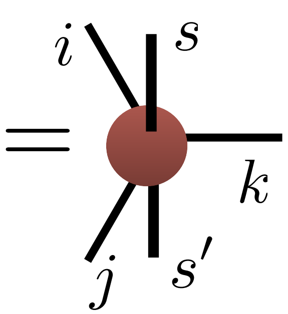
It is given by "loop gas" operator.

$P \propto$



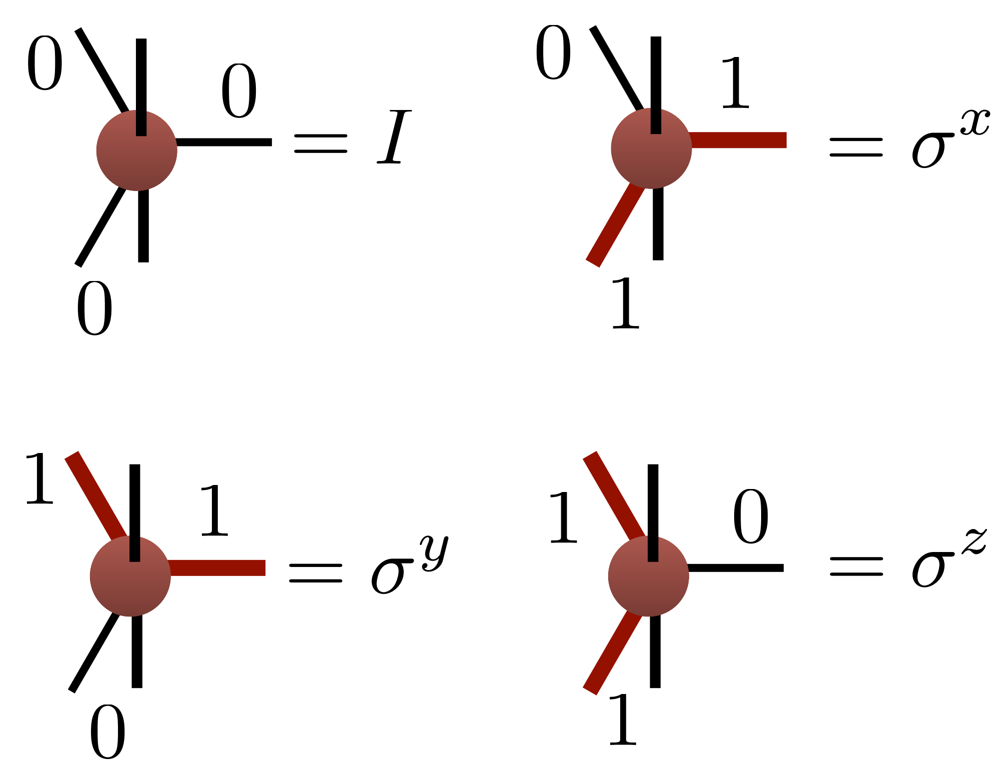
(D=2, TPO)

$Q^{ss'}_{ijk} =$



$i, j, k = 0, 1$

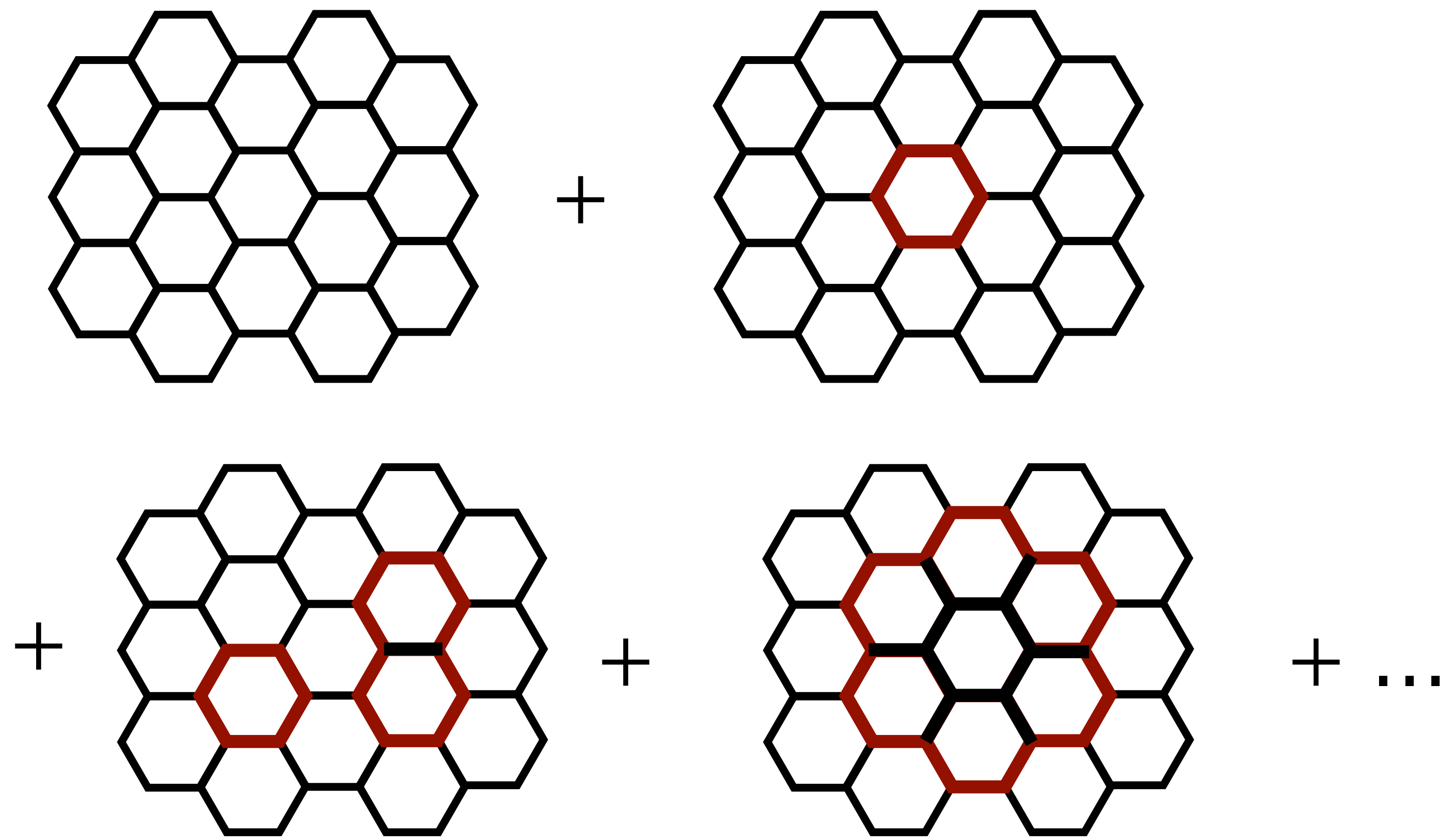
Non zero elements:

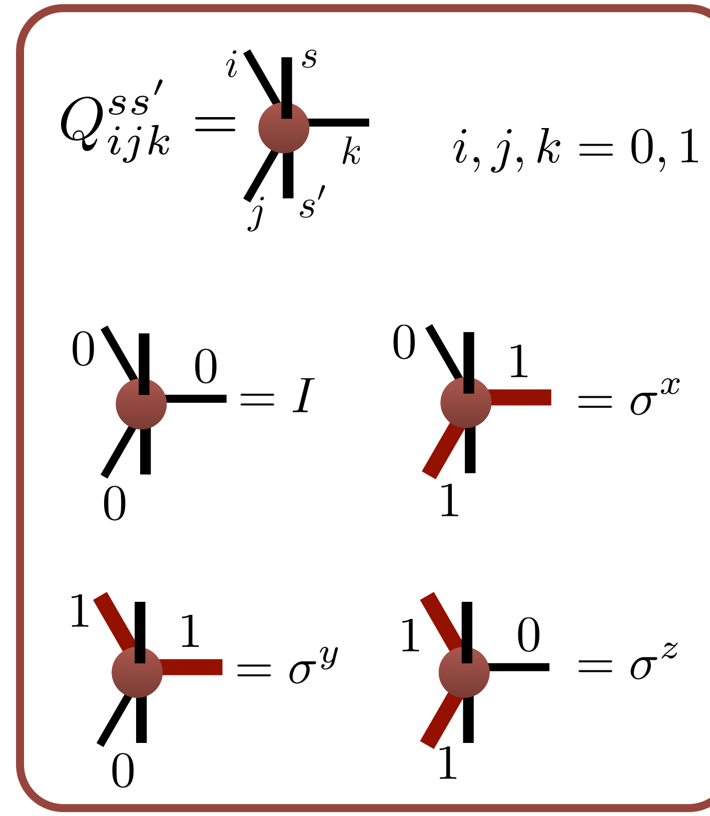


Loop structure of the operator

H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

$$\mathrm{tTr}\prod Q =$$

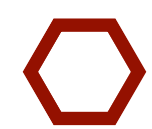


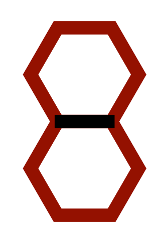


Sum over the all closed loops!

$$= \prod_p (I + W_p) \quad = N_G P$$

$N_G = 2^{N_p}$:# of graphs

Notice:  $= W_p$

 $= W_p W'_p$

…

Loop gas state: a vortex free state

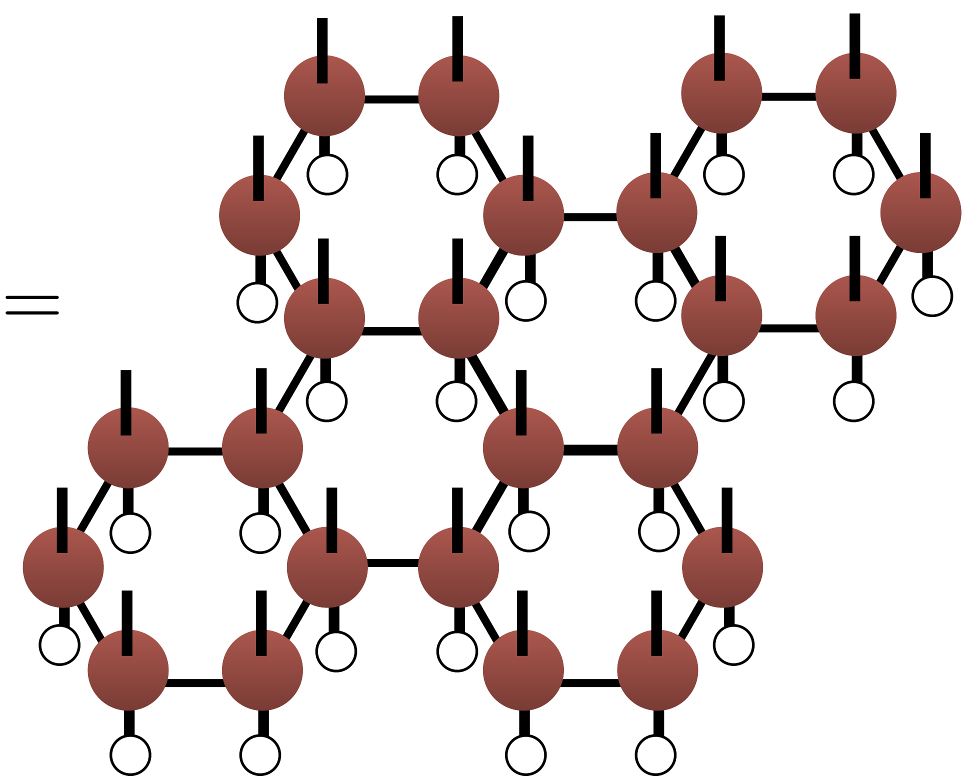
H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

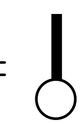
A simple vortex free state corresponding to the isotropic Kitaev model:

$$|\mathrm{LGS}\rangle = \hat{Q}_{LG} \prod_i \otimes |111\rangle_i$$

Ferromagnetic state pointing (1,1,1) direction.

$|\mathrm{LGS}\rangle =$



$|111\rangle =$ 

$$\langle 111|\sigma^{\gamma}|111\rangle = \frac{1}{\sqrt{3}}$$

D=*2*, TPS

Properties of the LGS

H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

$$|\mathrm{LGS}\rangle = \hat{Q}_{LG} \prod_i \otimes |111\rangle_i$$

Symmetries:

From the symmetries of *Q* and |111>, LGS is symmetric under

- Lattice translation
- C_6 lattice rotation (+ spin rotation)
- Reflection + Times reversal

* Single reflection or time reversal symmetry is broken due to underlying |111> state, although it can be recovered by considering a linear combination of Q|111> and Q|-1-1-1>.

Magnetism

Vortex free condition ensures that the LGS is non-magnetic.

→ Qualitatively very similar to the Kitaev spin liquid.

Criticality of the LGS

$$|\mathrm{LGS}\rangle = \hat{Q}_{LG} \prod_i \otimes |111\rangle_i$$

H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

Criticality of the gapless KSL:

- It belongs to so called conformal quantum point.

cf. E. Ardonne, P. Fendley, and E. Fradkin, Ann. Phys. 310, 493 (2004).

→ The wave function itself shows criticality (in 2d).

- It belongs c=1/2 Ising universality class.

(eg. K. Meichanetzidis et al, Phys. Rev. B **94**, 115158 (2016))

↓

If a wave function $|\phi\rangle$ is adiabatically connected to the Kitaev spin liquid, $\langle\phi|\phi\rangle$ should show critical behavior which belongs to the Ising universality.

Criticality of the LGS

$$|\mathrm{LGS}\rangle = \hat{Q}_{LG} \prod_i \otimes |111\rangle_i$$

H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

LGS is mapped to classical loop gas:

$$\langle \mathrm{LGS}|\mathrm{LGS}\rangle = N_G \langle 111|\hat{Q}_{LG}|111\rangle \qquad (\hat{Q}_{LG}^2 = N_G \hat{Q}_{LG})$$

$$= N_G \sum_{G \in \text{closed loop}} \langle 111|Q_G|111\rangle$$

Q_G :product of σ^γ corresponding to the graph G

$$\langle 111|\sigma^\gamma|111\rangle = \frac{1}{\sqrt{3}}$$

$$= N_G \sum_{G \in \text{closed loop}} \left(\frac{1}{\sqrt{3}}\right)^{l_G}$$

l_G :loop length

Identical wit the partition function of the classical loop gas model with fugacity $1/\sqrt{3}$.

On the honeycomb lattice, it is exactly solvable.

(B. Nienhuis Phys. Rev. Lett. **49** 1062 (1982).)

It is actually the critical point of the loop gas model, ant its criticality belongs to the Ising universality class.

LGS : a simple Kitaev spin liquid like state?

H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

Qualitative properties of LGS: $|\mathrm{LGS}\rangle = \hat{Q}_{LG} \prod_i \otimes |111\rangle_i$

- ☑ It satisfies the symmetries common with (gapless) KSL.
  - Lattice translation
  - C_6 lattice rotation (+ spin rotation)
  - Reflection + Times reversal
- ☑ It is vortex free, and therefore nonmagnetic.
- ☑ It shows the same criticality with KSL.

➡ One can consider LGS as the simplest example of KSL.

(It might be similar to the case of AKLT sate against the Haldane phase.)

Systematic improvement of LGS

H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

Energy of LGS for the Kitaev model: $\mathcal{H} = -\sum_{\gamma,\langle i,j\rangle_\gamma} J_\gamma S_i^\gamma S_j^\gamma$

When we calculate the energy of LGS, it is

$$E = \frac{\langle \mathrm{LGS}|\mathcal{H}|\mathrm{LGS}\rangle}{\langle \mathrm{LGS}|\mathrm{LGS}\rangle} \simeq -0.16349 \quad \Longleftrightarrow \quad E_{exact} \simeq -0.19682$$

Large discrepancy

Is is possible to improve the energy without spoiling nice properties of LGS?

→ Yes! We can systematically construct
a family of LGS by using tensor network.

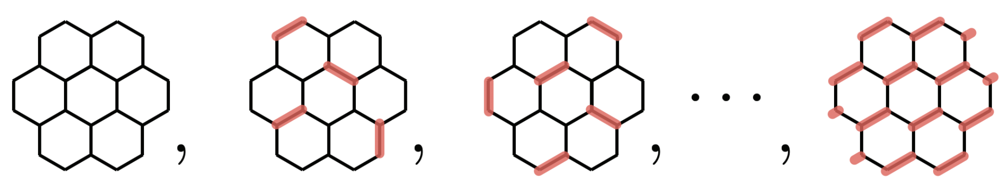
Dimer gas operator

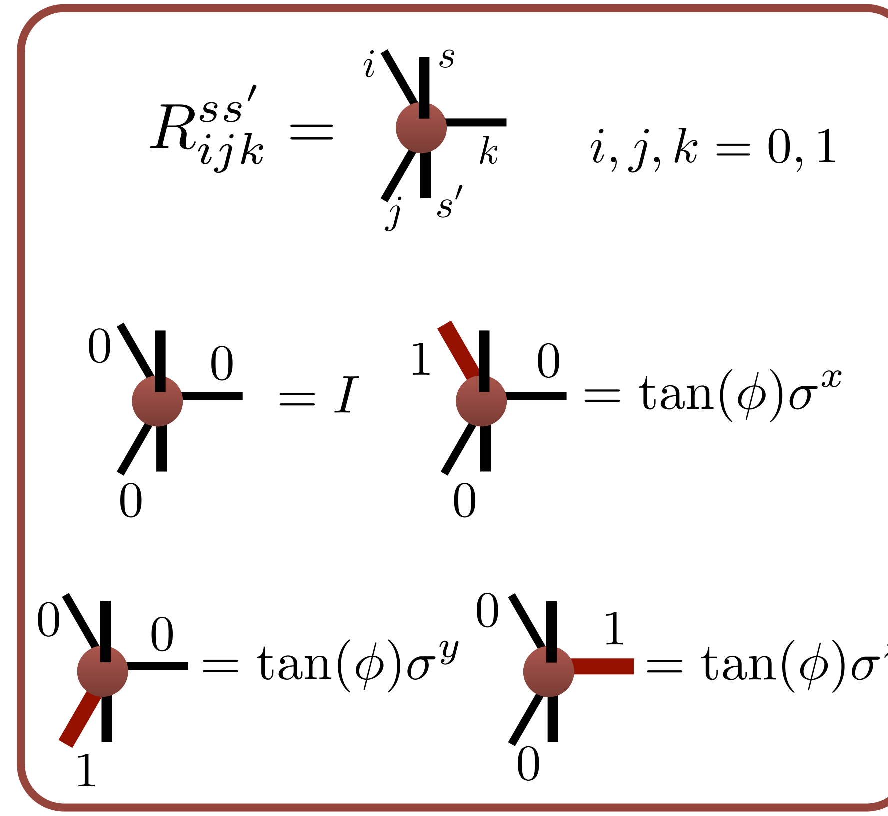
H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

$$\hat{R}_{ijk}(\phi) = \sum_{s,s'} R_{ijk}(\phi)|s\rangle\langle s'|$$

$$\hat{R}_{DG}(\phi) = \mathrm{tTr}\prod_{\alpha} \hat{R}_{i_\alpha j_\alpha k_\alpha}(\phi)$$

$$= \sum_{G \in \Gamma_D} (\tan(\phi))^{l_G} Q_G$$

$\Gamma_{\mathrm{D}} =$ 



We can show $[\hat{R}_{DG}(\phi), \hat{Q}_{LG}] = 0$

, and it satisfies all symmetries same with LGO.

So, application of DG operator does not spoil the properties of LGO.

String gas states: energies

H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRL **123**, 087203 (2019)

*n*th-order string gas state (SGS)

$$|\psi_n\rangle = \left[\prod_i^n \hat{R}_{DG}(\phi_i)\right] |\mathrm{LGS}\rangle$$

	$\lvert\psi_0\rangle = \lvert\mathrm{LGS}\rangle$	$\lvert\psi_1\rangle$	$\lvert\psi_2\rangle$	Exact
D	2	4	8	
# of parameters	0	1	2	
E/J	-0.16349	-0.19643	-0.19681	-0.19682
$\Delta E/E_{ex}$	0.17	0.02	0.0007	-

By using only two variational parameters,
we can obtain very accurate energy.

By LGS and SGS, we can accurately represent the gapless Kitaev spin liquid qualitatively and quantitatively!

LGS for chiral spin liquids

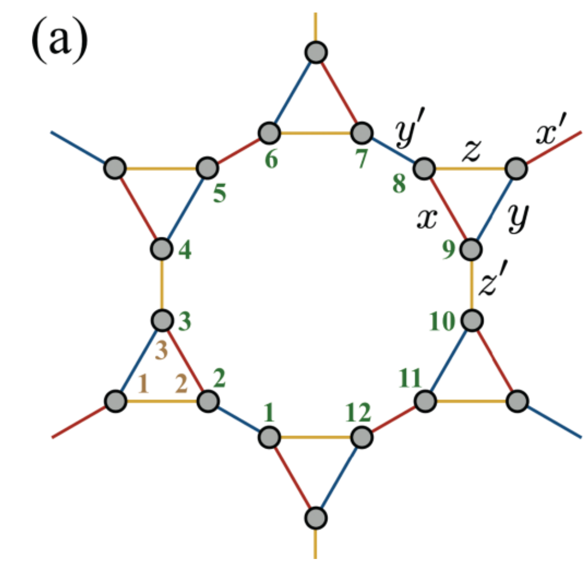
H.-Y. Lee, R. Kanako, T.O. and N. Kawashima, PRB **101**, 035140 (2020)

Kitaev model on the star lattice

$$\hat{\mathcal{H}} = -\frac{J}{4}\sum_{\langle ij\rangle\in\gamma}\hat{\sigma}_i^{\gamma}\hat{\sigma}_j^{\gamma} - \frac{J'}{4}\sum_{\langle ij\rangle\in\gamma'}\hat{\sigma}_i^{\gamma'}\hat{\sigma}_j^{\gamma'},$$

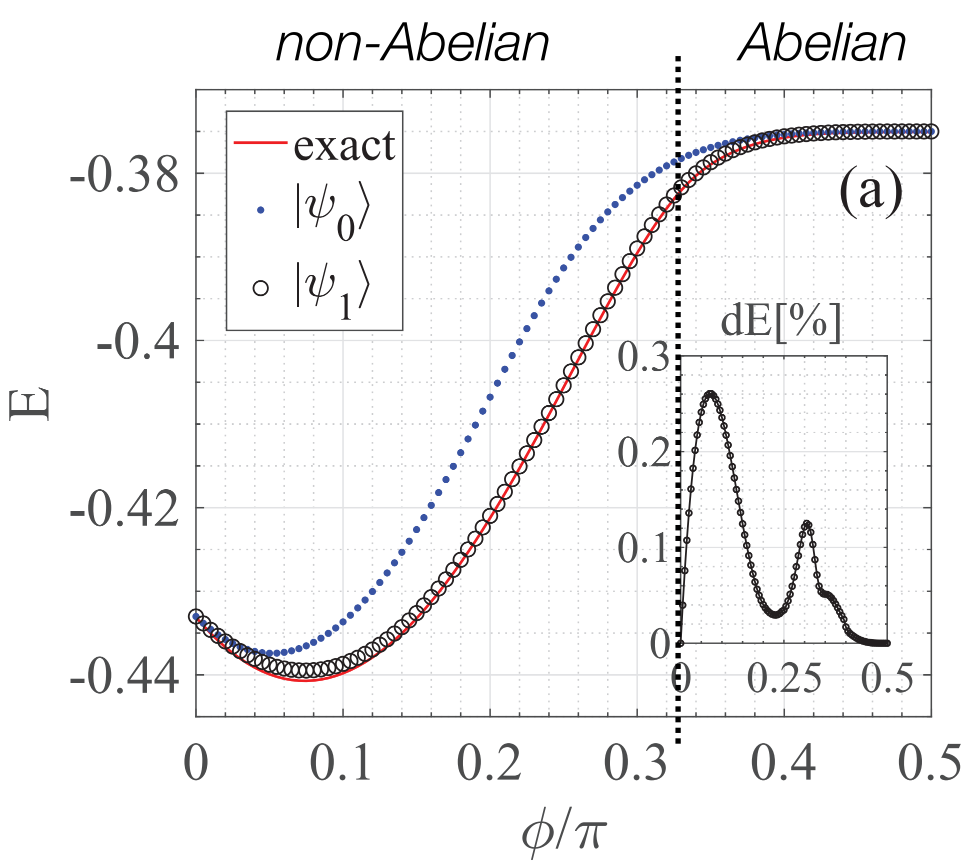
Ground state is a chiral spin liquid.

Star lattice

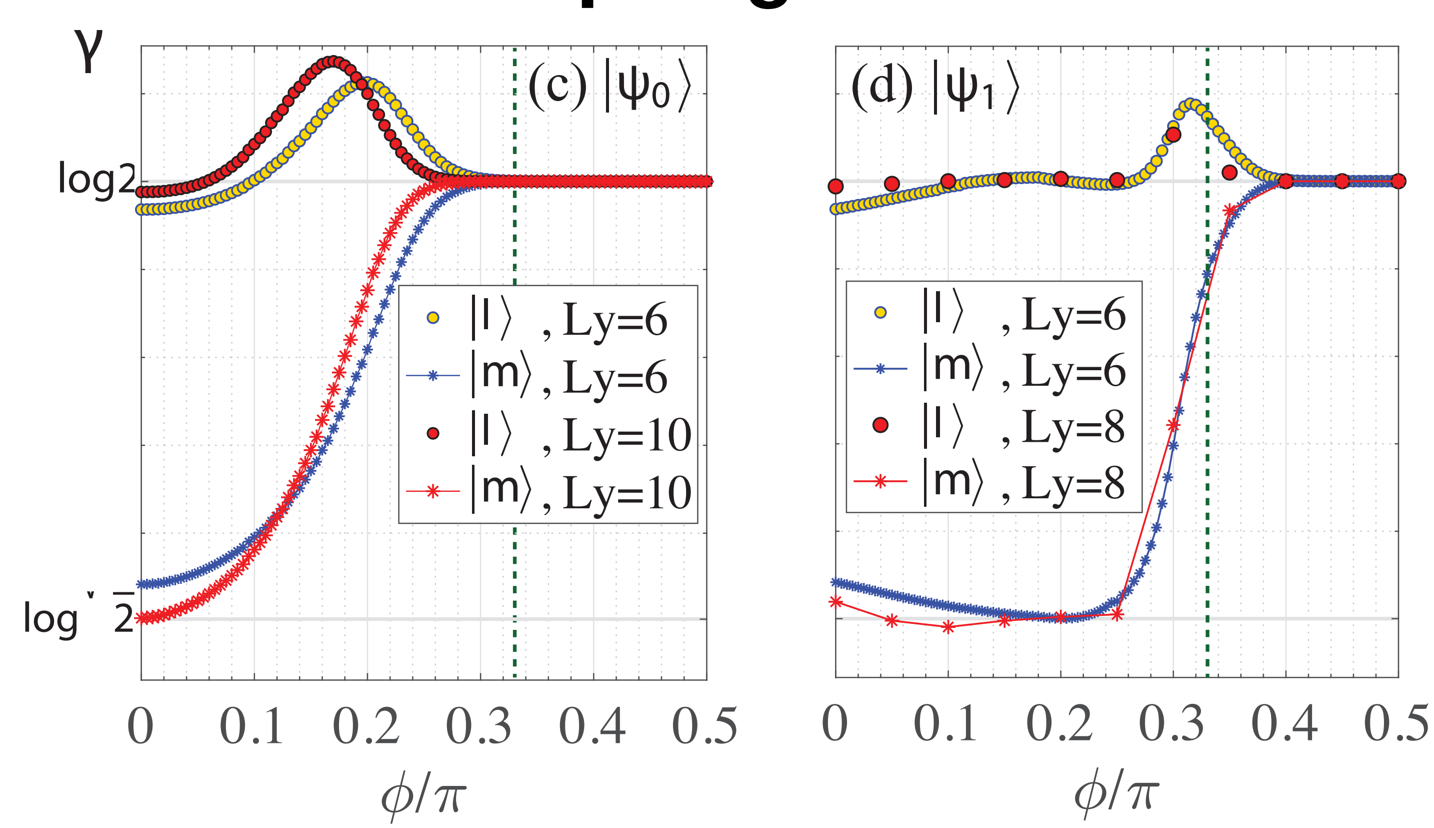


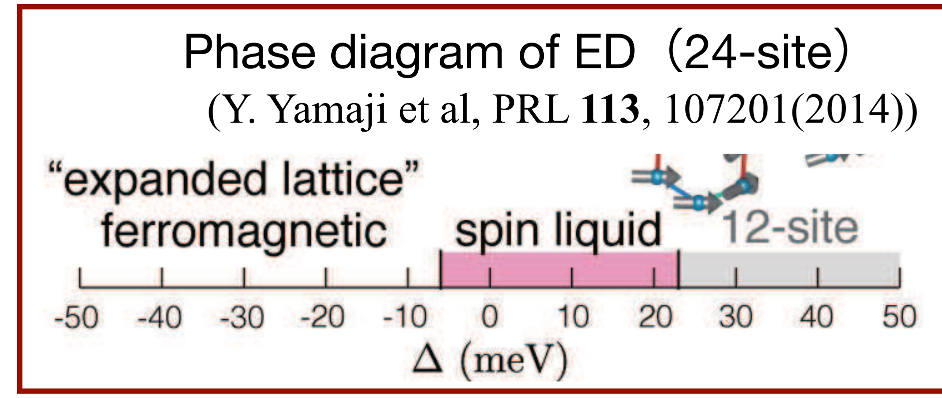
$J/J' = \tan\phi$

Energy



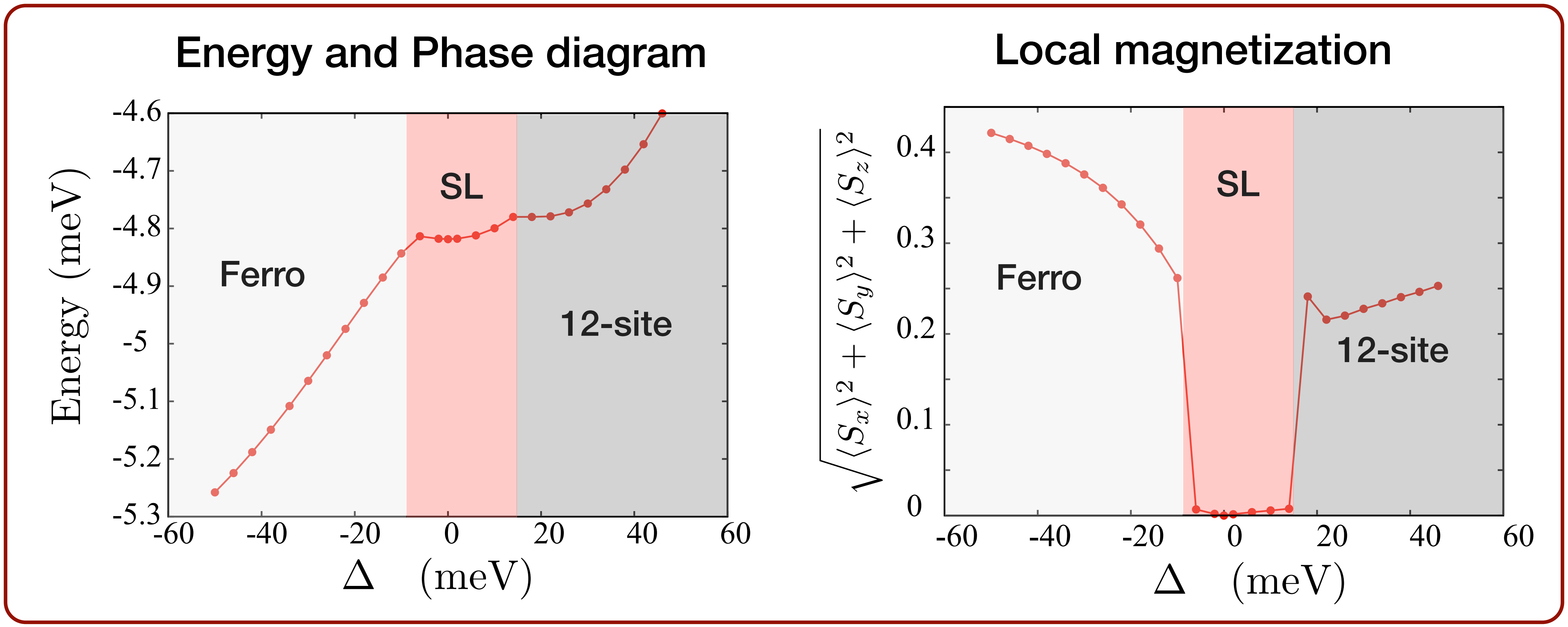
Topological EE





LGS as initial states

ab initio Hamiltonian for Na_2IrO_3 (with lattice expansion)



- iTPS phase diagram is qualitatively consistent with the ED.
  - Around Δ=0, a Kitaev spin liquid phase is clearly stabilized.

Contents

- Introduction
  - Tensor network representation for quantum states
  - Honeycomb lattice Kitaev model
- Compact tensor network representation for the gapless Kitaev spin liquid
- Finite temperature simulation (on going)
- Summary

Finite temperature calculation

Expectation value

$$\langle \hat{O} \rangle_\beta = \mathrm{Tr}[\rho(\beta)\hat{O}]$$

Density matrix $\rho(\beta) = \frac{1}{\mathcal{Z}} e^{-\beta \mathcal{H}}$

Partition function $\mathcal{Z} = \mathrm{Tr}\ e^{-\beta \mathcal{H}}$

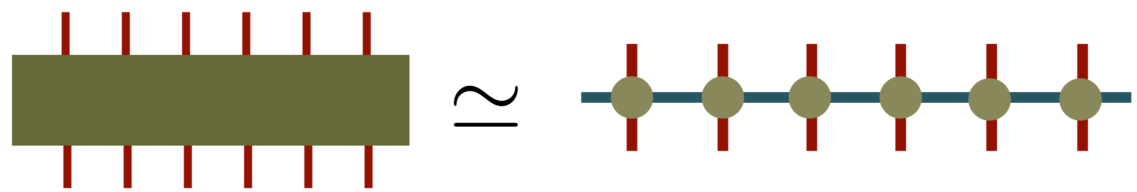
How can we calculate the expectation value?

1. Full diagonalization: $$\langle \hat{O} \rangle_\beta = \frac{\sum_n \langle n | e^{-\beta E_n} \hat{O} | n \rangle}{\sum_n \langle n | e^{-\beta E_n} | n \rangle}$$
   - Size is limited due to $O(e^N)$ dimension of the Hilbert space
2. QMC: MCMC sampling of world line configurations
   - We can treat large size. But, application of QMC is limited due to the sign problem.
3. Typical pure states (Restricted to finite size systems)
4. Approximation of density operator

Tensor network representation of density matrix

Possible two representations of the density matrix as TNs.

1. Direct TPO representation (cf. A. Kshetrimayum et al, PRL **122**, 070502 (2019))

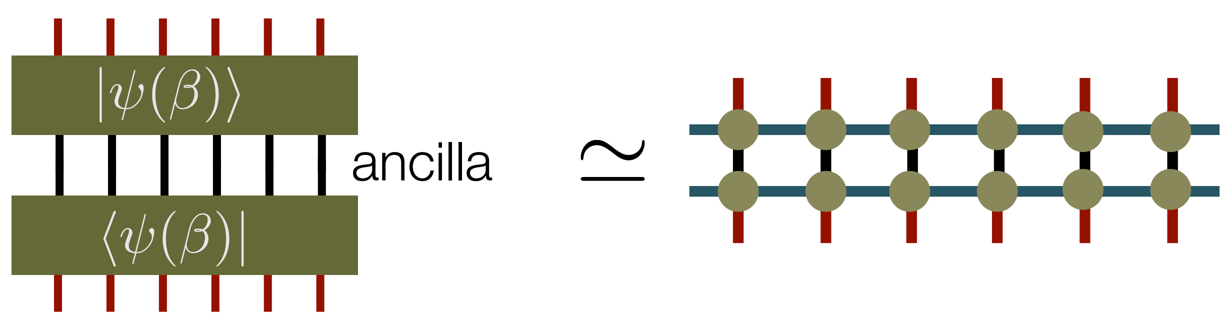
$\rho(\beta) =$ 

This talk

Pros:
- Algorithm becomes simpler.

Cons:
- Approximate density matrix may contain negative (or complex) eigenvalues.
- For full update, we need much cost.

2. Local purification (cf. Czarnik et al, PRB **99**, 035115 (2019))

$\rho(\beta) =$ 

Pros:
- The approximate density matrix is positive semi-definite.

Cons:
- Optimization of ancilla degree of freedoms seems to be complex.
- Bond dimensions can be much larger than the direct representation.

Gemma De las Cuevas et al, New J. Phys. **15**, 123021 (2014)

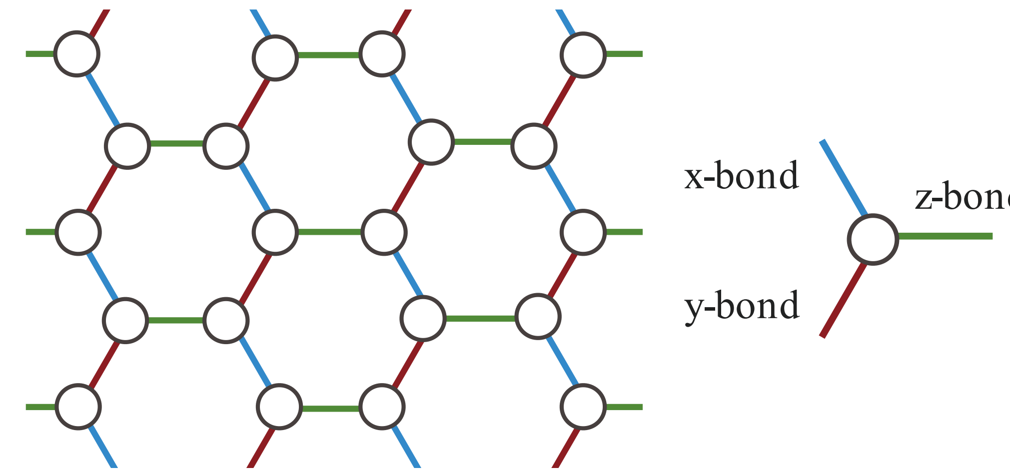
Target: Honeycomb lattice Kitaev Model

Kitaev model A. Kitaev, Annals of Physics 321, 2 (2006)

$$\mathcal{H} = -K \sum_{\gamma, \langle i,j \rangle_\gamma} S_i^\gamma S_j^\gamma$$

γ :bond direction

$\left(S = \frac{1}{2}\right)$

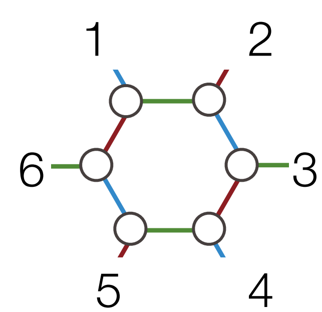


- Ground state is gapless spin liquid

  It satisfies the vortex free condition:

$$^\forall p, W_p = 1$$

p: plaquette



Flux: $W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$

$$[\mathcal{H}, W_p] = 0, [W_p, W_p'] = 0$$

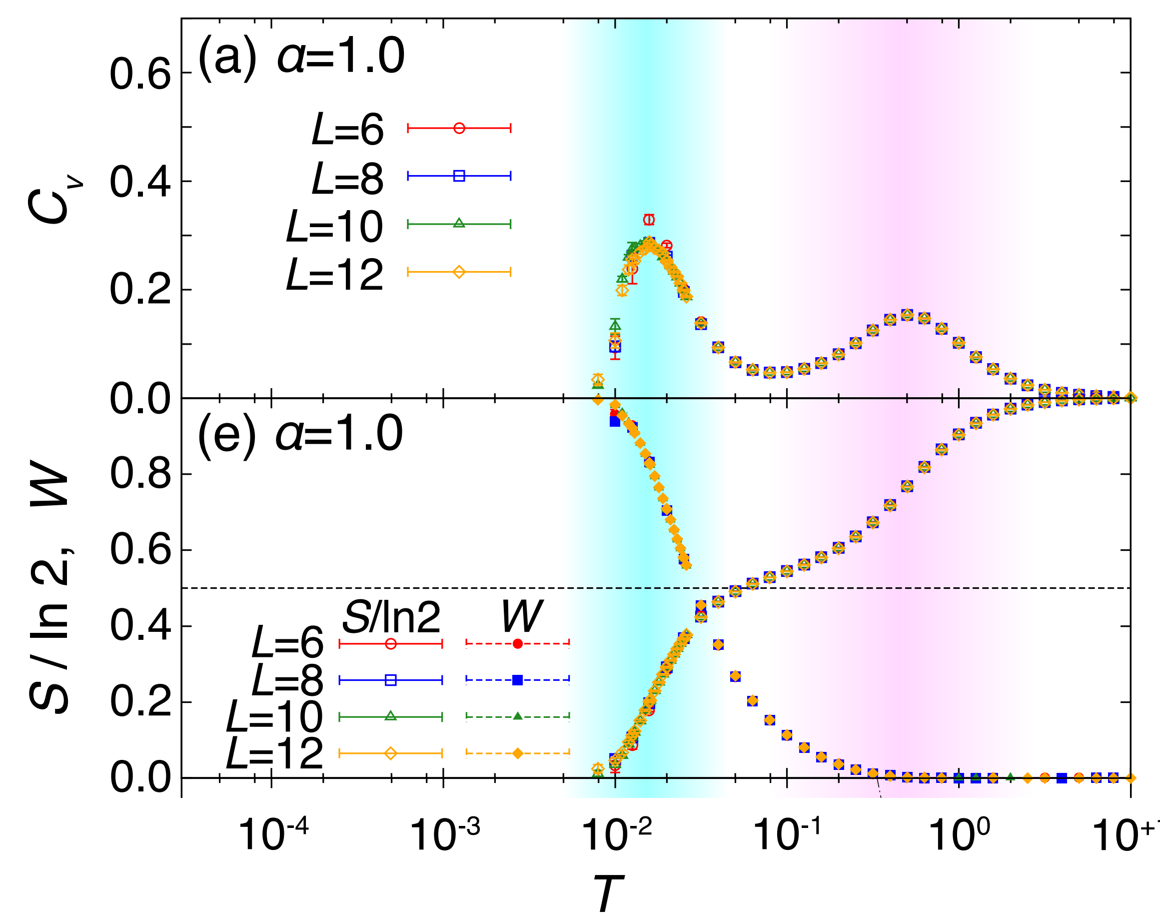
(cf. H.-Y. Lee, et al, PRL (2019))

- At finite temperature, double peaks structure is expected in the specific heat.

  The low temperature peak corresponds to the development of the flux.

Can we reproduce it by iTPO method?

J. Nasu et al PRB **92**, 115122 (2015) (QMC)

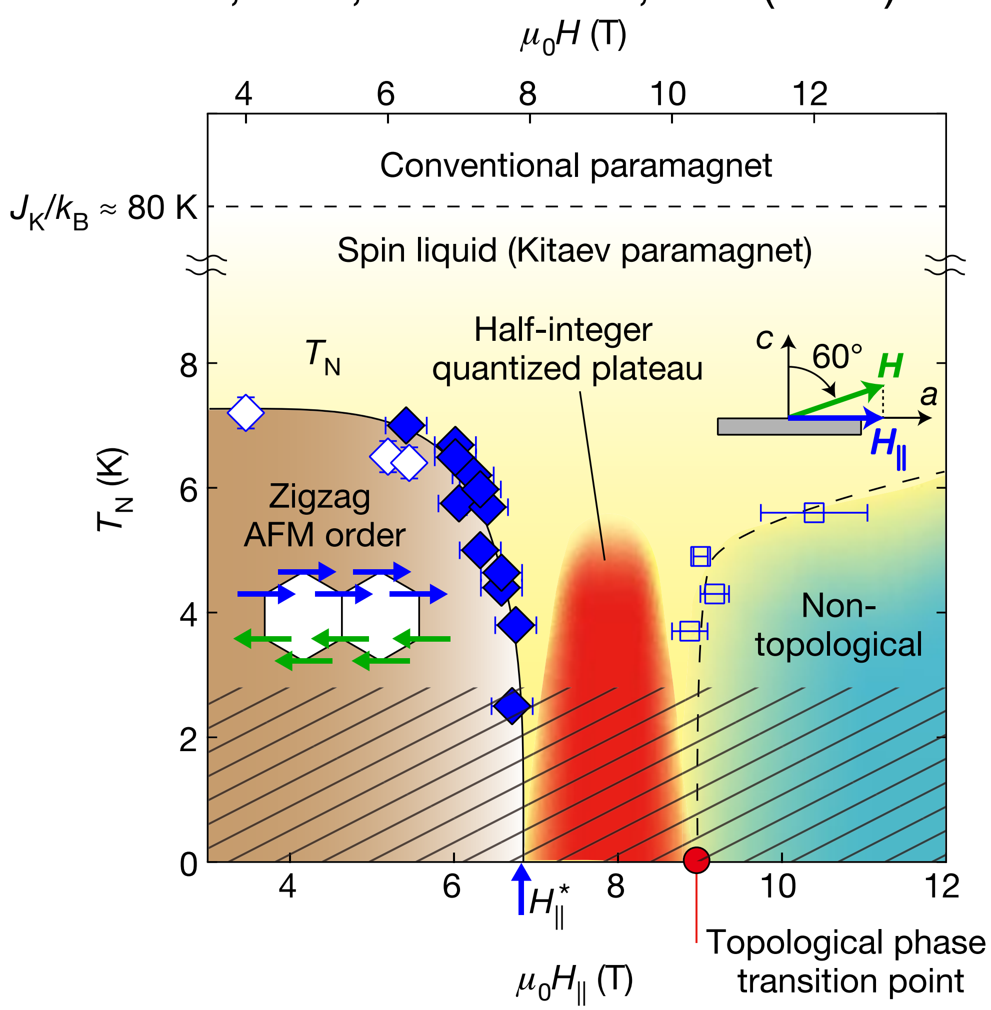


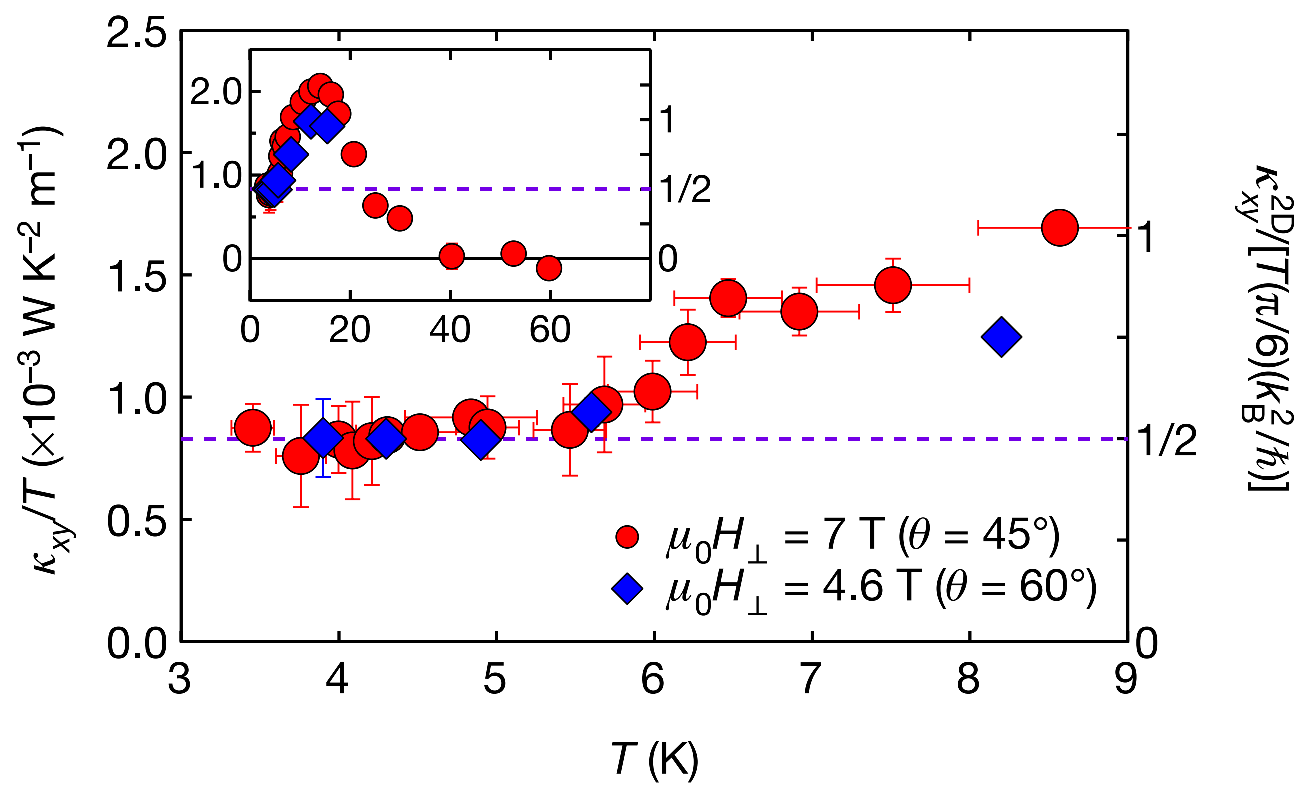
Another motivation: Kitaev material

α-RuCl₃ :candidate of Kitaev spin liquid under a magnetic field

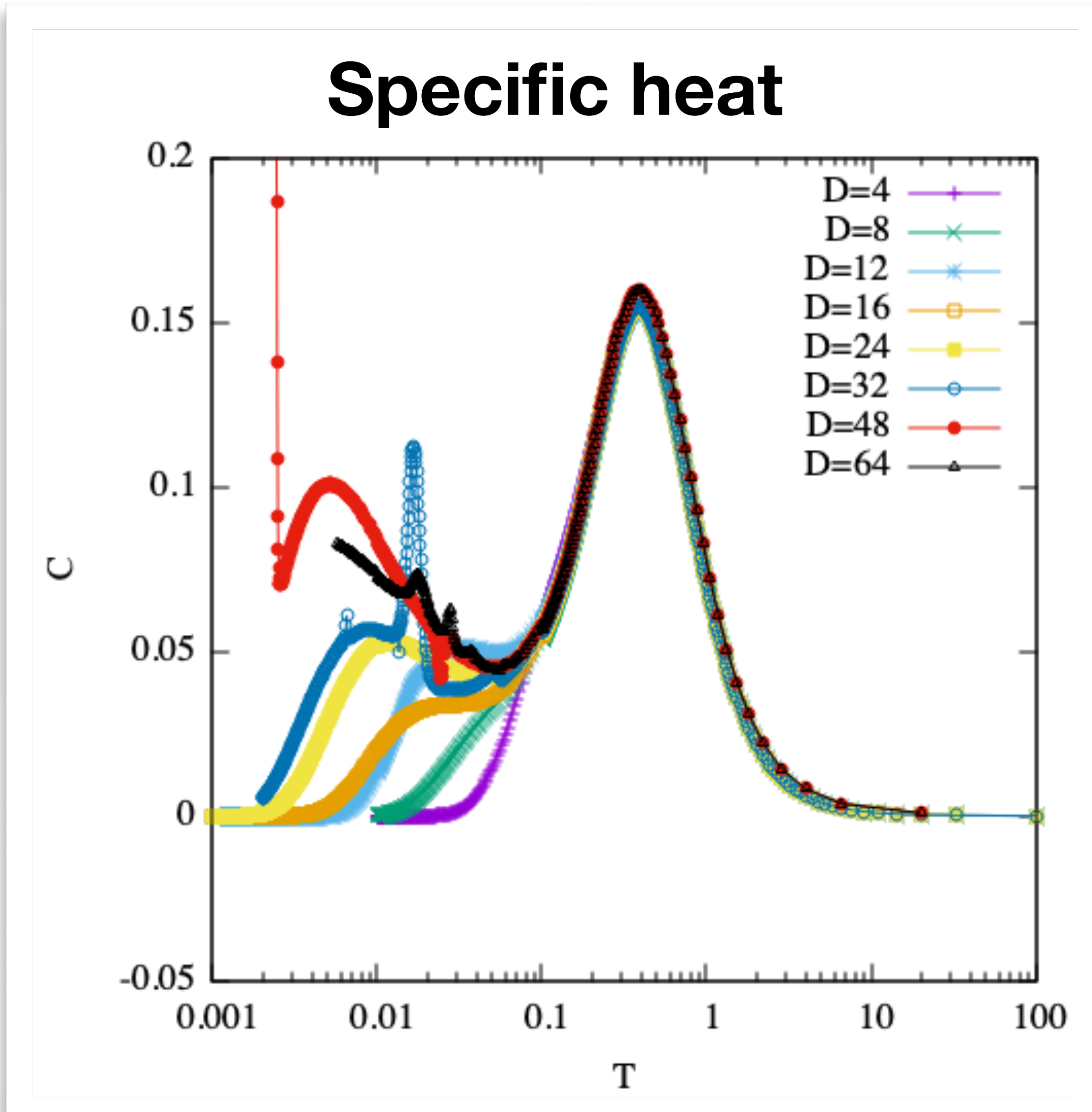
- Its ground state is Zigzag state at zero magnetic field.
- Under a moderate magnetic field, the magnetic order seems to disappear.
- In this "phase", they observed half quantized thermal Hall conductivity.

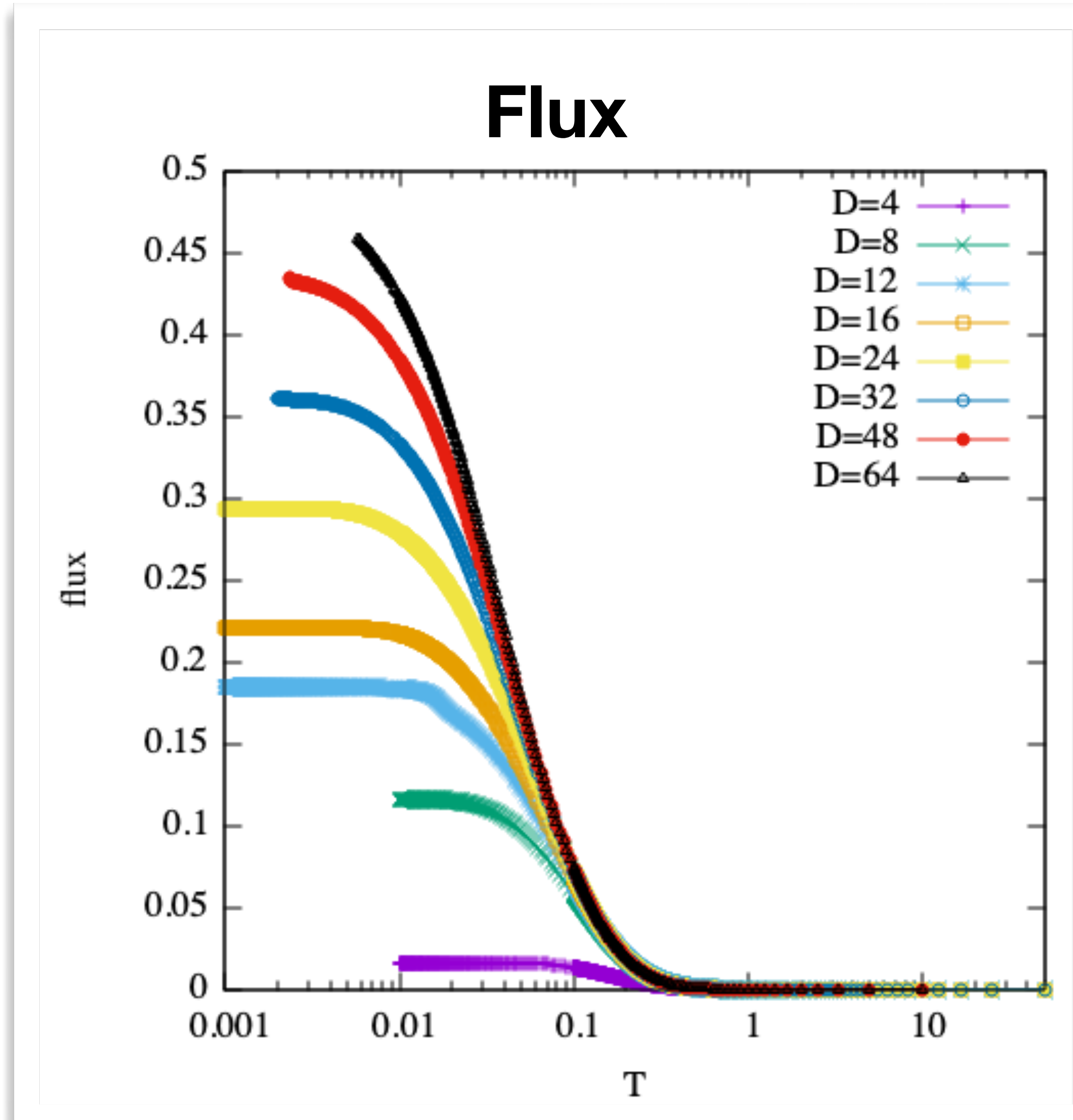
Y. Kasahara, et al, Nature **559** , 227 (2018).





Results: specific heat and flux



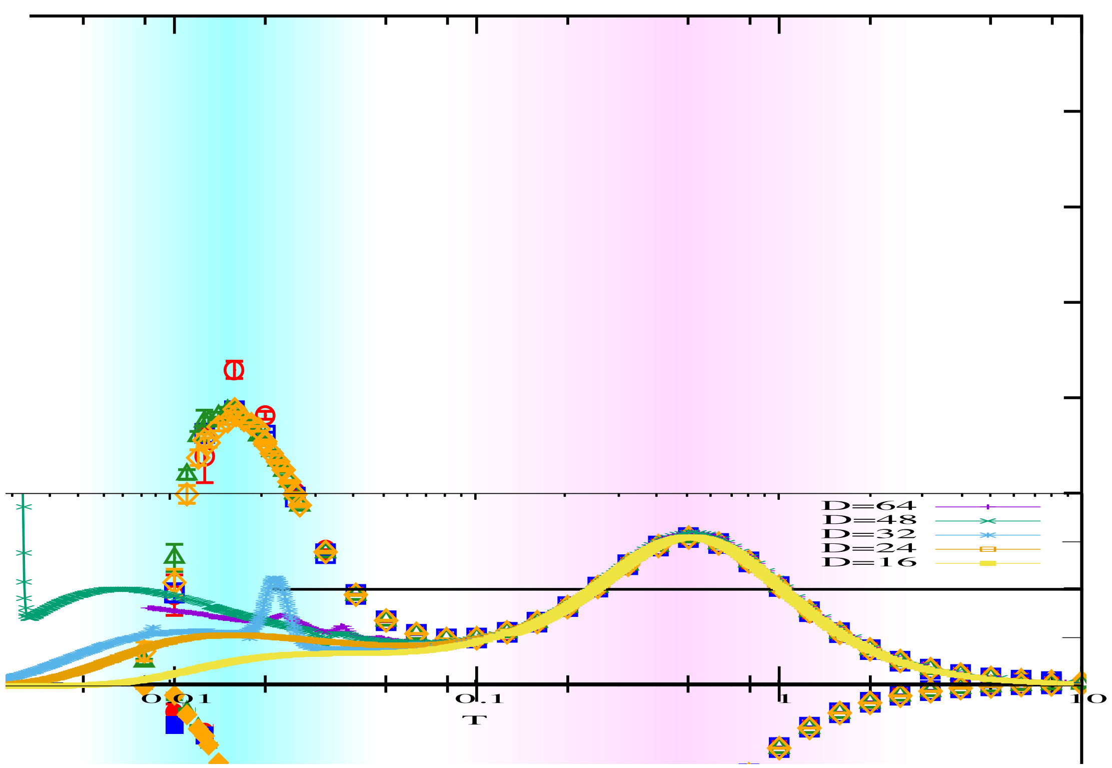


- Small *D*, we do not see two peak structure.
- As *D* is increased, the second peak becomes visible.
  - It corresponds to the increase of the flux.

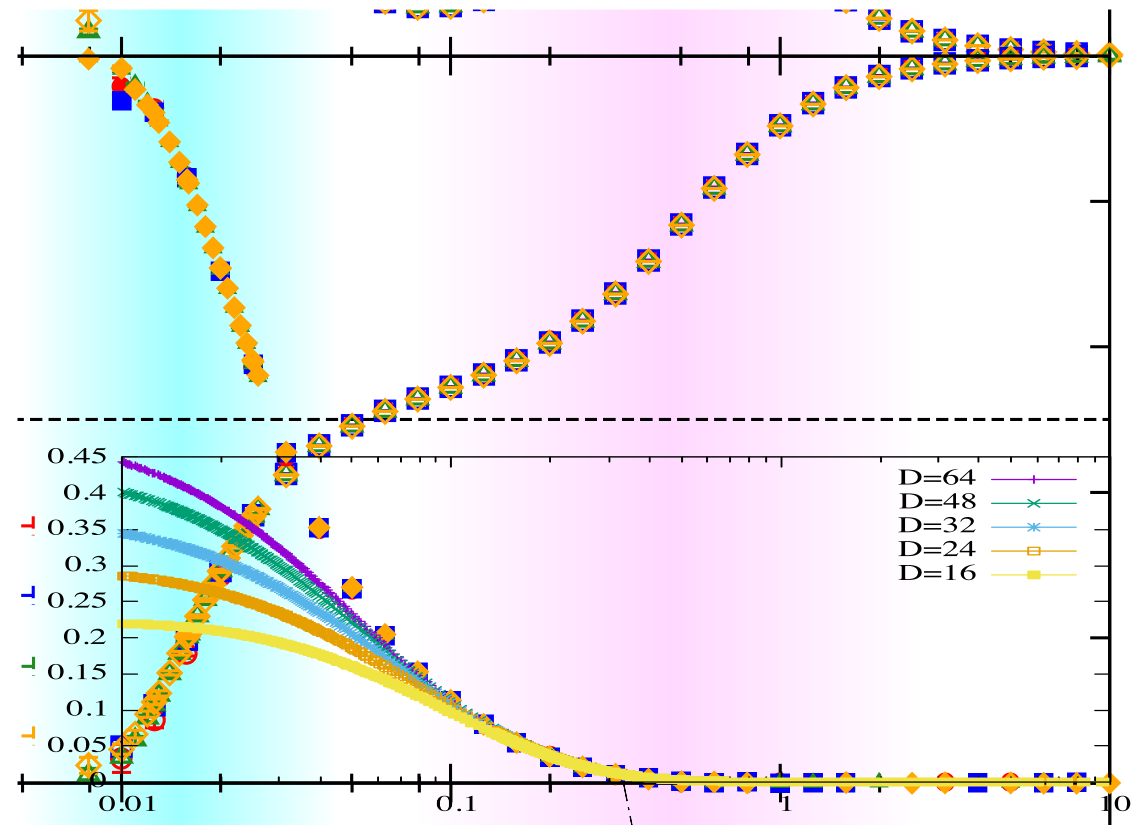
Comparison between iTPO and QMC

J. Nasu et al PRB **92**, 115122 (2015) (QMC)

Specific heat



Flux



Compared with QMC, TPO method could not capture the quantitative nature of Kitaev spin liquid at $T < 0.1$.

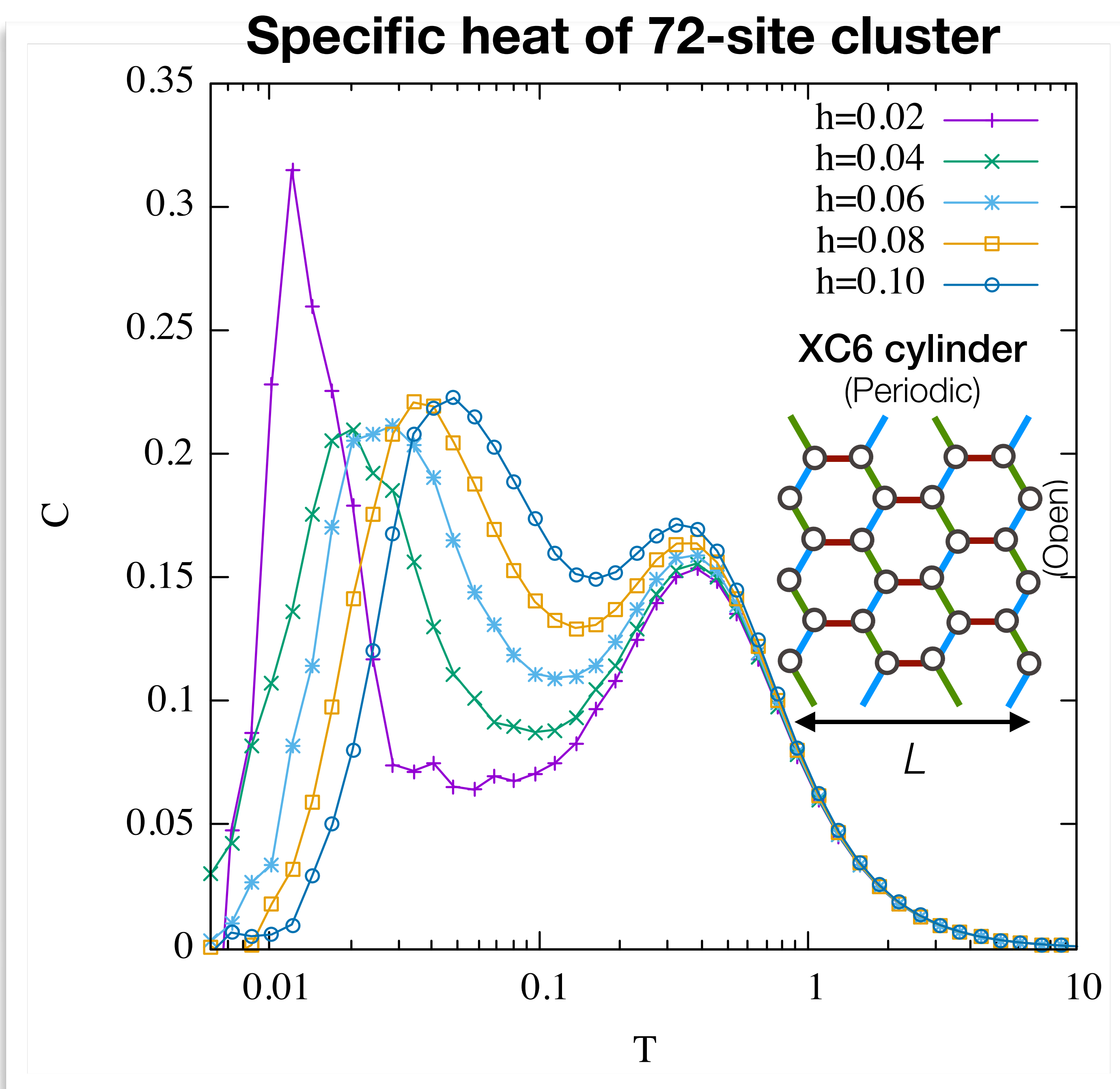
This is probably due to the difficulty of optimization for infinite TPS.

When we consider finite size systems, optimization becomes easier.

Kitaev model under a magnetic field (preliminary)

(In collaboration with Y. Motome, J. Nasu and T. Misawa)

- Instead of the infinite 2d system, we consider a finite cylinder.
- For this setup, MPO representation of the density matrix works well.
 (cf. H. Li et al, arXiv:2006.02405)
- We can accurately calculate finite temperature properties even at low temperature.
    - 2nd peak of the specific heat.
- We can discuss interesting properties, such as the thermal current.
    - It will be reported in the next JPS meeting.



Summary

- Tensor networks are useful tool to investigate quantum many-body problems
  - We can investigate a variety of frustrated spin systems by iTPS.
- We proposed compact tensor network representations for the gapless Kitaev spin liquid.
  - They are represented by loop gas or string gas configurations.
  - They satisfy common symmetries with the Kitaev model.
  - They are critical and belong to the Ising universality class.
- We can extend the tensor network method to finite temperature.
  - For the infinite Kitaev model, accuracy becomes worse at a low temperature.
  - For a finite size cluster, we can obtain reliable result by using MPO representation.

TeNeS: Tensor Network Solver

We are developing a open source software for massively parallel tensor network solver for 2D quantum lattice system.

https://github.com/issp-center-dev/TeNeS

- ☑ Ground state calculation of infinite 2d quantum spin (or boson) models
- ☑ Easy calculation for standard 2D lattices
  - You can also calculate models on general 2D lattices
- ☑ Support of parallel calculations