Kitaev Physics in Strongly Correlated Electron Systems with Spin-Orbit Coupling

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Collaboration with

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University of Tokyo

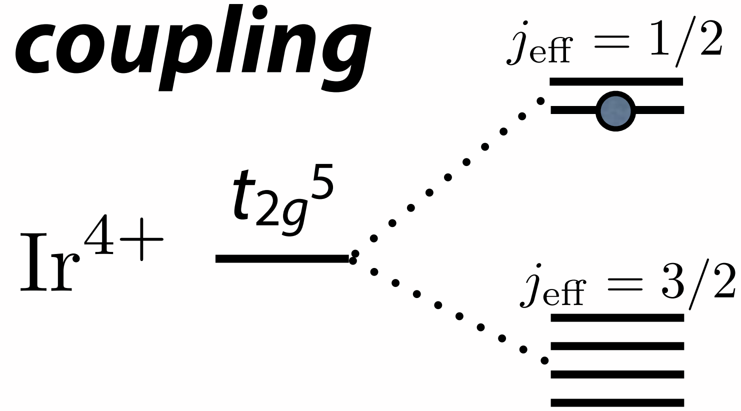
JN, T. Kaji, K. Matsuura, M. Udagawa, and Y. Motome, Phys. Rev. B **89**, 115125 (2014)

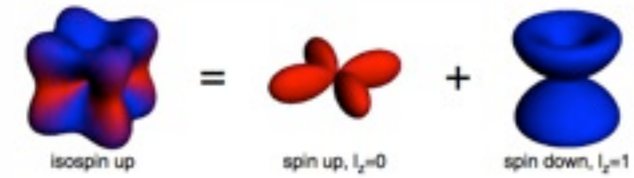
JN and Y. Motome, to be published in Phys. Rev. B

JN, M. Udagawa, and Y. Motome, arXiv:1406.5415

Kitaev Physics in Transition Metal Oxides

Strong spin-orbit coupling





$j_{\rm eff}$=1/2 localized spin

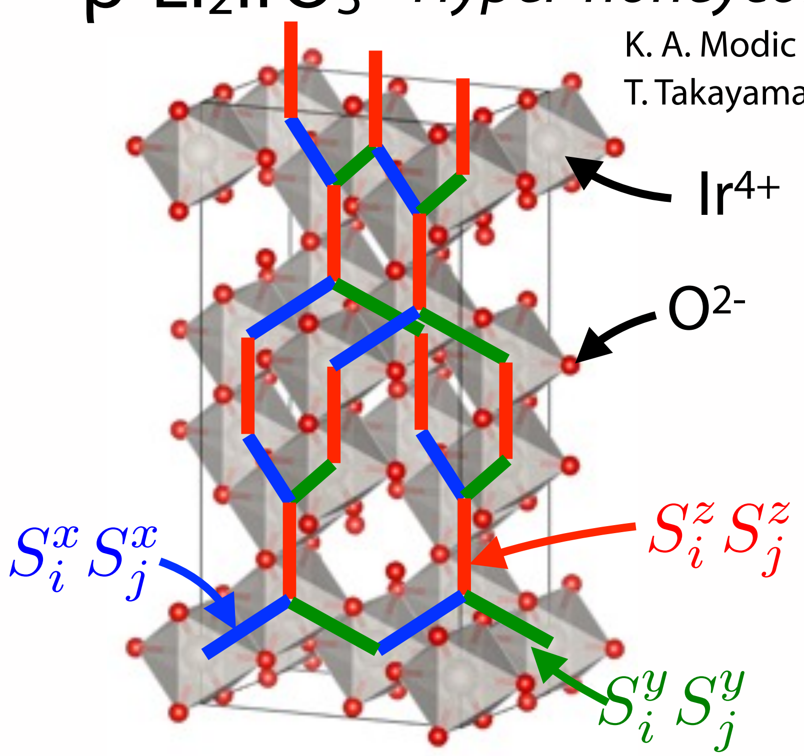
G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009)

→ ***Kitaev-type interaction***

(bond-dependent Ising-type interaction)

β-Li_2IrO_3 *Hyper-honeycomb lattice*

K. A. Modic et al., Nat. comm. **5**, 4203 (2014).
T. Takayama et al., arXiv:1403.3296.

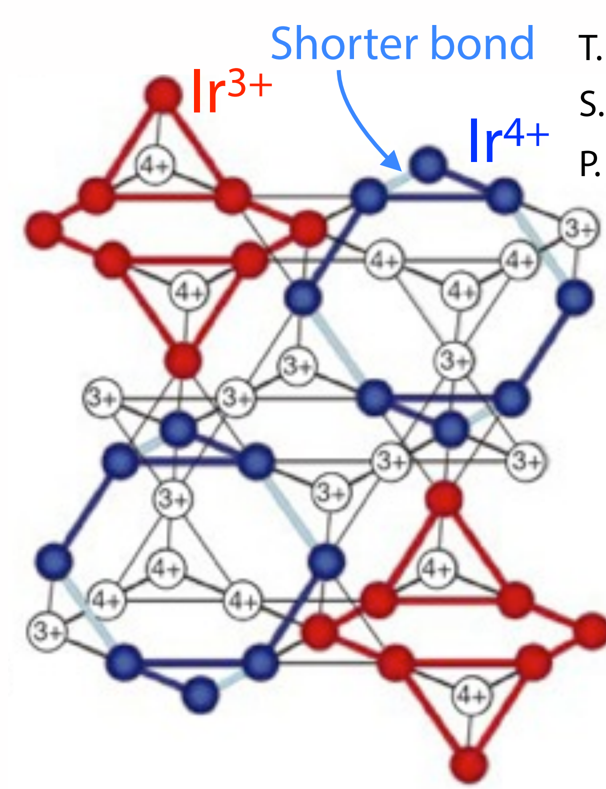


Finite-*T* phase transition to quantum spin liquid

JN *et al.*, Phys. Rev. B **89**, 115125 (2014)
JN, M. Udagawa, and Y. Motome, arXiv:1406.5415

$CuIr_2S_4$ *Spinel* (Ir^{4+} *form octamer*)

T. Furubayashi *et al.*, JPSJ **63**, 3333 (1994).
S. Nagata *et al.*, Phys. Rev. B **58**, 6844 (1998).
P. G. Radaelli *et al.*, Nature **416**, 155 (2002).



Remnant paramagnetism at low *T*

JN and Y. Motome, to be published in Phys. Rev. B

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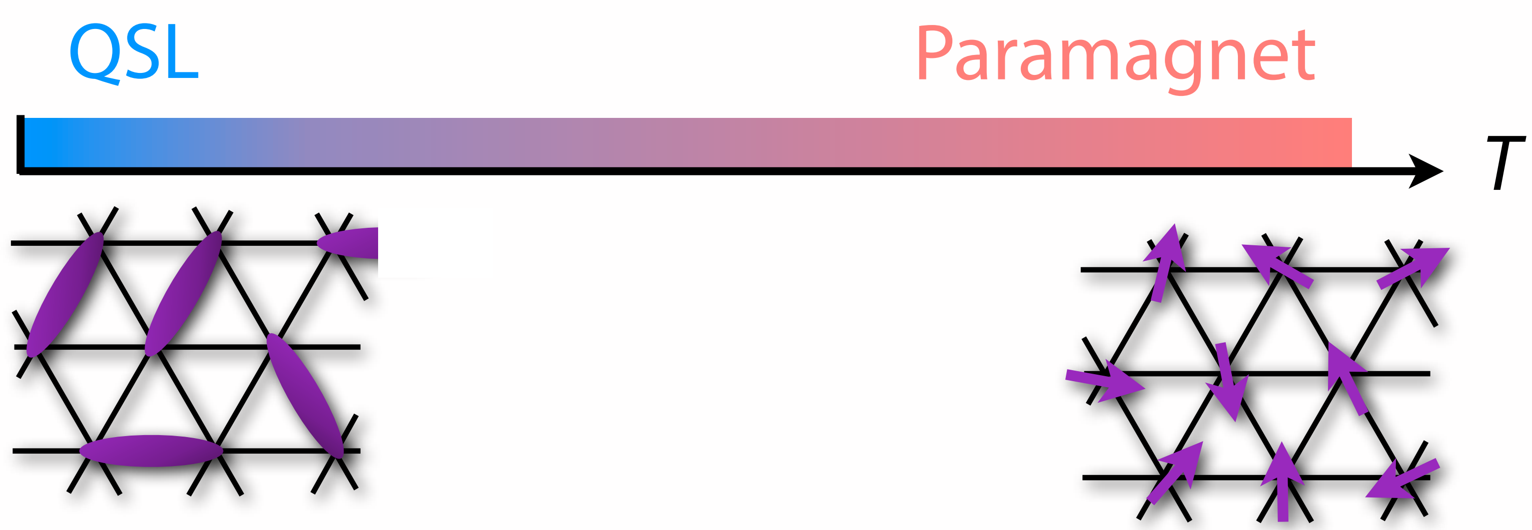
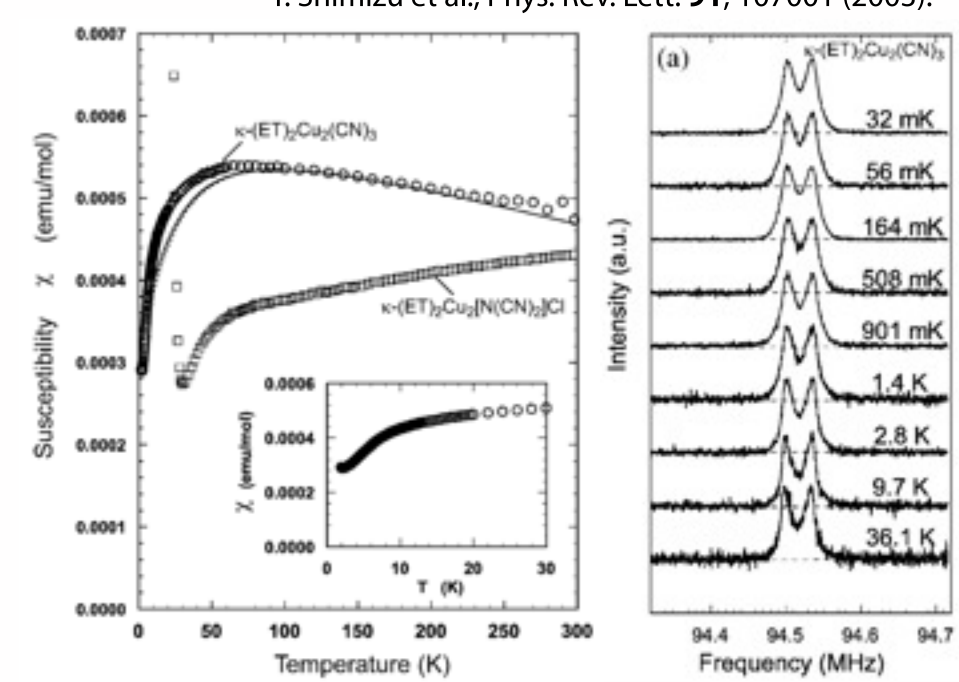
Quantum Spin Liquid (QSL)



Quantum fluctuation disturbs orderings.

Y. Shimizu et al., Phys. Rev. Lett. **91**, 107001 (2003).



Quantum spin liquid (QSL):

- No singularity in C_v or χ
- No apparent symmetry breakings down to low *T*

Theory for QSL

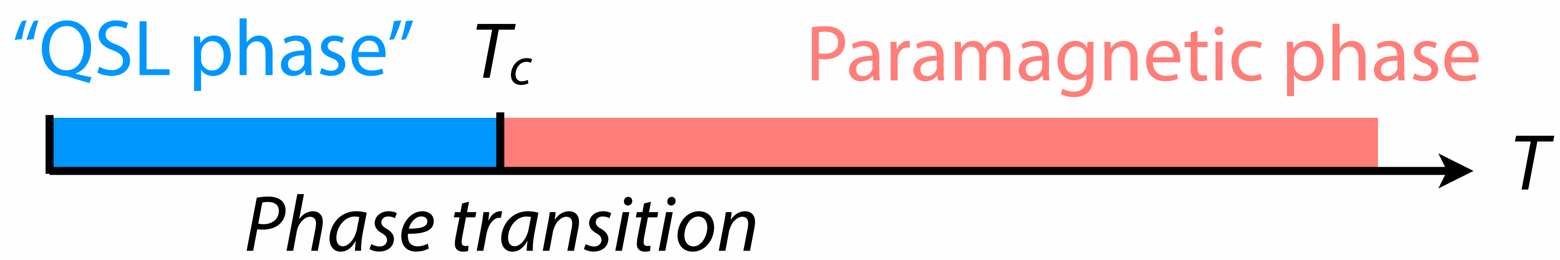
QSL is *numerically* confirmed to be realized in Heisenberg and Hubbard models on *frustrated lattices*.

Triangular, kagome, J_1-J_2 models ...

H. Morita et al., J. Phys. Soc. Jpn. **71**, 2109 (2002).
S. Yan et al., Science **332**, 1173 (2011).
H.-C. Jiang et al., Phys. Rev. B **86**, 024424 (2012). etc.

Thermodynamics in Quantum Spin Liquid

Can we distinguish paramagnet and QSL, particularly at finite T?



A model with QSL ground state will be useful for studying the thermodynamics.

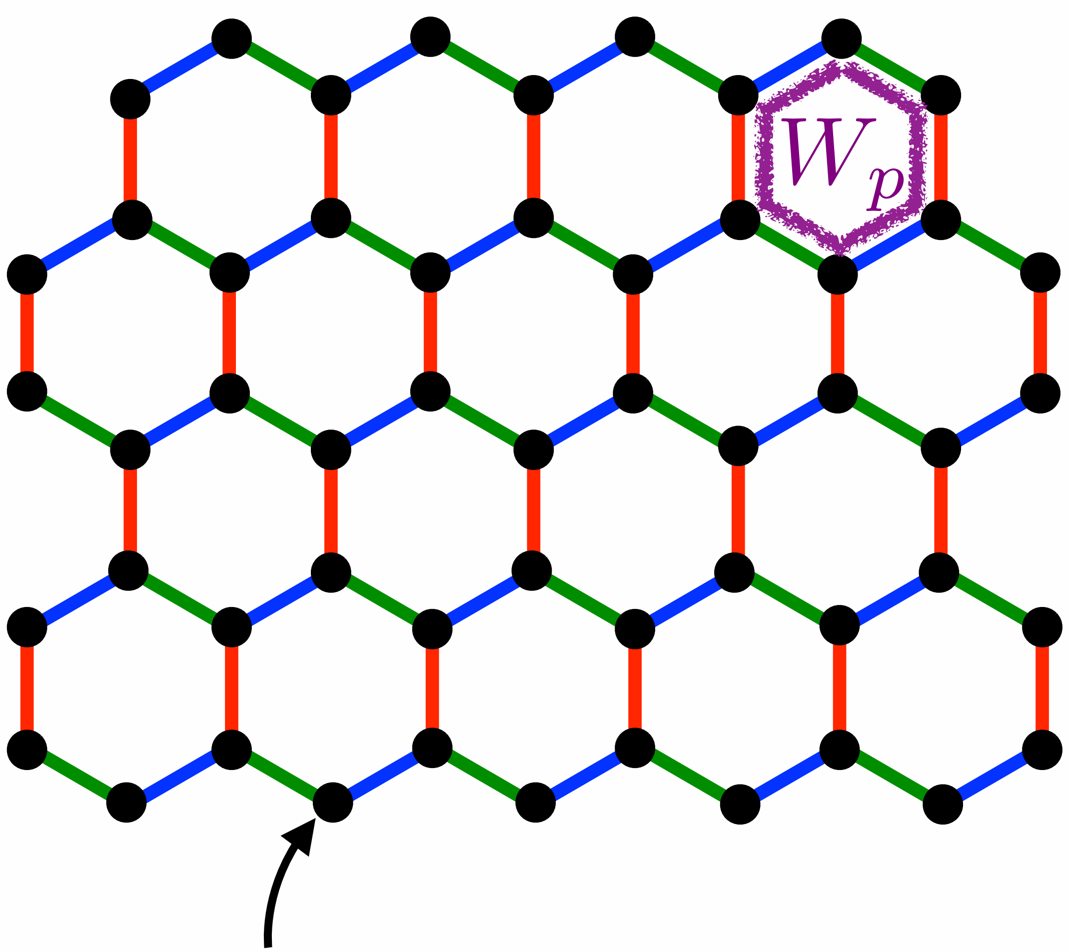
***Kitaev model*: exactly solvable and QSL ground state**

→ a good starting point

Kitaev Model

$$\mathcal{H} = -J_x \sum_{<ij>_x} \sigma_i^x \sigma_j^x - J_y \sum_{<ij>_y} \sigma_i^y \sigma_j^y - J_z \sum_{<ij>_z} \sigma_i^z \sigma_j^z$$

Honeycomb lattice



S=1/2 spin

- Bond-dependent interaction

  ⇒ *Frustration*

  ⇒ *Novel ground state*

- Local conserved quantity W_p

- **Ground state:**
  Quantum spin liquid (Exact solution)

- **Stabilized at *zero temperature***

A. Kitaev, Ann. Phys. **321**, 2 (2006).

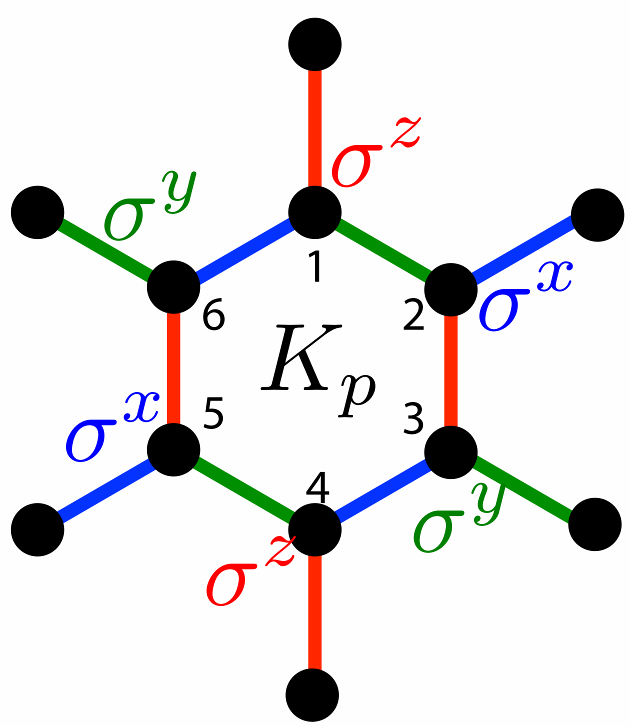
C. Castelnovo and C. Chamon, Phys. Rev. B **76**,184442 (2007).

Z. Nussinov and G. Ortiz, Phys. Rev. B **77**, 064302 (2008).

Local conserved quantity

$$\mathcal{H} = -J_x \sum_{<ij>_x} \sigma_i^x \sigma_j^x - J_y \sum_{<ij>_y} \sigma_i^y \sigma_j^y - J_z \sum_{<ij>_z} \sigma_i^z \sigma_j^z$$

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



- $W_p^2 = 1$
- $[\mathcal{H}, W_p] = 0$
  since $[\sigma_1^y \sigma_2^y, W_p] = 0$
- $[W_p, W_{p'}] = 0 \qquad p \neq p'$

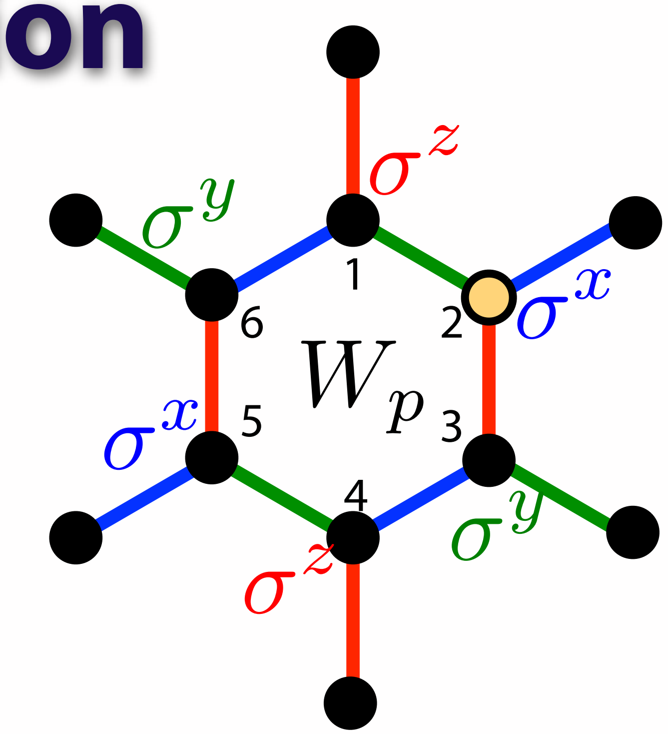
Eigenstates of Kitaev model are characterized by $\{W_p = \pm 1\}$

⇒ Solvable by introducing Majorana fermions

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

Spin Correlation Function

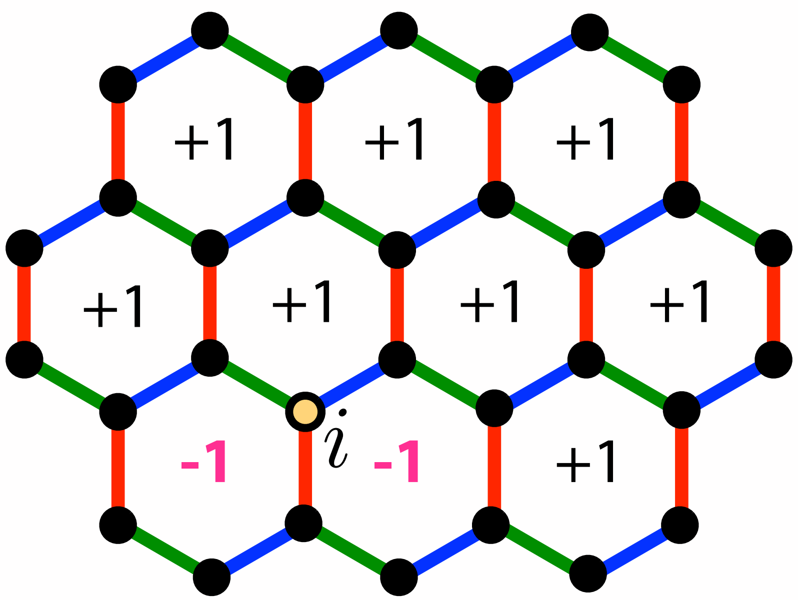
Ground state : all of W_p =+1



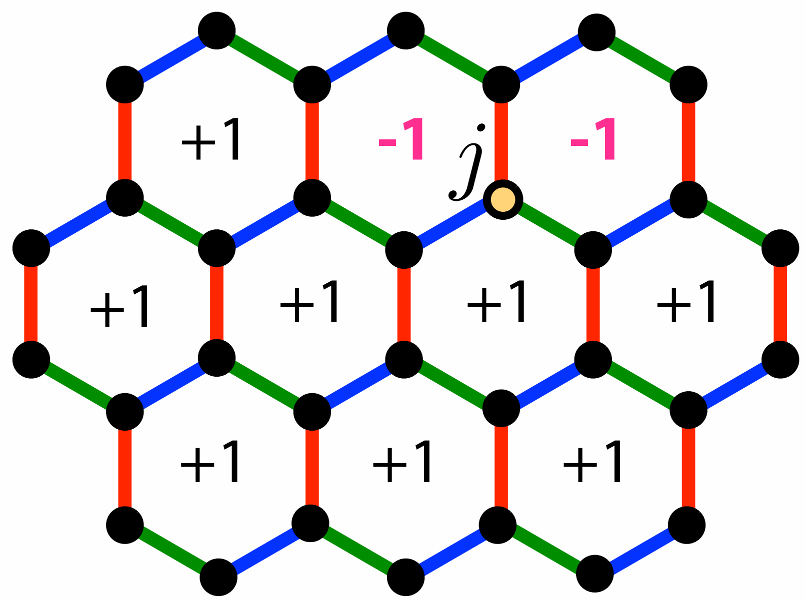
$$W_p \sigma_2^z = -\sigma_2^z W_p$$

$$\Rightarrow W_p |\sigma_2^z \Phi_0\rangle = -|\sigma_2^z \Phi_0\rangle$$

$|\sigma_i^z \Phi_0\rangle$



$|\sigma_j^z \Phi_0\rangle$



$$\langle \Phi_0 | \sigma_i^z \sigma_j^z | \Phi_0 \rangle$$

$$= \langle \sigma_i^z \Phi_0 | \sigma_j^z \Phi_0 \rangle$$

$$= 0$$

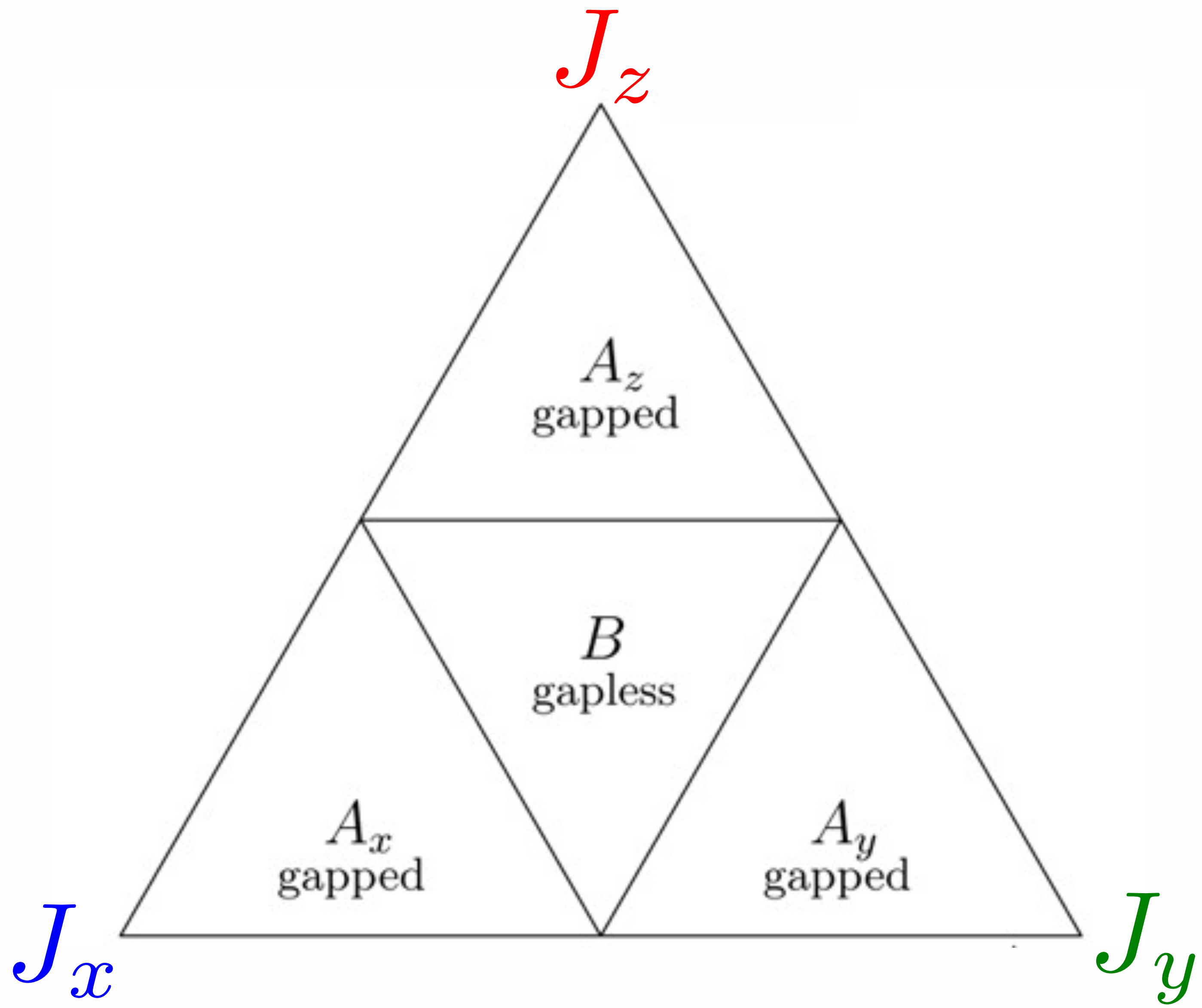
(except for NN bonds)

Anticommutation between spin and conserved quantity leads to the state without spin correlations. ⇒ ***Quantum spin liquid***

G. Baskaran, S. Mandal, and R. Shankar, Phys. Rev. Lett. **98**, 247201 (2007).

Phase diagram of Kitaev Model

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



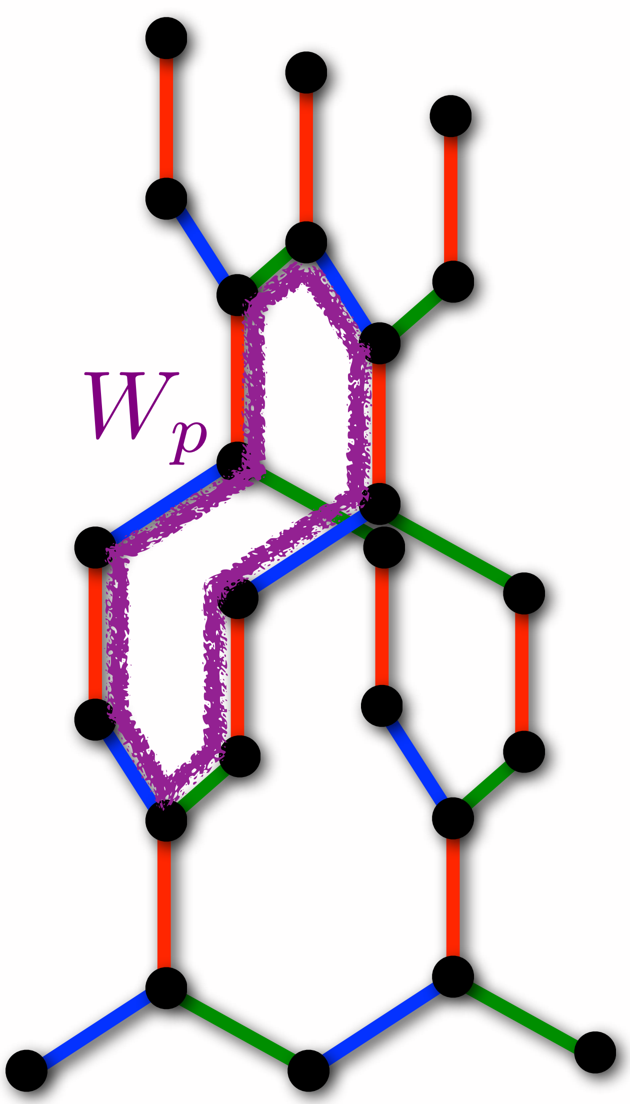
- Phase diagram is depicted on a plane with $J_x + J_y + J_z = 1$
- There are *gapped* and *gapless* **quantum spin liquids**.
- Phase boundary: $J_z = J_x + J_y$, etc.

3D Extension of Kitaev Model

$$\mathcal{H} = -J_x \sum_{<ij>_x} \sigma_i^x \sigma_j^x - J_y \sum_{<ij>_y} \sigma_i^y \sigma_j^y - J_z \sum_{<ij>_z} \sigma_i^z \sigma_j^z$$

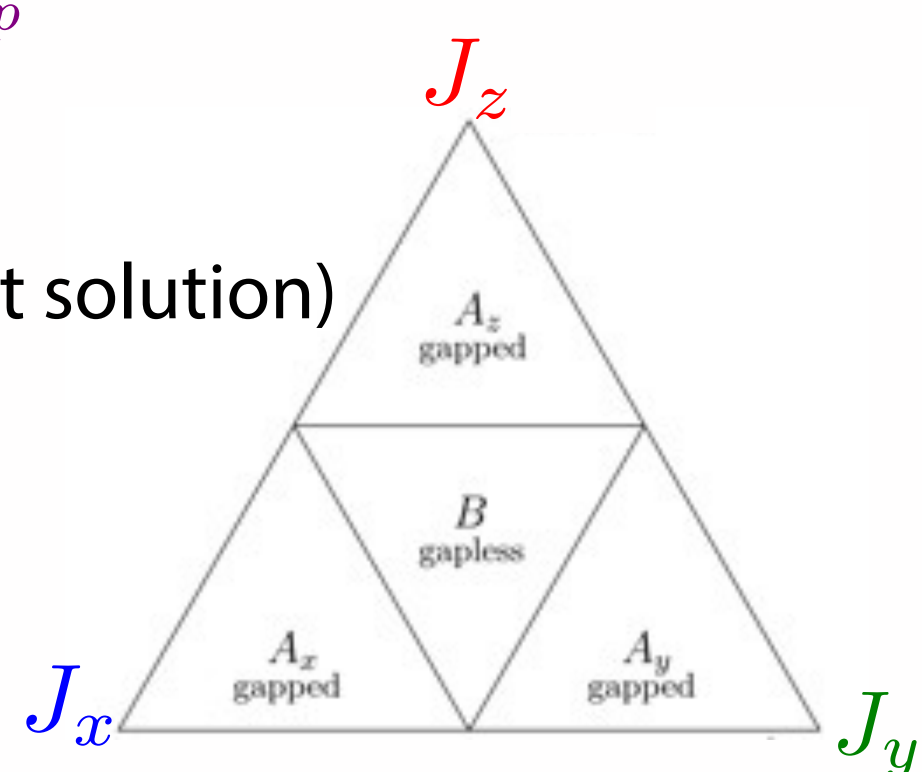
S. Mandal and N. Surendran, Physical Review B **79**, 024426 (2009).

Hyper-honeycomb lattice



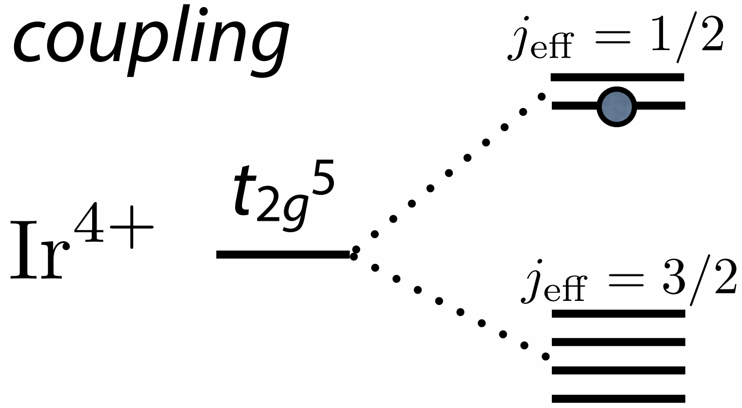
Common properties to 2D Kitaev model

- Local conserved quantity W_p
- **Ground state:**
  Quantum spin liquid (Exact solution)
- Ground state phase diagram



Relevance to Real Materials

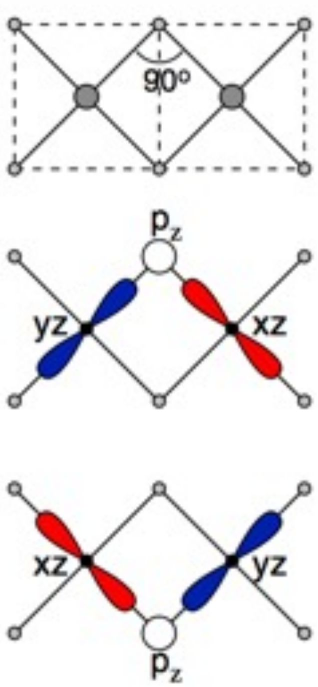
Strong spin-orbit coupling



$j_{\rm eff}$=1/2 localized spin

G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009)

Superexchange interaction in ***edge sharing case***



dpd hopping on a *xy* plane

$-JS_i^zS_j^z$: *Ising interaction on xy plane*

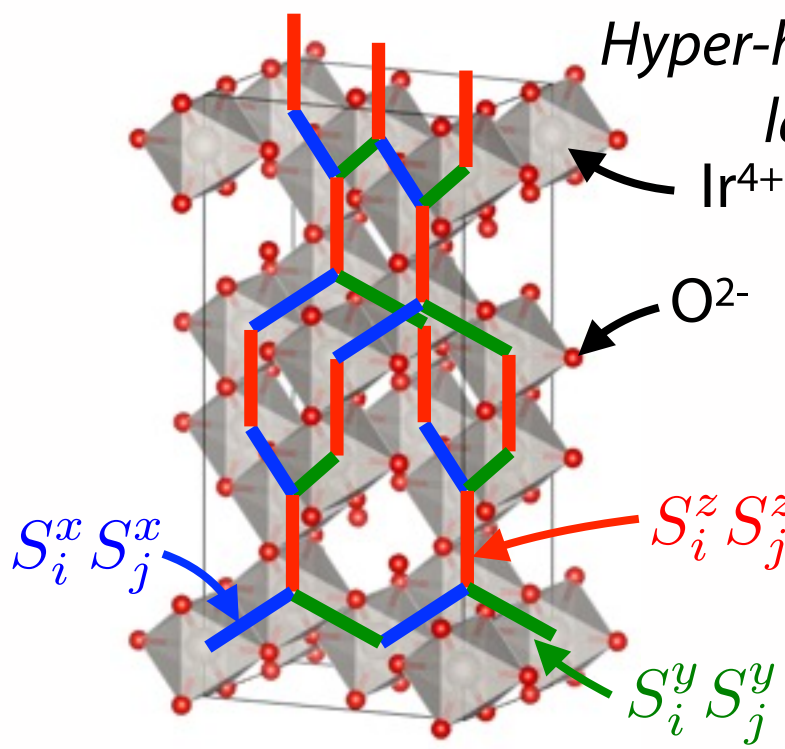
$-JS_i^xS_j^x$ *on yz plane*

$-JS_i^yS_j^y$ *on zx plane*

bond-dependent interaction due to orbital anisotropy

Recently found iridate β-Li_2IrO_3

K. A. Modic et al., Nat. comm. **5**, 4203 (2014).
T. Takayama et al., arXiv:1403.3296.

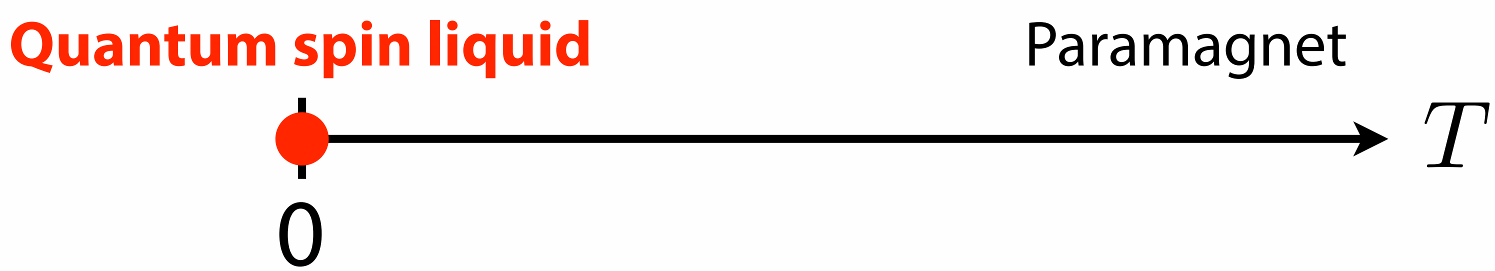


Theoretical studies for Kitaev-Heisenberg model

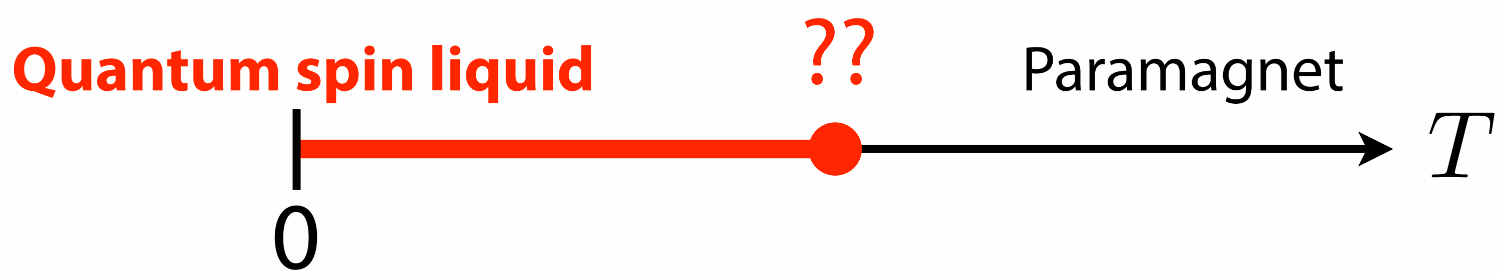
E. K.-H. Lee et al., Phys. Rev. B **89**, 045117 (2014).
S.B. Lee et al., Phys. Rev. B **89**, 014424 (2014).
I. Kimchi et al., arXiv:13091171.
J. Nasu et al., Phys. Rev. B **89**, 115125 (2014).

Purpose

2D Kitaev model (Totic code limit)



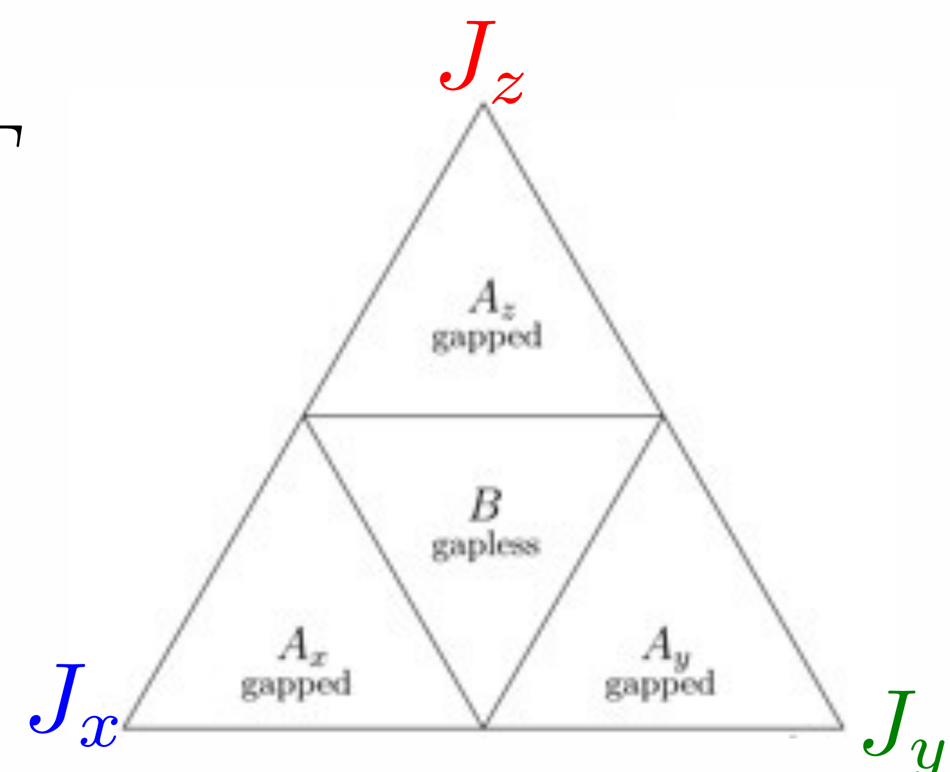
3D Kitaev model



Finite-*T* phase transition ??

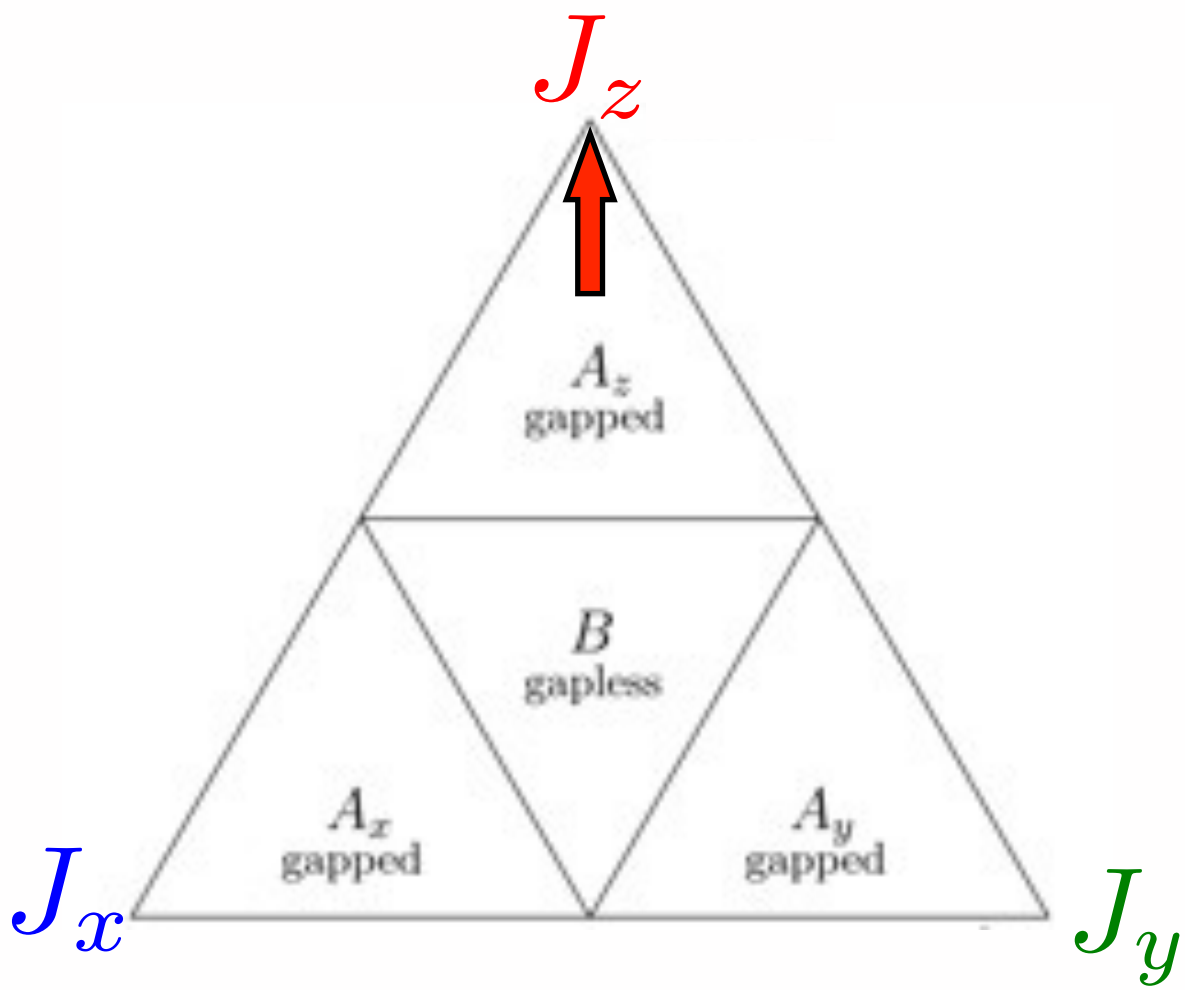
Characterization of phase transition

Magnetic properties

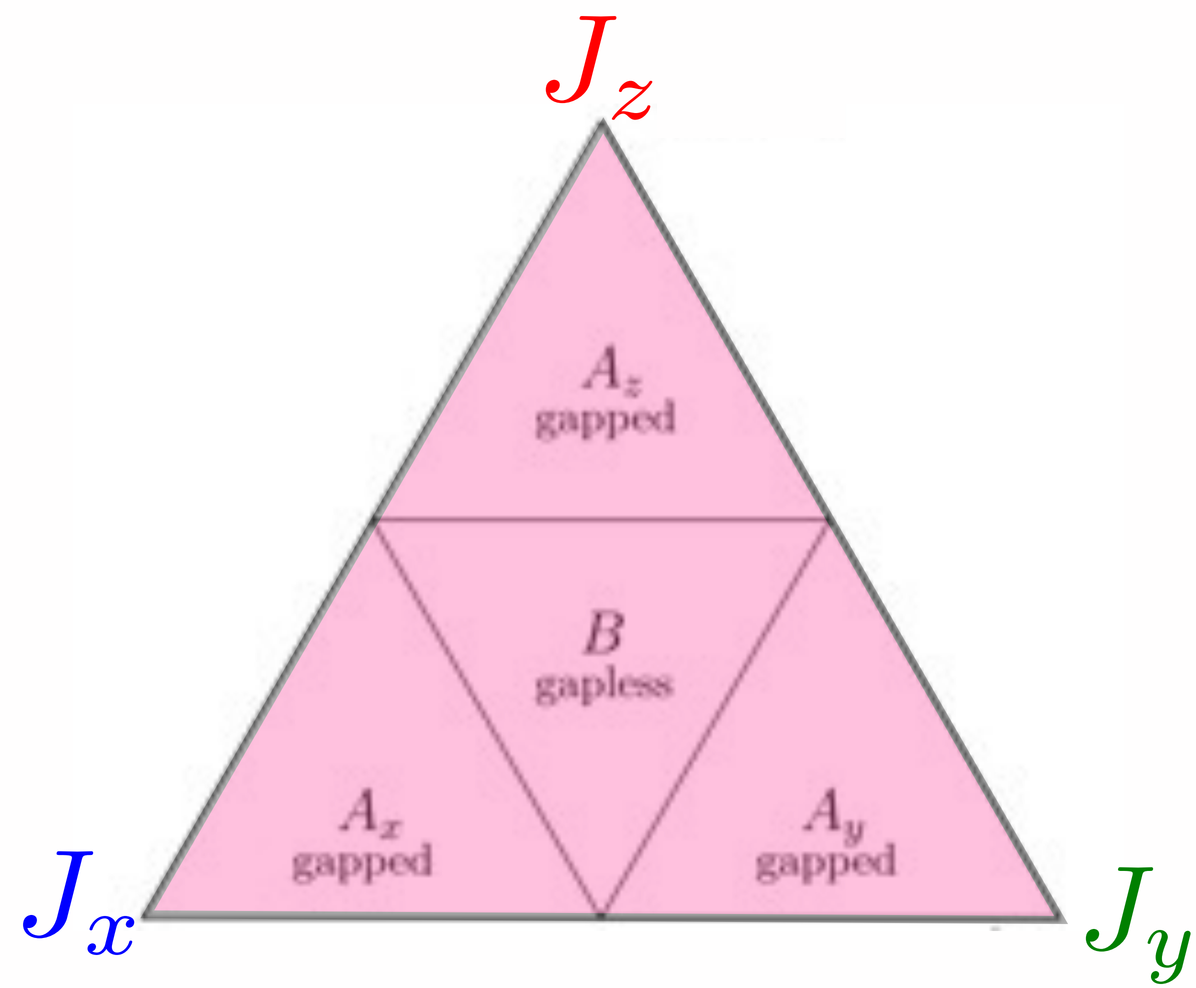


Parameter Space

- $J_z \gg J_x, J_y$ ***Totic code limit***

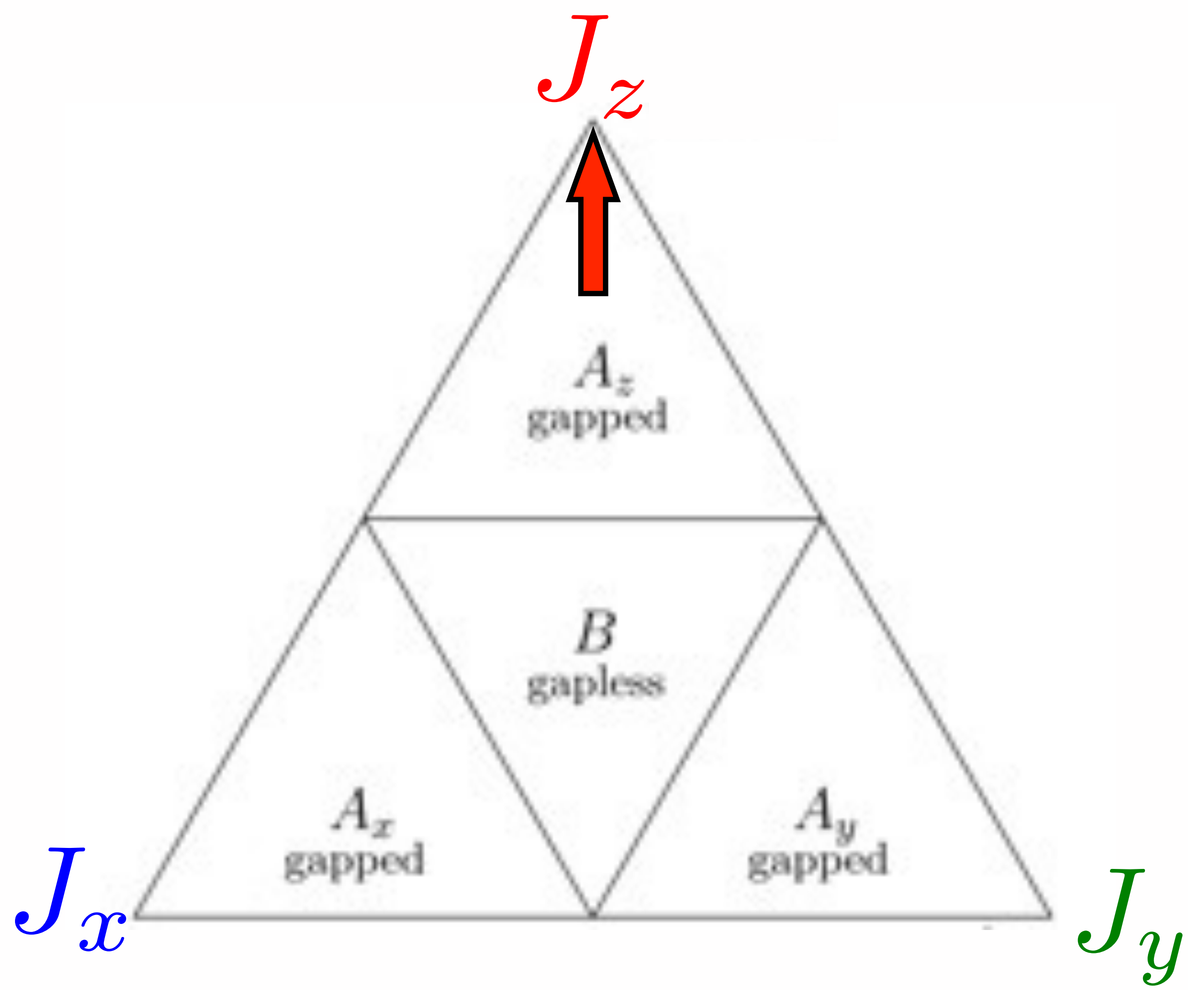


- Original Kitaev model



Anisotropic limit

$J_z \gg J_x, J_y$ ***Totic code limit***

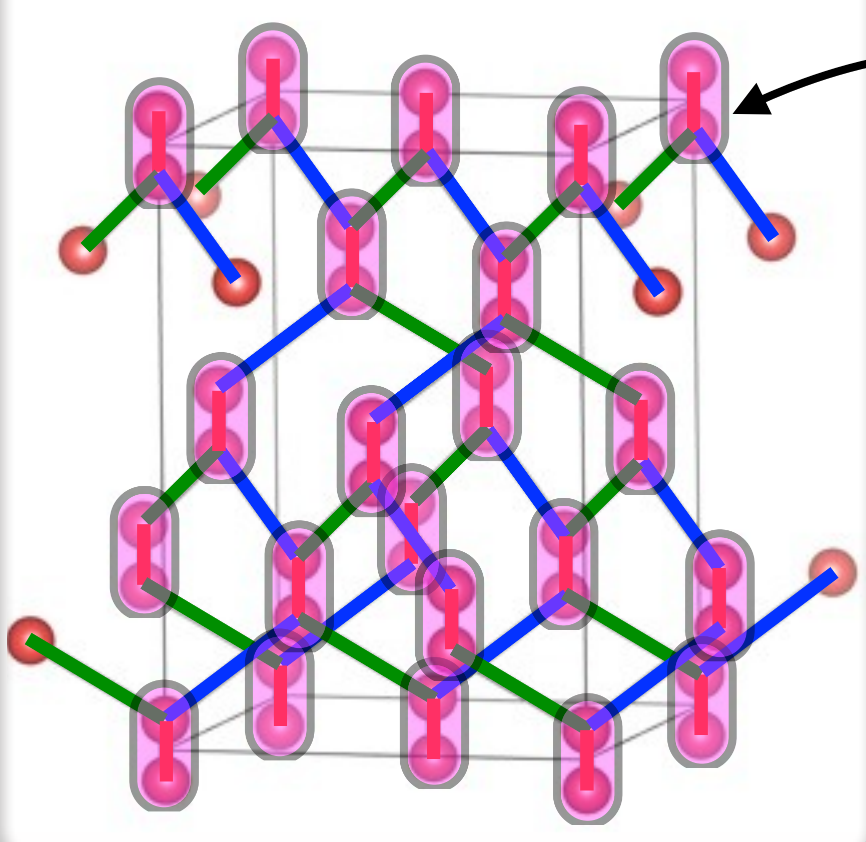


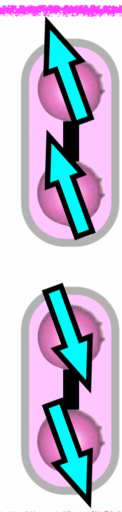
Large J_z Limit (Gapped phase)

$$\mathcal{H} = -J_x \sum_{<ij>_x} \sigma_i^x \sigma_j^x - J_y \sum_{<ij>_y} \sigma_i^y \sigma_j^y - J_z \sum_{<ij>_z} \sigma_i^z \sigma_j^z$$

For $J_z >> J_x, J_y$

Hyper-honeycomb lattice

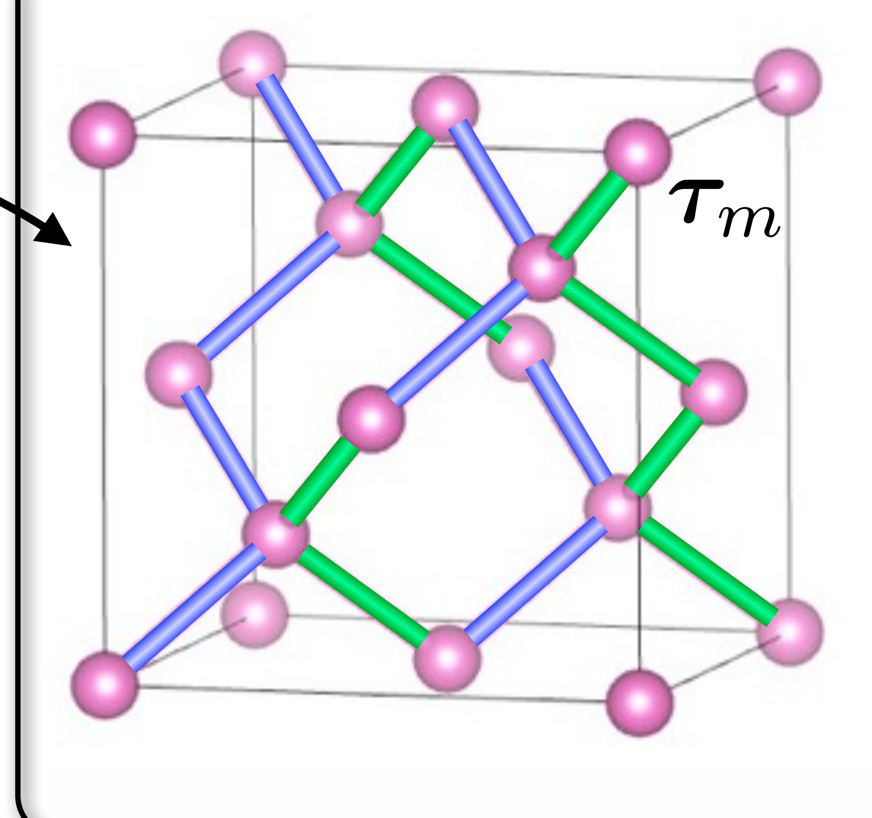




$$|\Uparrow\rangle = |\uparrow\uparrow\rangle$$

$$|\Downarrow\rangle = |\downarrow\downarrow\rangle$$

Diamond lattice



Pseudo spin

$$\tau^z|\Uparrow\rangle = +|\Uparrow\rangle$$

$$\tau^z|\Downarrow\rangle = -|\Downarrow\rangle$$

Perturbation expansion for J_x and J_y

→ Interaction between τ_m

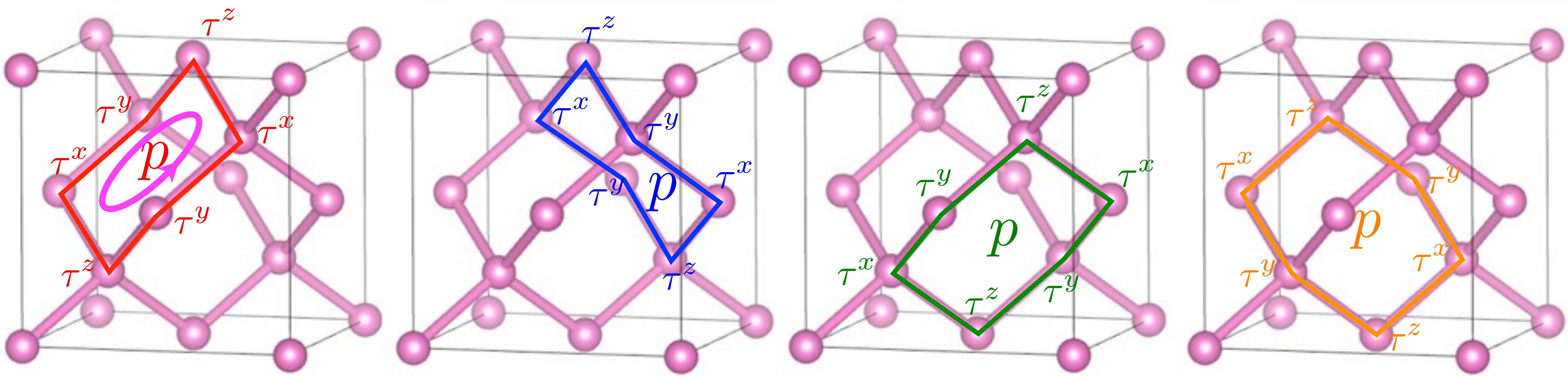
Effective Model

Sixth order perturbation expansion for $J_z \gg J_x, J_y$

$$\mathcal{H}_{\text{eff}} = -J_{\text{eff}} \sum_p B_p \qquad J_{\text{eff}} = \frac{7}{256} J^6 / J_z^5$$

$$J = J_x = J_y$$

Ring exchange interactions on four kinds of 6-site plaquettes



$B_p = \tau_1^z \tau_2^y \tau_3^x \tau_4^z \tau_5^y \tau_6^x$ $\quad B_p = \tau_1^z \tau_2^y \tau_3^x \tau_4^z \tau_5^y \tau_6^x$ $\quad B_p = \tau_1^z \tau_2^y \tau_3^x \tau_4^z \tau_5^y \tau_6^x$ $\quad B_p = \tau_1^z \tau_2^y \tau_3^x \tau_4^z \tau_5^y \tau_6^x$

$$[B_p, B_{p'}] = 0$$
$$[\mathcal{H}_{\text{eff}}, B_p] = 0$$
$$B_p^2 = 1$$

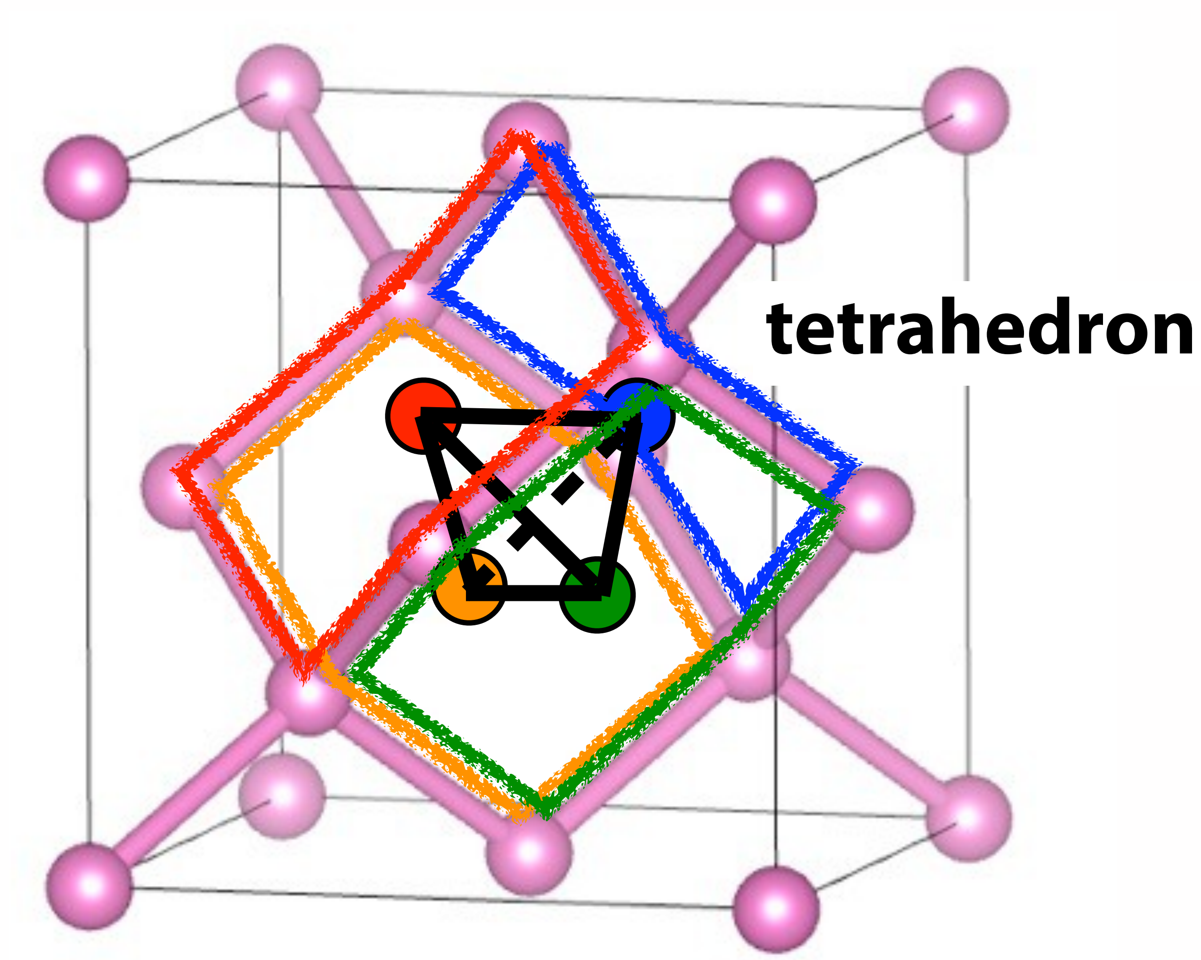
Eigenstate ⟺ Ising degree of freedom $\{B_p = \pm 1\}$

Characteristic of Effective Model

$$\mathcal{H}_{\rm eff} = -J_{\rm eff} \sum_p B_p$$: *Free* Ising model with magnetic field

$$B_p = \pm 1$$

B_p form a pyrochlore lattice



Product of four B_p

$$B_p \, B_p \, B_p \, B_p = 1$$

Local constraint

+ global constraints

S. Mandal and N. Surendran, Physical Review B **79**, 024426 (2009).

Correlation effect due to local constraints

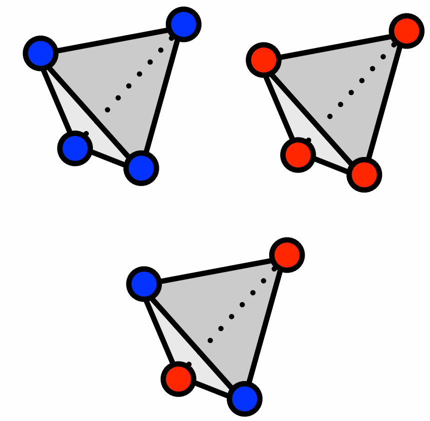
→ **Finite-*T* phase transition??**

Local Constraint in Effective Model

$$\mathcal{H}_{\text{eff}} = -J_{\text{eff}} \sum_p B_p$$

Ising-type degree of freedom $B_p = \pm 1$
on a pyrochlore lattice

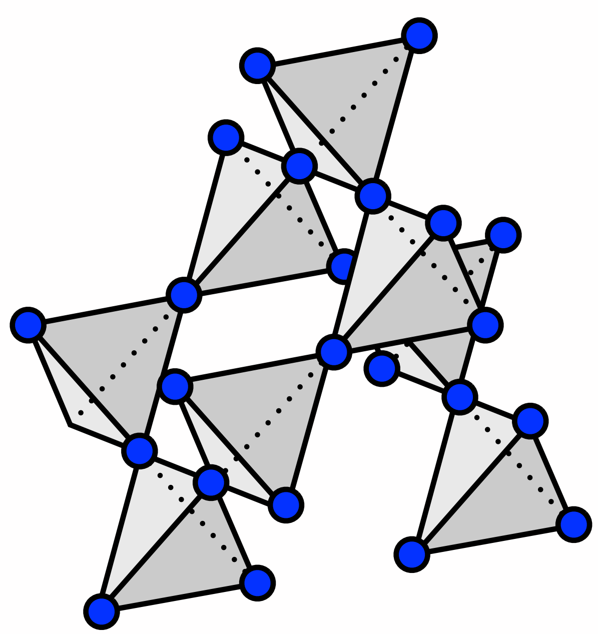
Local constraint



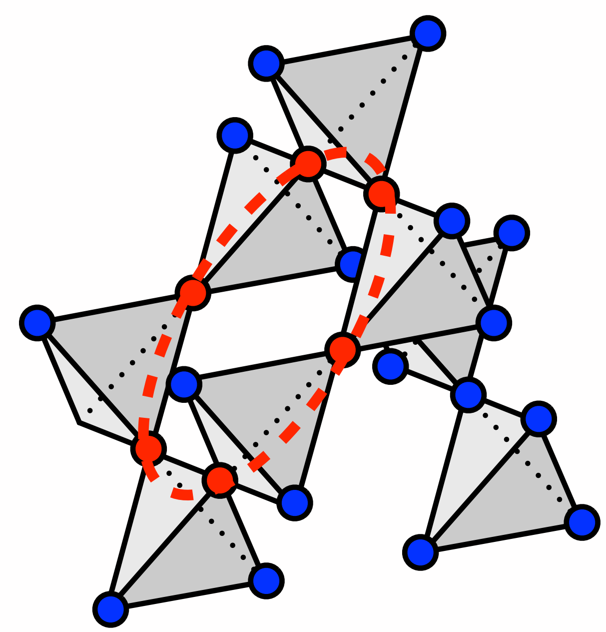
● $B_p = +1$
● $B_p = -1$

Number of $B_p = -1$
is even.

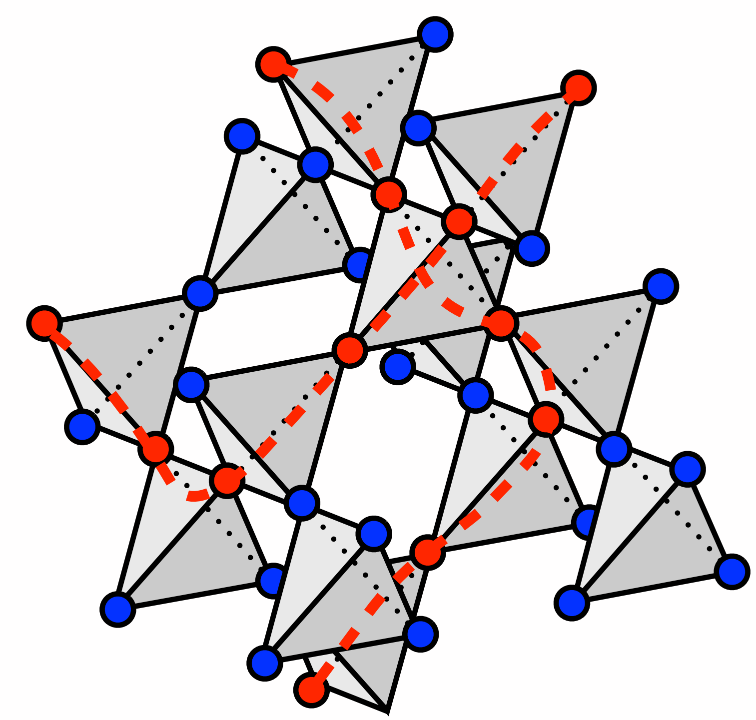
Ground state



Excited states



Loop excitation

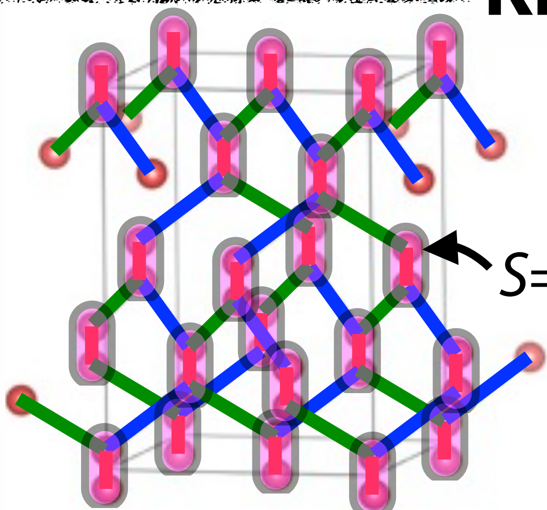


Loop crossing is allowed.

Excitation energy is propotional to sum of loop lengths

Short summary: from 3D Kitaev model to Loop model

Kitaev model on a hyper-honeycomb lattice

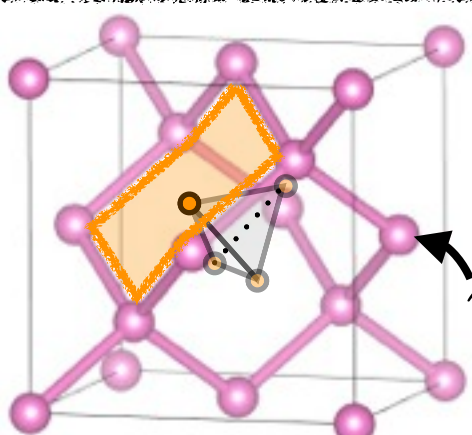


S=1/2 spin

$$\mathcal{H} = -J_x \sum_{<ij>_x} \sigma_i^x \sigma_j^x - J_y \sum_{<ij>_y} \sigma_i^y \sigma_j^y - J_z \sum_{<ij>_z} \sigma_i^z \sigma_j^z$$

$J_z \gg J_x, J_y$

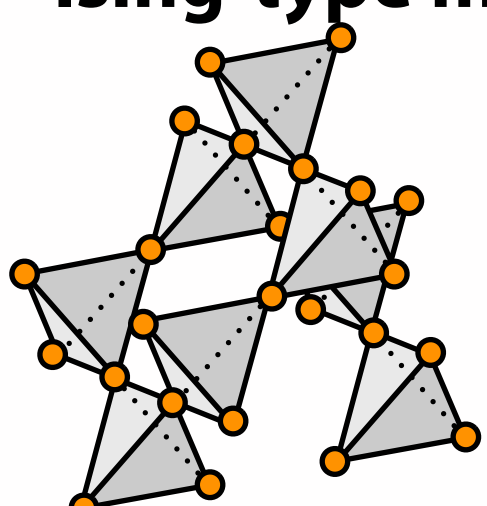
Effective model on a diamond lattice



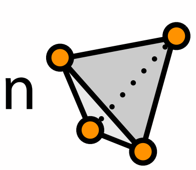
τ_i^l

$$\mathcal{H}_{\text{eff}} = -J_{\text{eff}} \sum_p \underbrace{\tau_{i_1}^{l_1} \tau_{i_2}^{l_2} \tau_{i_3}^{l_3} \tau_{i_4}^{l_4} \tau_{i_5}^{l_5} \tau_{i_6}^{l_6}}_{B_p}$$

Ising-type model on a pyrochlore lattice

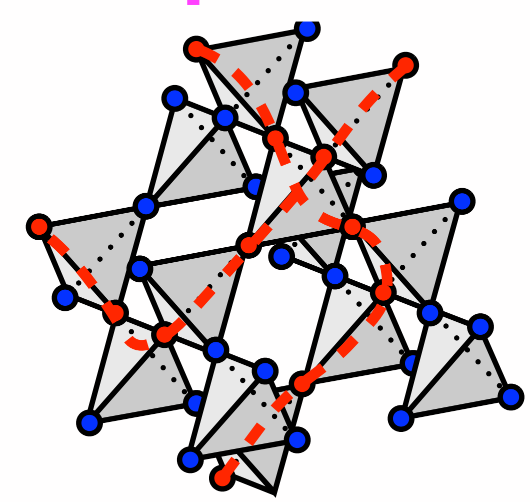


$$\mathcal{H}_{\text{eff}} = -J_{\text{eff}} \sum_p B_p$$

+ Local constraint in 

Ising degree of freedom $B_p = \pm 1$

Loop model



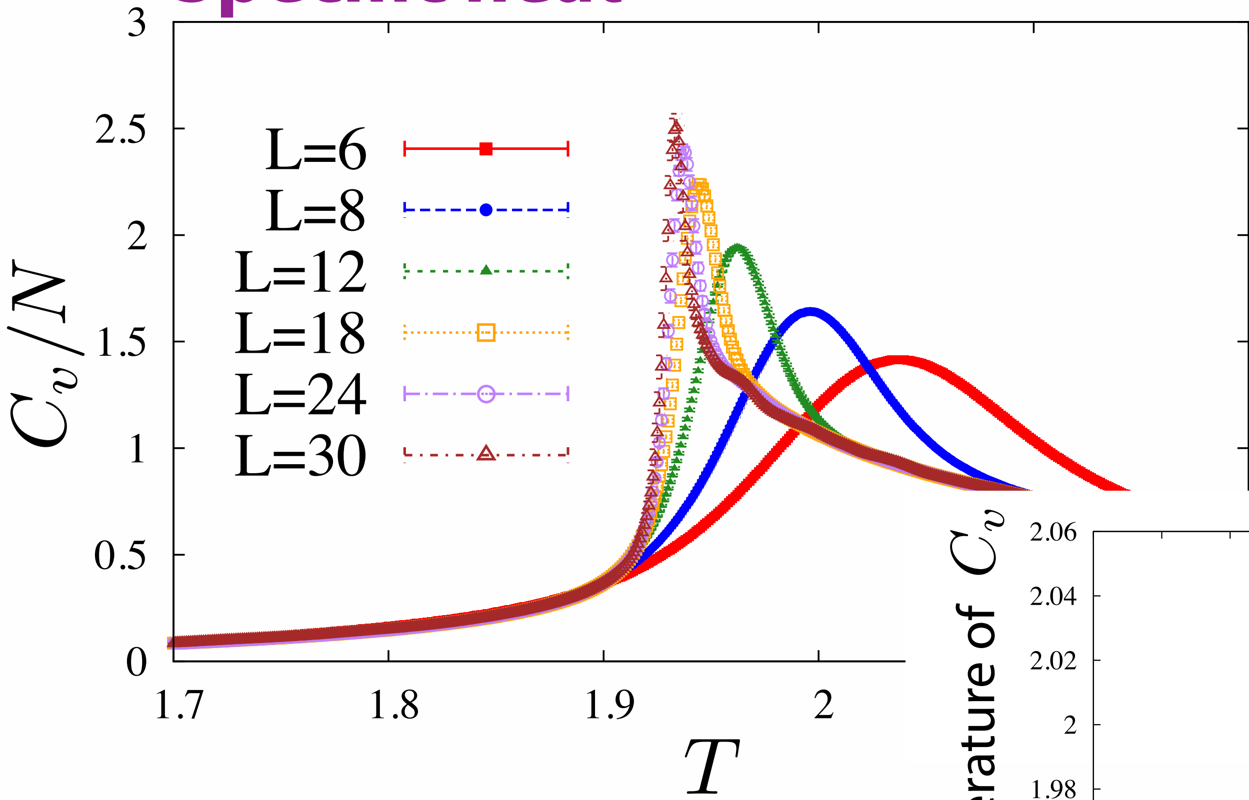
Monte Carlo simulation

$$\mathcal{H}_{\rm eff} = -J_{\rm eff}\sum_p B_p$$ with local constraints & global constraints

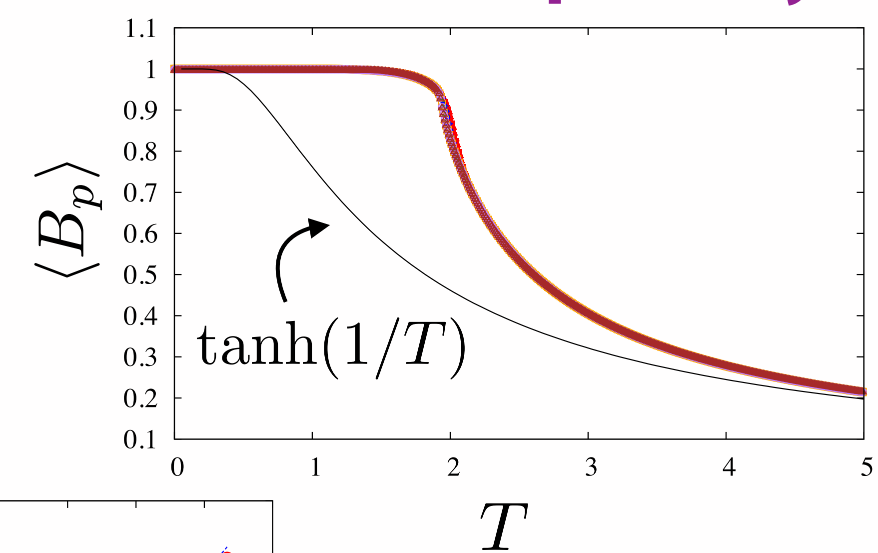
N=LxLxLx4
L<= 30
N<~100,000
$J_{\rm eff} = 1$

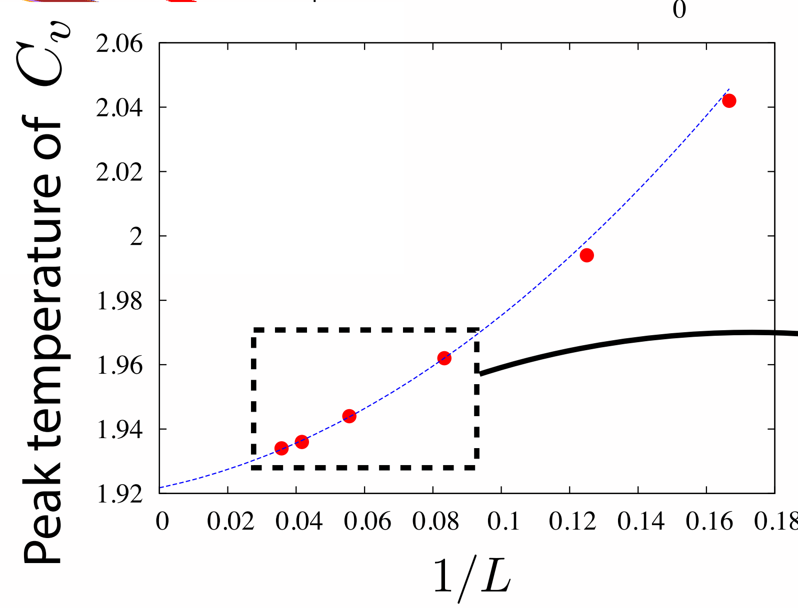
Periodic boundary condition

Specific heat



Local conserved quantity





Fit by quadratic function

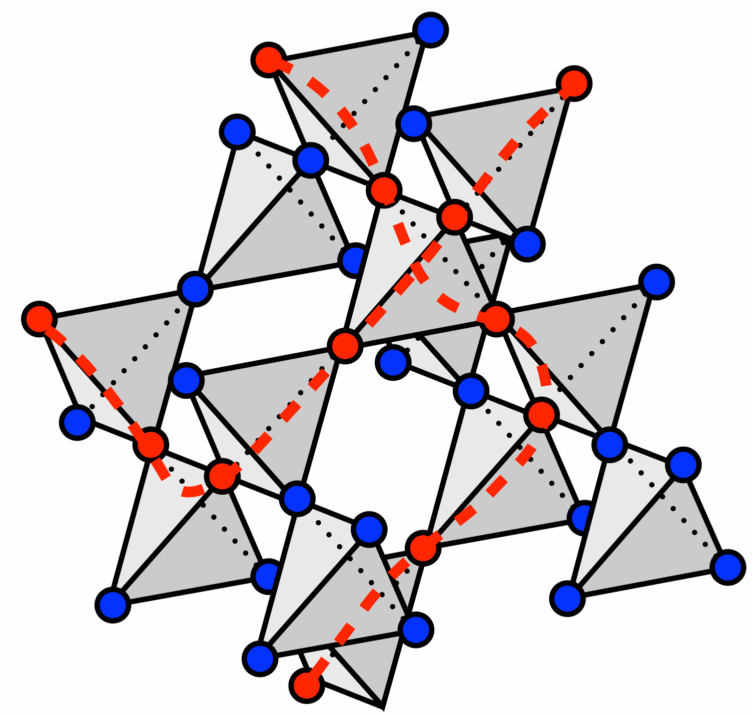
$T_c = 1.922(4)$

With increasing temperature, B_p decreases and cusp-like feature appears and the peak in Cv grows near T=1.92.

Correspondence to Ising model

Model Hamiltonian: $\mathcal{H}_{\rm eff} = -J_{\rm eff}\sum_p B_p$

Excitation energy is propotional to sum of loop lengths



Ising degree of freedom $B_p = \pm 1$

on a pyrochlore lattice

⇒ Ising degree of freedom

on the bond of a diamond lattice

Partition function of Ising model on *a diamond lattice*: $Z_{\rm Ising}(\beta')$

High temperature expansion

$J=1, \quad N_d = N/2$: site number of the diamond lattice

$$Z_{\rm Ising}(\beta') = \cosh^{zN_d/2}\beta' \sum_{\sigma_1}\cdots\sum_{\sigma_{N_d}}\prod_{<ij>}(1+\sigma_i\sigma_j\tanh\beta')$$

$$= 2^{N_d}\cosh^{zN_d/2}\beta' \sum_{{\rm loop}:l}\exp[l\ln\tanh\beta']$$

sum of loops on the diamond lattice

Correspondence to Ising model

Partition function of Ising model on a diamond lattice: $Z_{\rm Ising}(\beta')$

Partition function of the present loop model: $Z(\beta)$

(without the global constraints)

High temperature expansion for Ising model

$$Z_{\rm Ising}(\beta') = 2^{N_d} \cosh^{zN_d/2} \beta' Z(-1/2 \ln \tanh \beta') e^{\beta' z N_d/2}$$

・For T_c $\quad \beta_c = -1/2 \ln \tanh \beta'_c = 1/1.9249$

In Ising model on a diamond lattice $\quad 1/\tanh \beta'_c = 2.82641(10)$

D. S. Gaunt and M. F. Sykes, J. Phys.: Math., Nucl. Gen., **6** 1517 (1973).

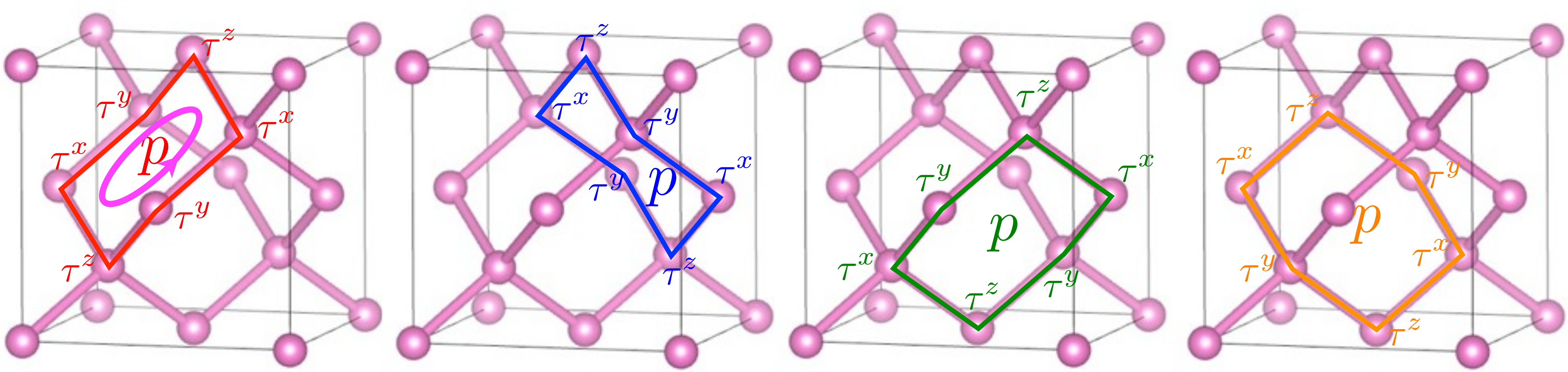
・Second order phase transition

belonging to the 3D Ising universality class

Magnetic susceptibility

$$\chi_{ij}^{zz} = \int_0^\beta d\lambda \langle e^{\lambda \mathcal{H}_{\text{eff}}} \tau_i^z e^{-\lambda \mathcal{H}_{\text{eff}}} \tau_j^z \rangle$$

Two kinds of B_p $\begin{cases} B_p \text{ commuting with } \tau_i^z \\ B_p \text{ anticommuting with } \tau_i^z \end{cases}$ the set of B_p: $\mathcal{A}_i$



$B_p = \tau_1^z \tau_2^y \tau_3^x \tau_4^z \tau_5^y \tau_6^x$ $B_p = \tau_1^z \tau_2^y \tau_3^x \tau_4^z \tau_5^y \tau_6^x$ $B_p = \tau_1^z \tau_2^y \tau_3^x \tau_4^z \tau_5^y \tau_6^x$ $B_p = \tau_1^z \tau_2^y \tau_3^x \tau_4^z \tau_5^y \tau_6^x$

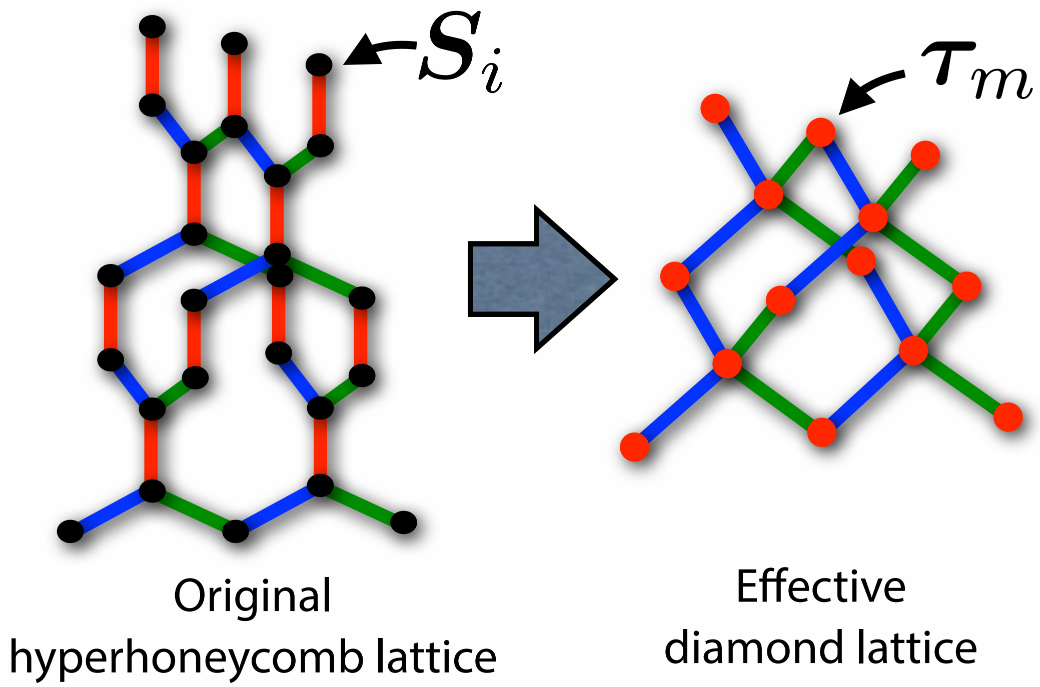
$$\chi_{ij}^{zz} = \int_0^\beta d\lambda \langle \exp[-2\lambda J_{\text{eff}} \sum_{p \in \mathcal{A}_i} B_p] \tau_i^z \tau_j^z \rangle = \int_0^\beta d\lambda \langle \exp[-2\lambda J_{\text{eff}} \sum_{p \in \mathcal{A}_i} B_p] \rangle \delta_{ij}$$

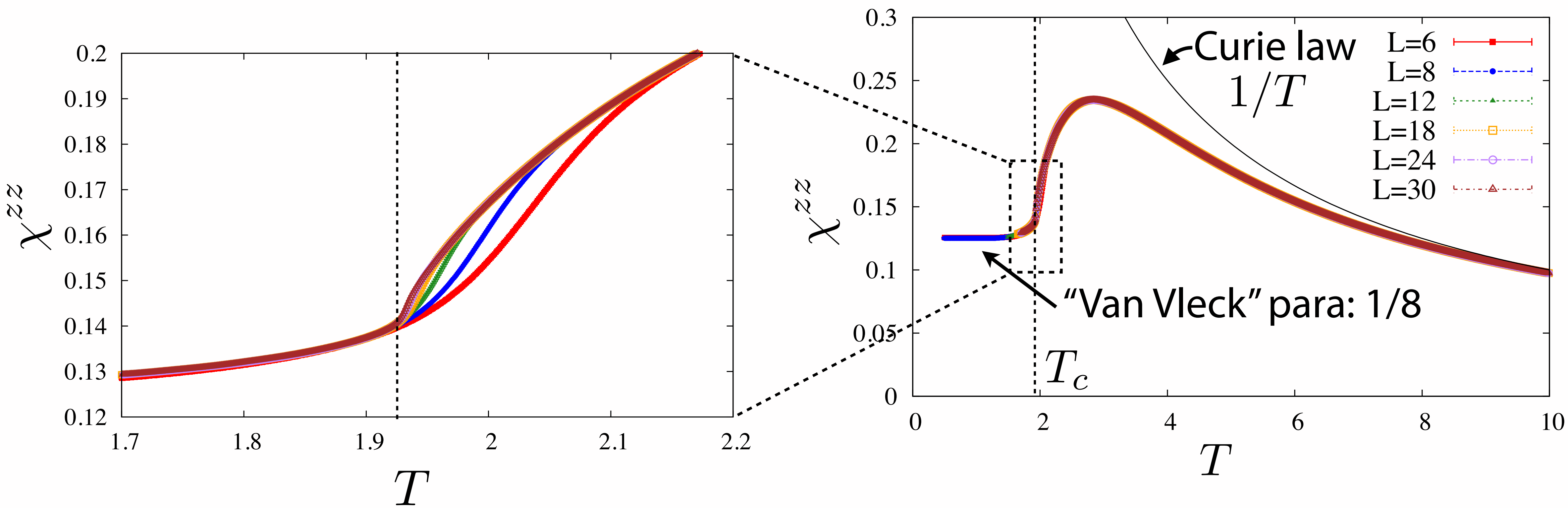
N.B. equal-time correlation $\langle \tau_i^z \tau_j^z \rangle = \delta_{ij}$

Magnetic susceptibility

$$\chi^{zz} = \frac{2}{N}\sum_{ij}\int_0^\beta d\lambda \langle e^{\lambda\mathcal{H}} S_i^z e^{-\lambda\mathcal{H}} S_j^z \rangle$$
$$= \frac{1}{N_d}\sum_{mn}\int_0^\beta d\lambda \langle e^{\lambda\mathcal{H}_{\rm eff}} \tau_m^z e^{-\lambda\mathcal{H}_{\rm eff}} \tau_n^z \rangle$$

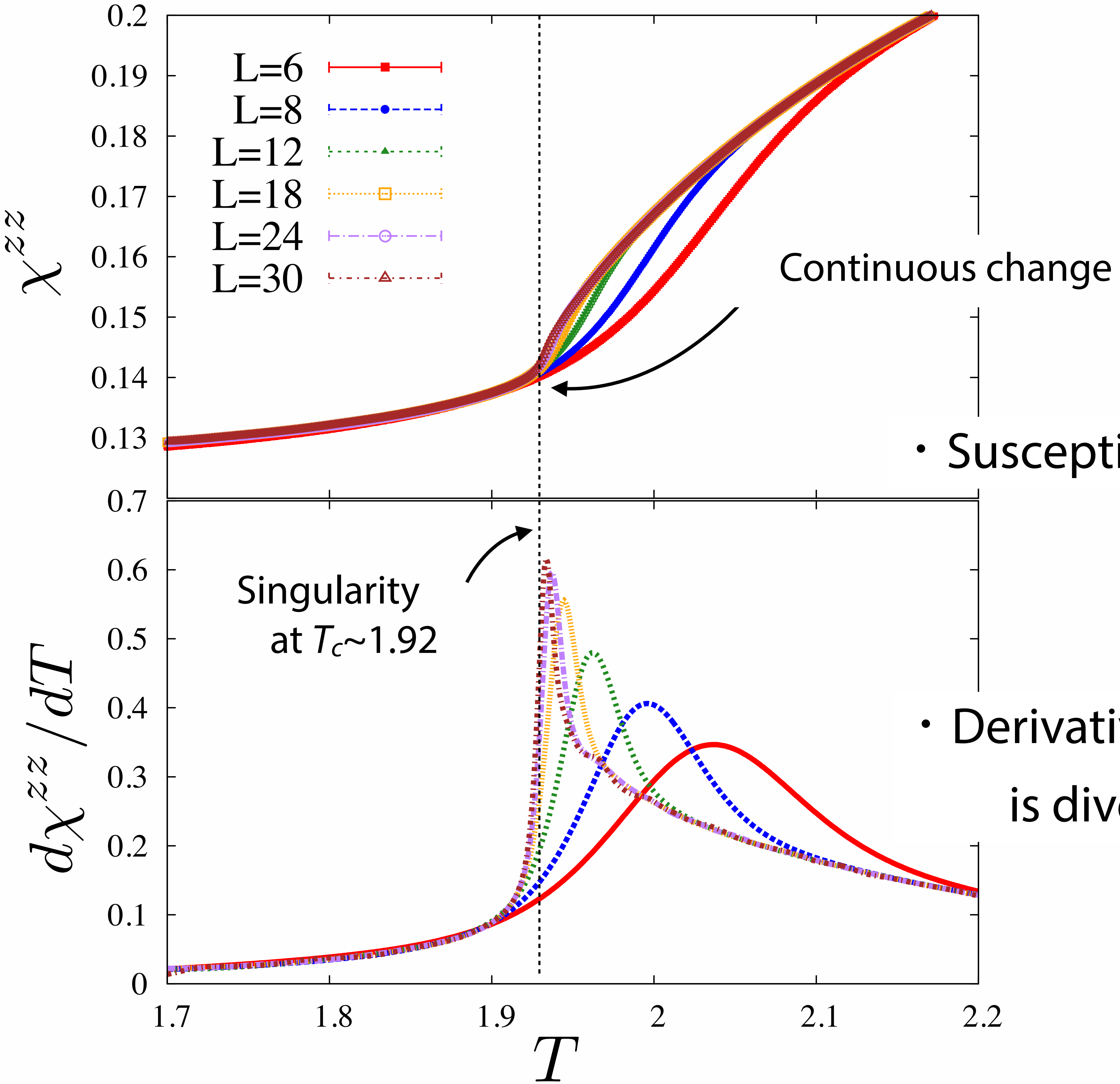
in terms of ***original quantum spin***





- Curie law due to $\langle \tau_i^z \tau_j^z \rangle = \delta_{ij}$
- *"Van Vleck"* paramagnetism at low *T*

T-derivative of susceptibility



- Susceptibility is continuous at Tc.
- Derivative of the suspeptibility is divergent at Tc.

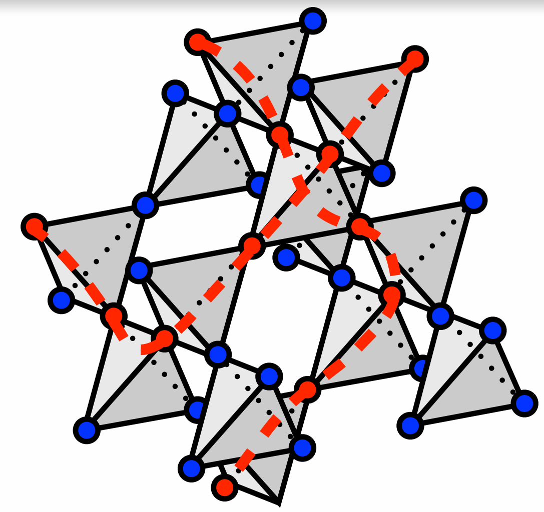
Topological characterization of the transition

Loops are composed by flipped B_p.

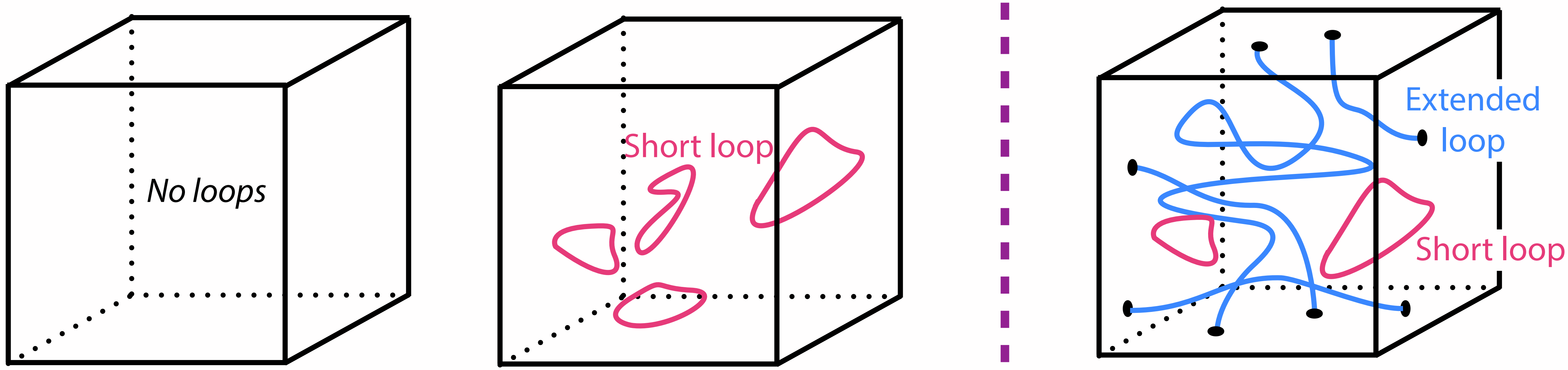
$$\mathcal{H}_{\mathrm{eff}} = -J_{\mathrm{eff}} \sum_p B_p$$

● $B_p = +1$

● $B_p = -1$



Zero temperature | Low temperature | High temperature



Quantum spin liquid

Paramagnet

Finite-T phase transition

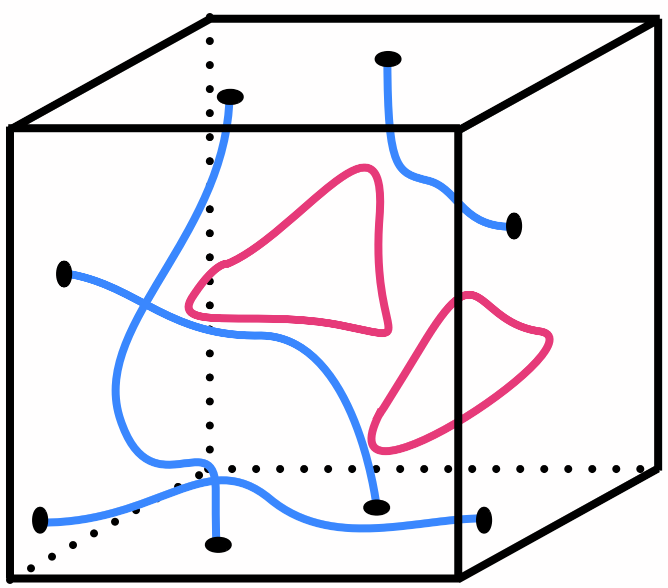
Characterization by <u>Extended loops</u> **"Topology of loops"**

Winding number (Flux)

$$\phi_i^x = \oint_{C_i} \boldsymbol{e}_x \cdot d\boldsymbol{s}/L_x \qquad C_i \text{ :loop}$$

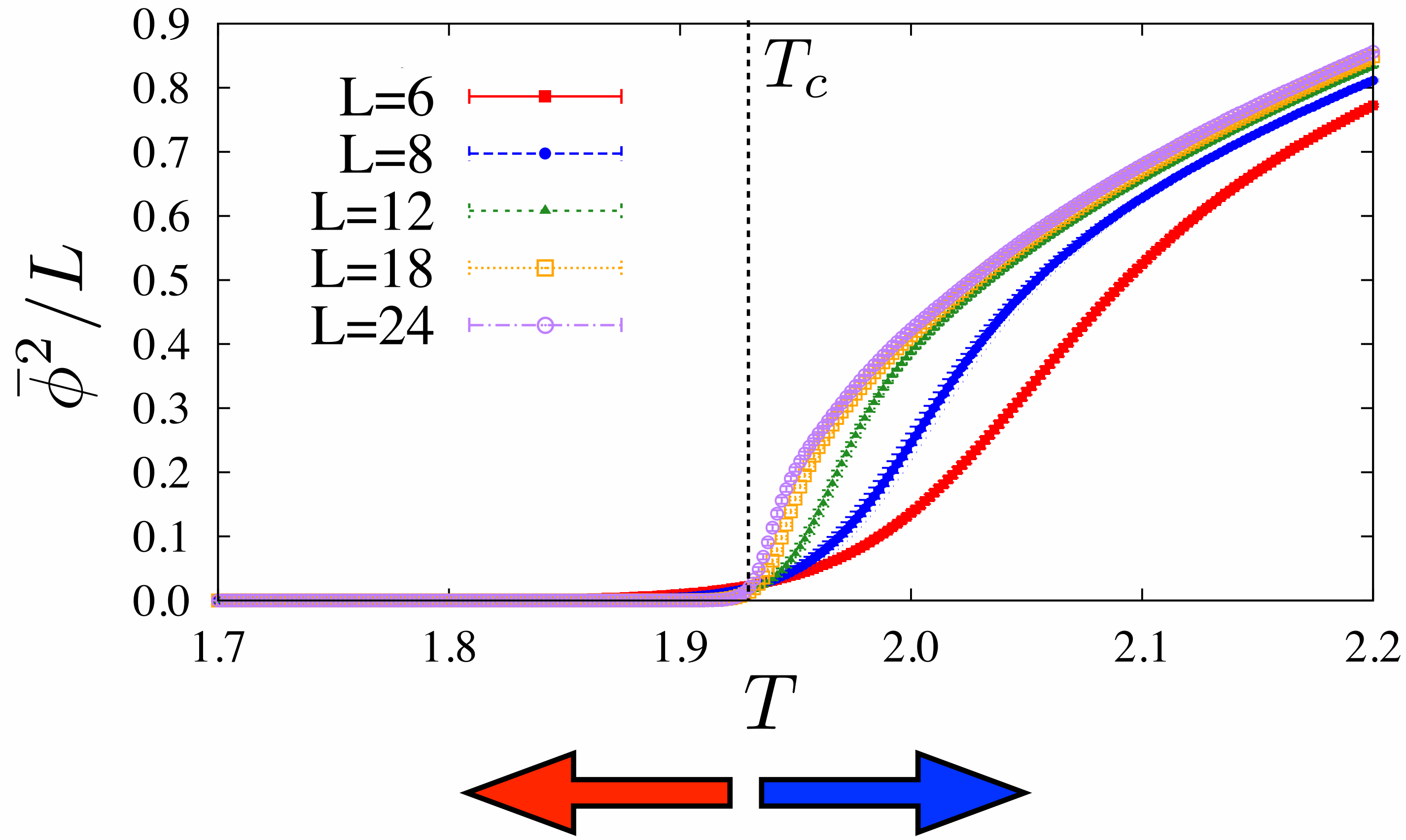
Flux density : $\bar{\phi}^2/L = \sum_i \langle (\phi_i^x)^2 + (\phi_i^y)^2 + (\phi_i^z)^2 \rangle / L$

F. Alet, G. Misguich, V. Pasquier, R. Moessner, and J. Jacobsen, Phys. Rev. Lett. **97**, 030403 (2006).



Extended loops : non-zero flux

Short loops : zero flux

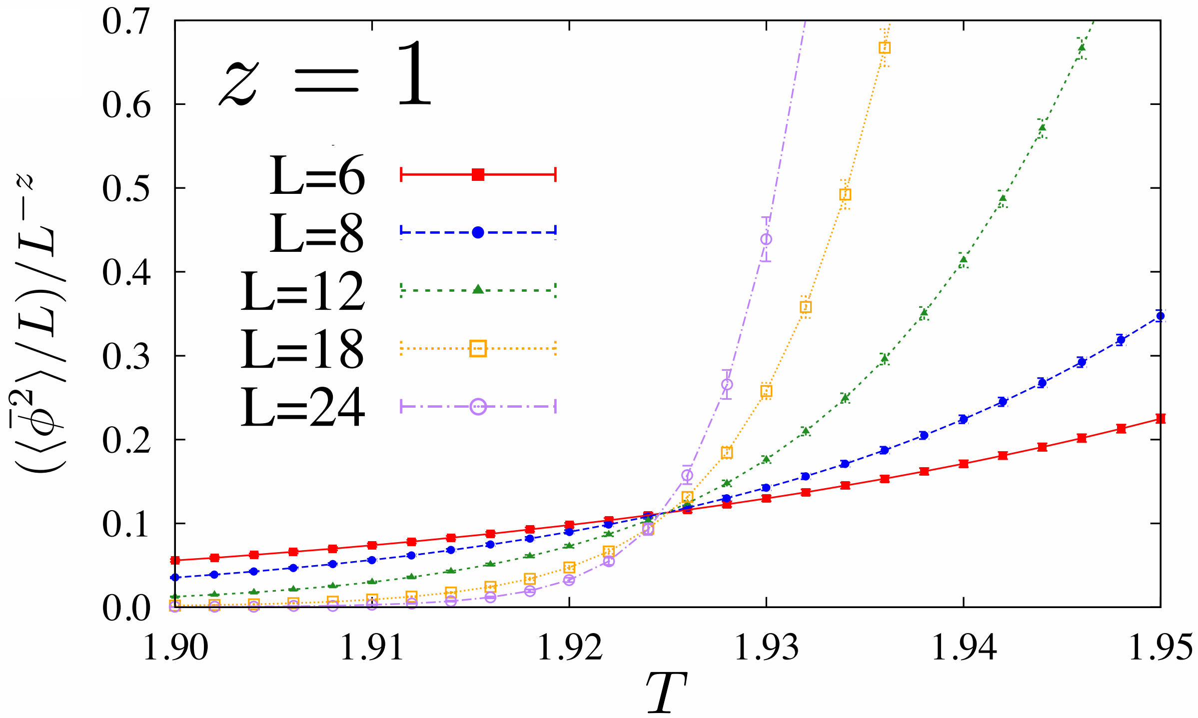


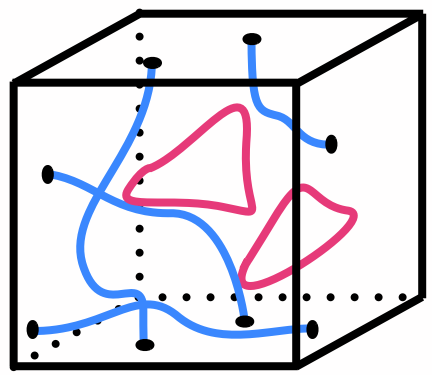
zero flux phase non-zero flux phase

Quantum spin liquid ***Paramagnet***

Finite size scaling

$\bar{\phi}^2/L$: Density of loop flux

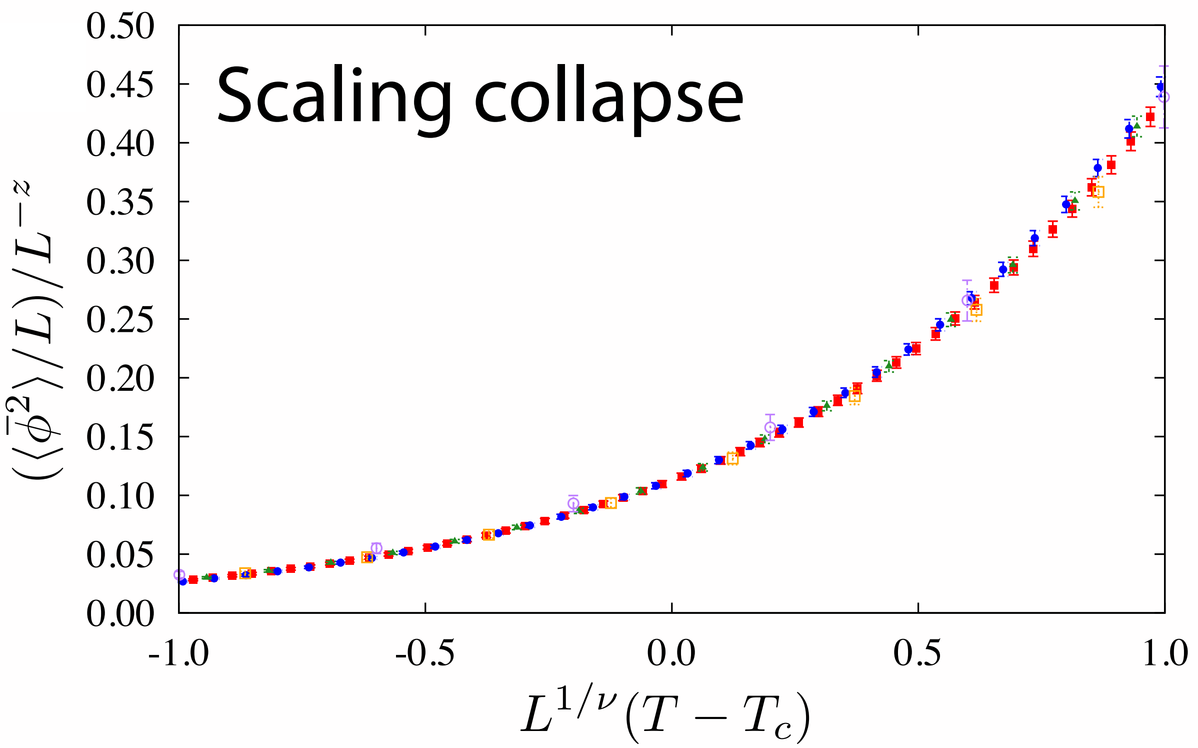




Blue lines contribute to the loop flux.

Assuming *z* as a exponent of density of loop flux,

all the data collapse onto a single curve with $\nu = 0.60(5)$ $T_c^{\text{eff}} = 1.925(1)$



If neglecting *global constraints*...

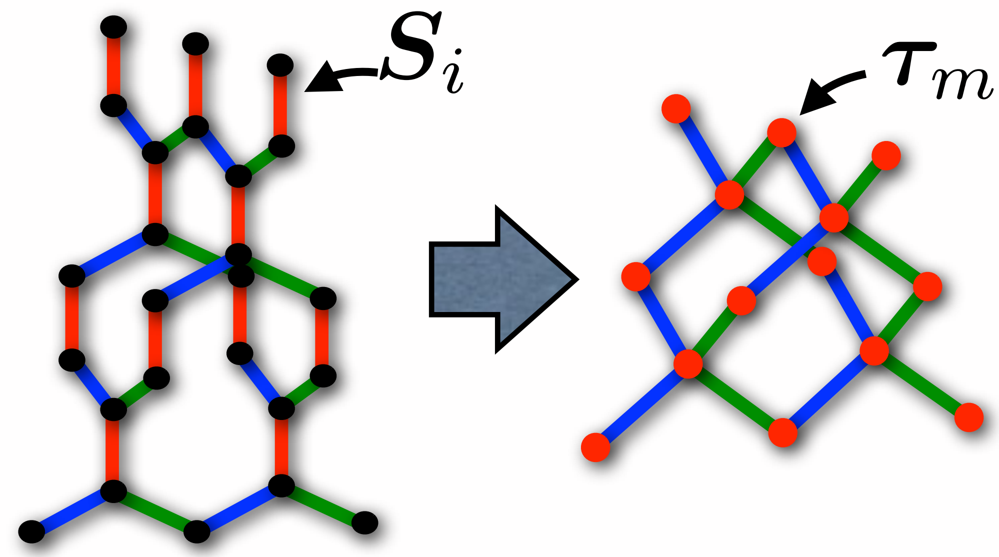
The loop model

⟺ High-*T* expansion in *the Ising model* on a diamond lattice

3D Ising universality class

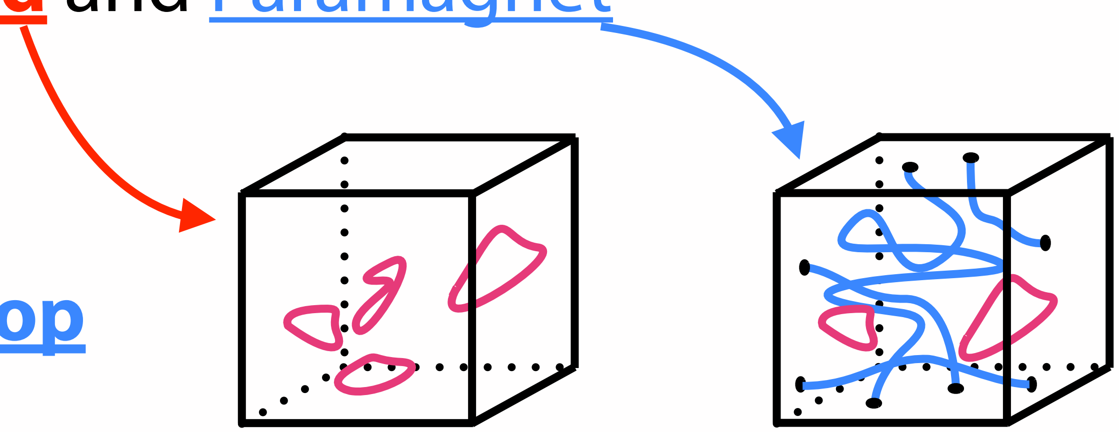
Summary for Anisotropic case

$$\mathcal{H} = -J_x \sum_{<ij>_x} \sigma_i^x \sigma_j^x - J_y \sum_{<ij>_y} \sigma_i^y \sigma_j^y - J_z \sum_{<ij>_z} \sigma_i^z \sigma_j^z$$



- Monte Carlo simulation in $J_z \gg J_x, J_y$

- Finite-*T* phase transition
  between **Quantum spin liquid** and Paramagnet



zero-flux phase   non-zero flux phase

- Characterization by **Extended loop**

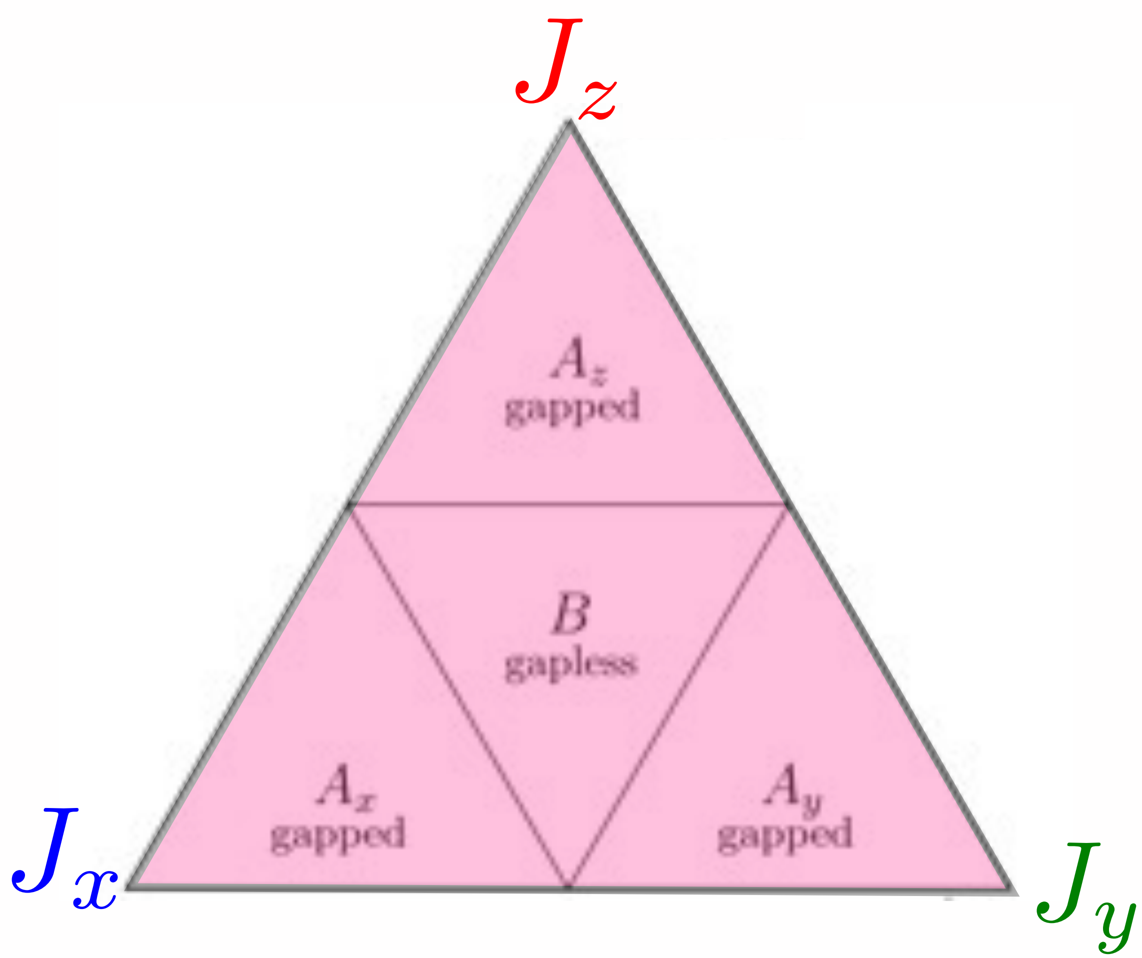
  "Topology of loops"

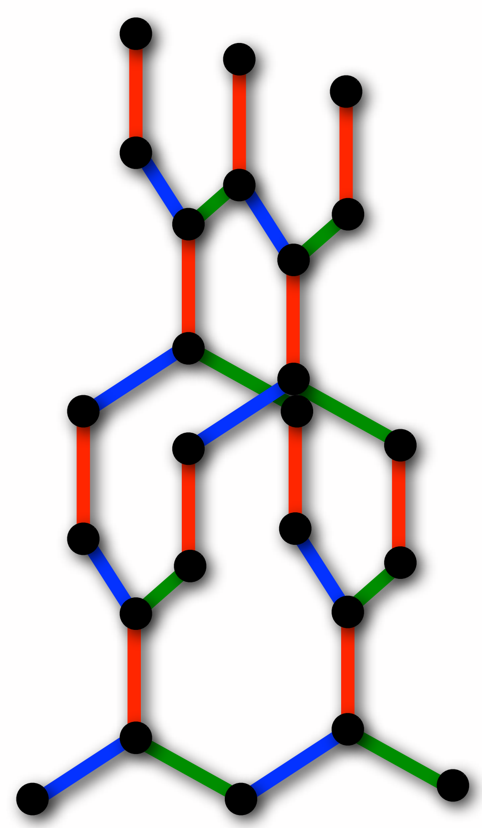
- Continuous phase transition belonging to 3D Ising universality class

- Susceptibility: "Van Vleck" para. at low *T*, and Curie law at high *T*

Numerical Simulation for Original Kitaev Model

- Gapped and Gapless phases -



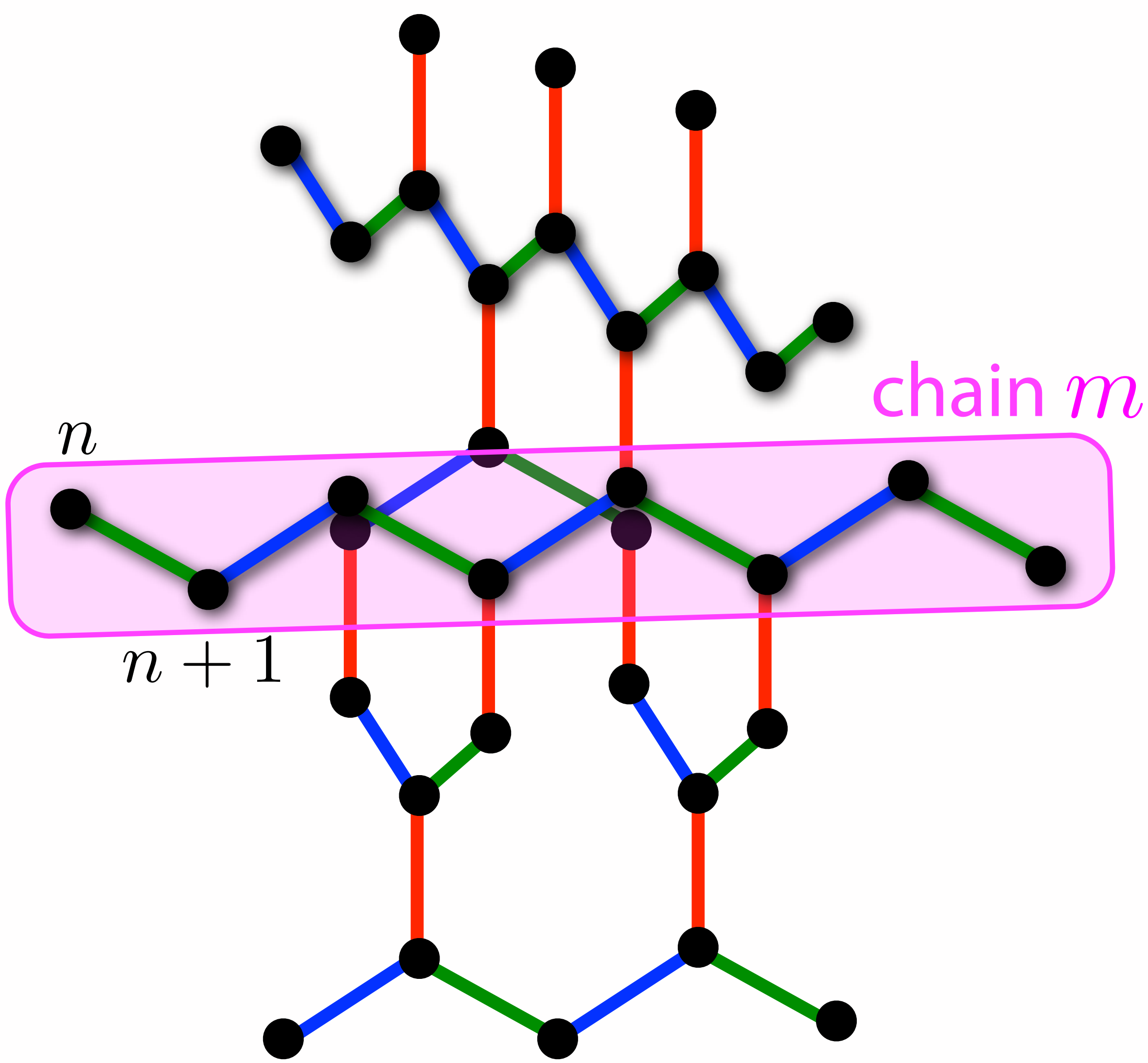


Jordan-Wigner Transformation

$$\mathcal{H} = -J_x \sum_{<ij>_x} \sigma_i^x \sigma_j^x - J_y \sum_{<ij>_y} \sigma_i^y \sigma_j^y - J_z \sum_{<ij>_z} \sigma_i^z \sigma_j^z$$

Hyperhoneycomb lattice:

zigzag *xy* chains connected by *z*-bonds



Jordan-Wigner transformation

$$S^+_{m,n} = (S^-_{m,n})^\dagger = \prod_{n'=1}^{n-1} (1 - 2n_{m,n'}) a^\dagger_{m,n}$$

$$\sigma^x_{m,n}\sigma^x_{m,n+1} = -(a_{m,n} - a^\dagger_{m,n})(a_{m,n+1} + a^\dagger_{m,n+1}),$$

$$\sigma^y_{m,n}\sigma^y_{m,n+1} = (a_{m,n} + a^\dagger_{m,n})(a_{m,n+1} - a^\dagger_{m,n+1}),$$

$$\sigma^z_{m,n}\sigma^z_{m',n'} = (2n_{m,n} - 1)(2n_{m',n'} - 1).$$

H.-D. Chen and J. Hu, Physical Review B **76**, 193101 (2007).
X. Y. Feng, G.-M. Zhang, and T. Xiang, Phys. Rev. Lett. **98**, 087204 (2007).
H.-D. Chen and Z. Nussinov, J. Phys. A Math. Theor. **41**, 075001 (2008).

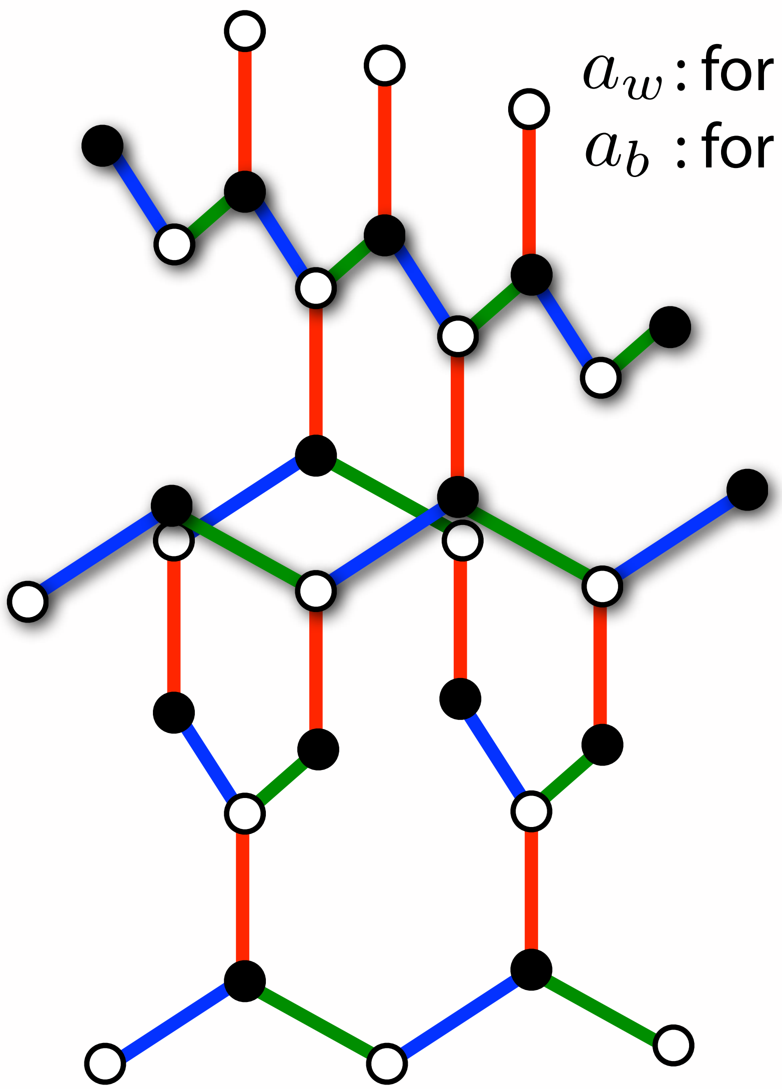
Majorana Representation

$$\mathcal{H} = -J_x \sum_{<ij>_x} \sigma_i^x \sigma_j^x - J_y \sum_{<ij>_y} \sigma_i^y \sigma_j^y - J_z \sum_{<ij>_z} \sigma_i^z \sigma_j^z$$

Jordan-Wigner Transformation

$$\mathcal{H} = J_x \sum_{x \text{ bonds}} (a_w - a_w^\dagger)(a_b + a_b^\dagger) - J_y \sum_{y \text{ bonds}} (a_b + a_b^\dagger)(a_w - a_w^\dagger) - J_z \sum_{z \text{ bonds}} (2n_b - 1)(2n_w - 1)$$

Interaction



a_w : for ***white*** sites

a_b : for ***black*** sites

Introducing *Majorana fermions*

$$c_w = (a_w - a_w^\dagger)/\mathrm{i}, \quad \bar{c}_w = a_w + a_w^\dagger,$$

$$c_b = a_b + a_b^\dagger, \quad \bar{c}_b = (a_b - a_b^\dagger)/\mathrm{i}$$

$$\mathcal{H} = \mathrm{i}J_x \sum_{x \text{ bonds}} c_w c_b - \mathrm{i}J_y \sum_{y \text{ bonds}} c_b c_w + J_z \sum_{z \text{ bonds}} \bar{c}_b \bar{c}_w c_b c_w$$

$$[\bar{c}_b \bar{c}_w, \mathcal{H}] = 0$$

$\eta_r \equiv i\bar{c}_b \bar{c}_w$: *local conserved quantity*

$$\mathcal{H} = \mathrm{i}J_x \sum_{x \text{ bonds}} c_w c_b - \mathrm{i}J_y \sum_{y \text{ bonds}} c_b c_w - \mathrm{i}J_z \sum_{z \text{ bonds}} \eta_r c_b c_w$$

Monte Carlo Simulation

$$\mathcal{H} = -J_x \sum_{<ij>_x} \sigma_i^x \sigma_j^x - J_y \sum_{<ij>_y} \sigma_i^y \sigma_j^y - J_z \sum_{<ij>_z} \sigma_i^z \sigma_j^z$$

⇩

$$\mathcal{H} = \mathrm{i}J_x \sum_{x \text{ bonds}} c_w c_b - \mathrm{i}J_y \sum_{y \text{ bonds}} c_b c_w - \mathrm{i}J_z \sum_{z \text{ bonds}} \eta_r c_b c_w$$

$\eta_r = \pm 1$ on *z* bonds

Free **Majorana system coupled to the Ising variables**

(Similar to *the double-exchange model*)

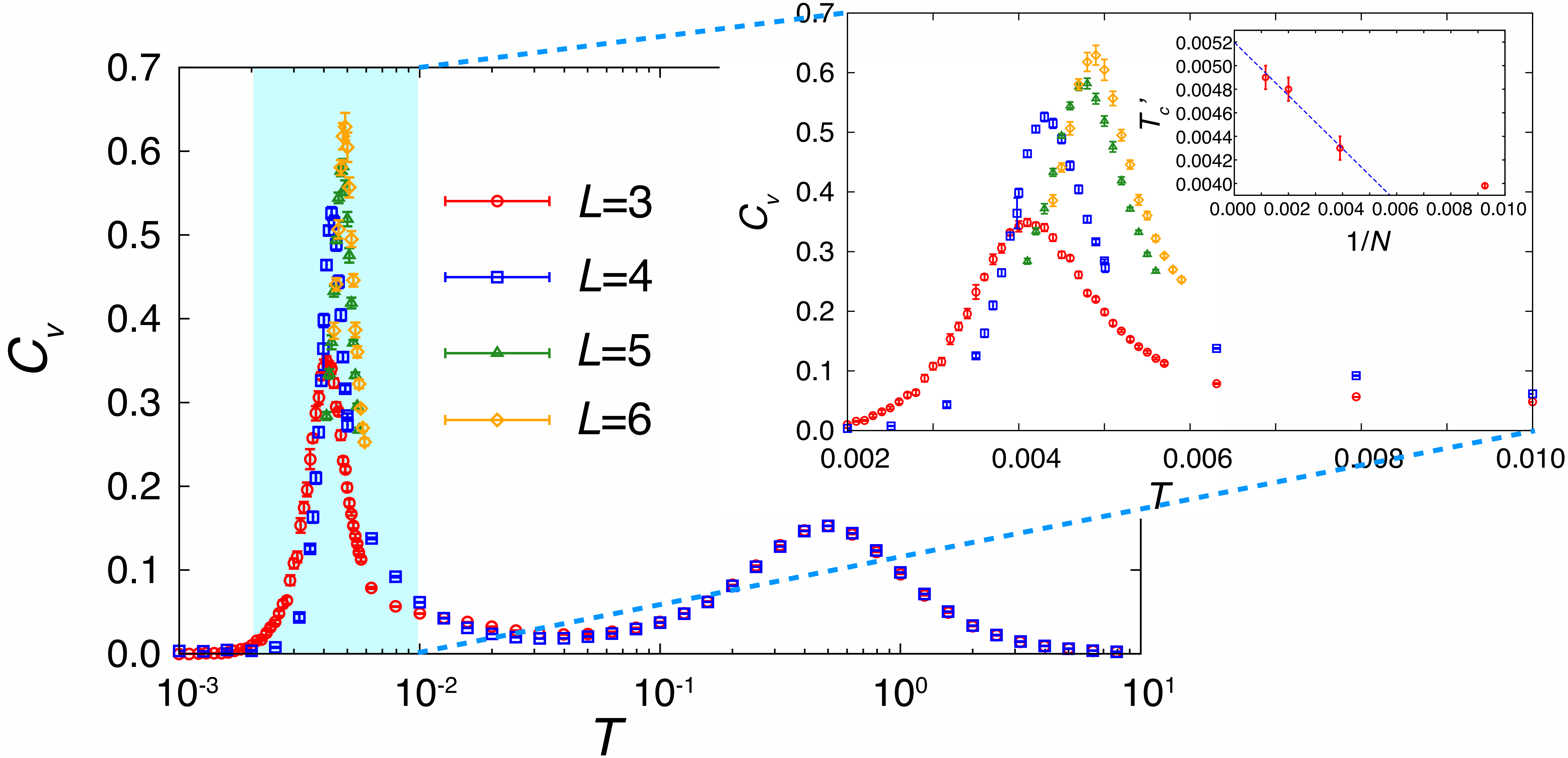
- Partition function: $Z = \mathrm{Tr}_{\{\eta_r\}} \mathrm{Tr}_{\{c_i\}} e^{-\beta \mathcal{H}} = \mathrm{Tr}_{\{\eta_r\}} e^{-\beta F_f(\{\eta_r\})}$

  $F_f(\{\eta_r\}) = -T \ln \mathrm{Tr}_{\{c_i\}} e^{-\beta \mathcal{H}(\{\eta_r\})}$ calculated by exact diagonalization

- $\{\eta_r\}$ are updated so as to reproduce the distribution $e^{-\beta F_f(\{\eta_r\})}$
- System size 4xL^3 up to L=6 (864sites)
- Conditions: 40,000 (10,000) MC steps for L=3,4,5 (L=6), parallel tempering (16 replicas)
- We impose an open boundary condition to avoid the boundary terms from JW transformation

Specific Heat in isotropic case

$J_x = J_y = J_z = 1/3$ ground state is gapless QSL



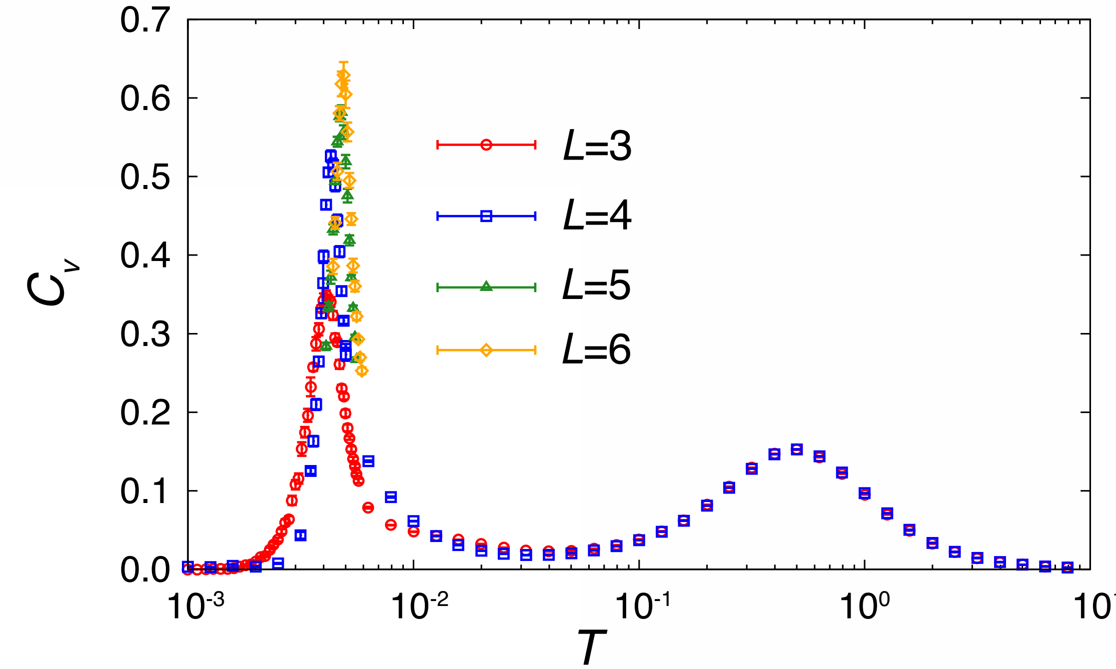
High temperature peak (Size independent)

Low temperature peak (Size dependent)

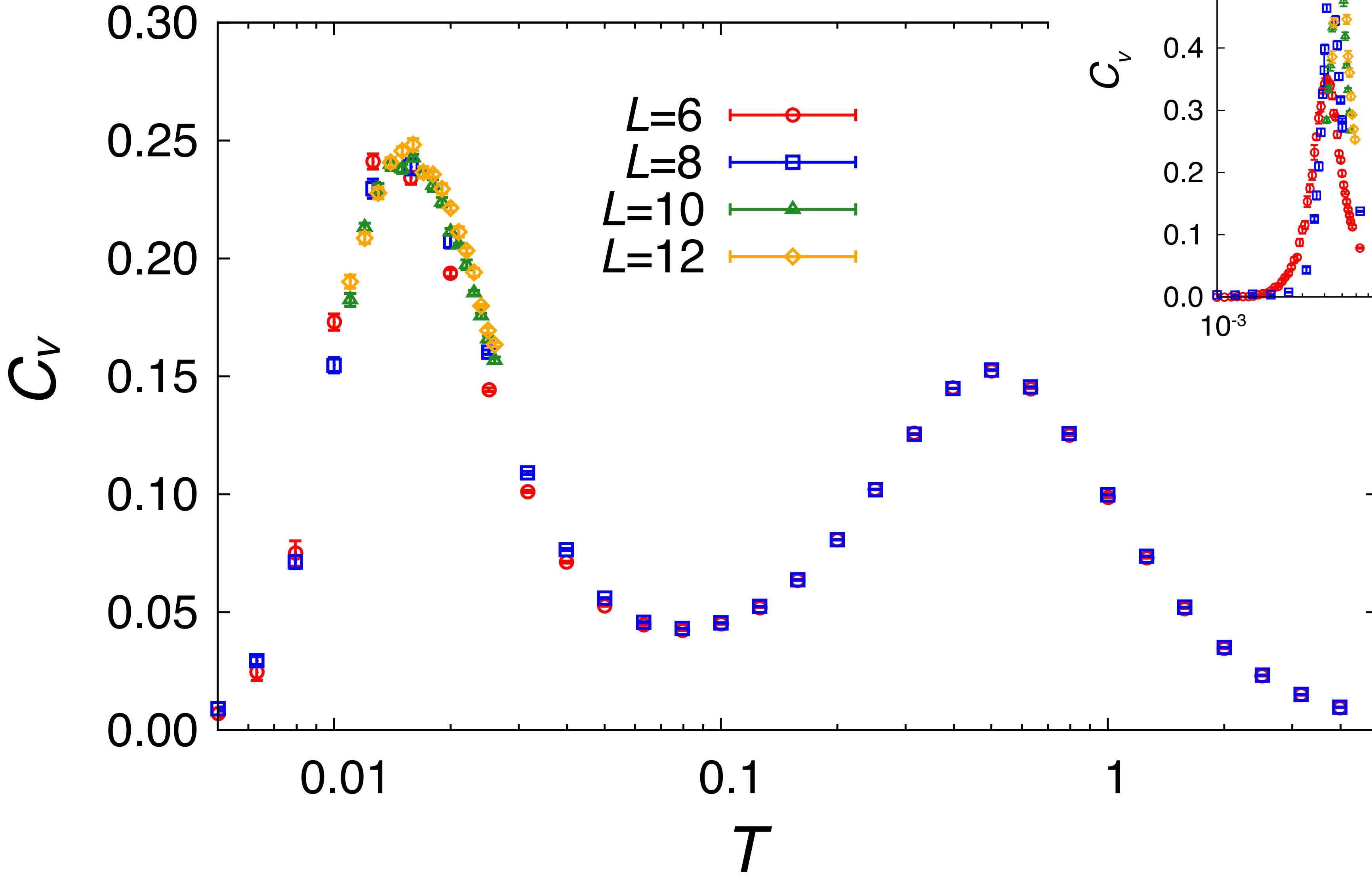
→ ***Phase transition*** **(T_c~ 0.0052)**

Specific Heat in 2D Kitaev model

3D Kitaev model



2D Kitaev model

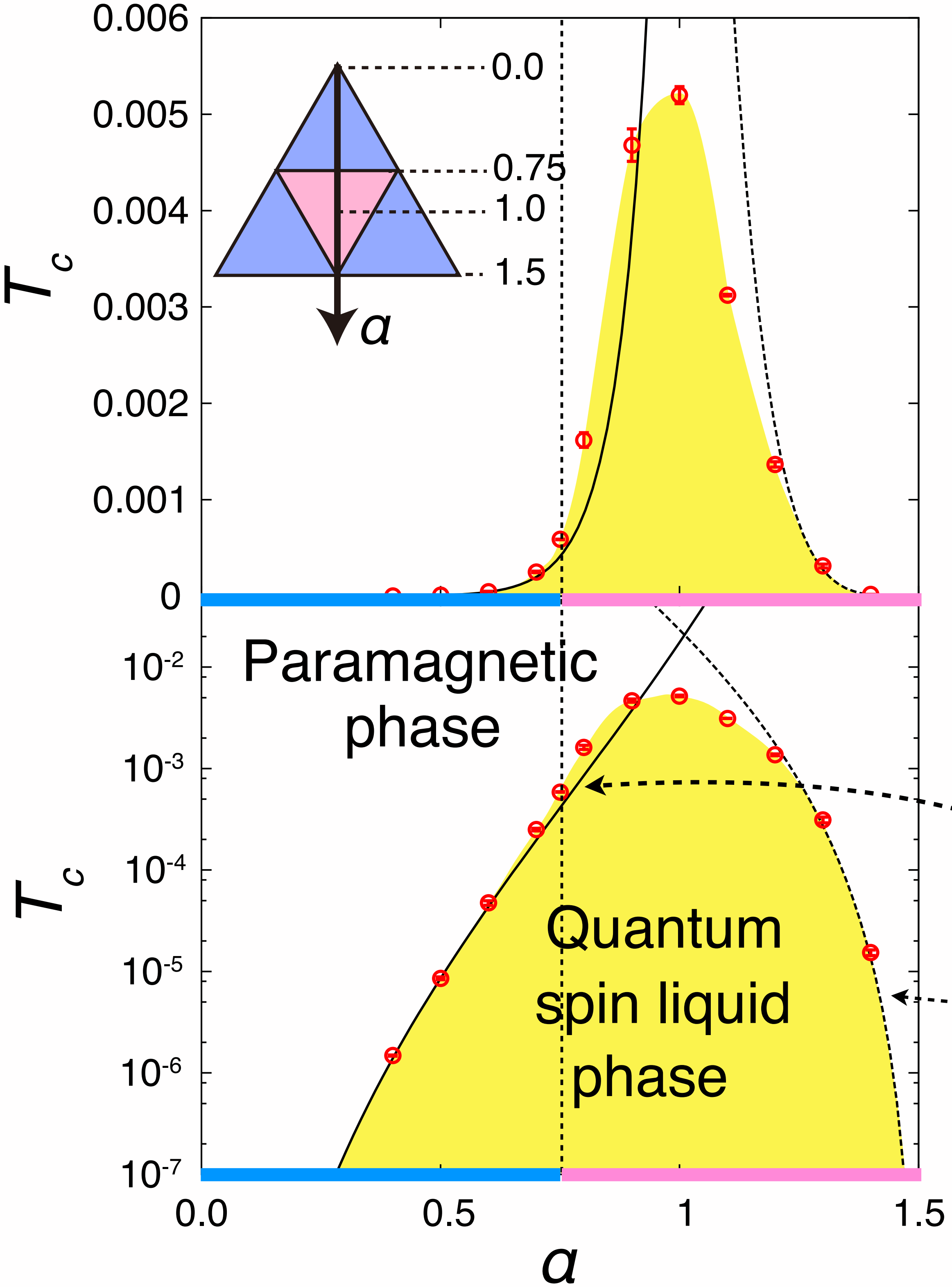


Low temperature peak does not grow with increasing *L*.

→ **No phase transition in 2D case**

Phase Diagram

Parameters: $J_x = J_y = \frac{\alpha}{3}, \; J_z = 1 - \frac{2\alpha}{3}$



- T_c is determined by extrapolating the peak temperatures of C_v. (L=4,5,6)
- T_c *continuously changes* at gapless/gapped boundary.
- T_c takes maximum at $J_x = J_y = J_z$.
  Frustration stabilizes the QSL.
- Two limits:

$J_z \gg J_x, J_y$

$$T_c = 1.925(1) \times \frac{7}{256} \frac{J^6}{J_z^5}$$

$J_z \ll J_x, J_y$

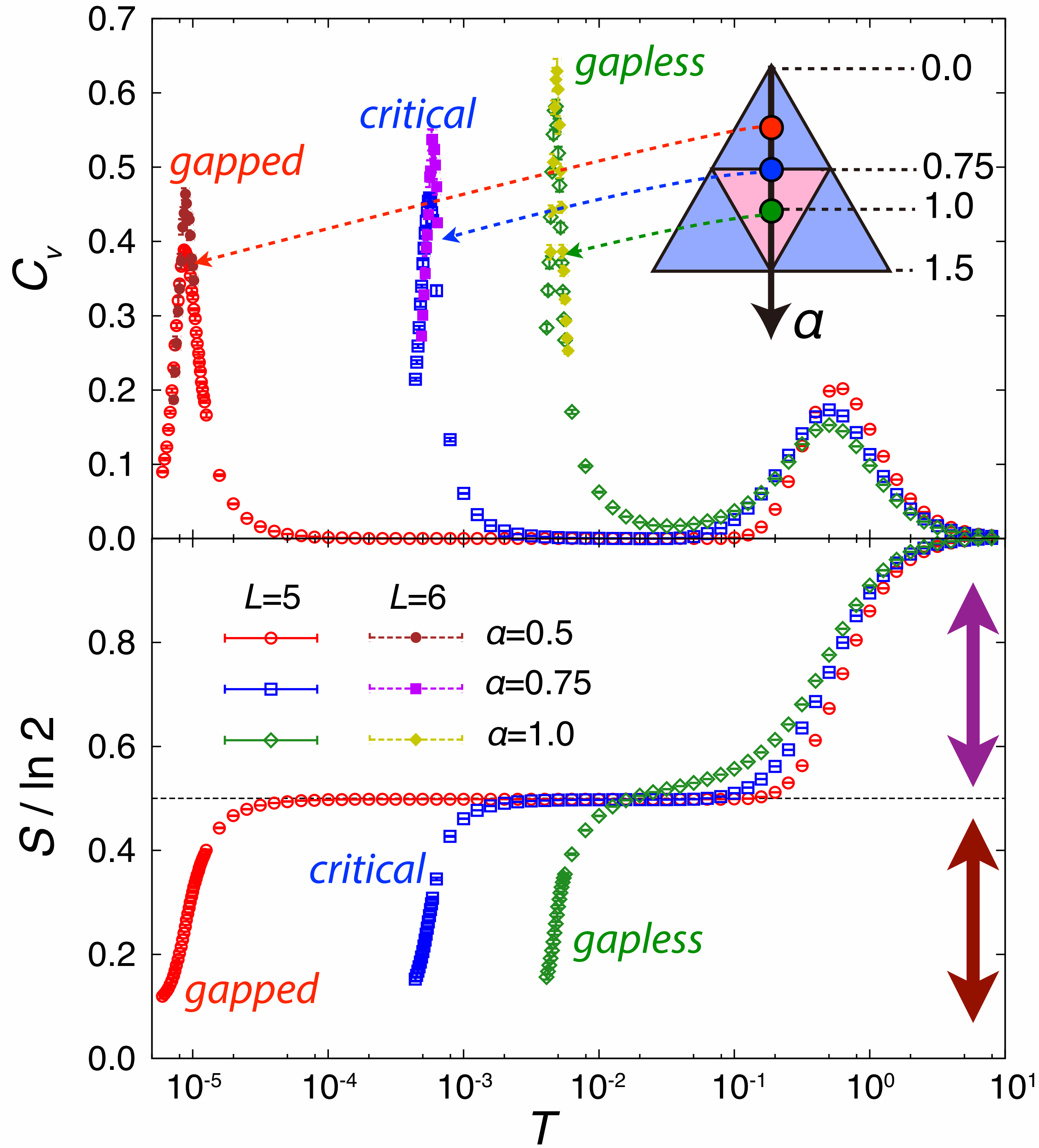
$$T_c \propto \frac{J_z^4}{J^3}$$

- Asymptotic behaviors of T_c agree with the perturbation results.

Separation of two energy scale

$$\mathcal{H} = \mathrm{i}J_x \sum_{x \text{ bonds}} c_w c_b - \mathrm{i}J_y \sum_{y \text{ bonds}} c_b c_w + J_z \sum_{z \text{ bonds}} \bar{c}_b \bar{c}_w c_b c_w$$

$\bar{c}_b \bar{c}_w \rightarrow \eta_r$



S=1/2 spin ⟹ two Majorana fermions

S_i → c_i **forms free fermion system**

S_i → $\bar{c}_i$ **forms a Z_2 variable** η_r

Entropy release for ***itinerant Majorana fermions*** c_i (Kinetic energy~ $J_x+J_y+J_z=1$)

(Anisotropy independent)

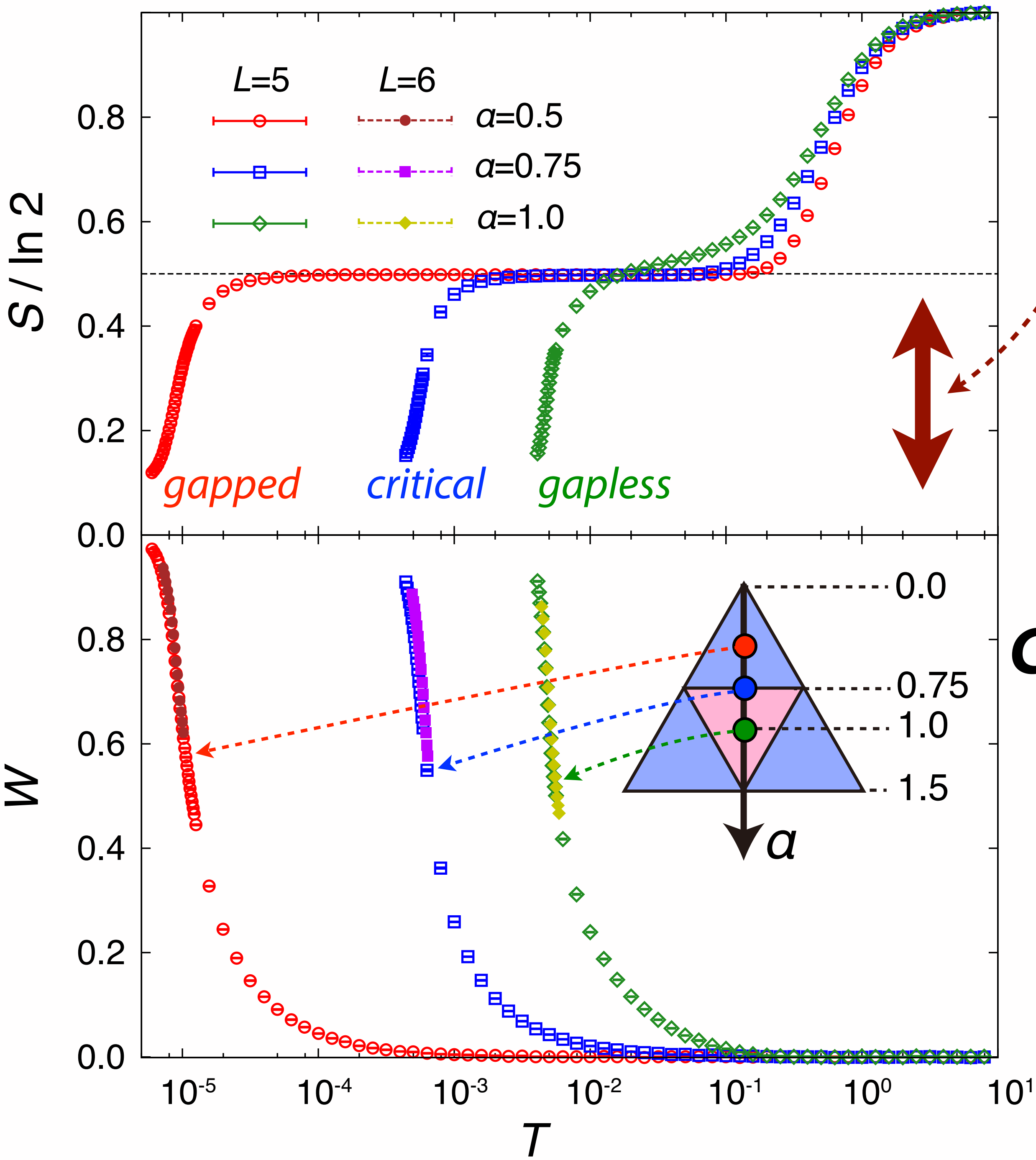
Entropy release for ***localized Majorana fermions*** $\bar{c}_i$

⟹ ***Phase transition***

(Anisotropy dependent)

Temperature Dependence of W_p

$$\mathcal{H} = \mathrm{i}J_x \sum_{x\text{ bonds}} c_w c_b - \mathrm{i}J_y \sum_{y\text{ bonds}} c_b c_w + J_z \sum_{z\text{ bonds}} \underbrace{\bar{c}_b \bar{c}_w}_{\eta_r} c_b c_w$$



Entropy release for ***localized Majorana fermions***

$\eta_r = i\bar{c}_b\bar{c}_w$

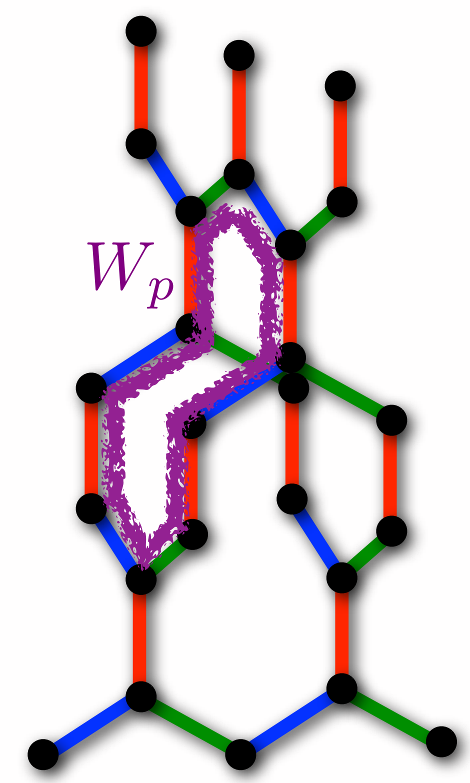
Local conserved quantity: $W_p = \prod_{r\in\text{loop}:p} \eta_r$

Coherent growth of the local conserved quantities

$$\tilde{W} = \frac{1}{N_p}\sum_p \langle W_p \rangle$$

N.B. **Not** order parameter

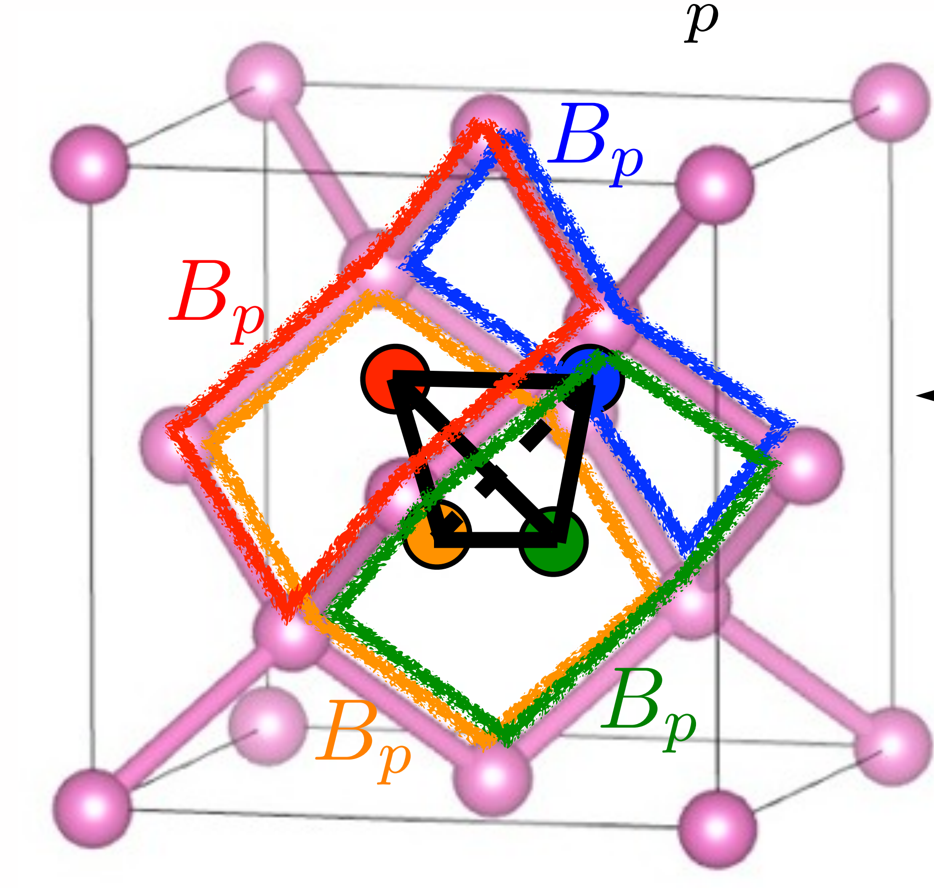
ground state: all $W_p = +1$



Local constraint for W_p

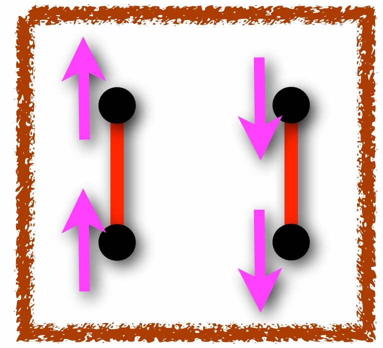
Effective model for $J_z \gg J_x, J_y$

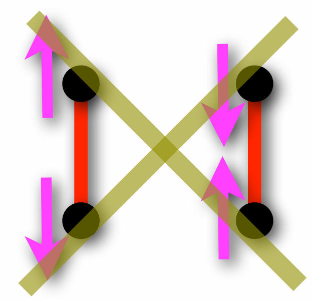
$$\mathcal{H}_{\rm eff} = -J_{\rm eff} \sum_p B_p$$



$$B_p \, B_p \, B_p \, B_p = 1$$

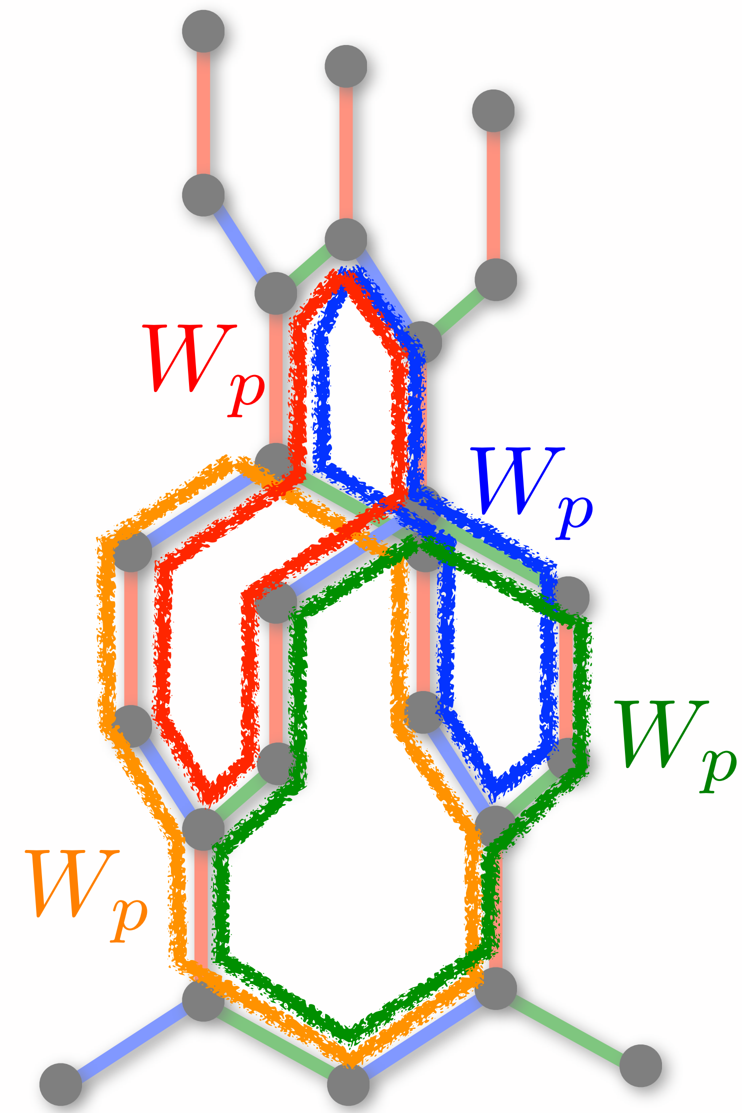
$\mathcal{P}$





$$B_p = \mathcal{P} W_p \mathcal{P}$$

Original Kitaev model



$$W_p W_p W_p W_p = 1$$

Local constraint for W_p in the original Kitaev model

→ Flipped W_p form a loop.

→ **Topological characterization** by W_p-loops.

Summary

Monte Carlo simulation is applied to the 3D Kitaev model

- ***Finite-T phase transition*** appears for both gapped & gapless QSL.
  from QSL to paramagnet
- The QSL phase is ***always*** separated from paramagnet.
- ***The frustration stabilizes the QSL***.
- The two kinds of energy scale.

S_i → ***Itinerant Majorana fermions*** ⇒ High-T(~1.0) crossover
S_i → ***Localized Majorana fermions*** ⇒ Low-T(~0.01) **phase transition**

- Asymptotic behavior of T_c agrees
  with the results in the anisotropic limit.
- The transition is characterized by ***the topological quantity***.
  The local constraint also exists for W_p in the original Kitaev model
  as well as for B_p in the toric code limit.

Thank you
for your attention