Quantum Monte Carlo Study of Thermodynamics in Kitaev Spin Liquids

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Message of this talk

Methodology: New quantum Monte Carlo (QMC) algorithm for Kitaev-type models based on the Majorana fermion representation

quantum spins → **Majorana fermions**

Jordan-Wigner transformation
+
Majorana representation

itinerant & localized

→ **unbiased QMC w/o negative sign problem !**

Physics: Quantum spin liquids in the Kitaev-type models are a good playground for hunting of Majorana fermions!

- Majorana representation is not just a mathematical tool, but has observable consequences.

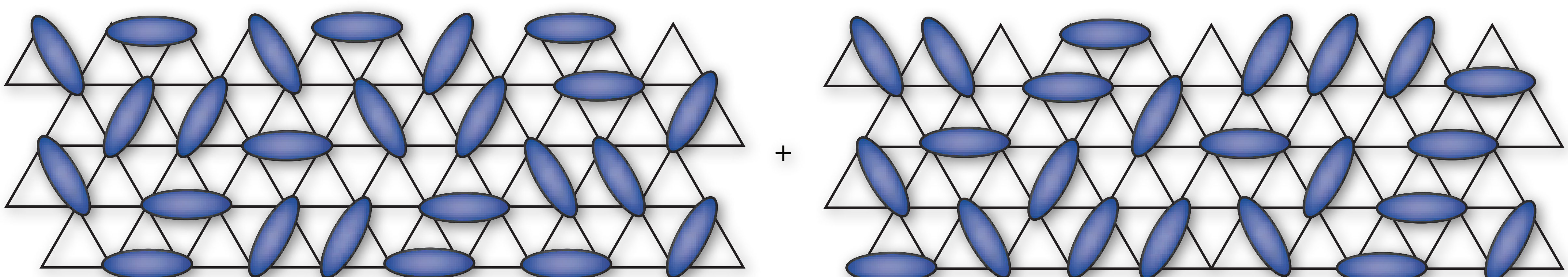
Outline

- **Introduction**
  - What is the quantum spin liquid (QSL)?
  - problems on the experimental and theoretical sides
  - our motivation and strategy
- **Model:** fundamentals of the Kitaev model and its extensions
- **Method:** QMC technique in Majorana fermion representation
- **Results**
  - thermal fractionalization of a quantum spin into Majorana fermions:
    a guide of Majorana hunting for experimentalists
  - "liquid-gas" phase transition in 3D:
    unconventional transition caused by proliferation of emergent loops
- **Summary and perspectives**

Introduction

Quantum spin liquid (QSL)

- **new state of matter in magnets**: magnetic state which does not “solidify” down to T=0 due to strong quantum fluctuations
  - magnetic analog of liquid helium (P. W. Anderson, 1973)
  - no long-range order down to T=0, same symmetry as paramagnet



Anderson’s RVB: figure is taken from L. Balents 2010

- QSLs have attracted much interest from not only condensed matter physics but also fundamental statistical physics and quantum information.

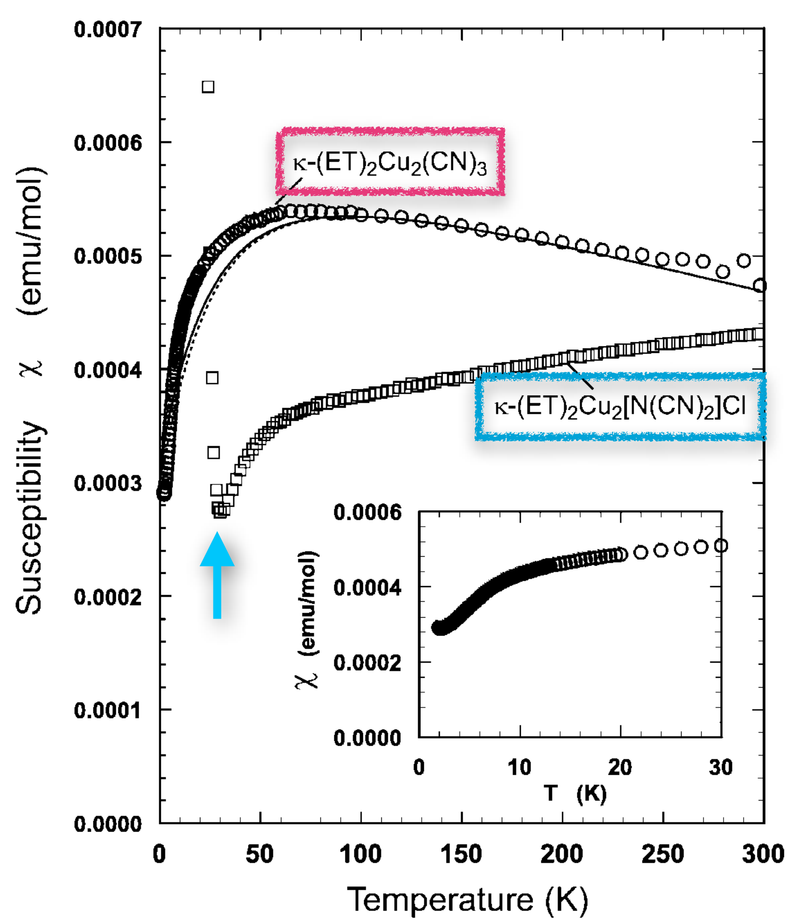
  e.g. topological computation by non-Abelian anyons (A. Kitaev, 2003)

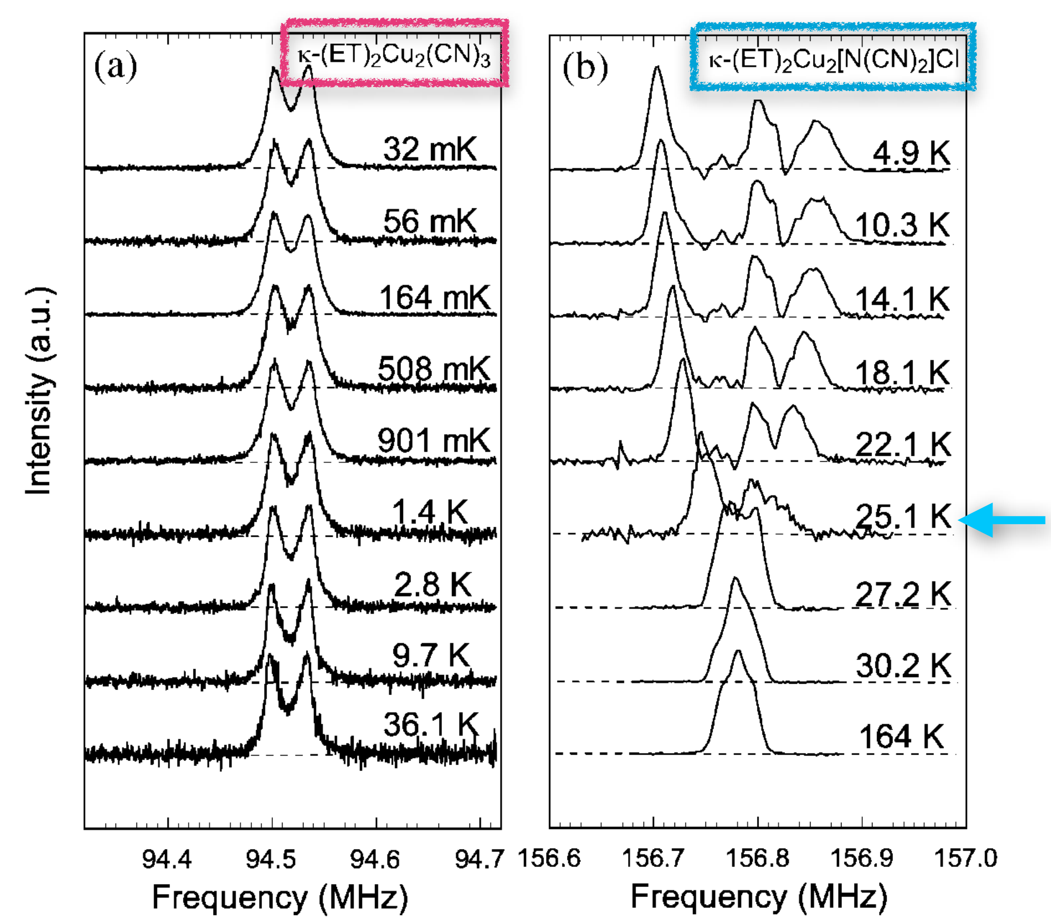
Problems in the study of QSLs

on the experimental side, there are several candidates, but...

- how to prove the existence of QSLs? necessary to prove "an alibi"?
- how to distinguish QSLs from paramagnet? any "positive" fingerprint?

✳ organic conductor κ-$(ET)_2Cu_2(CN)_3$: S=1/2 spins on a triangular layers





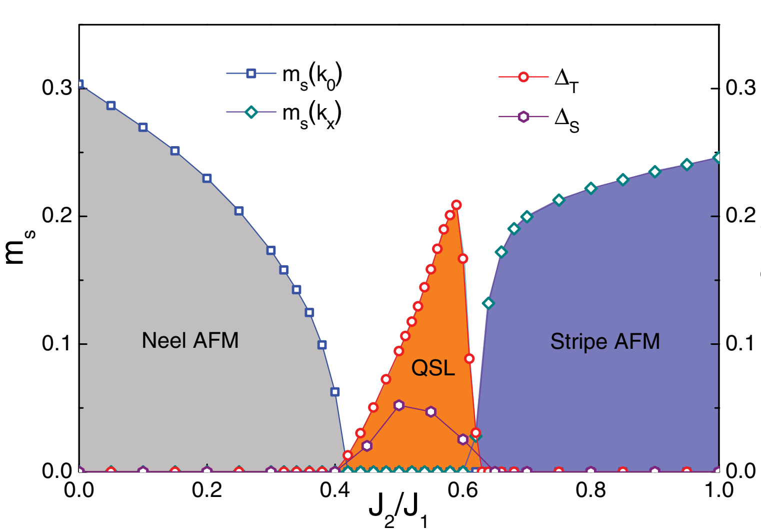
Y. Shimizu *et al.*, 2003

Problems in the study of QSLs

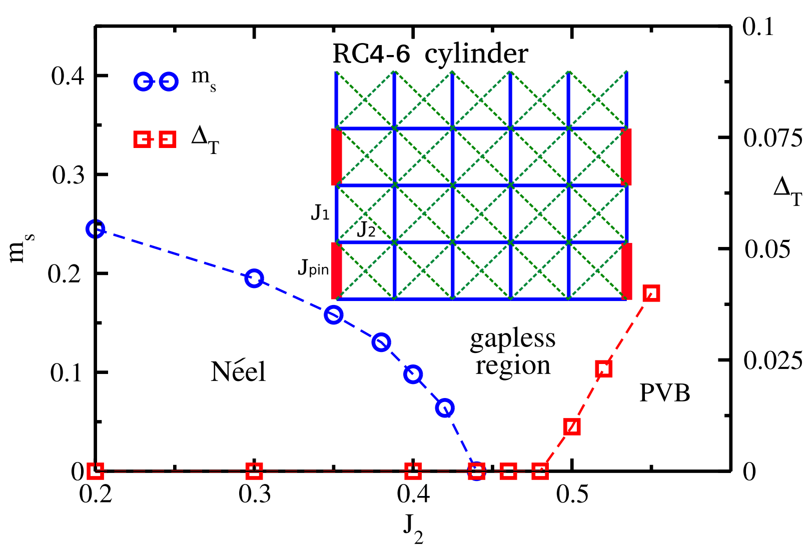
on the theoretical side...

- less examples of well-identified QSLs
  - need to prove the absence of “all” conventional long-range orders
- less choice of effective theoretical tools
  - Results often depend on the methods, even on the computational conditions (e.g., boundary conditions in finite-size clusters).

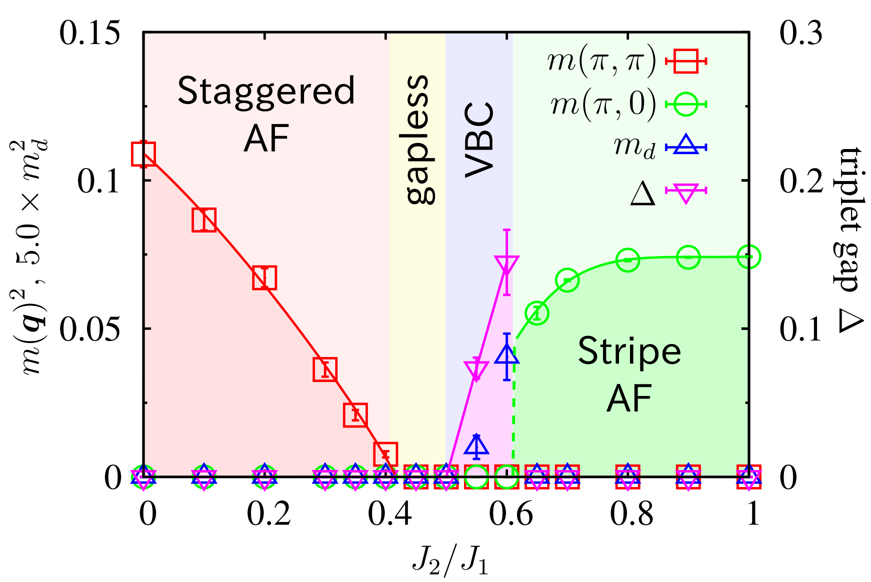
✳ S=1/2 J_1-J_2 Heisenberg model on a square lattice



H.-C. Jiang, H. Yao, and L. Balents, 2012



S.-S. Gong, W. Zhu, D. N. Sheng, O. I. Motrunich, and M. P. A. Fisher *et al.*, 2014



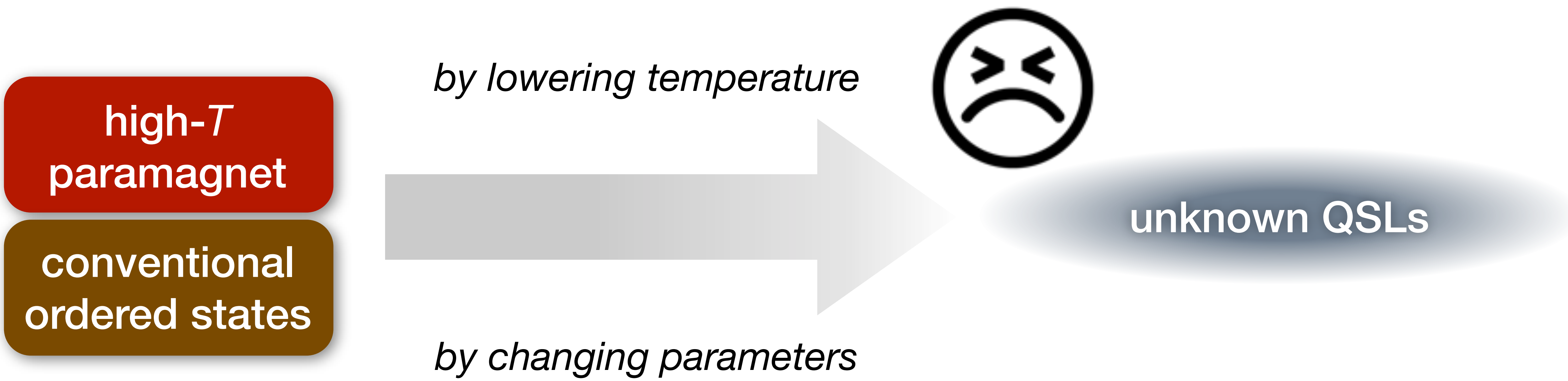
S. Morita, R. Kaneko, and M. Imada, 2015

Motivation and strategy

high-*T* paramagnet

conventional ordered states

Motivation and strategy



Motivation and strategy

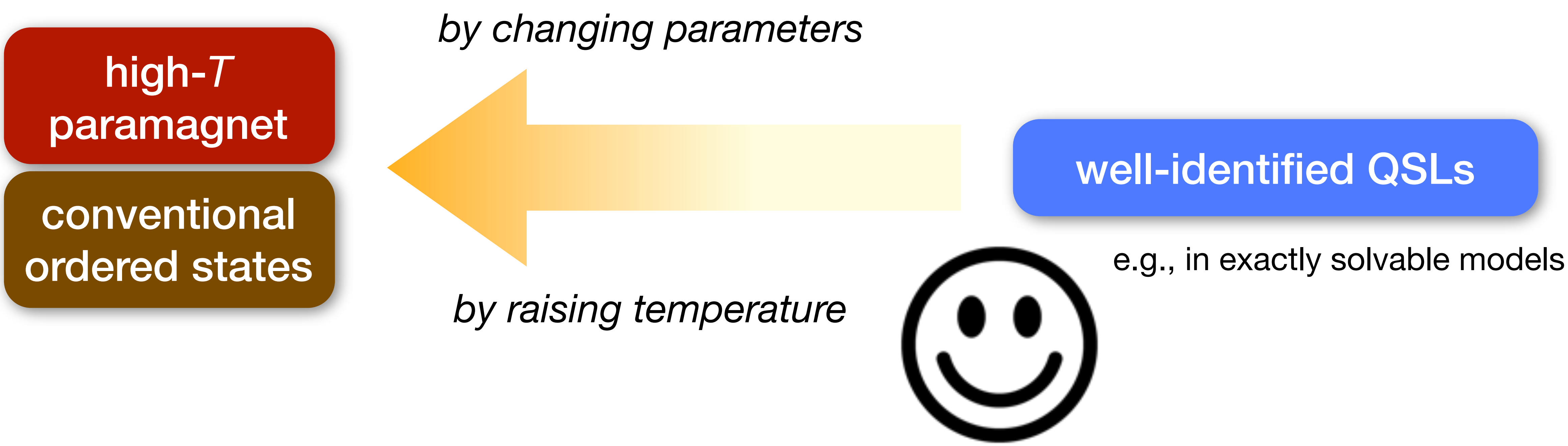
high-*T* paramagnet

conventional ordered states

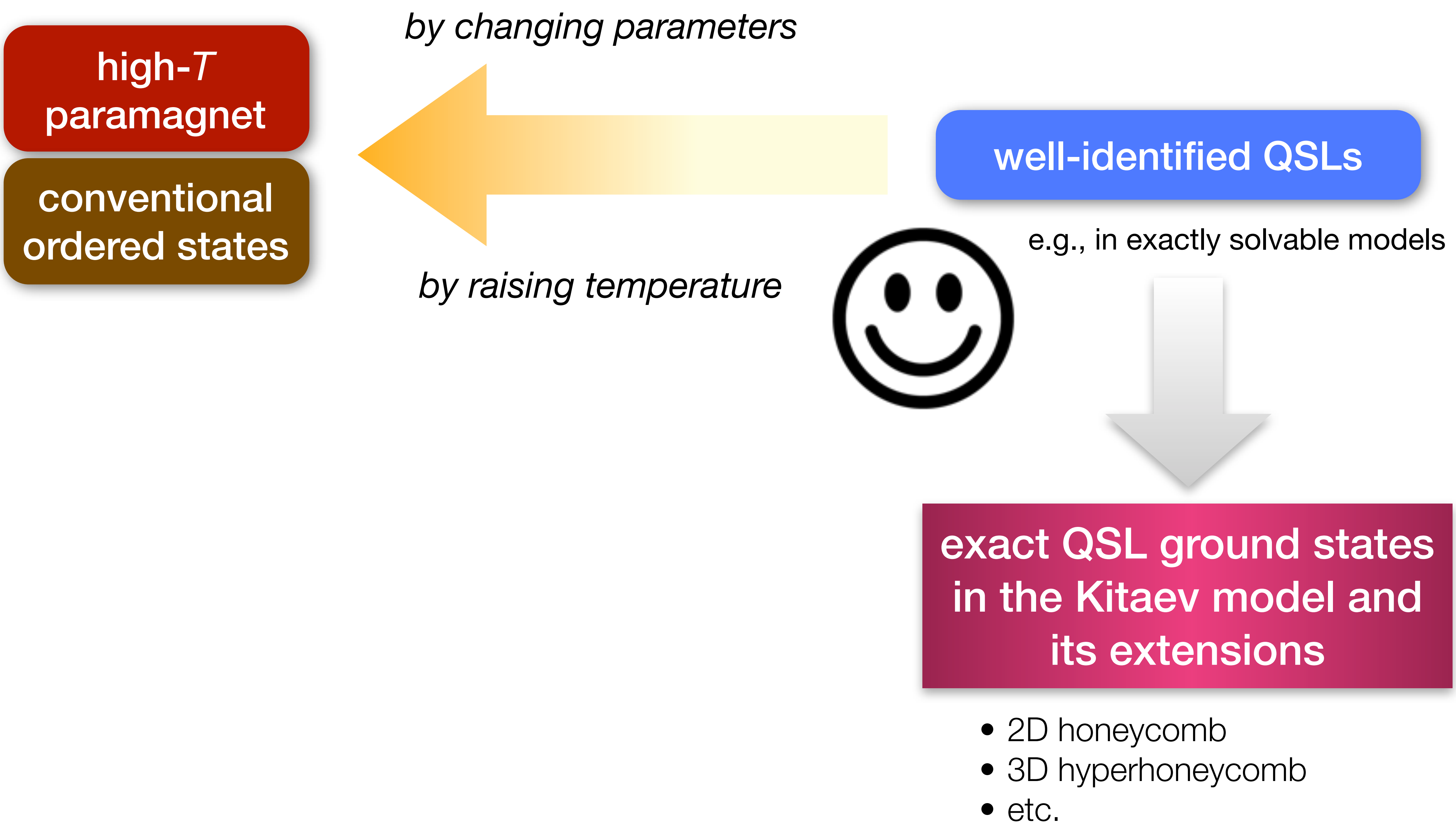
well-identified QSLs

e.g., in exactly solvable models

Motivation and strategy



Motivation and strategy



Motivation and strategy

high-*T* paramagnet

conventional ordered states

by changing parameters

by raising temperature

well-identified QSLs

e.g., in exactly solvable models

unbiased quantum Monte Carlo simulation without negative-sign problem

new method on the basis of Majorana fermion representation

exact QSL ground states in the Kitaev model and its extensions

- 2D honeycomb
- 3D hyperhoneycomb
- etc.

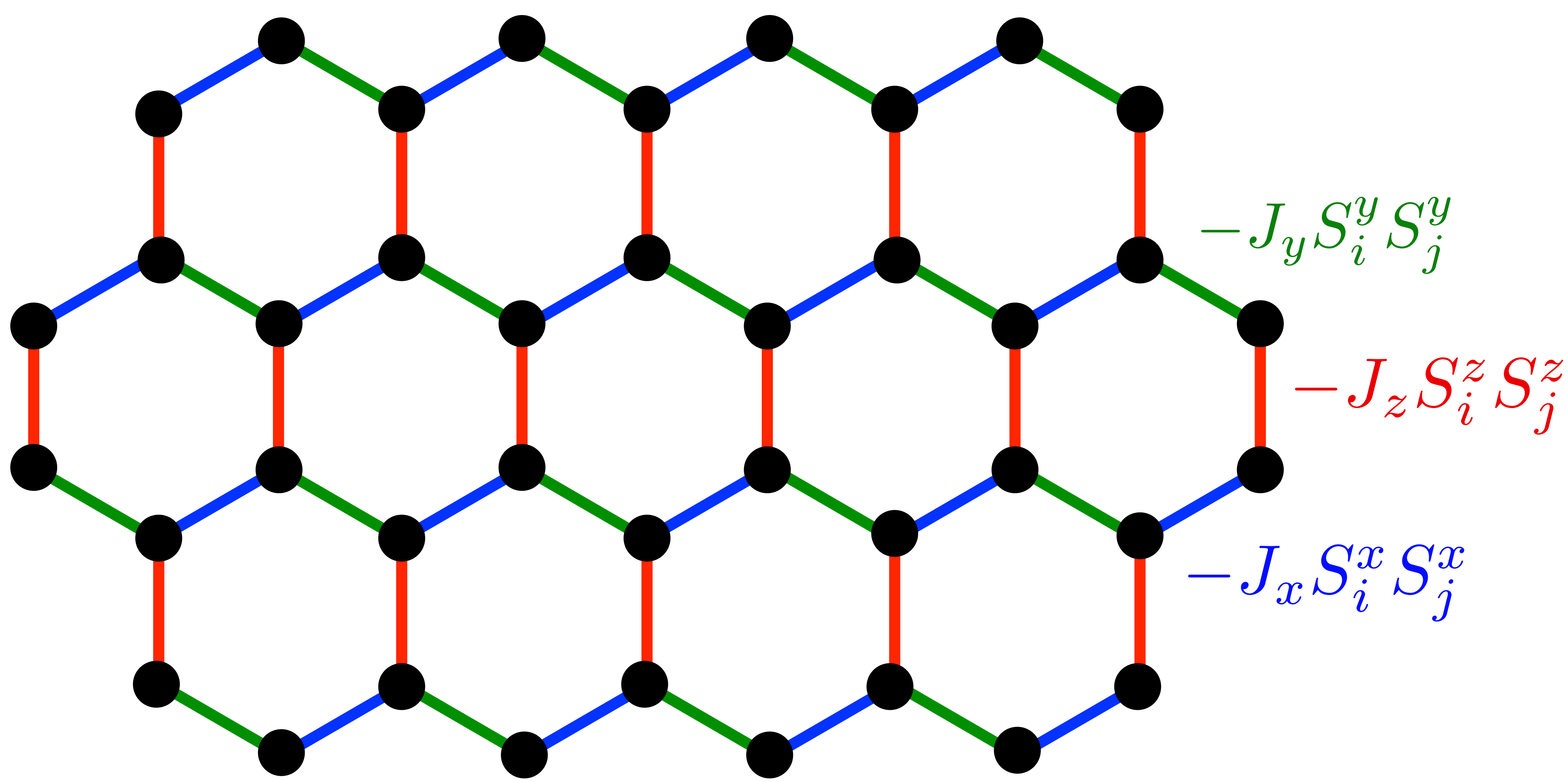
Model

Fundamentals of the Kitaev models

Kitaev model: exactly solvable model for QSL

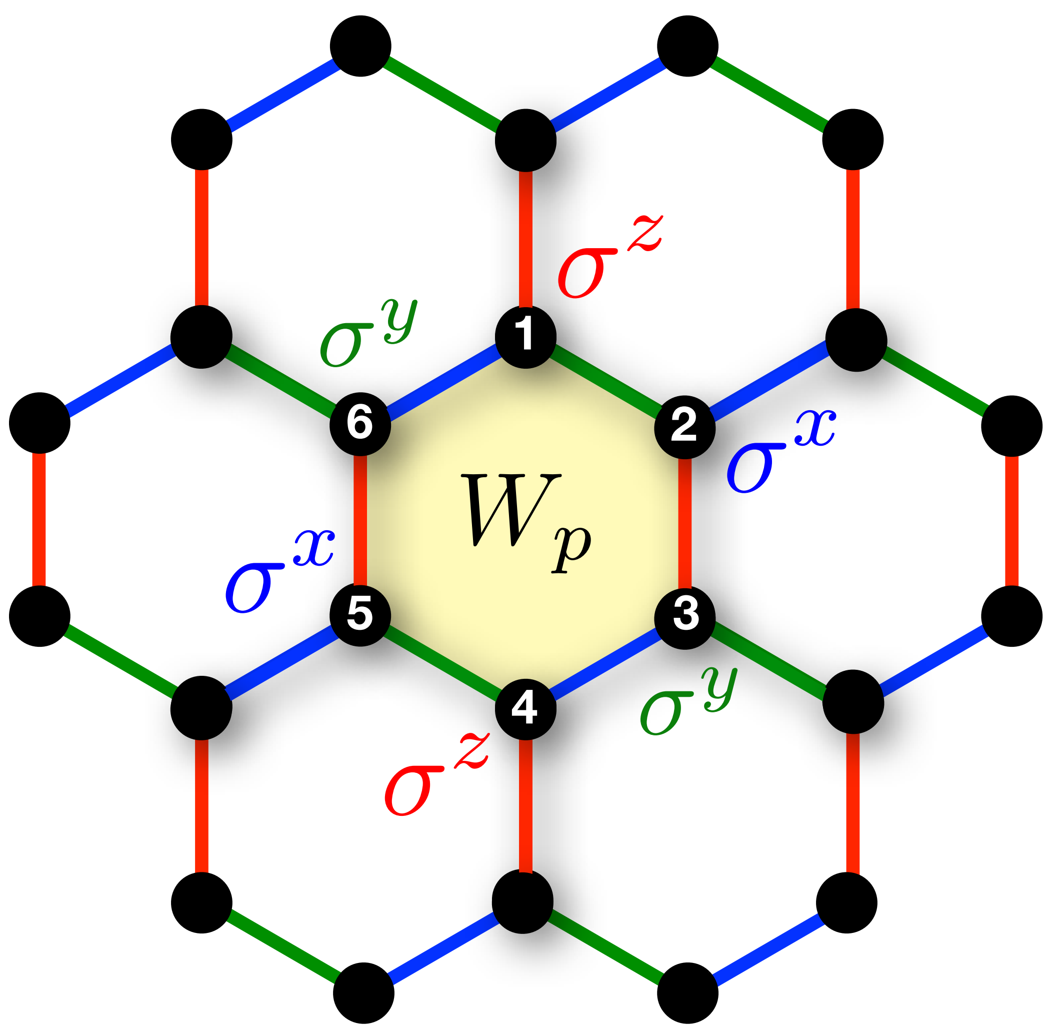
- S=1/2 quantum spin model on a 2D honeycomb lattice (A. Kitaev, 2006)

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



bond dependent interactions ➡ *frustration*

Kitaev model: local conserved quantity



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

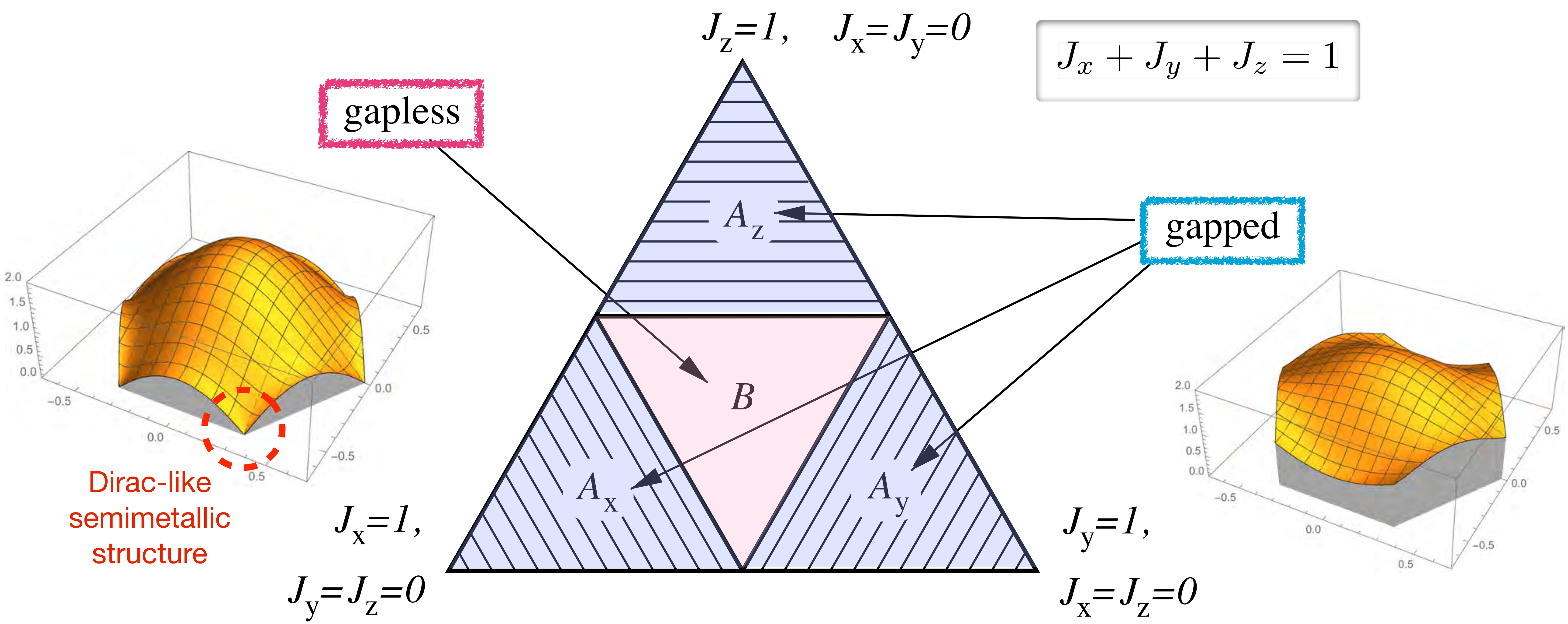
- ✓ $[\mathcal{H}, W_p] = 0$
- ✓ $[W_p, W_p'] = 0 \quad \text{for } p \neq p'$
- ✓ $W_p^2 = 1$

➡ Z_2 variable $W_p = \pm 1$
(termed "flux")

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

➡ solvable by introducing Majorana fermions (A. Kitaev, 2006): ground state is given by all W_p=+1

Kitaev model: *T*=0 phase diagram



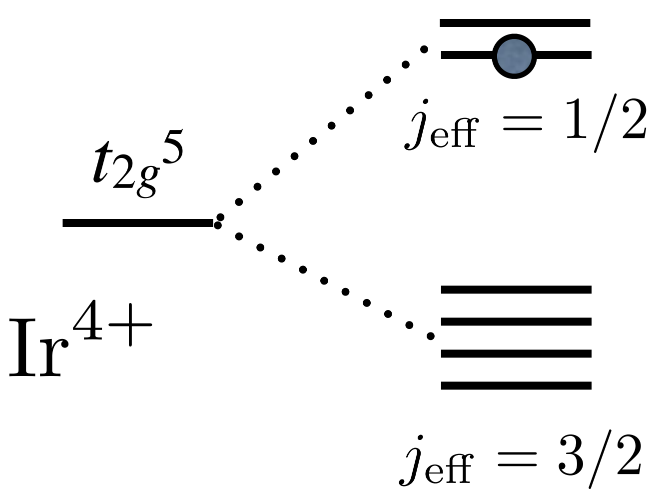
QSL ground states in the entire parameter region:
gapless and gapped QSLs depending on the anisotropy

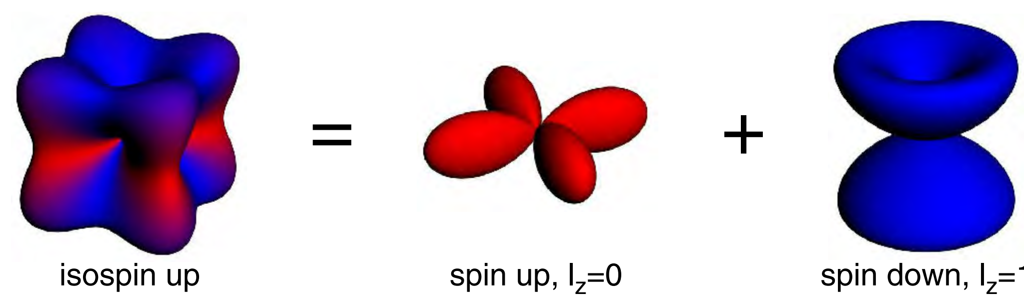
topological order, extremely short-range spin correlation, non-abelian anyons, quantum computation, ...

A. Kitaev, 2006; G. Baskaran, S. Mandal, and R. Shanker, 2007; C. Castelnovo and C. Chamon, 2007; Z. Nussinov and G. Ortiz, 2008, ...

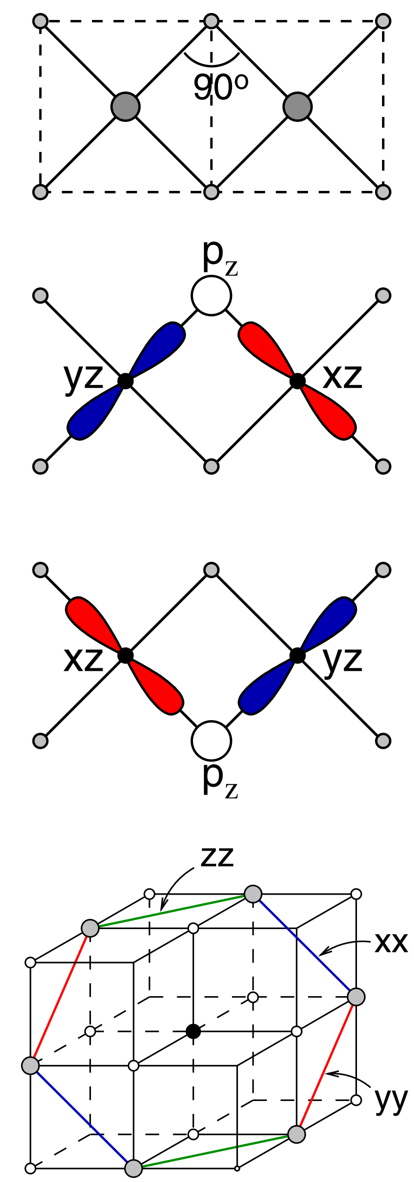
Kitaev model: experimental relevance

- An effective interaction for partially-filled t_{2g} levels under strong spin-orbit coupling may become Kitaev type (G. Jackeli and G. Khaliullin, 2009).





j_{eff}=1/2 isospin



- extension by including isotropic Heisenberg interaction

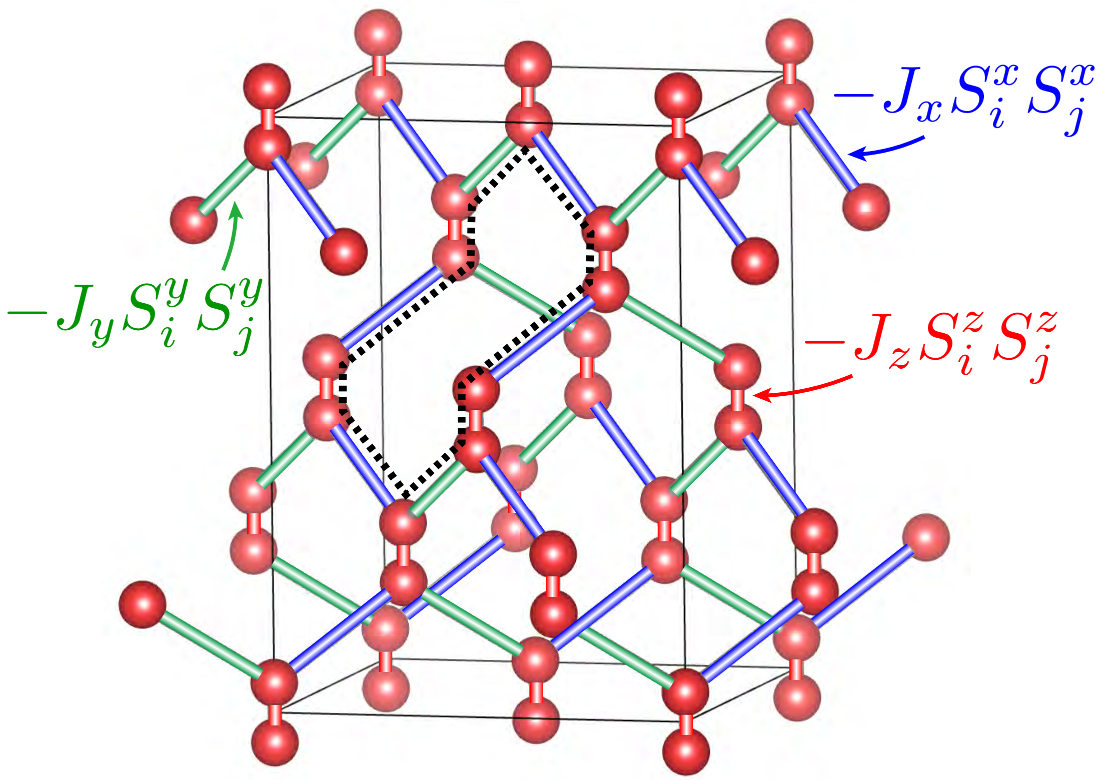
➡ Kitaev-Heisenberg models:

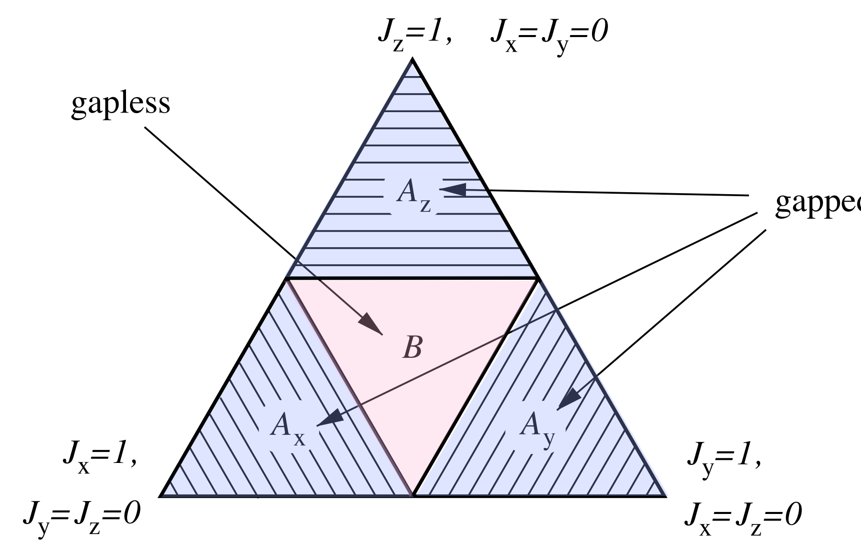
$$\mathcal{H} = -J_{\mathrm{Kitaev}} \sum_{\langle ij \rangle_l} S_i^l S_j^l + J_{\mathrm{Heis}} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

candidates: quasi-2D honeycomb compounds, Na_2IrO_3, Li_2IrO_3, ...
pyrochlore Ir_2O_4, hyperkagome $Na_4Ir_3O_8$, ...

3D extension

- S=1/2 quantum spin model on a 3D hyperhoneycomb lattice (S. Mandal and N. Surendran, 2009)





exactly the same T=0 phase diagram

QSL ground states in 3D

- new Iridates Li_2IrO_3: 3D honeycomb-type network of Ir^{4+} cations
  - harmonic honeycomb (K. A. Modic *et al*., 2014)
  - hyperhoneycomb (T. Takayama *et al*., 2015)

How to compute thermodynamics?

quantum Monte Carlo method in the Majorana fermion representation

Method

Method

- The conventional quantum Monte Carlo (QMC) methods on the basis of the world-line technique do not work because of the negative-sign problem:
  - Lattices are bipartite, but the interactions are frustrated.

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  - Lattices are bipartite, but the interactions are frustrated.

- Our solution:

interacting S=1/2 spins

↓ Jordan-Wigner transformation
Majorana fermion representation

non-interacting Majorana fermions coupled to thermally-fluctuating Z_2 fields

↓

QMC free from negative-sign problem

Method (details)

H.-D. Chen and J. Hu, 2007
X.-Y. Feng, G.-M. Zhang, and T. Xiang, 2007
H.-D. Chen and Z. Nussinov, 2008

step 1: Jordan-Wigner transformation

step 2: Majorana fermion representation

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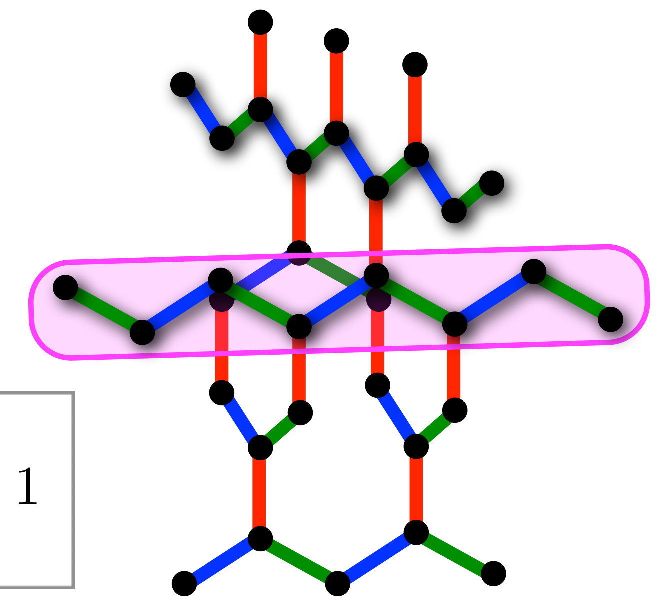
step 1: Jordan-Wigner transformation

- regard the system as an assembly of 1D chains (composed of x, y bonds) coupled by z bonds



$$S^+_{m,n} = (S^-_{m,n})^\dagger = \frac{1}{2}(\sigma^x_{m,n} + i\sigma^y_{m,n}) = \prod_{n'=1}^{n-1}(1-2n_{m,n'})a^\dagger_{m,n}, \quad \sigma^z_{m,n} = 2n_{m,n} - 1$$

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

step 2: Majorana fermion representation

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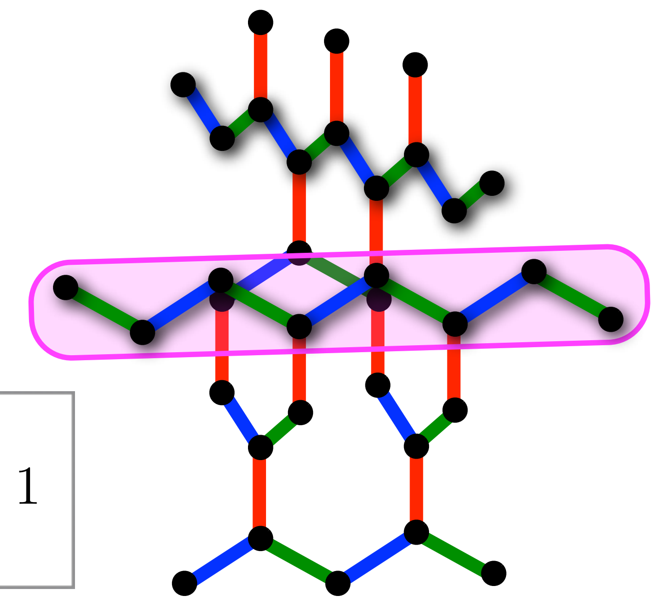

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step 2: Majorana fermion representation

$$c_w = (a_w - a^\dagger_w)/\mathrm{i}, \quad \bar{c}_w = a_w + a^\dagger_w, \qquad c_b = a_b + a^\dagger_b, \quad \bar{c}_b = (a_b - a^\dagger_b)/\mathrm{i}.$$

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

$\eta_r = \mathrm{i}\bar{c}_b\bar{c}_w = \pm 1$

: local conserved quantity (Z_2 variable) on each z bond

Simulation

$$\mathcal{H} = \mathrm{i}J_x \sum_{x \text{ bonds}} c_w c_b - \mathrm{i}J_y \sum_{y \text{ bonds}} c_b c_w - \mathrm{i}J_z \sum_{z \text{ bonds}} \eta_r c_b c_w \qquad \eta_r = \mathrm{i}\bar{c}_b \bar{c}_w = \pm 1$$

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- Formally, the model is similar to the double-exchange model with Ising spins.
  - ➡ MC simulation without fermion sign problem applicable
    - faithful representation of the original Hamiltonian: no approximation

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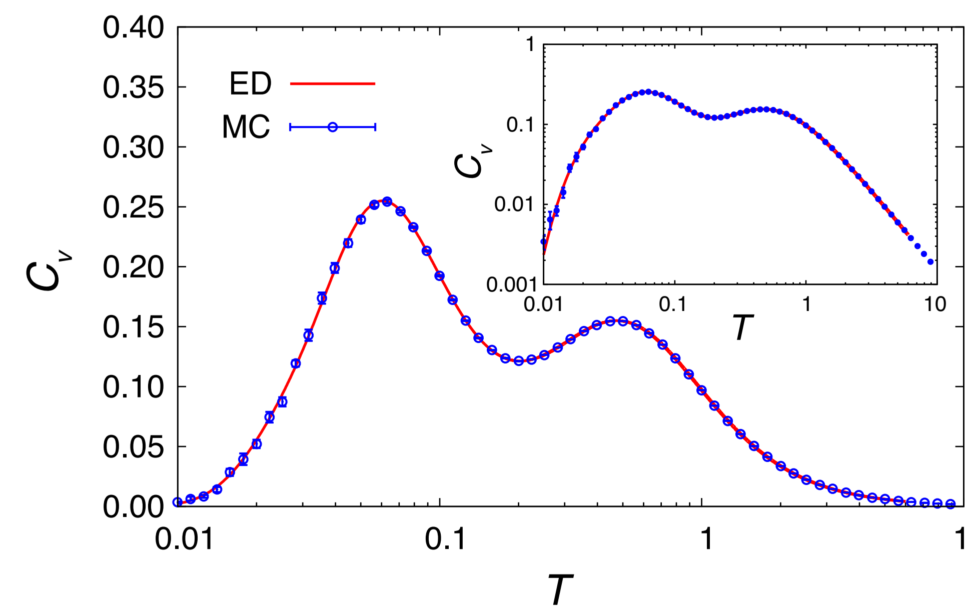
- benchmark for 2D honeycomb Kitaev model
  - 8 sites, isotropic case (J_x=J_y=J_z=1/3)
  - ED: exact diagonalization of the original Kitaev model with S=1/2 quantum spins
  - perfect agreement within the errorbars

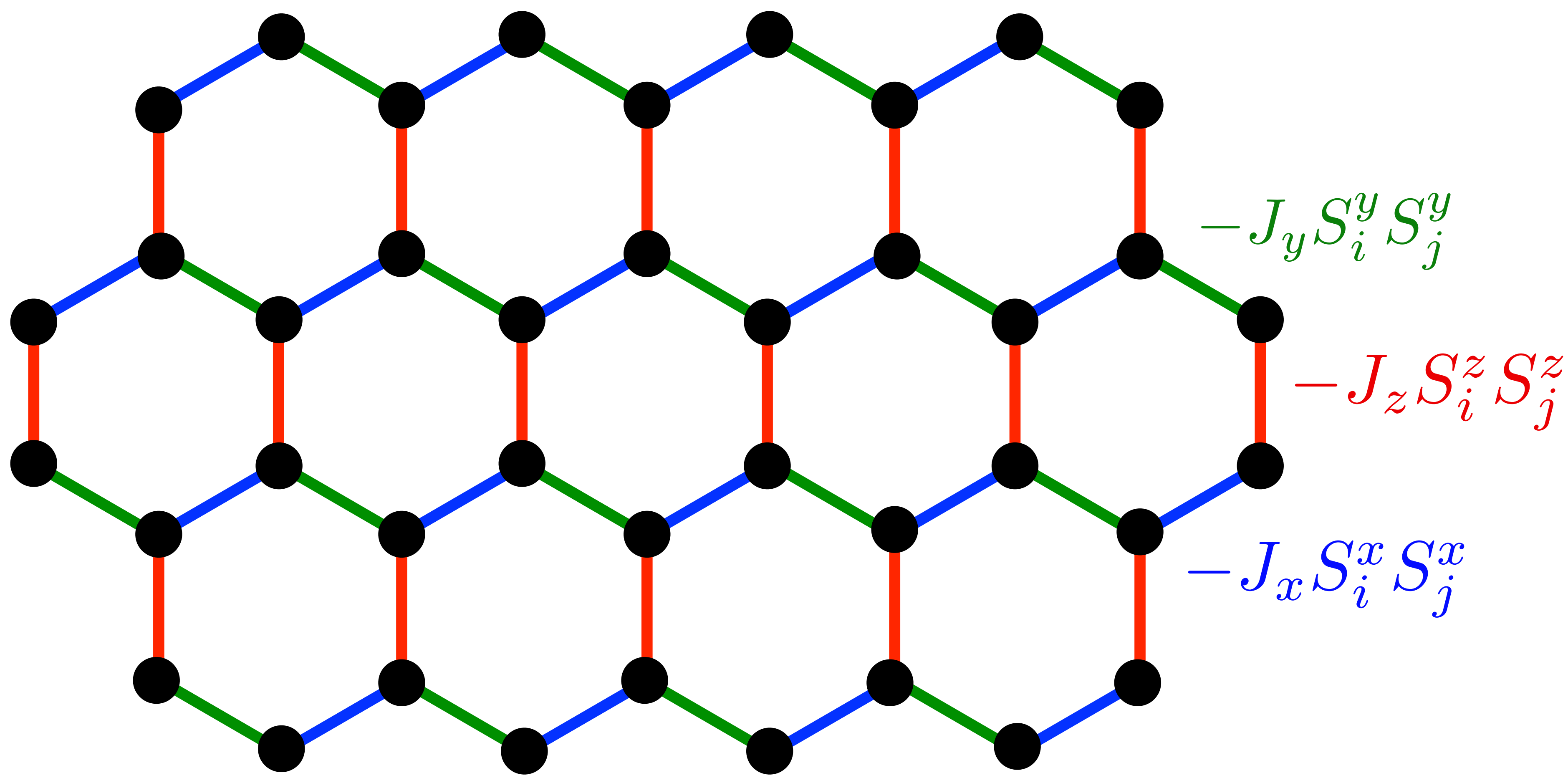


Thermal fractionalization of quantum spins into Majorana fermions

guide of Majorana hunting

2D honeycomb Kitaev model

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



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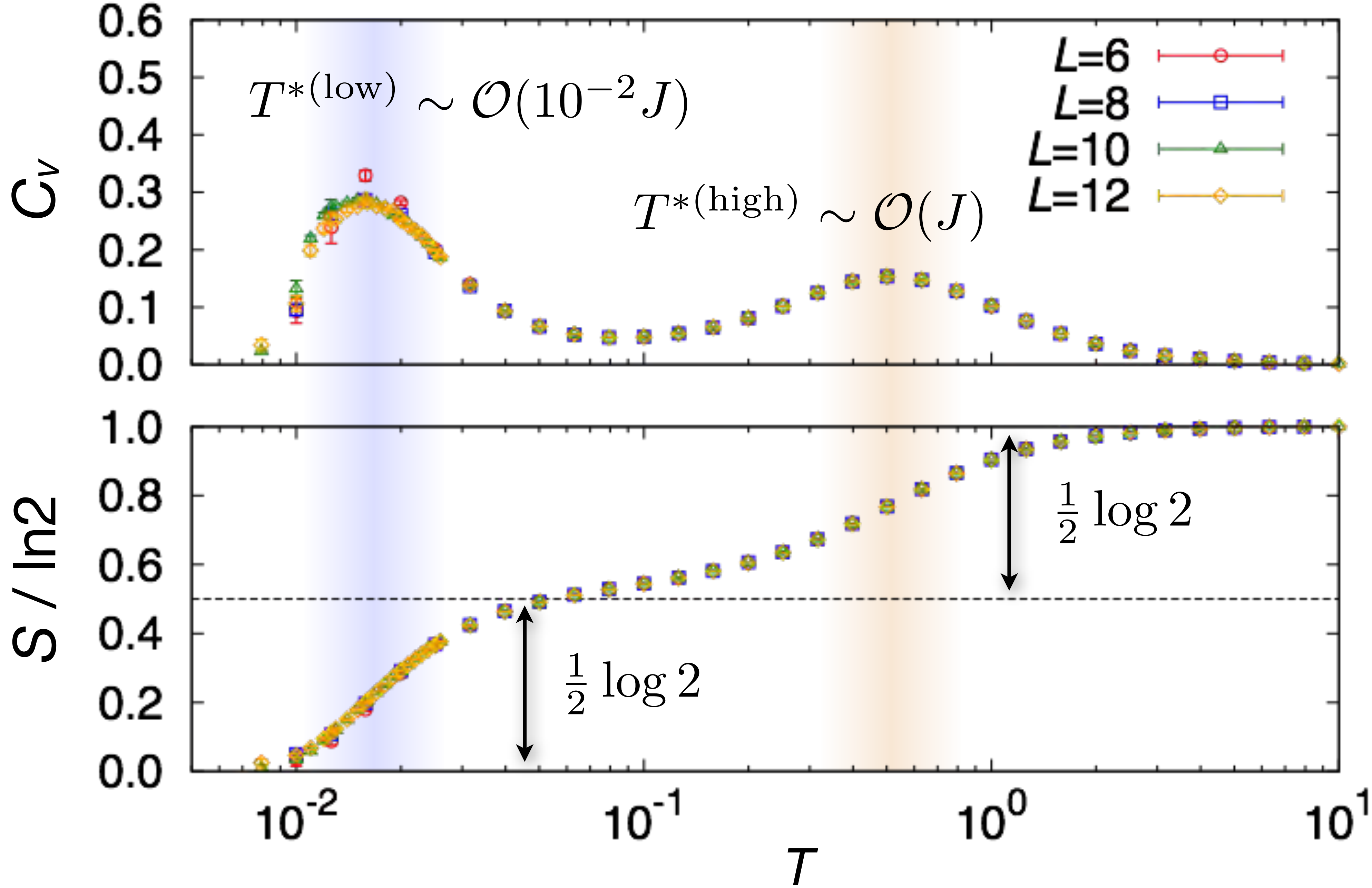
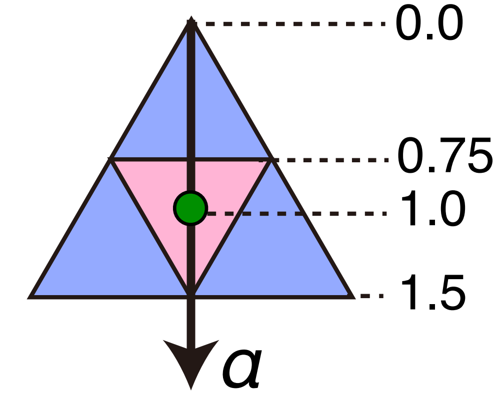
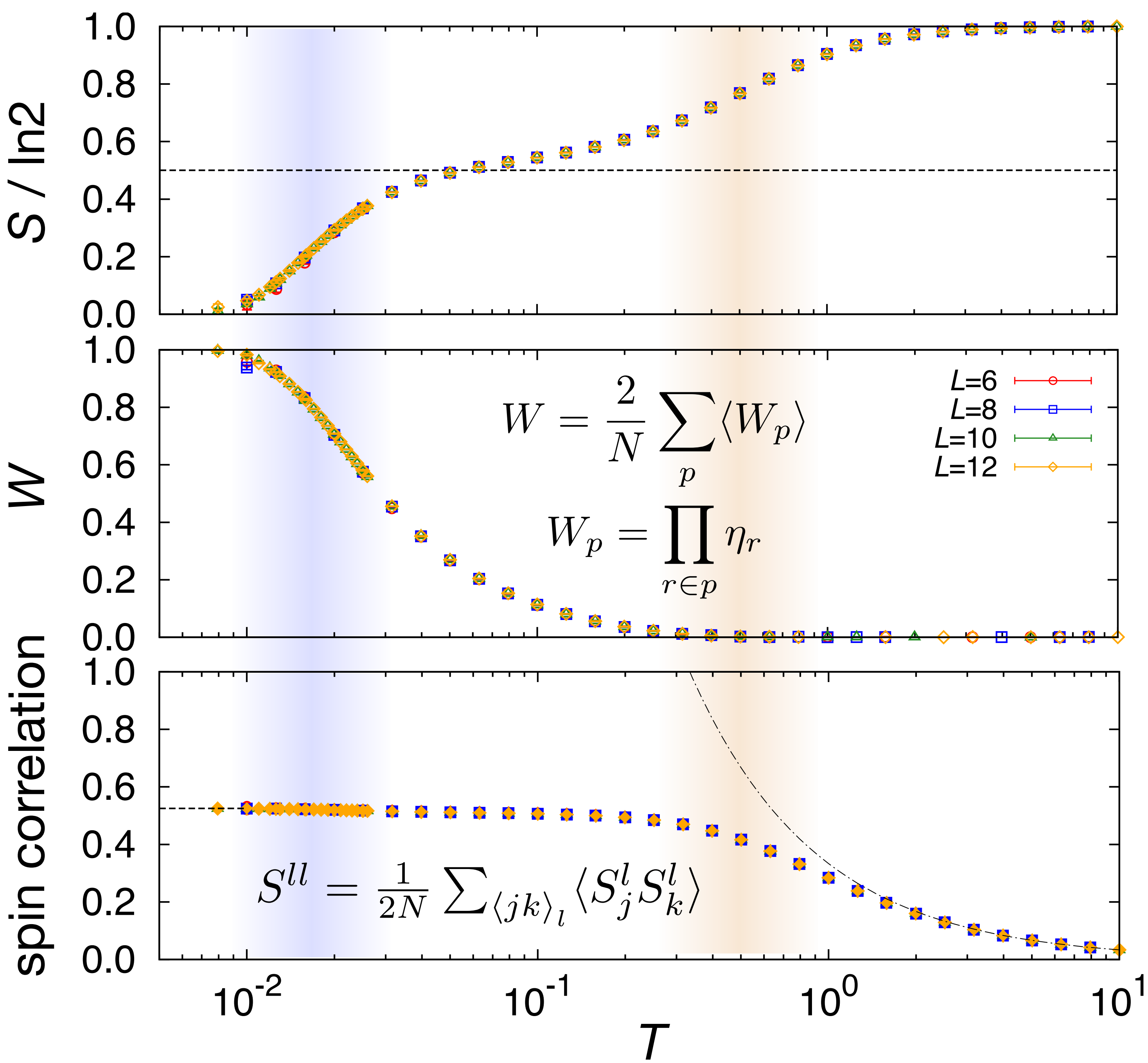
Specific heat and entropy

- two crossovers: successive release of 1/2(log2) entropy





Successive two crossovers



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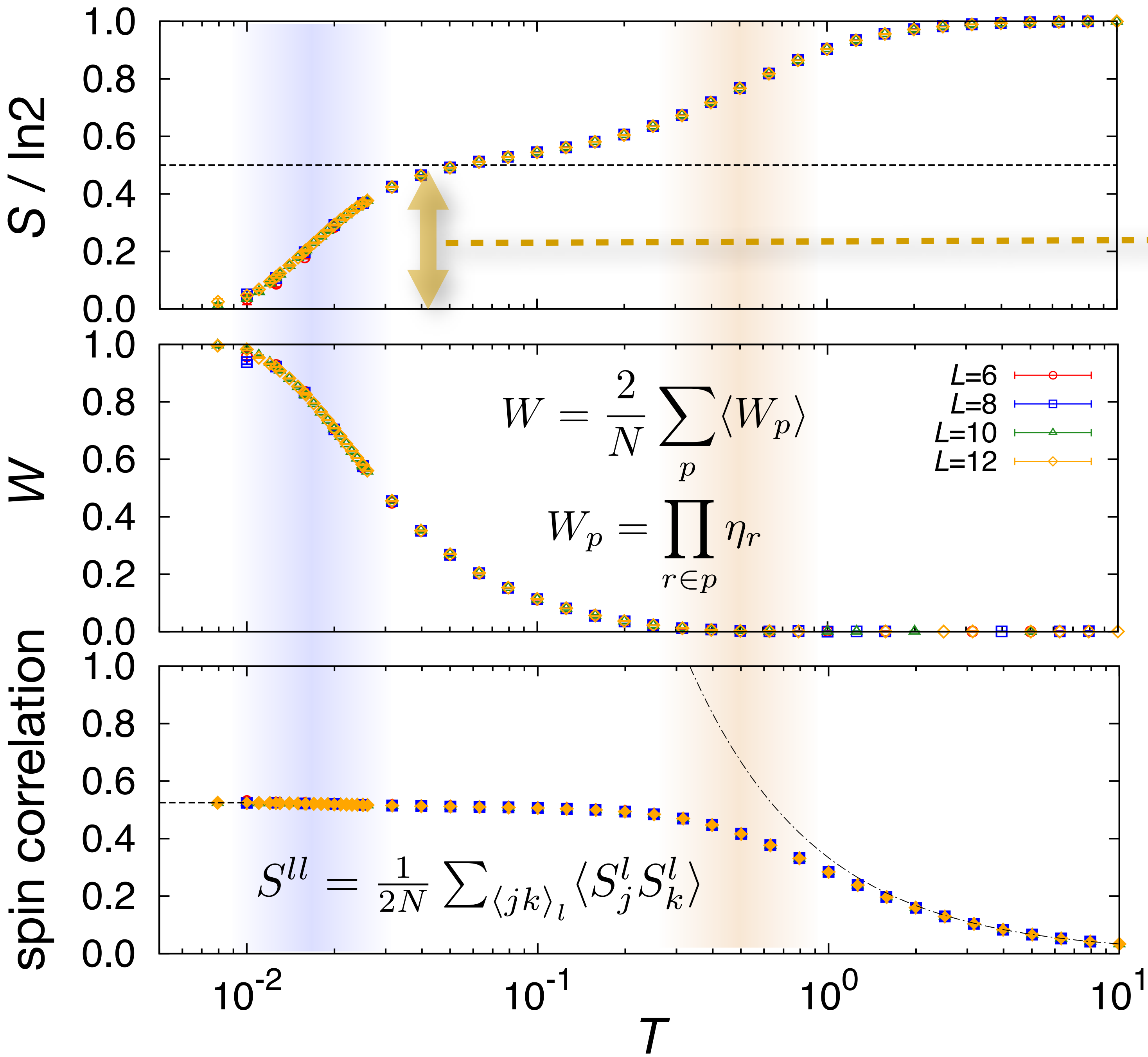
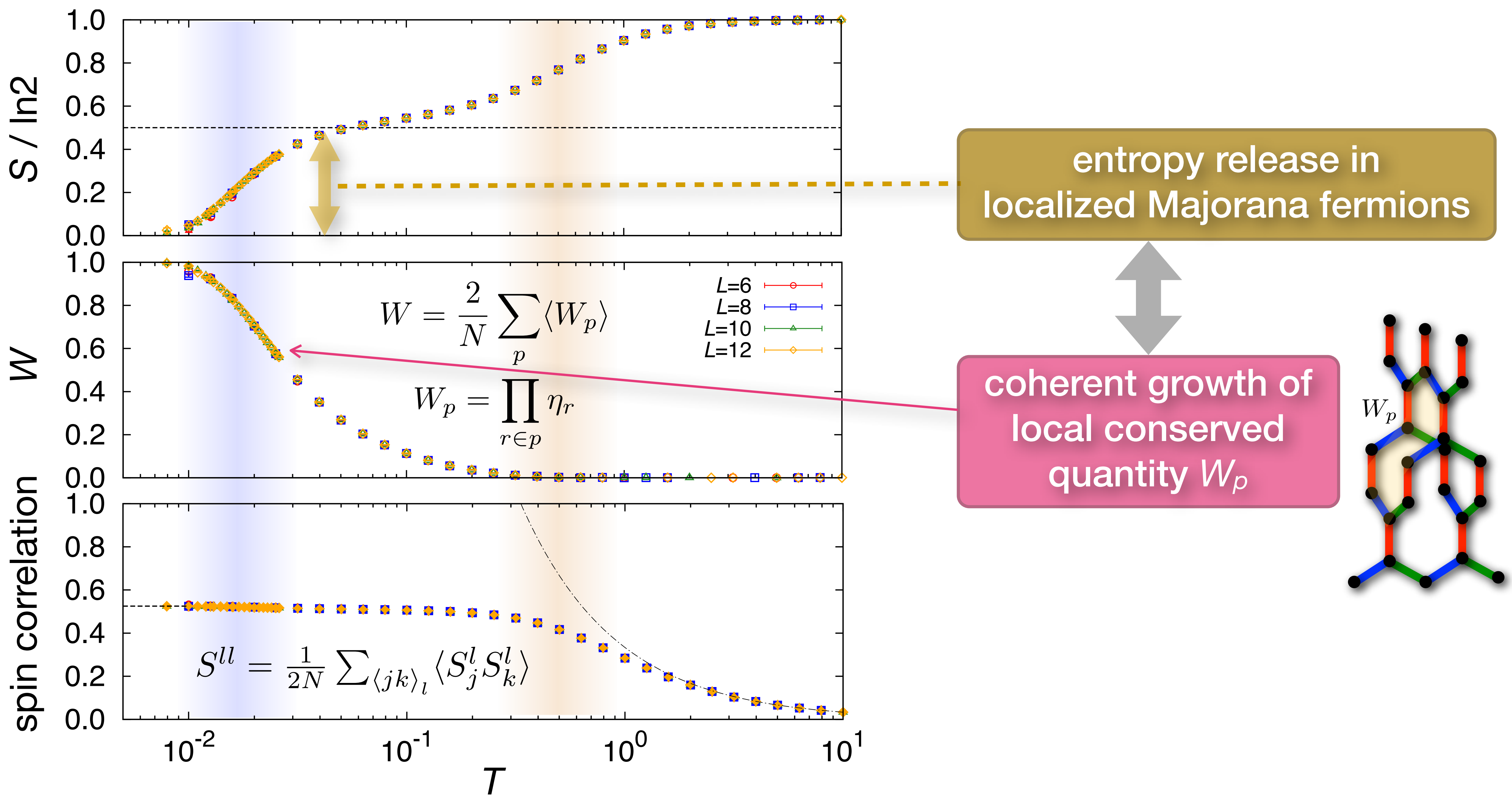
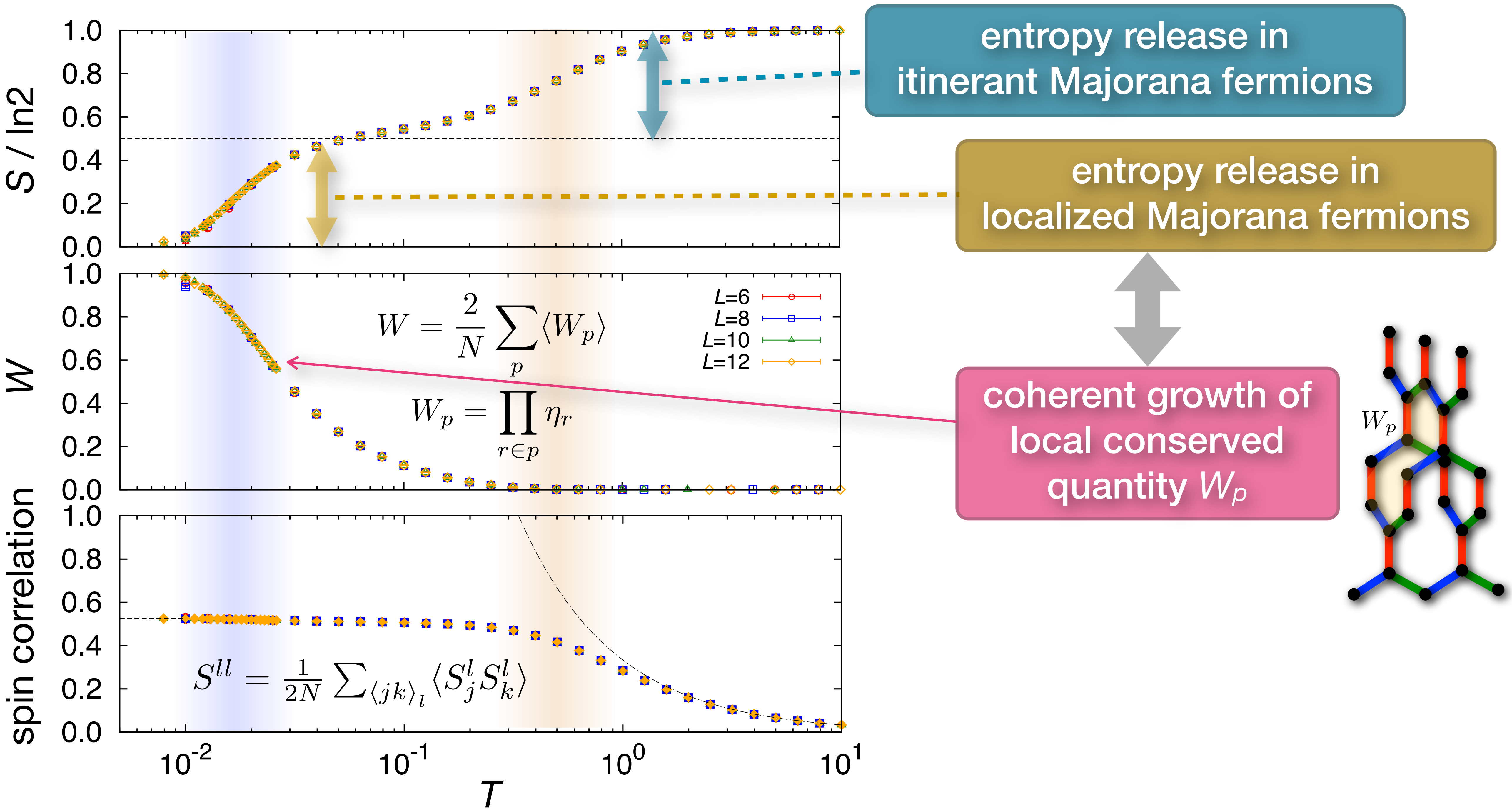


entropy release in localized Majorana fermions

Successive two crossovers



Successive two crossovers



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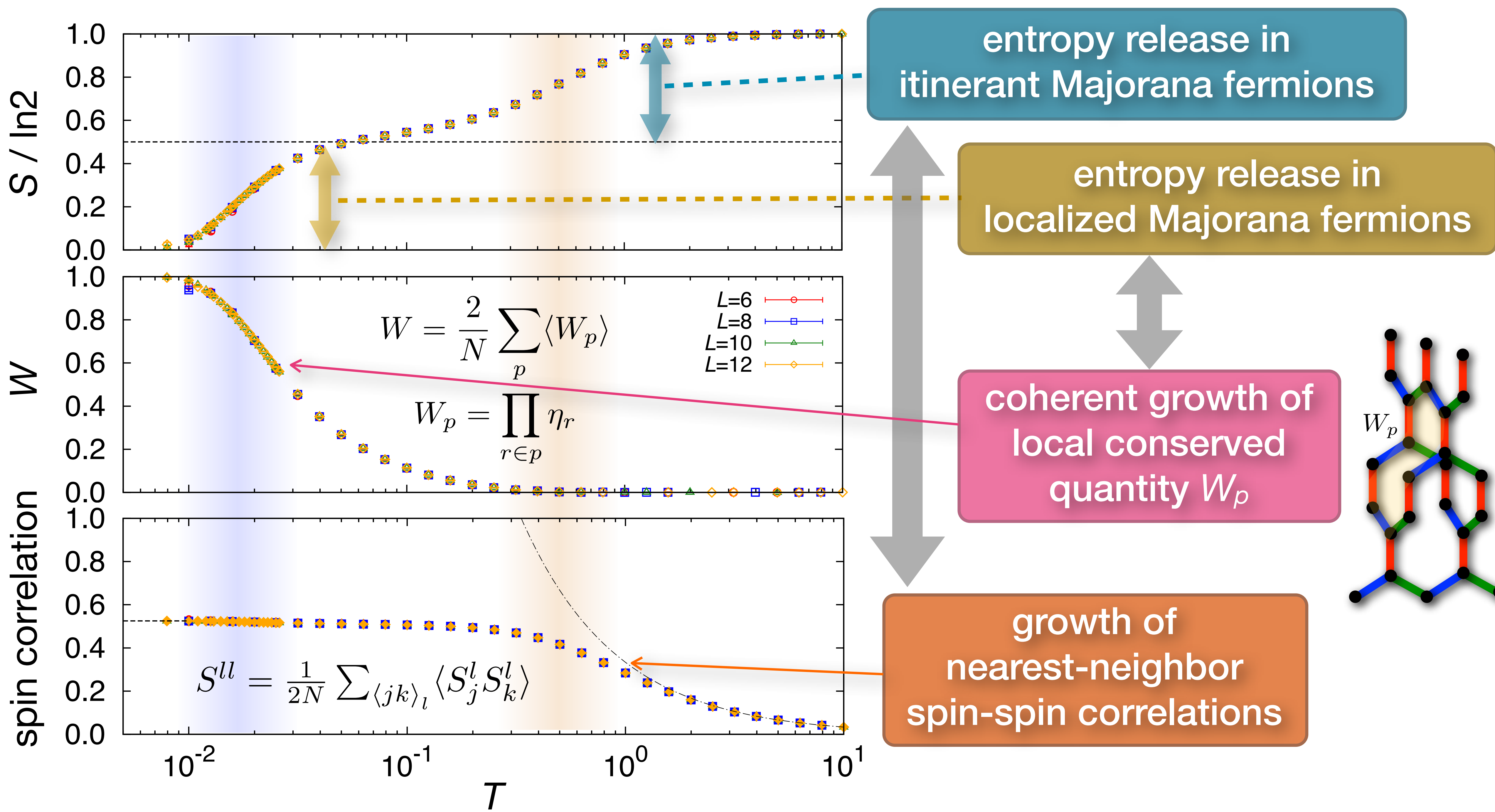

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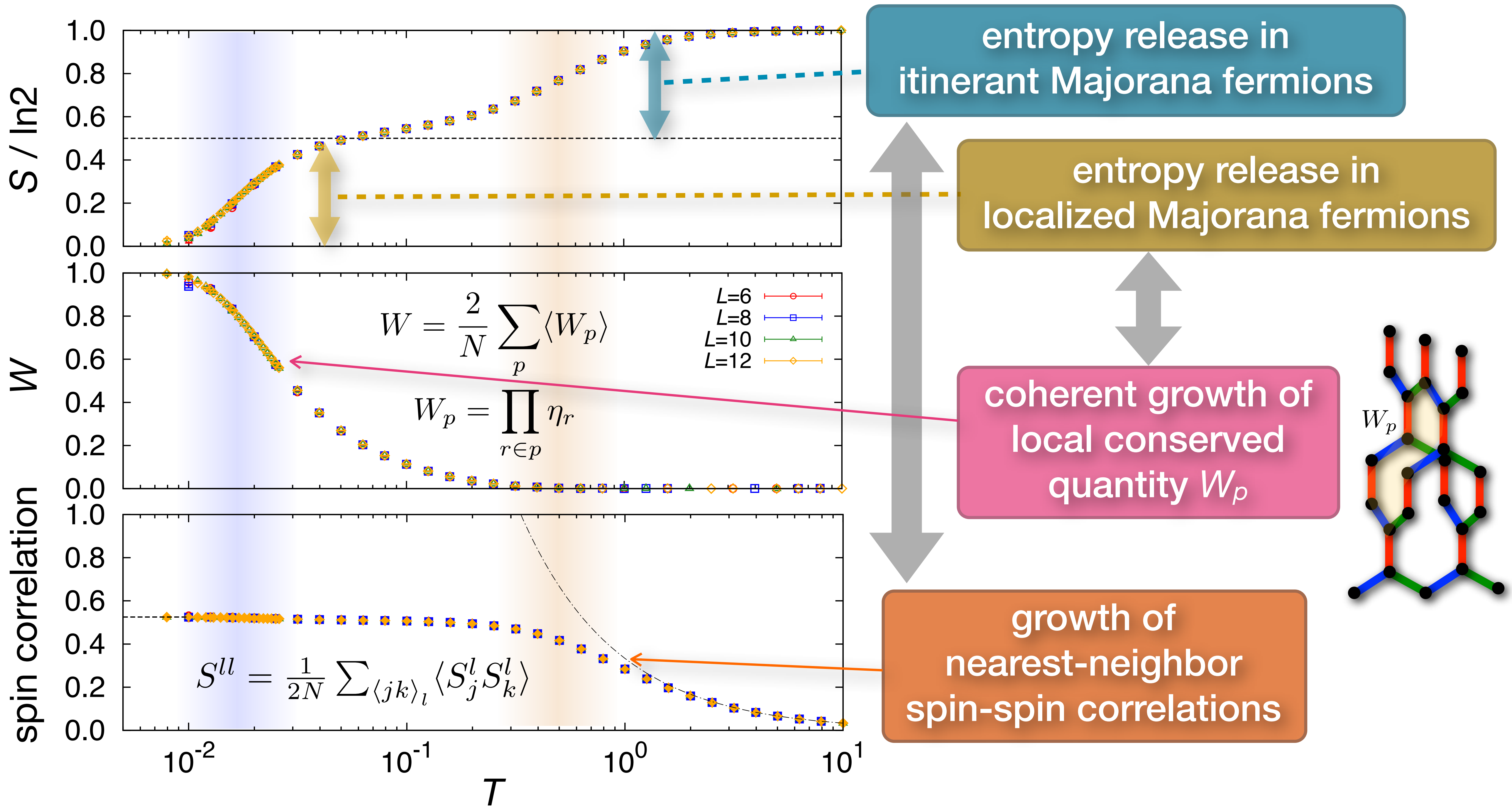
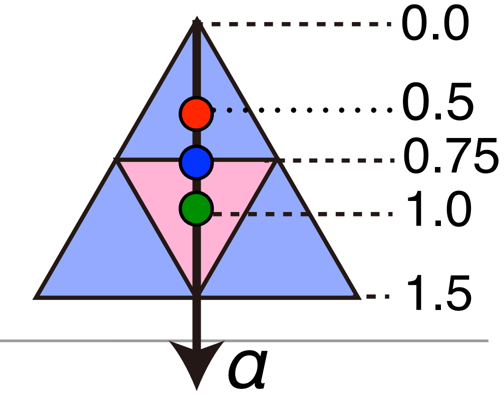
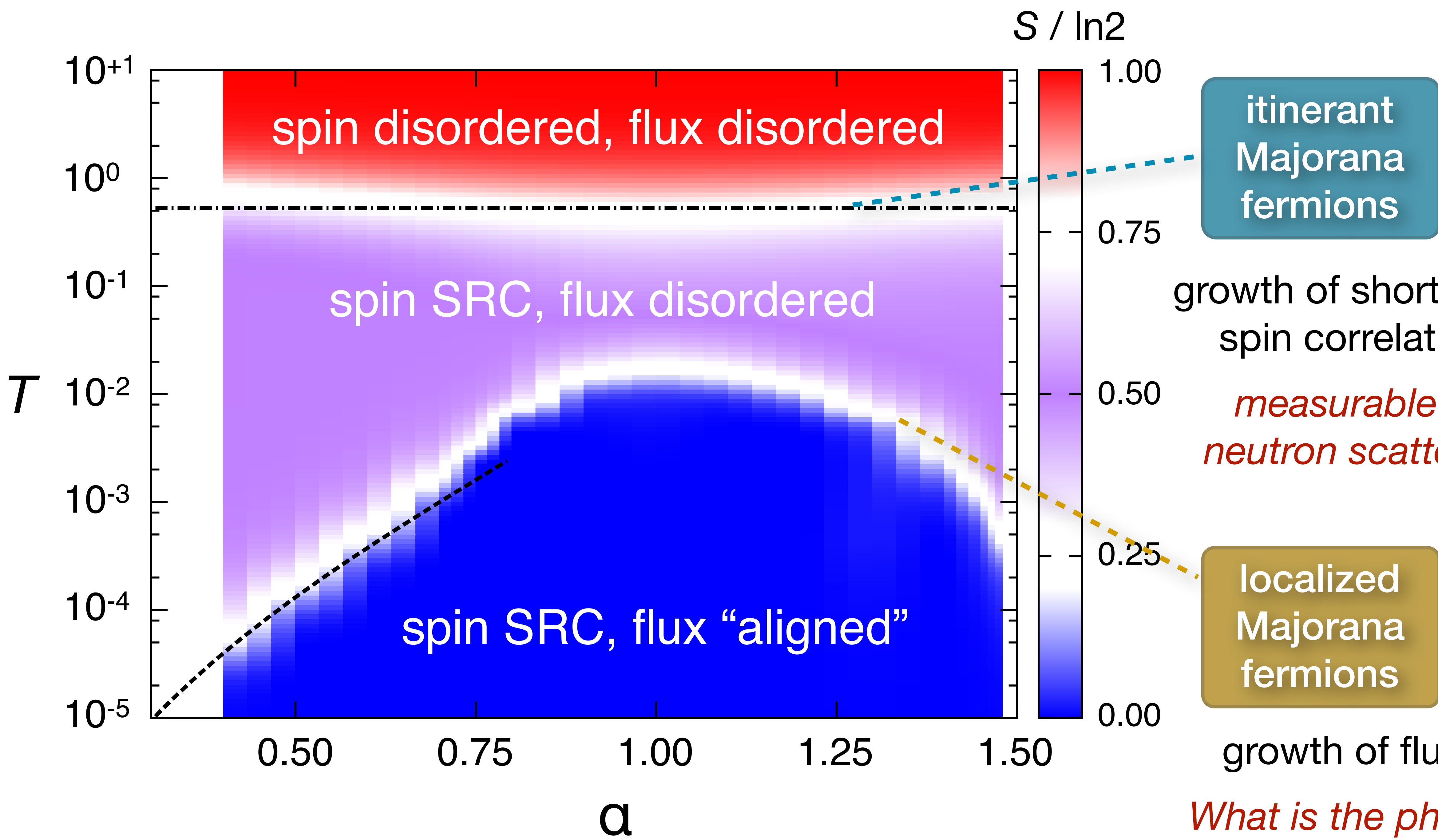


clear signatures of thermal fractionalization of quantum spins

Phase diagram in 2D





growth of short-range spin correlations

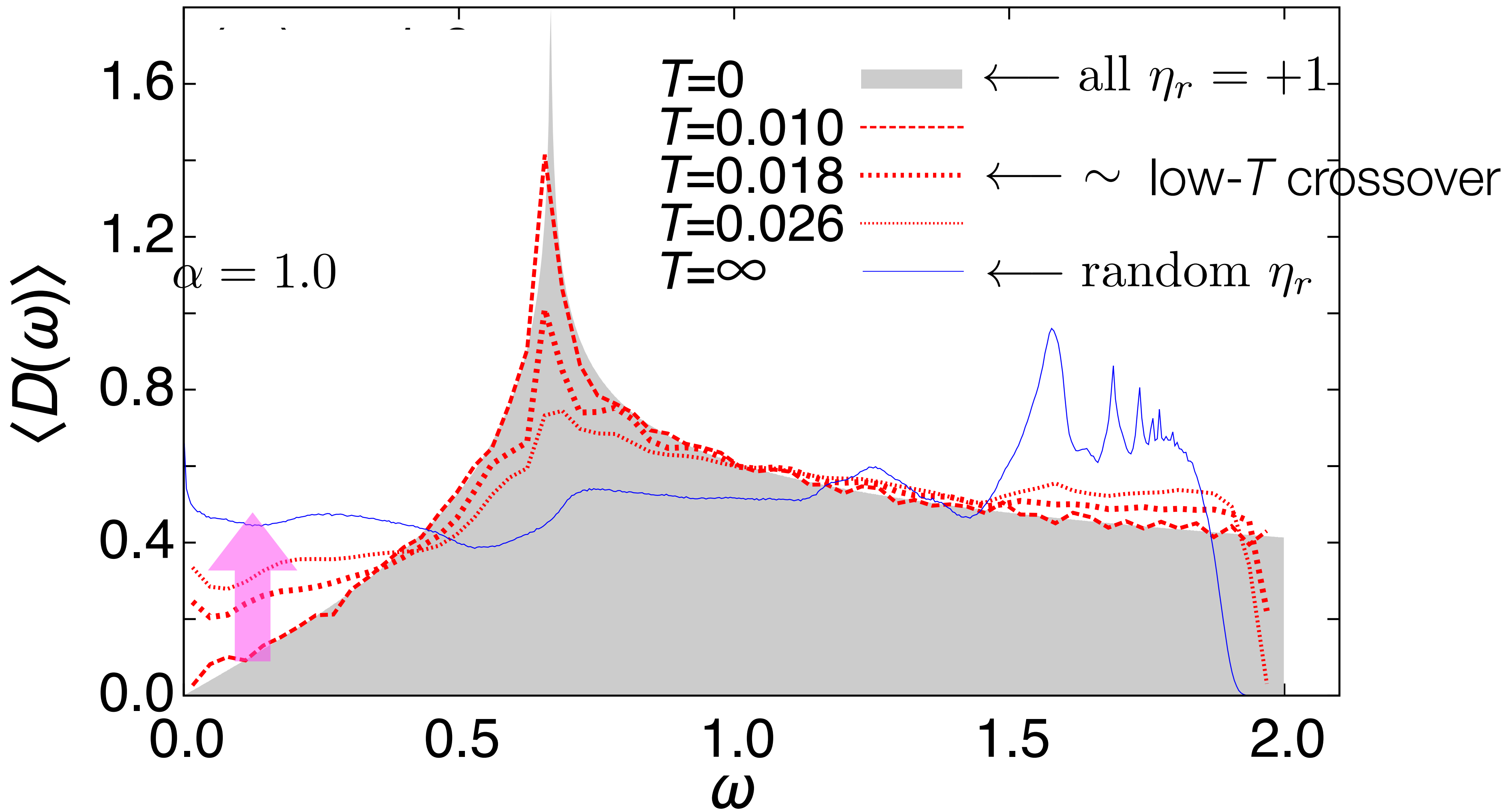
measurable by neutron scattering

growth of fluxes

What is the physical consequence?

DOS for itinerant Majorana fermions

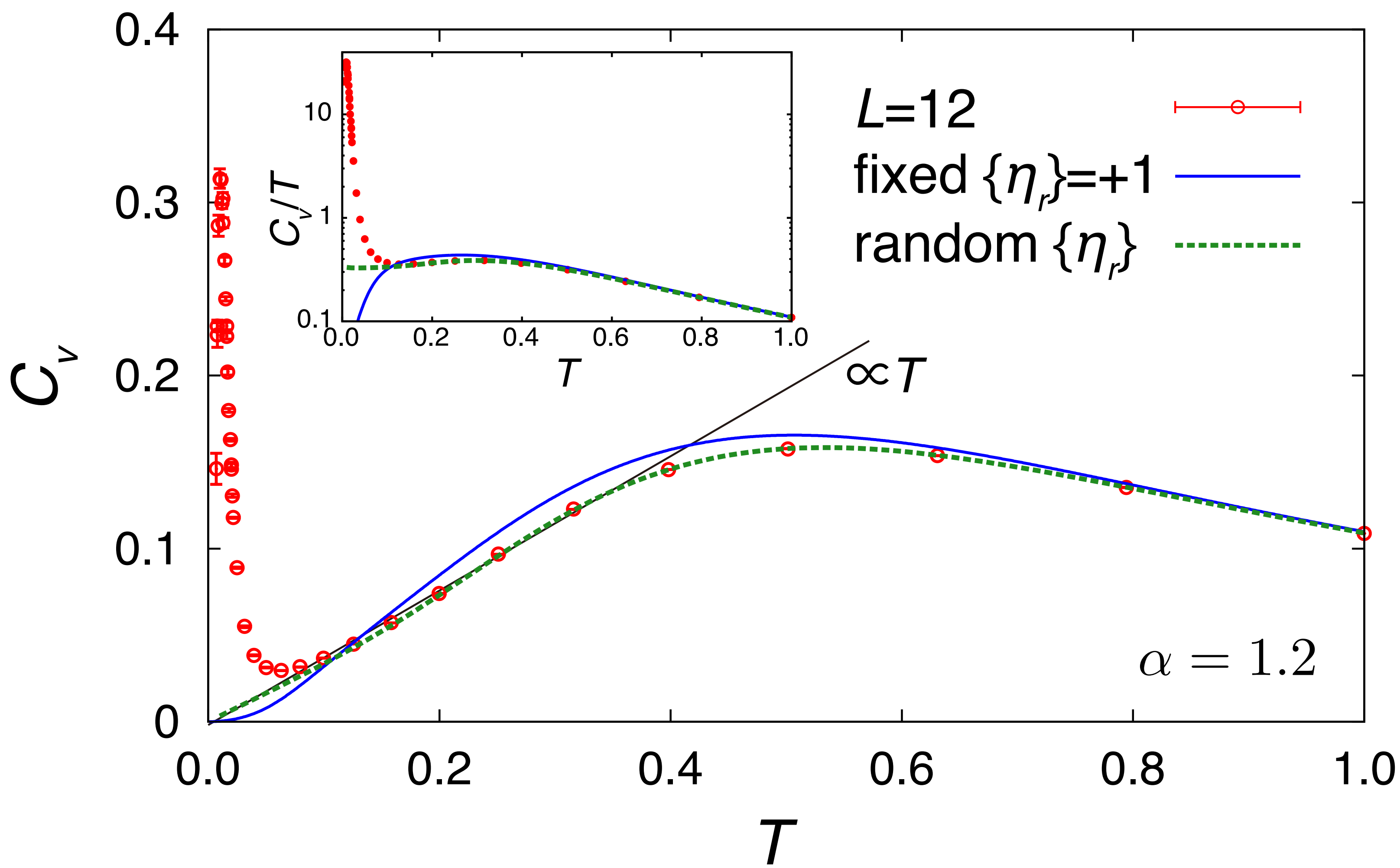
- Thermal fluctuations of the fluxes disturb the Majorana DOS.

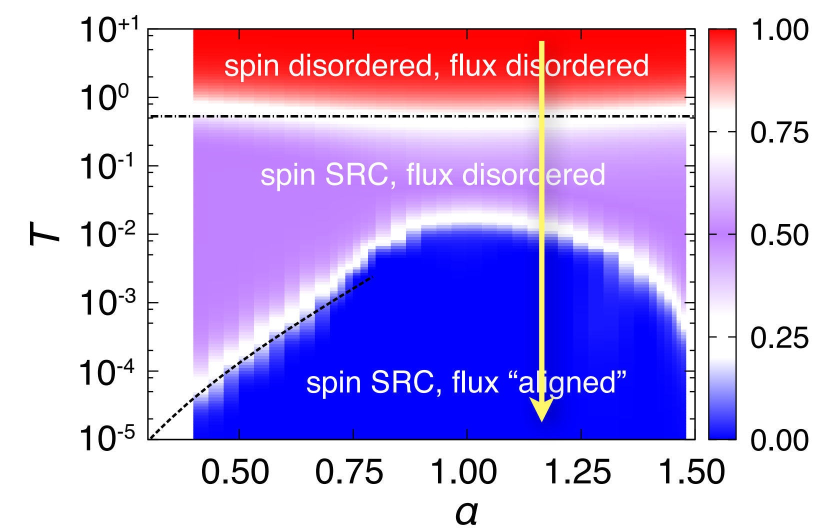


Dirac semimetal → "metal" above the low-T crossover by thermal fluctuations in fluxes (localized Majorana)

Apparent T-linear specific heat

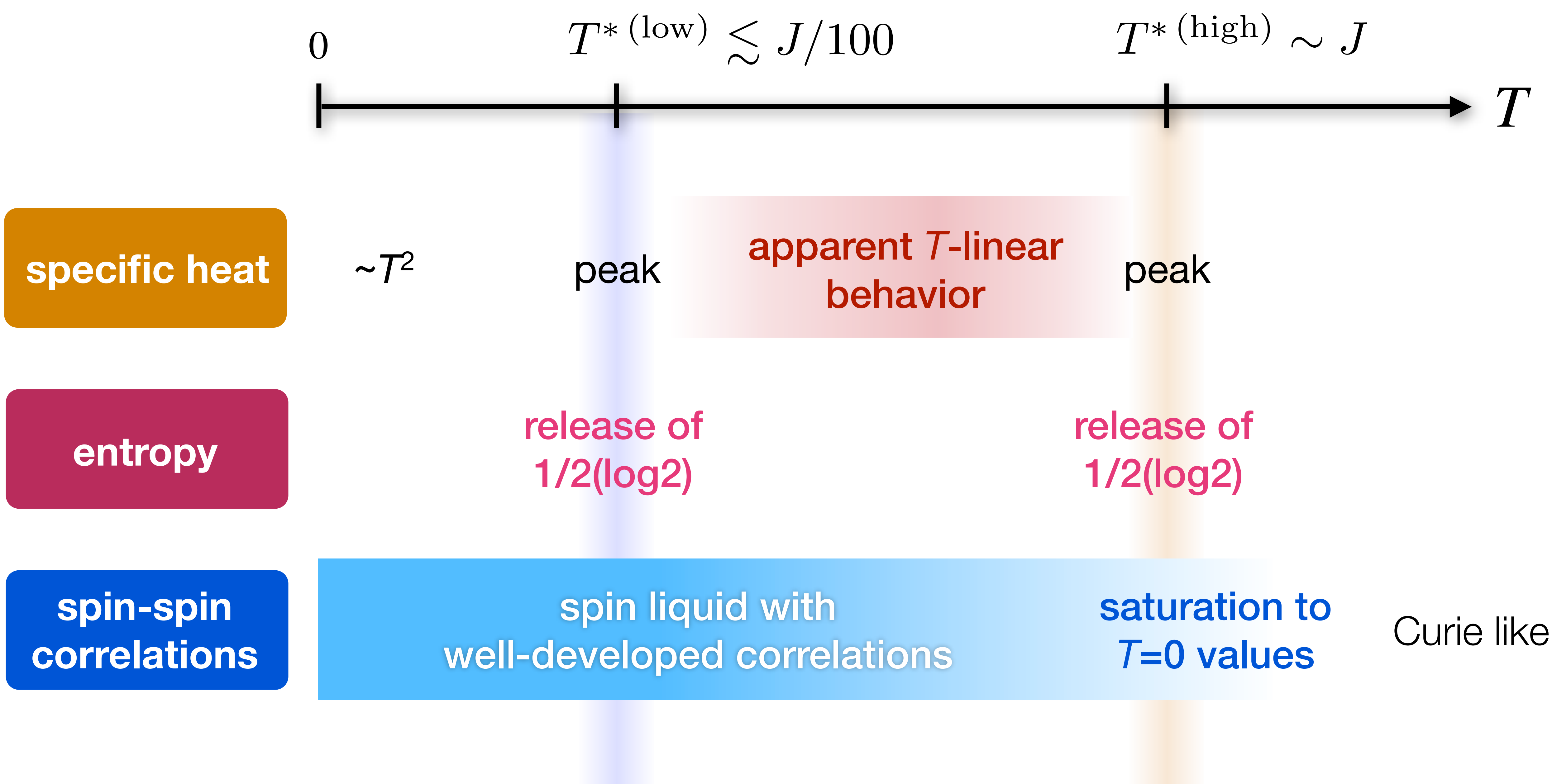
- Above the low-T crossover, the DOS becomes metallic, leading to apparent T-linear behavior in the specific heat, although T^2 behavior is expected for the Dirac semimetallic spectrum at T=0.



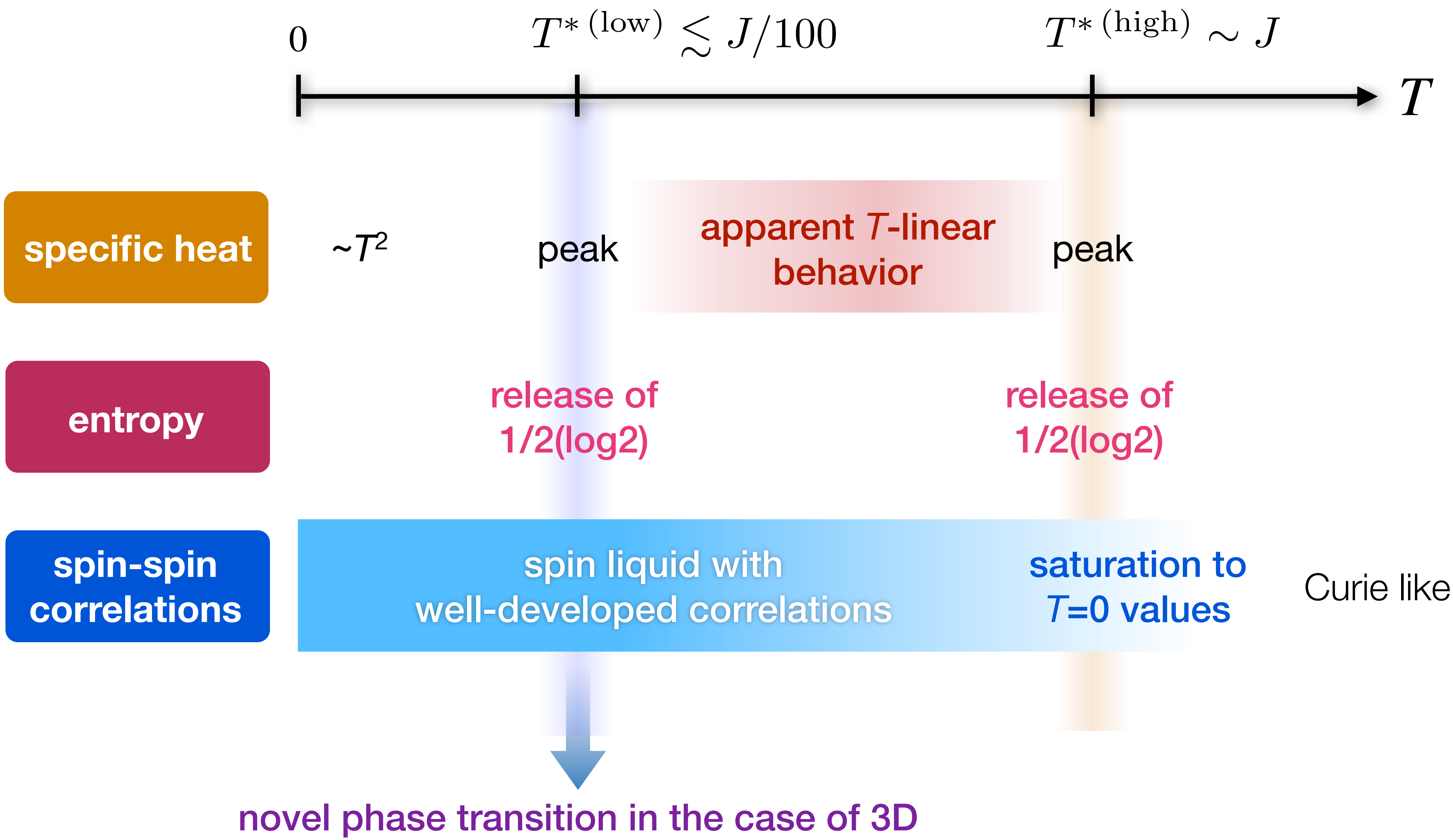


T-linear behavior for the "spin liquid" with well-developed spin correlations

Experimental implication



Experimental implication

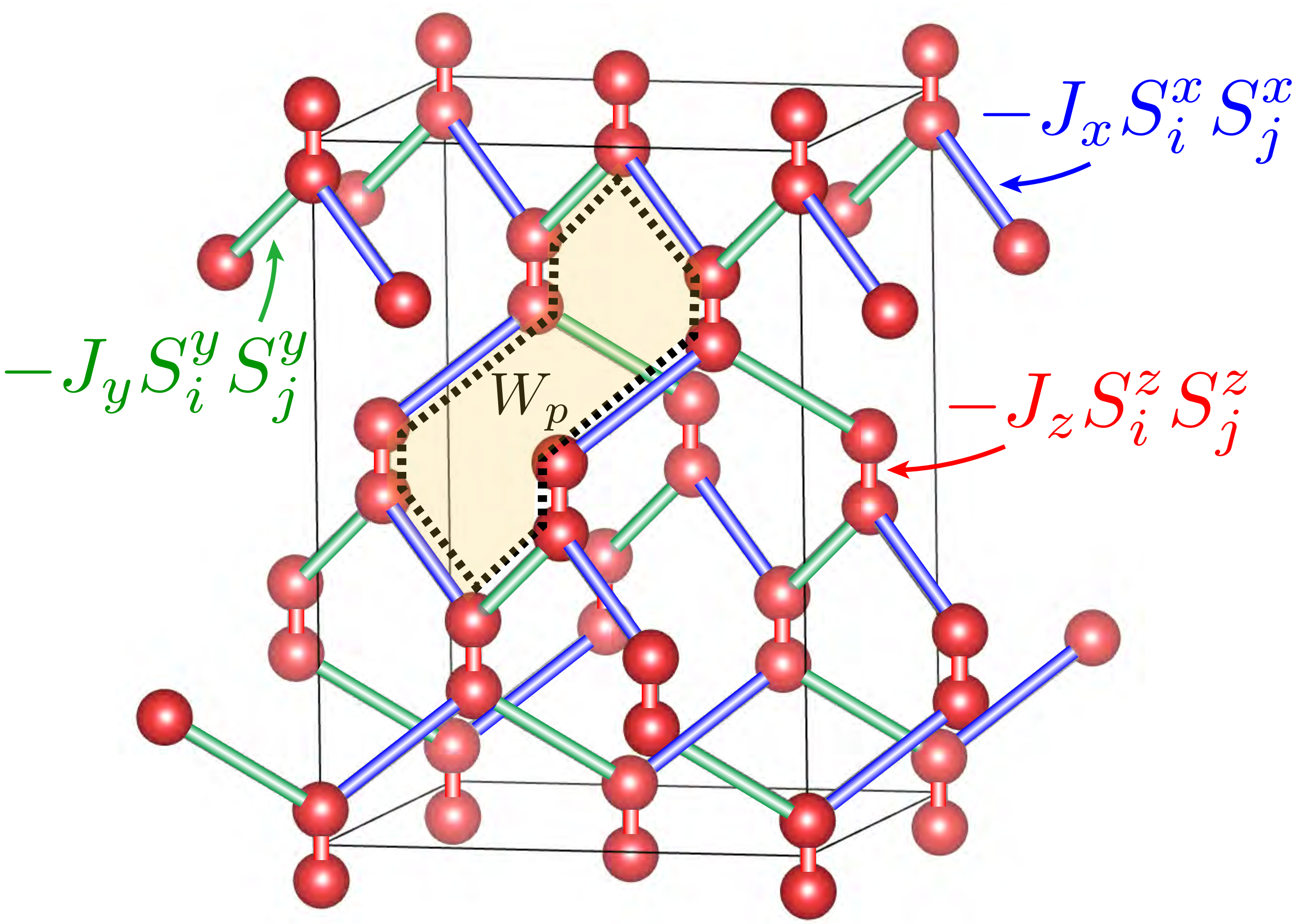


Finite-T "liquid-gas" transition in 3D

proliferation of flux loops

3D hyperhoneycomb Kitaev model

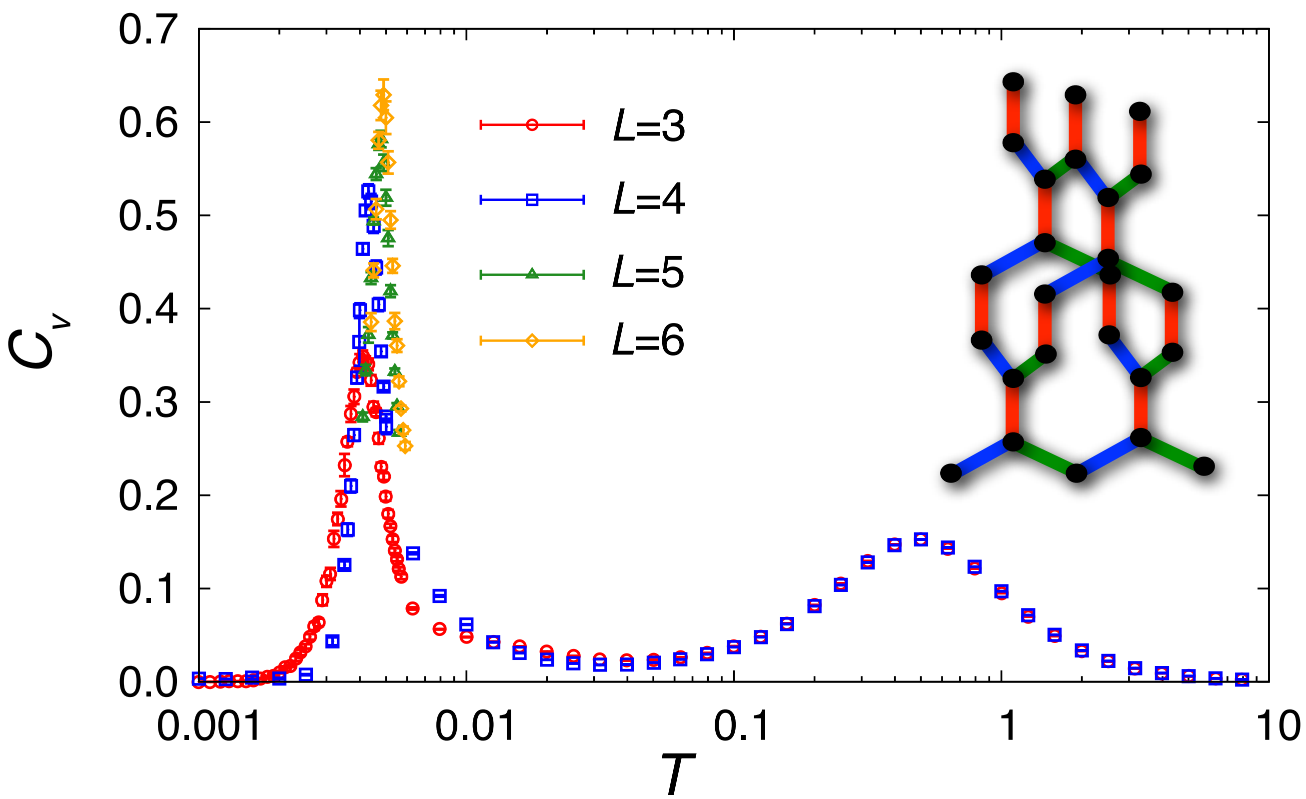
$$\mathcal{H} = -J_x \sum_{<ij>_x} S_i^x S_j^x - J_y \sum_{<ij>_y} S_i^y S_j^y - J_z \sum_{<ij>_z} S_i^z S_j^z$$



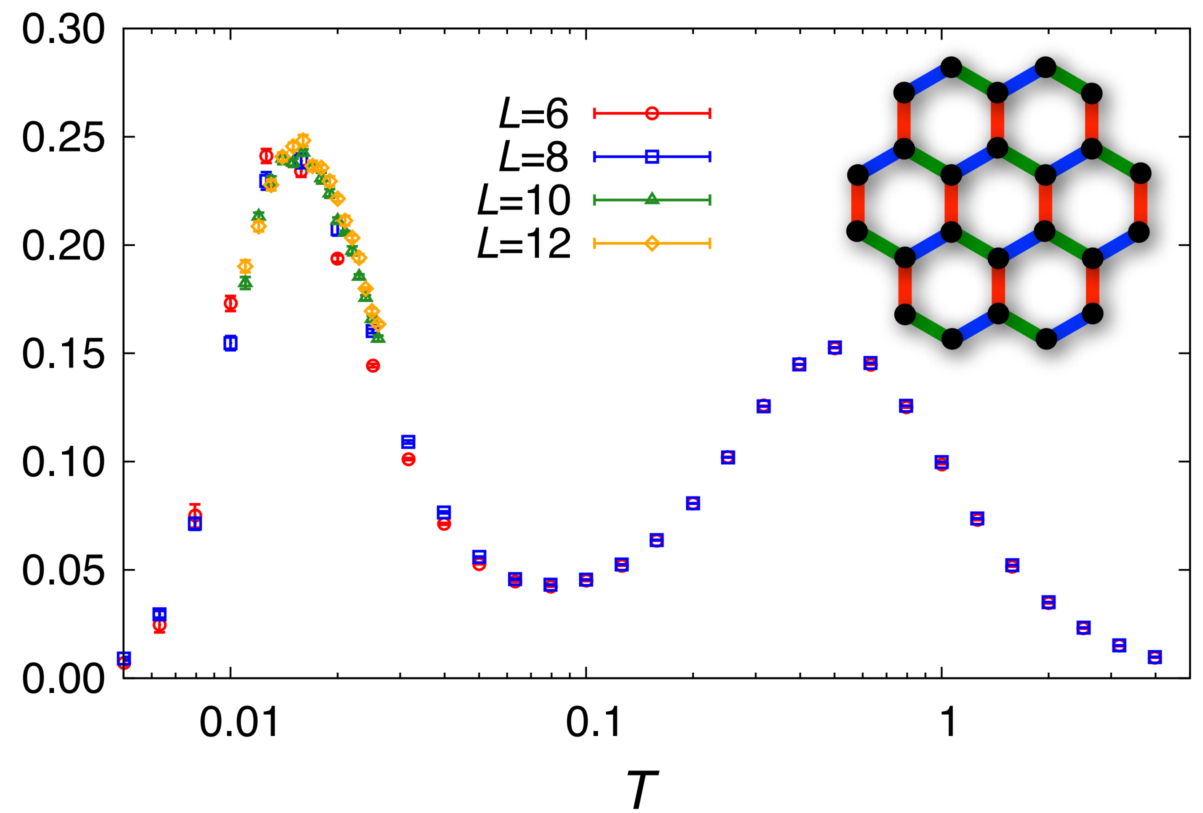
$$\mathcal{H} = \mathrm{i}J_x \sum_{x\text{ bonds}} c_w c_b - \mathrm{i}J_y \sum_{y\text{ bonds}} c_b c_w - \mathrm{i}J_z \sum_{z\text{ bonds}} \eta_r c_b c_w \qquad \eta_r = \mathrm{i}\bar{c}_b \bar{c}_w = \pm 1$$

Comparison between 3D and 2D

3D hyperhoneycomb



2D honeycomb



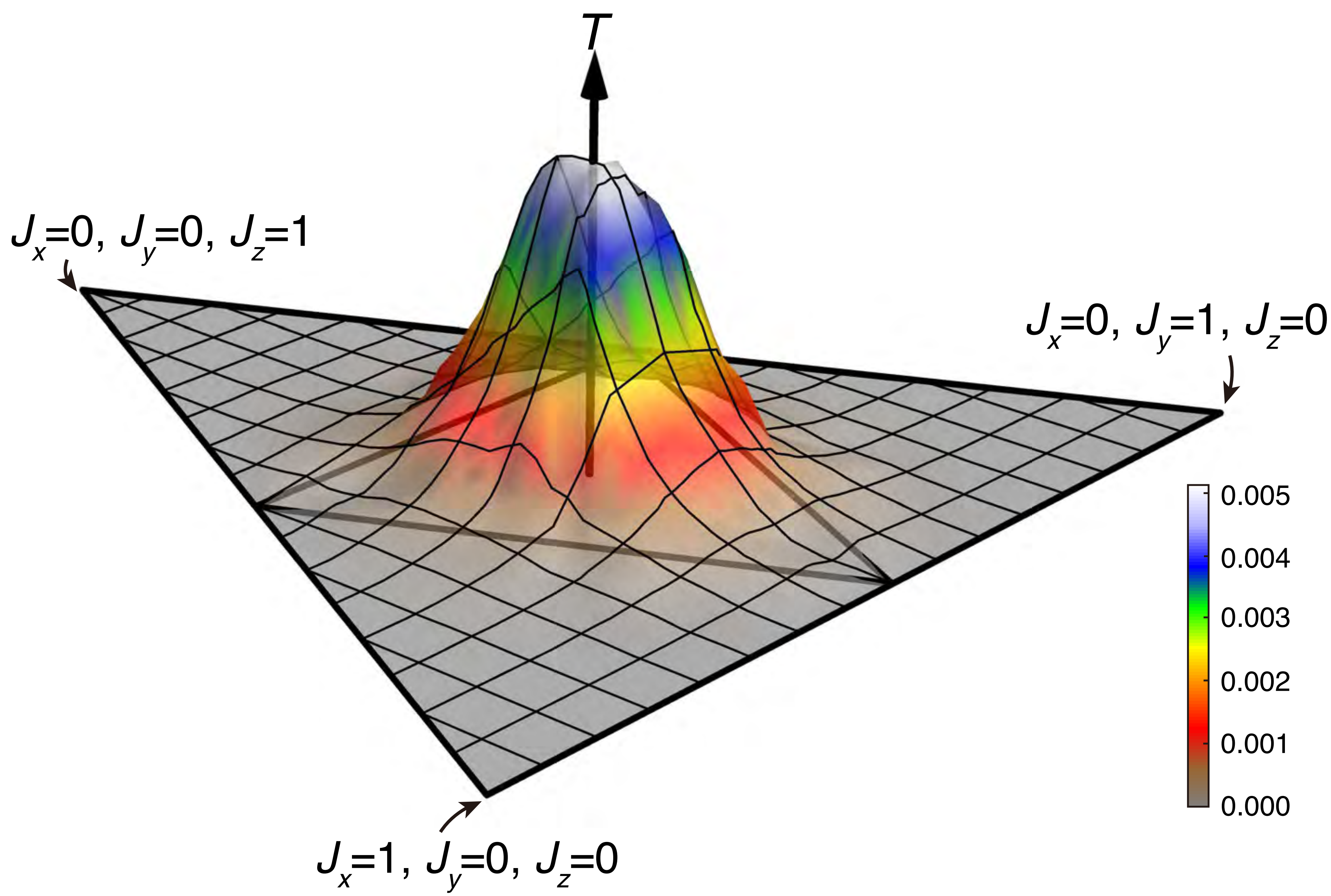
sharp peak growing and becoming narrower as the system size increases

➡ sign of a phase transition

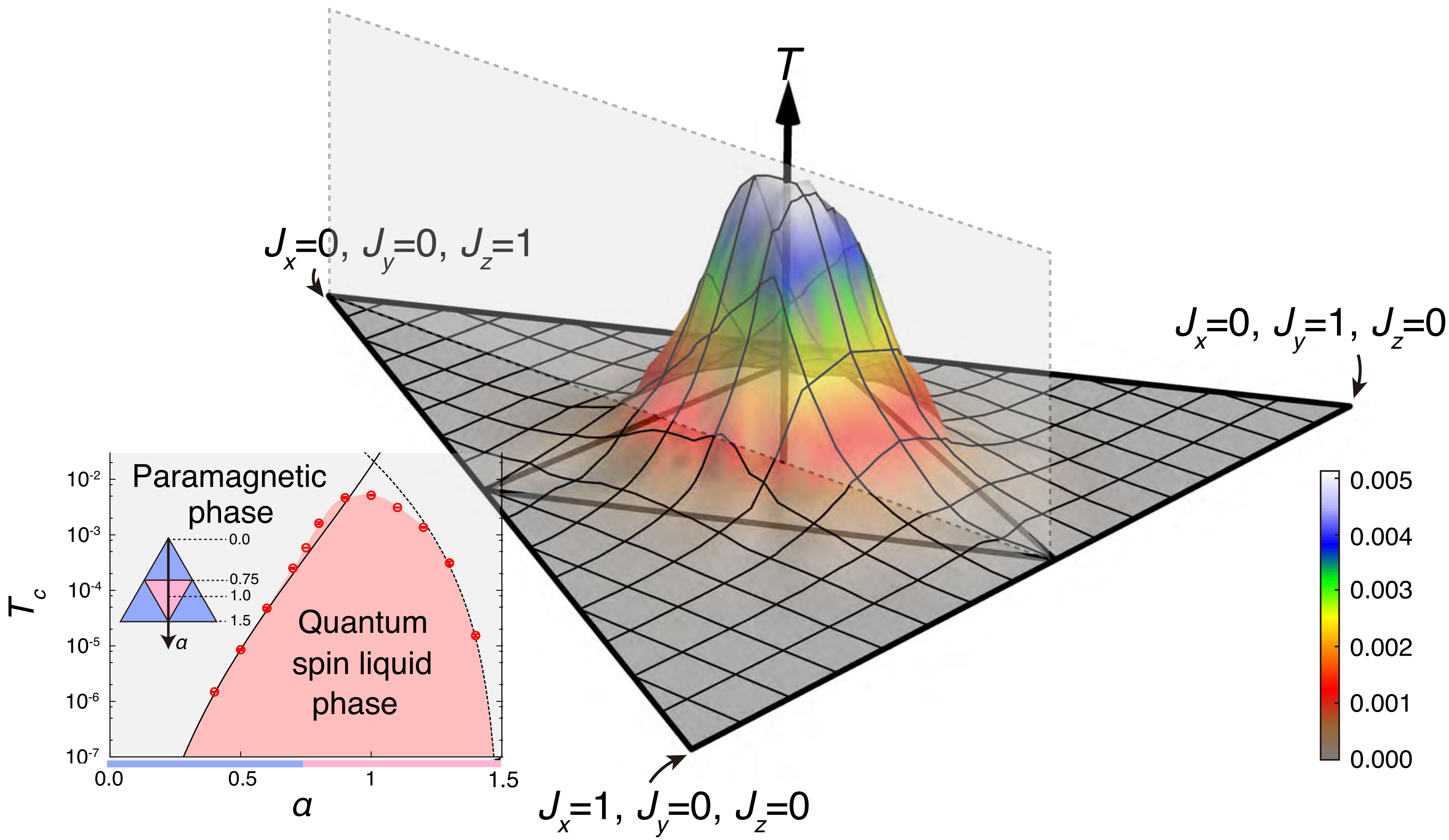
broad peak almost independent of the system sizes

➡ just a crossover

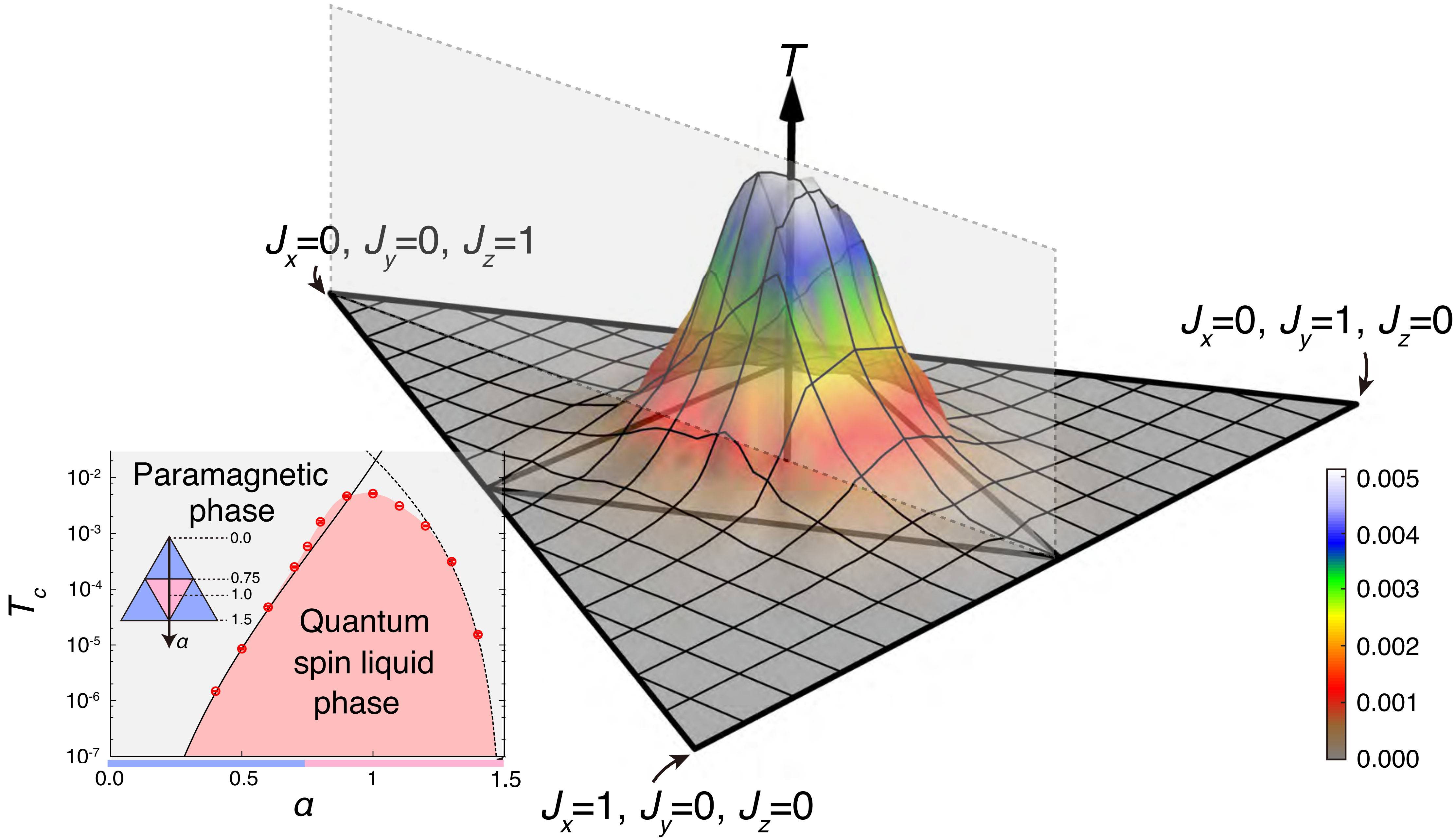
Phase diagram in 3D



Phase diagram in 3D



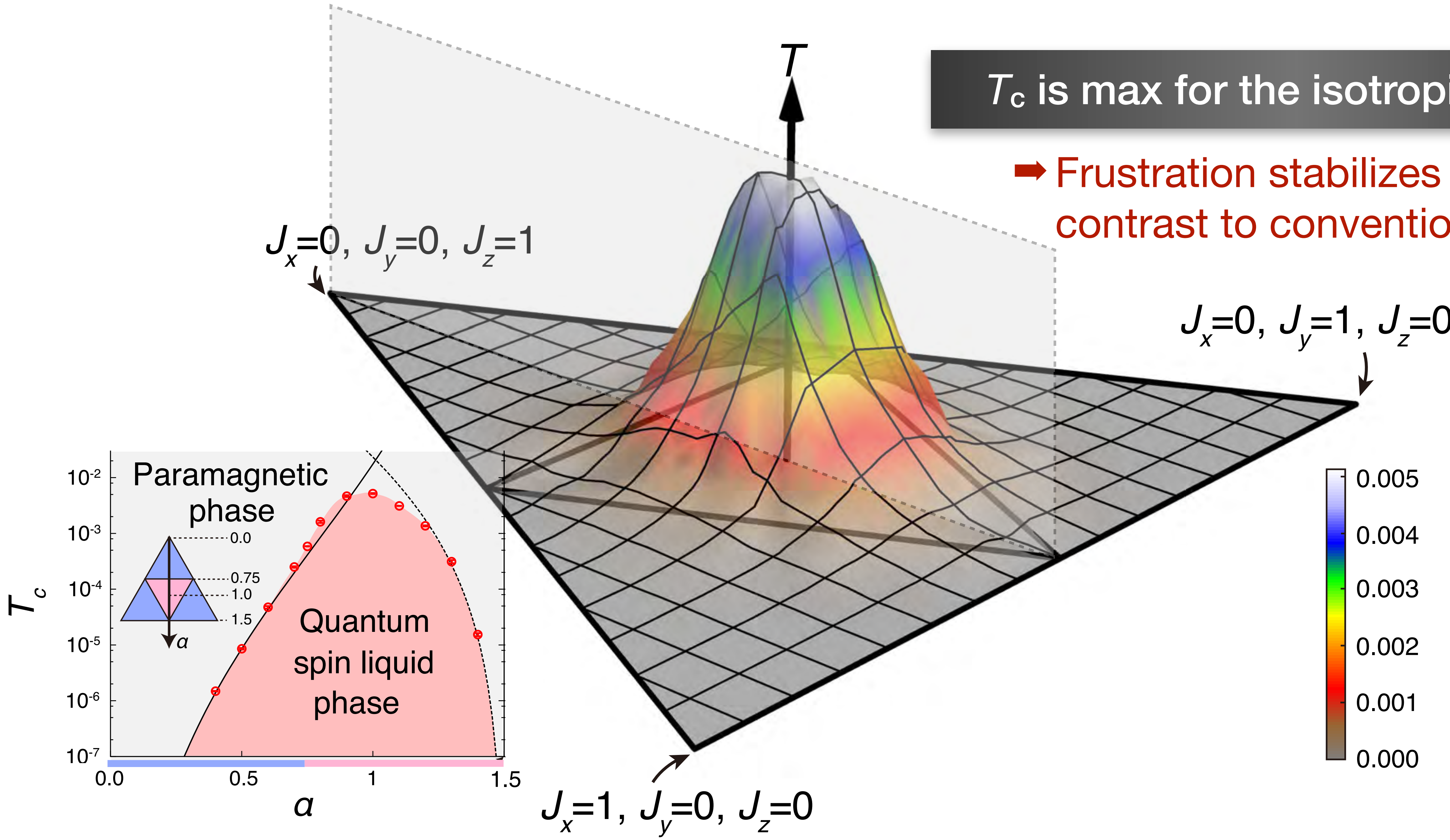
Phase diagram in 3D



All low-T QSLs are separated from high-T para by the phase transition.

➡ no adiabatic connection, qualitatively different from conventional fluids

Phase diagram in 3D



T_c is max for the isotropic case.

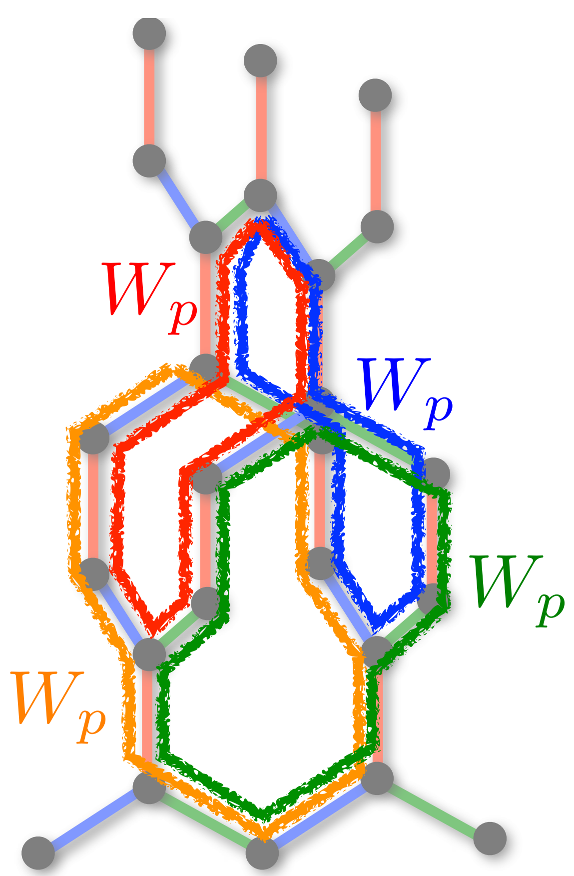
➡ Frustration stabilizes QSLs, in contrast to conventional orders.

All low-*T* QSLs are separated from high-*T* para by the phase transition.

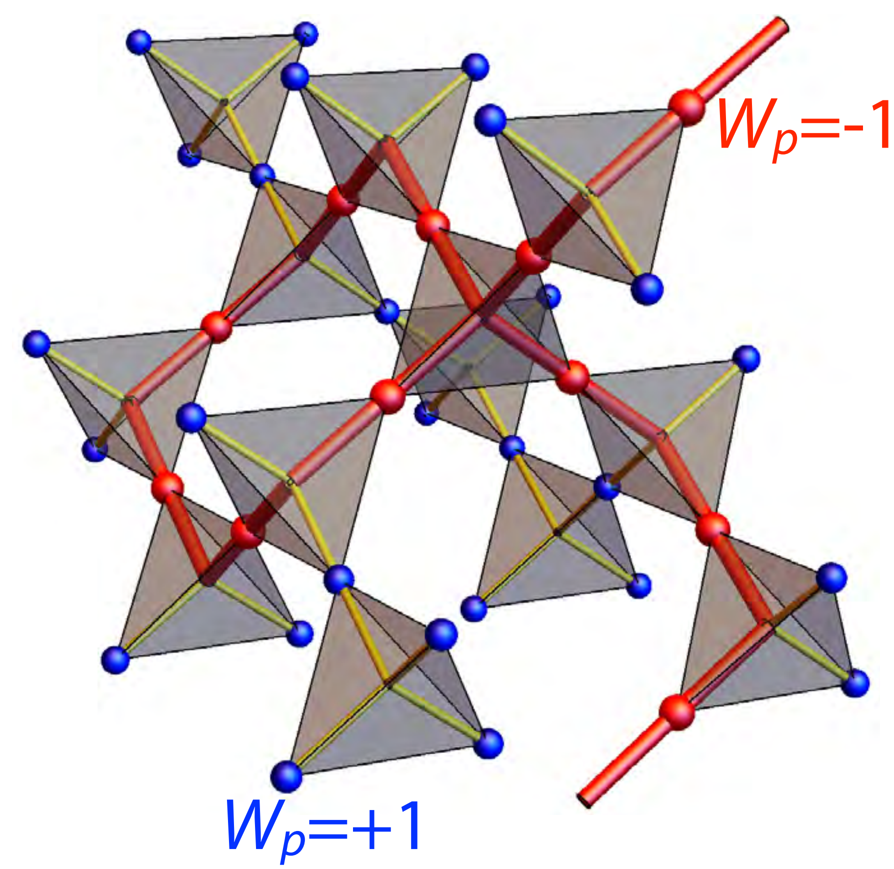
➡ no adiabatic connection, qualitatively different from conventional fluids

What is this phase transition?

- difference from 2D: W_p plaquettes form closed objects
  - ➡ local constraint for W_p: hard constraint by S=1/2 algebra
  - ➡ excited states include only closed loops of flipped W_p (at all T)



$$W_p\, W_p\, W_p\, W_p = 1$$

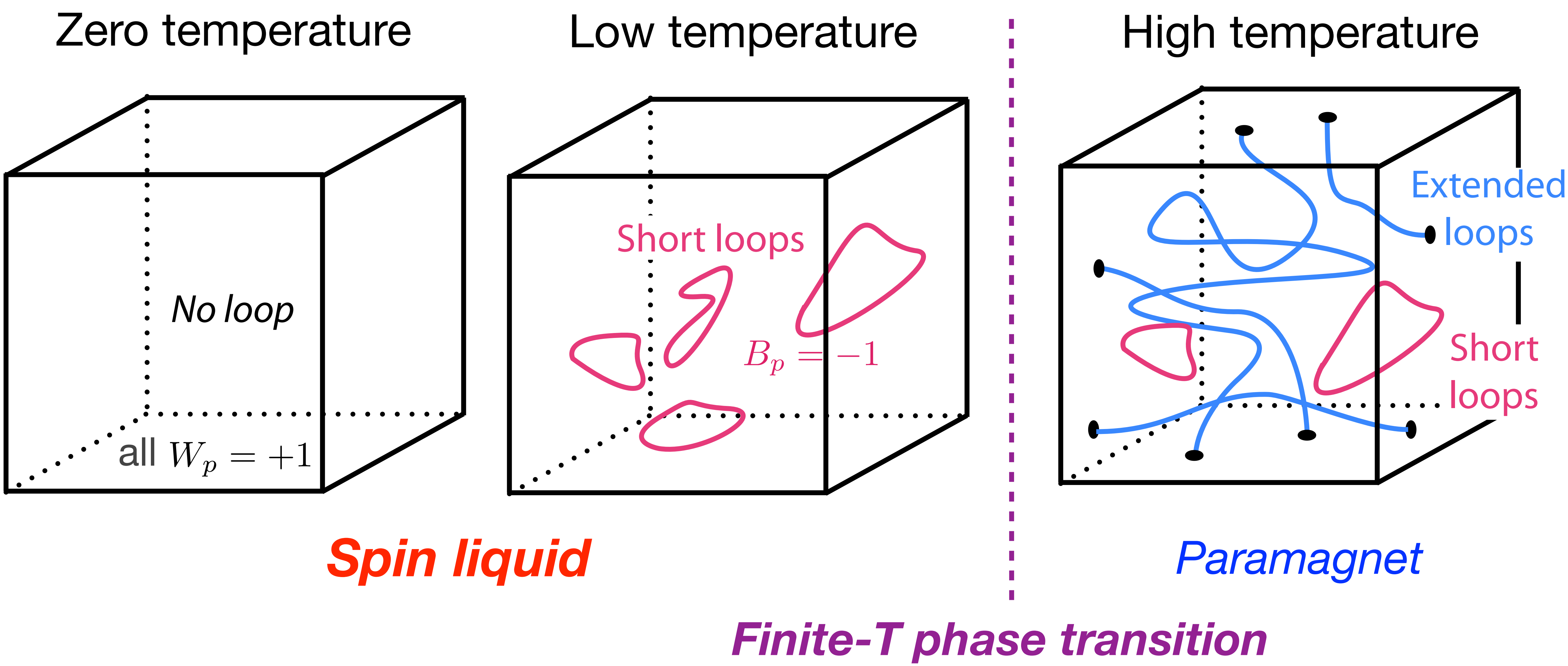


"2-in 2-out", "all-in", "all-out"

cf.) spin ice: soft constraint, only "2-in 2-out", no intersection

Proliferation of excited loops

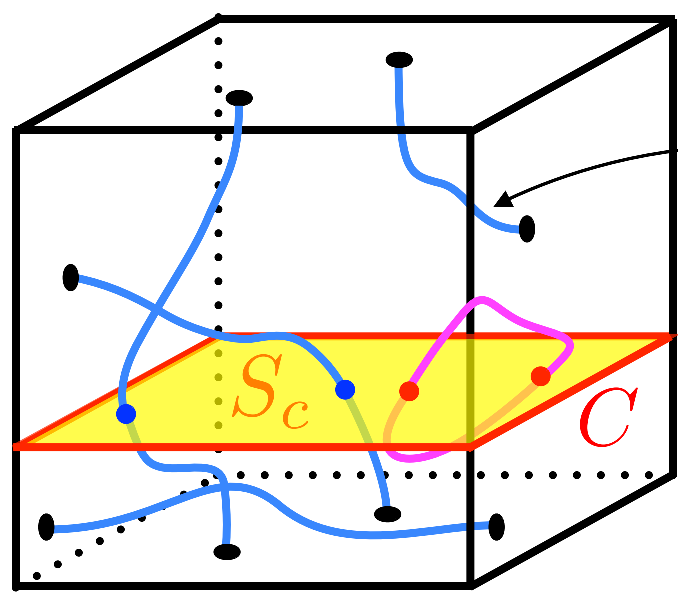
- observation from QMC snapshot: the phase transition might be related with the topological change of emergent loops



“confinement-deconfinement” type phase transition?

Characterization by Wilson loop

Loop operator (Wilson loop): $\mathcal{W}_C = \prod_{i \in C} \sigma_i^{l_i}$



flipped

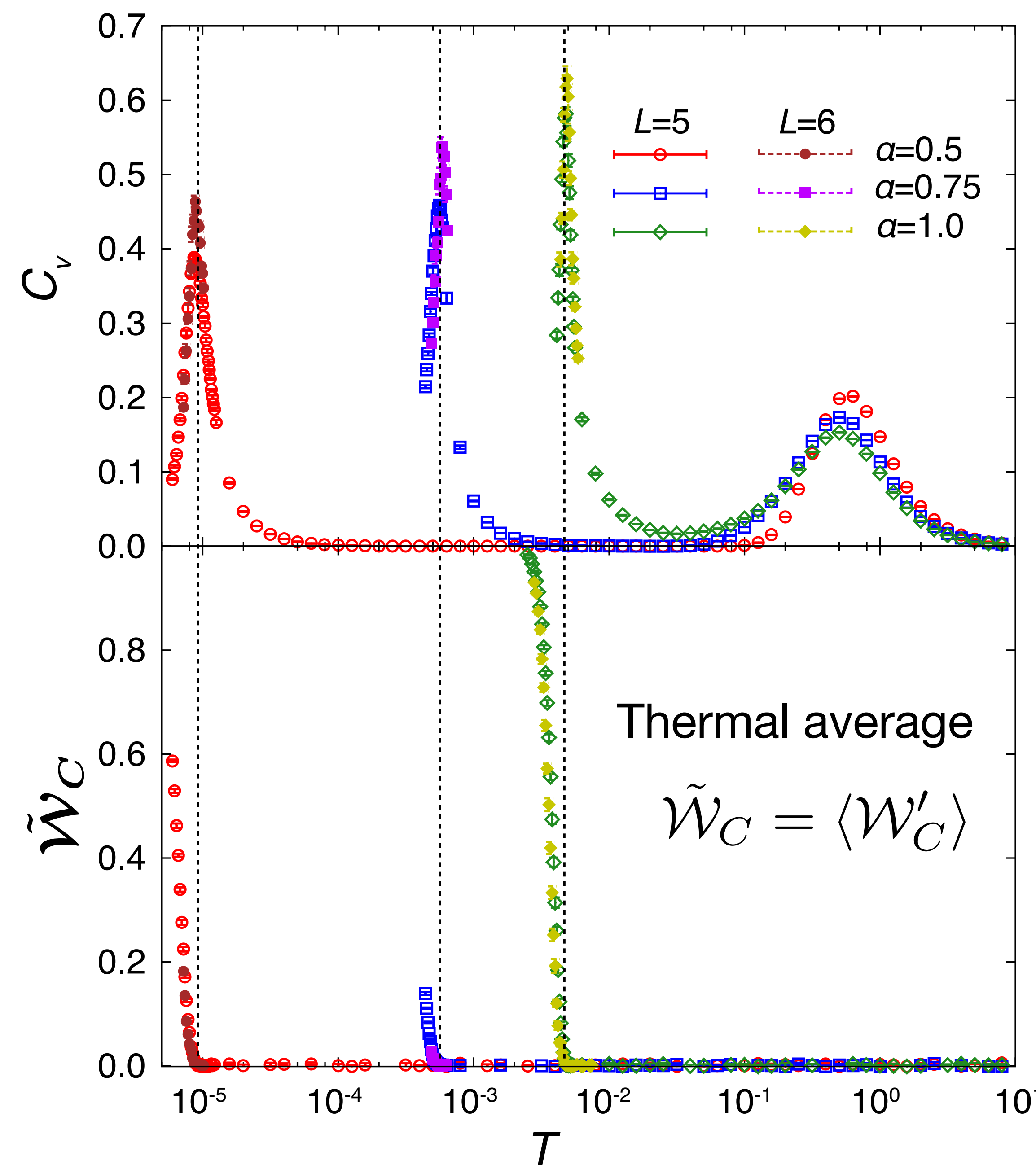
$W_p = -1$

$$\mathcal{W}_C = -\prod_{p \in S_C} W_p = -\prod_{r \in C} \eta_r \equiv -\mathcal{W}'_C$$

Extended loops : $\mathcal{W}_C = +1$ or -1

$\rightarrow \tilde{\mathcal{W}}_C = \langle \mathcal{W}'_C \rangle = 0$

Short loops : $\mathcal{W}_C = +1 \rightarrow \tilde{\mathcal{W}}_C = 1$



Wilson loop acts as an order parameter for this nonlocal transition.

Summary and perspective

Main results:

- thermal fractionalization of a quantum spin into Majorana fermions
- exotic "liquid-gas" phase transition by loop proliferation in 3D

QSLs may offer a good hunting place for Majorana fermions!

our results provides a guidebook for Majorana hunting

Open issues

- How universal is the Majorana physics in the zoo of QSLs?
- Any other direct smoking gun for the "Majorana-ness"?
- more inputs for/from experiments!
- etc.

References:

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