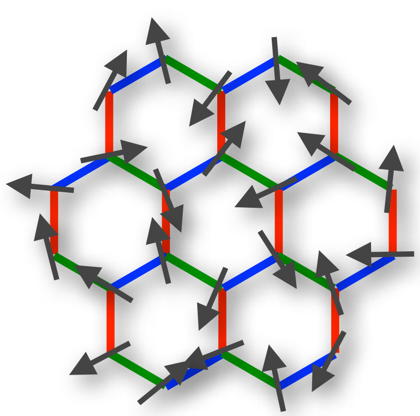
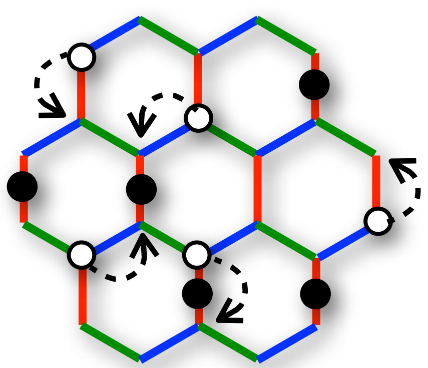
Hunting Majorana fermions in quantum spin liquids

Quantum Monte Carlo studies of Kitaev-type models

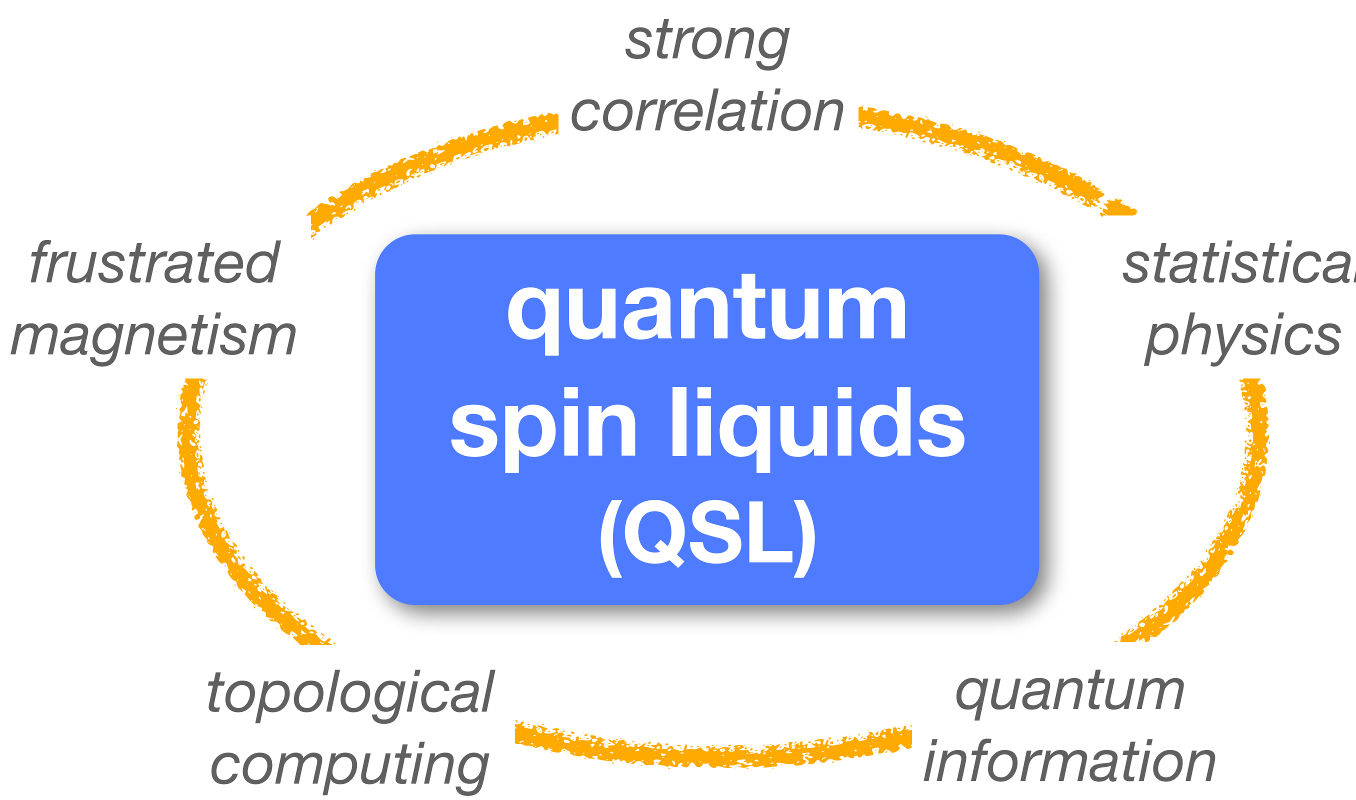


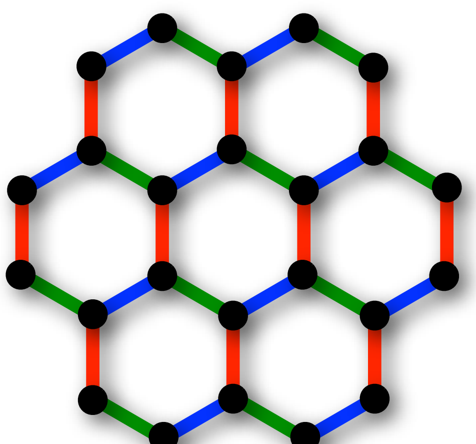


Yukitoshi Motome

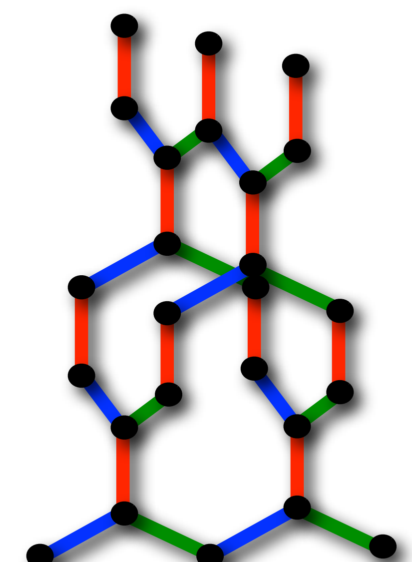
東京大学
THE UNIVERSITY OF TOKYO

Message of this talk





Kitaev-type models: **exact QSL at *T*=0**



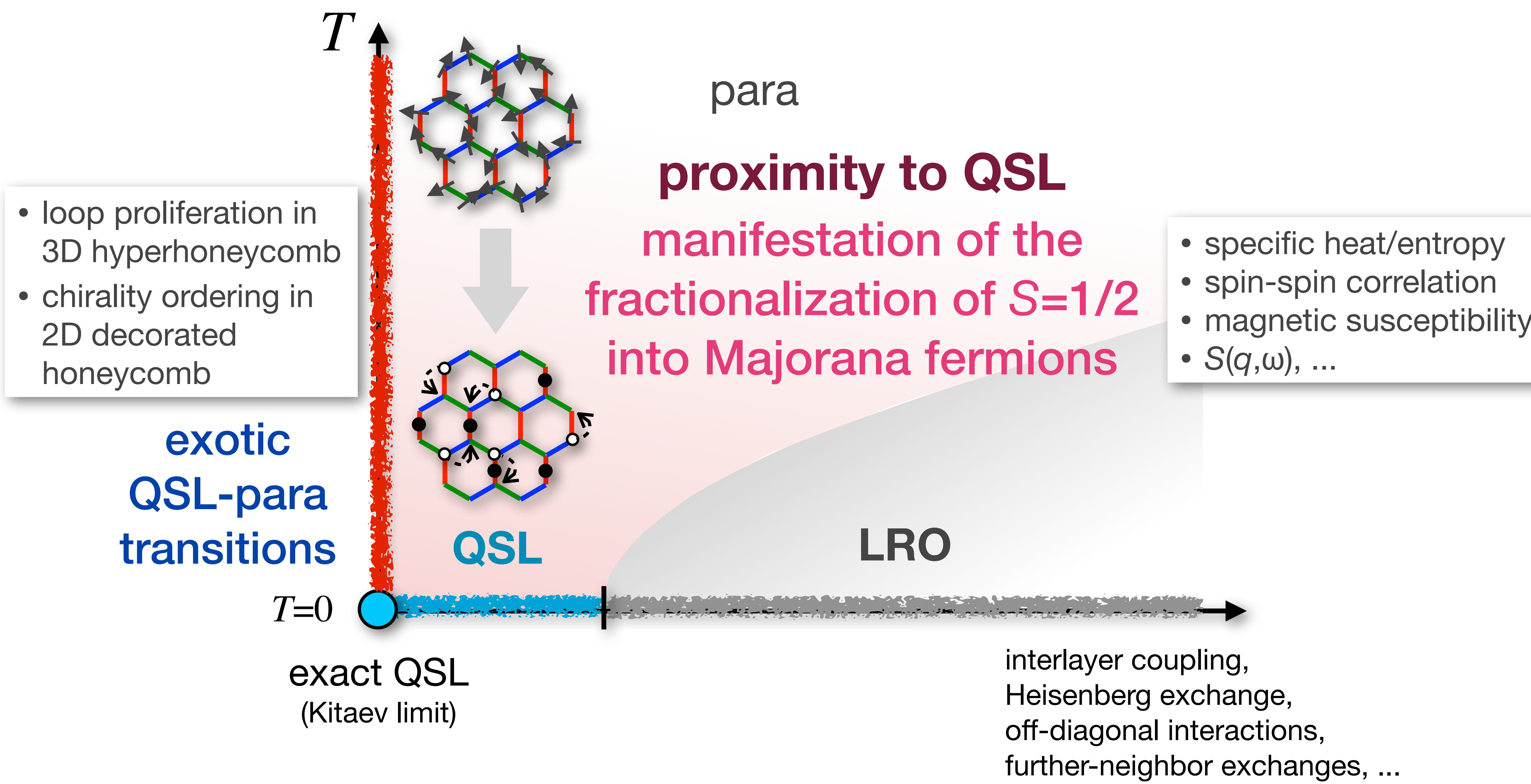
However, all the candidate materials show long-range orders (LRO) at low *T* so far.

Is this the end of the story?
No hope to see the sign of QSL?

Message of this talk

our answer **No!**

Many manifestations can be seen in high-*T* para



Collaborators

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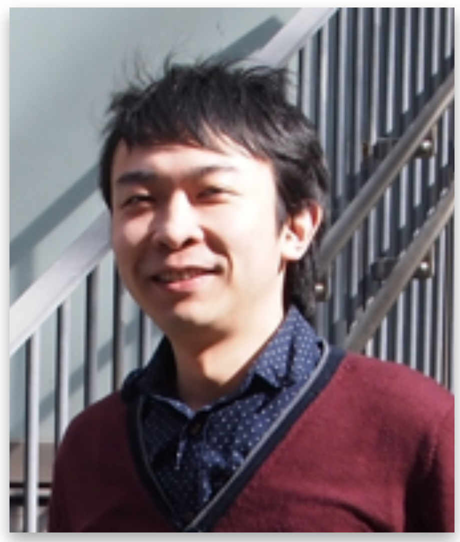

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(Univ. of Cambridge)

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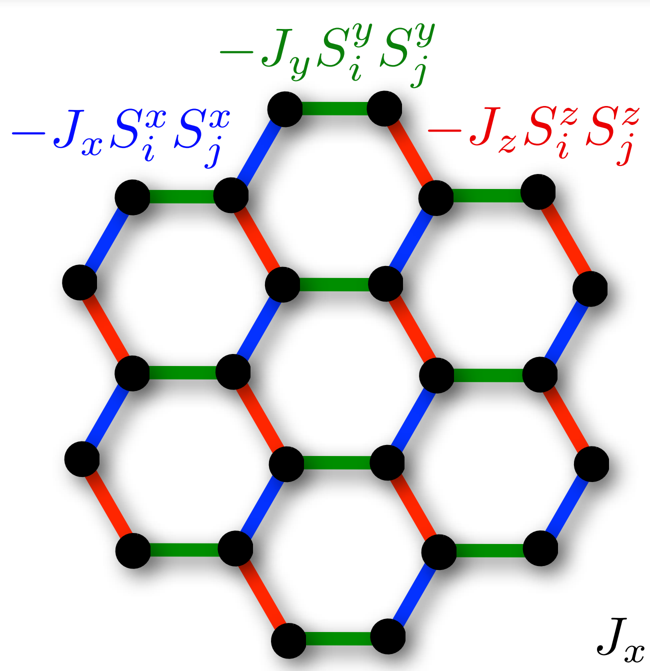
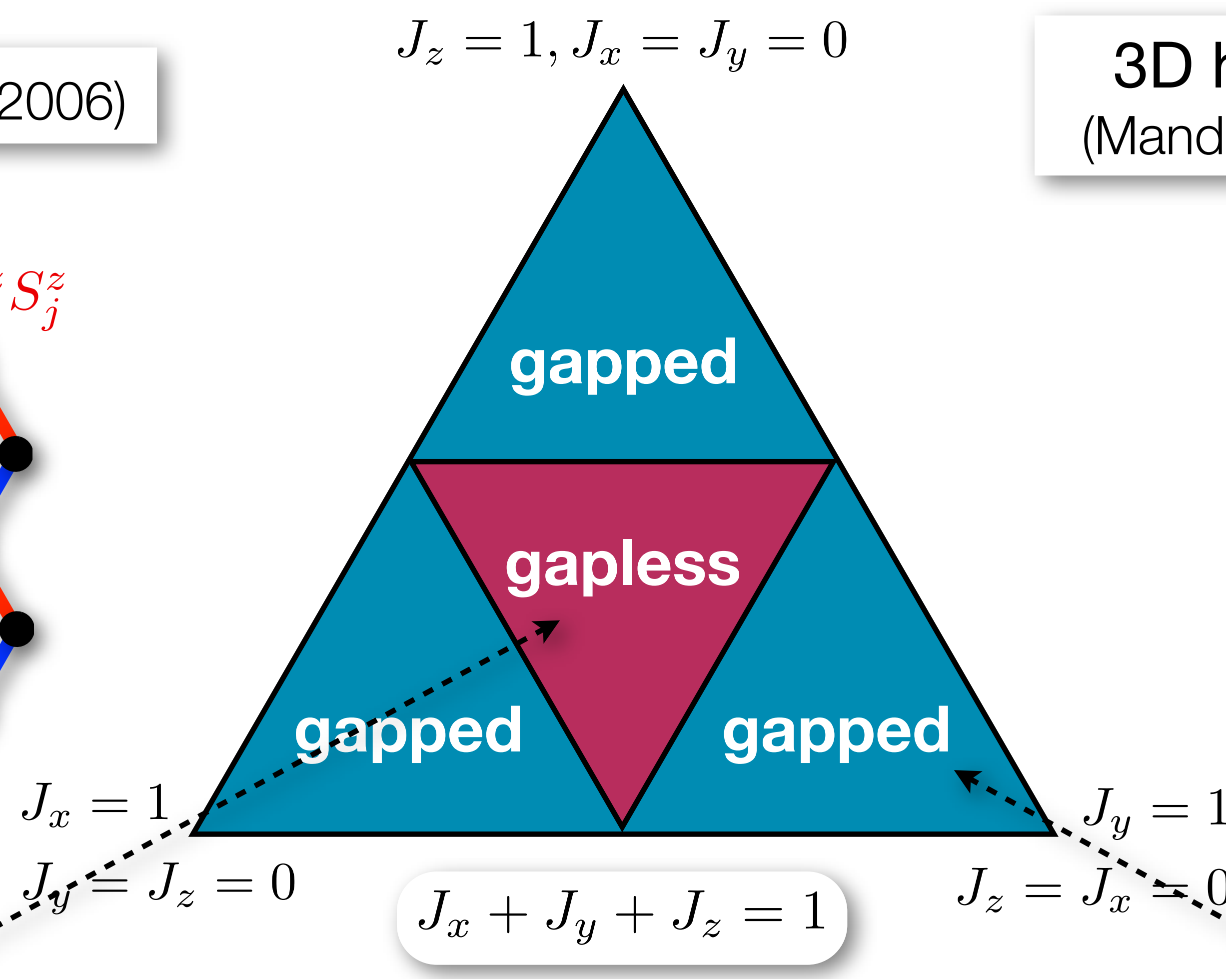
Exact QSLs in Kitaev-type systems

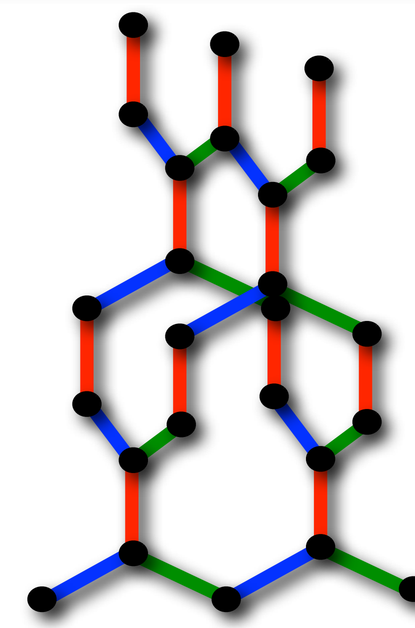
- *S*=1/2 spins on tri-coordinate lattices with bond dependent interactions

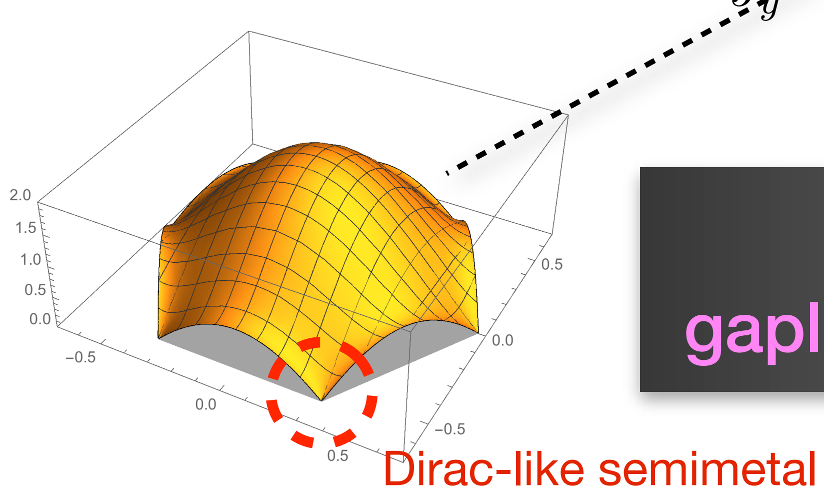
2D honeycomb (Kitaev 2006)



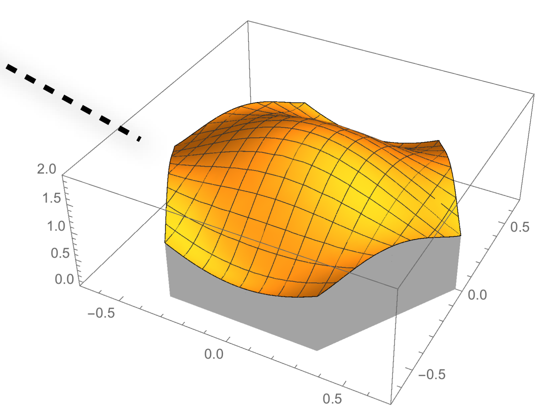


3D hyper-honeycomb
(Mandal and Surendran 2009)



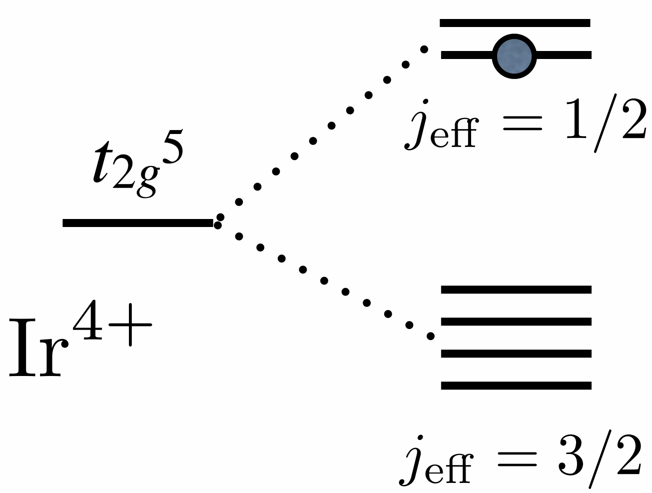


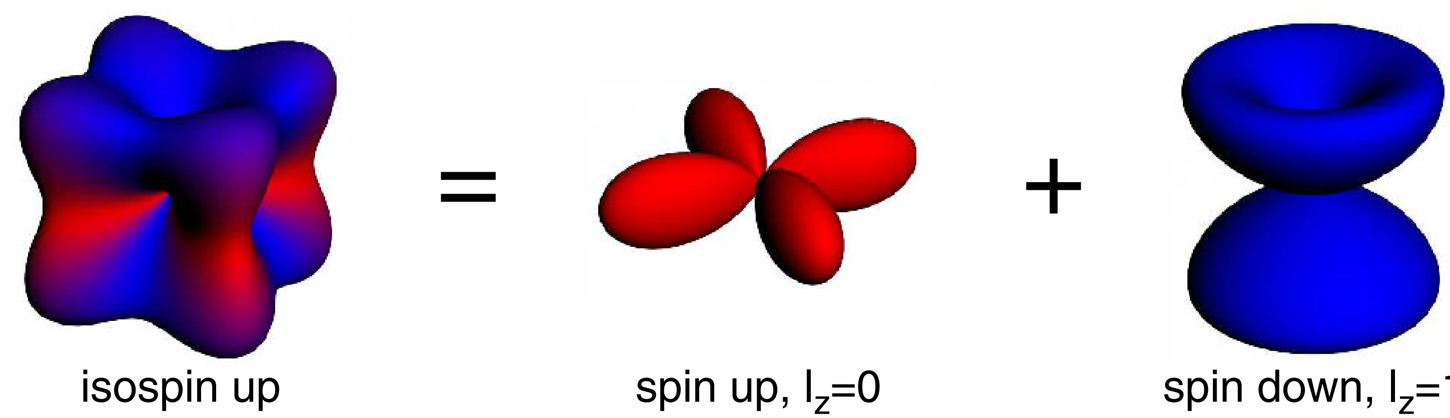
exact QSL ground states:
gapless and gapped dep. on parameters



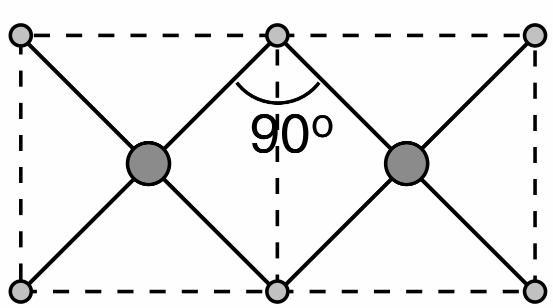
Experimental relevance

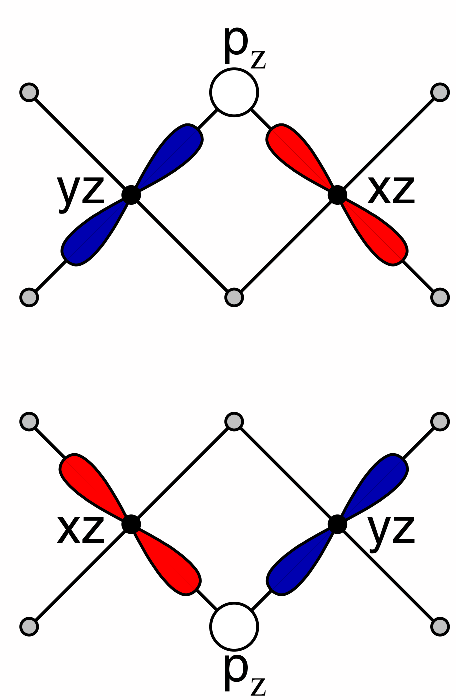
- Kitaev-type interactions may arise from partially-filled t_{2g} levels under strong spin-orbit coupling (G. Jackeli and G. Khaliullin, 2009)

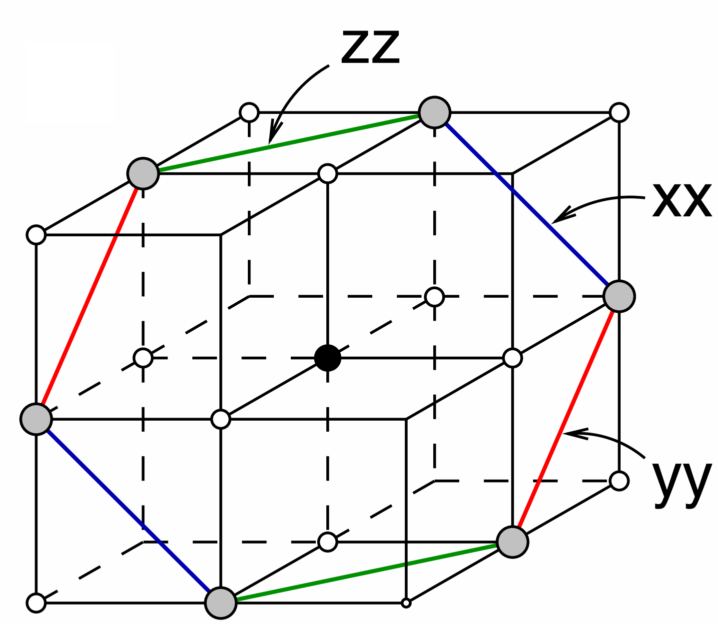




90-degree bond by edge-sharing octahedra

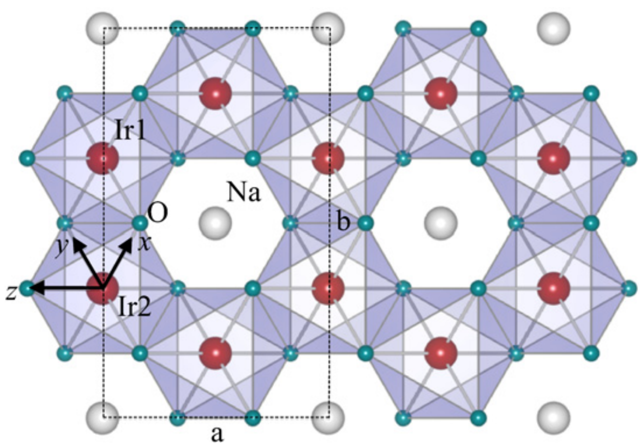






Candidate materials

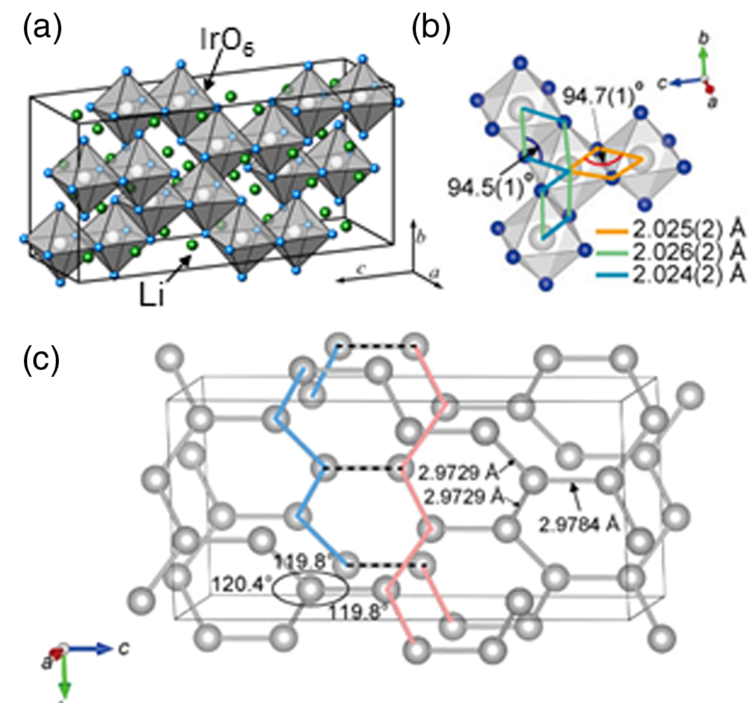
2D honeycomb



Na_2IrO_3, Li_2IrO_3,...

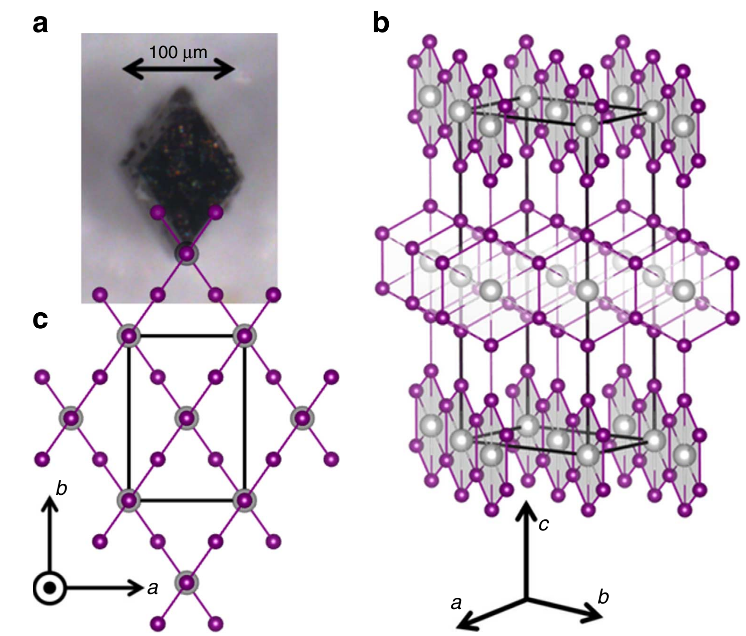
M. J. O'Malley *et al.*, 2008
Y. Singh and P. Gegenwart, 2010
Y. Singh *et al.*, 2012, ...

3D hyper-honeycomb



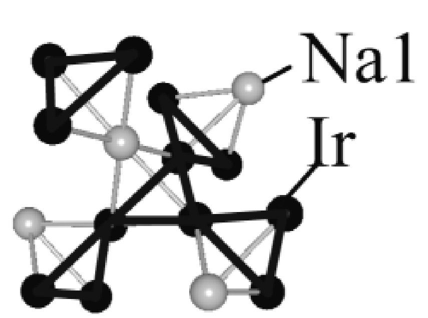
β-Li_2IrO_3 T. Takayama *et al.*, 2015

3D stripy-honeycomb



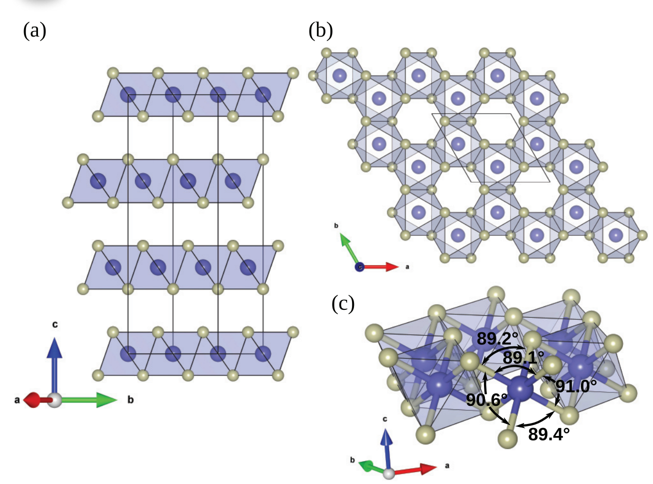
γ-Li_2IrO_3 K. A. Modic *et al.*, 2014

hyper-kagome



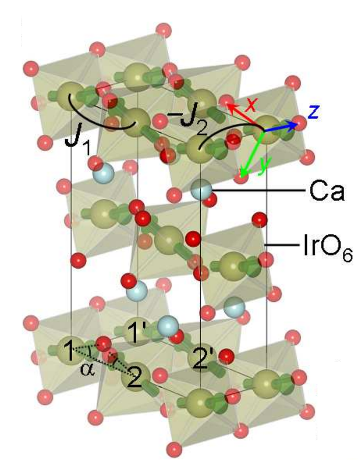
Y. Okamoto *et al.*, 2007

α-$RuCl_3$



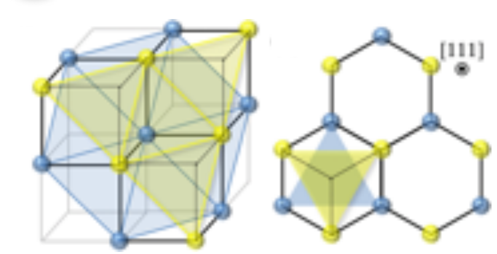
K. Plumb *et al.*, 2014
Y. Kubota *et al.*, 2015, ...

post-perovskite

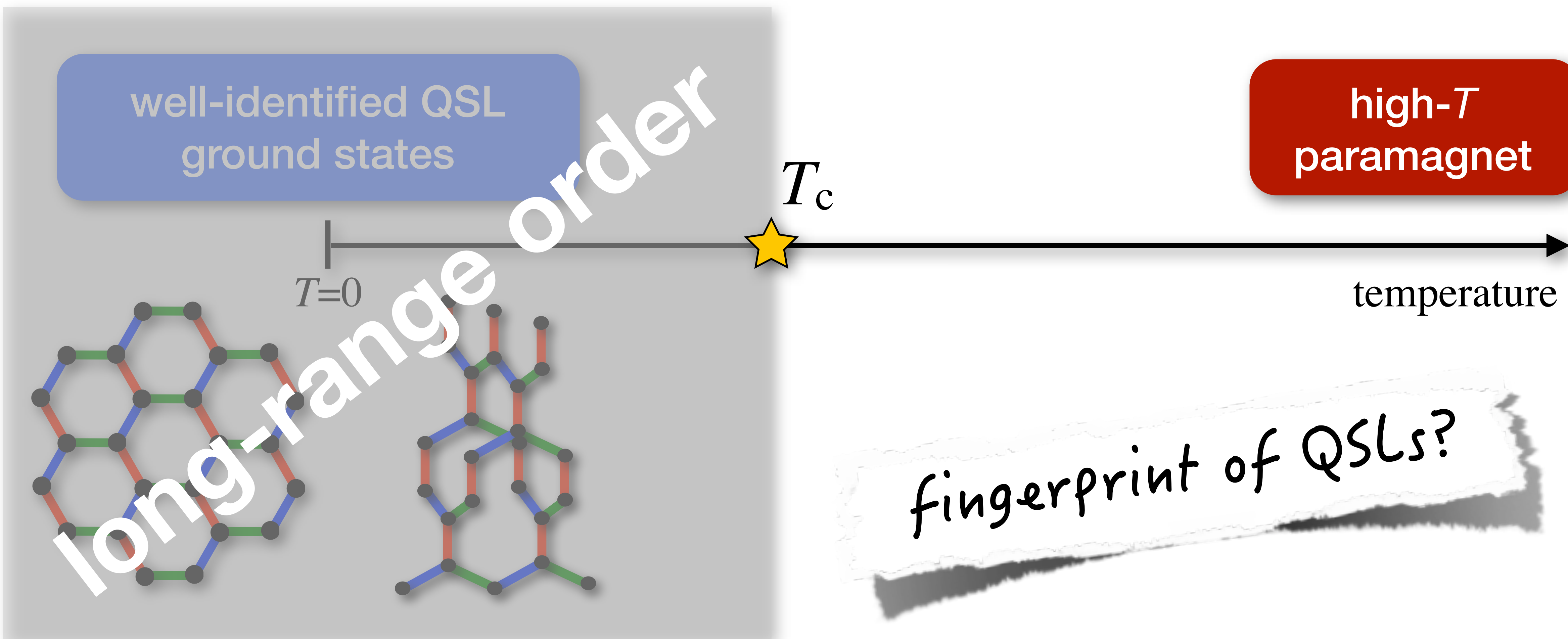


K. Ohgushi *et al.*, 2013, 2014

tailored films



D. Hirai *et al.*, 2015



How to compute thermodynamics?

Conventional quantum Monte Carlo (QMC)
on the basis of the world-line technique does not work
due to the negative sign problem...

New QMC method

- QMC on the basis of Majorana fermion representation

interacting S=1/2 spins

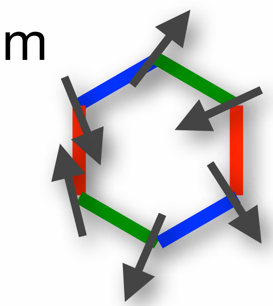
Jordan-Wigner transformation

Majorana fermion representation

H.-D. Chen and J. Hu, 2007
X.-Y. Feng *et al*., 2007
H.-D. Chen and Z. Nussinov, 2008

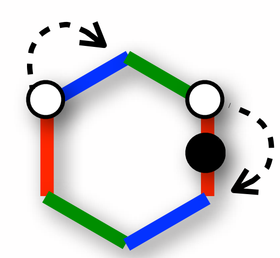
quantum spin

$\mathbf{S}_i$



itinerant Majorana c_i

localized Majorana $\bar{c}_i$



Z_2 variable

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

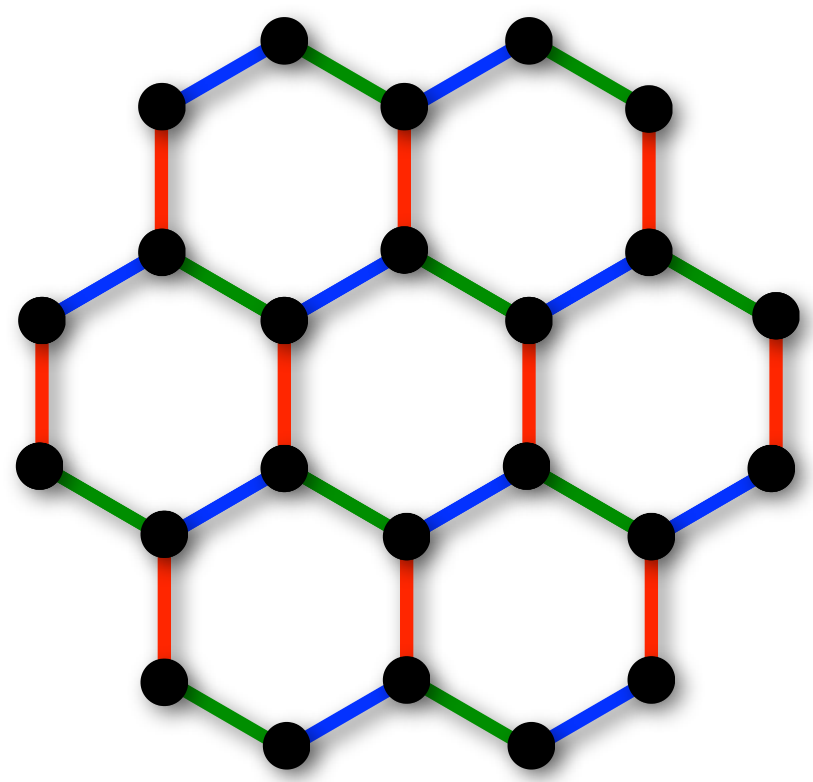
free Majorana fermions coupled to thermally-fluctuating Z_2 fields

formally, similar to the double-exchange model with Ising spins

→ unbiased QMC free from negative-sign problem!

Thermal fractionalization of S=1/2 into Majorana fermions:

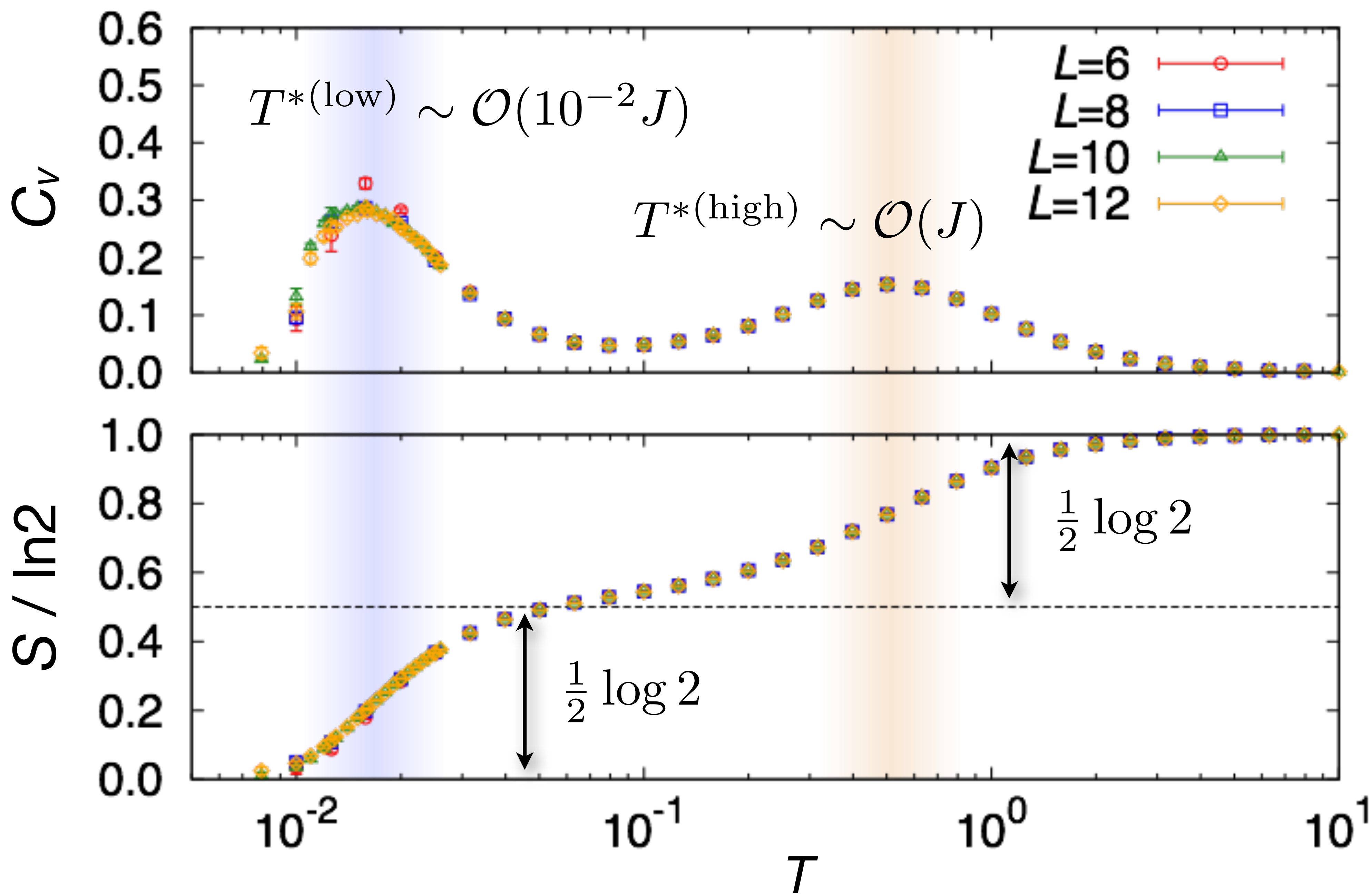
diagnostic in physical observables

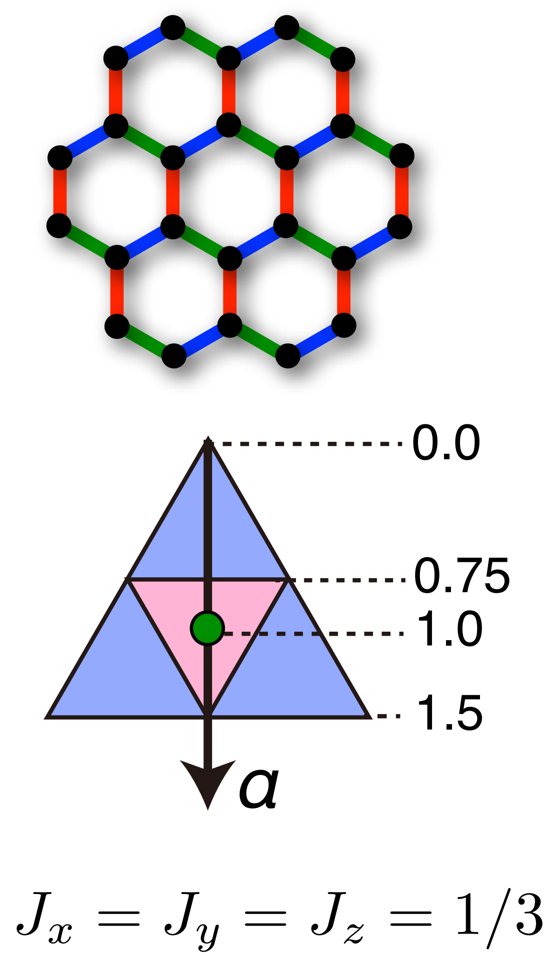


J. Nasu, M. Udagawa, and Y. Motome, preprint (arXiv:1504.01259)

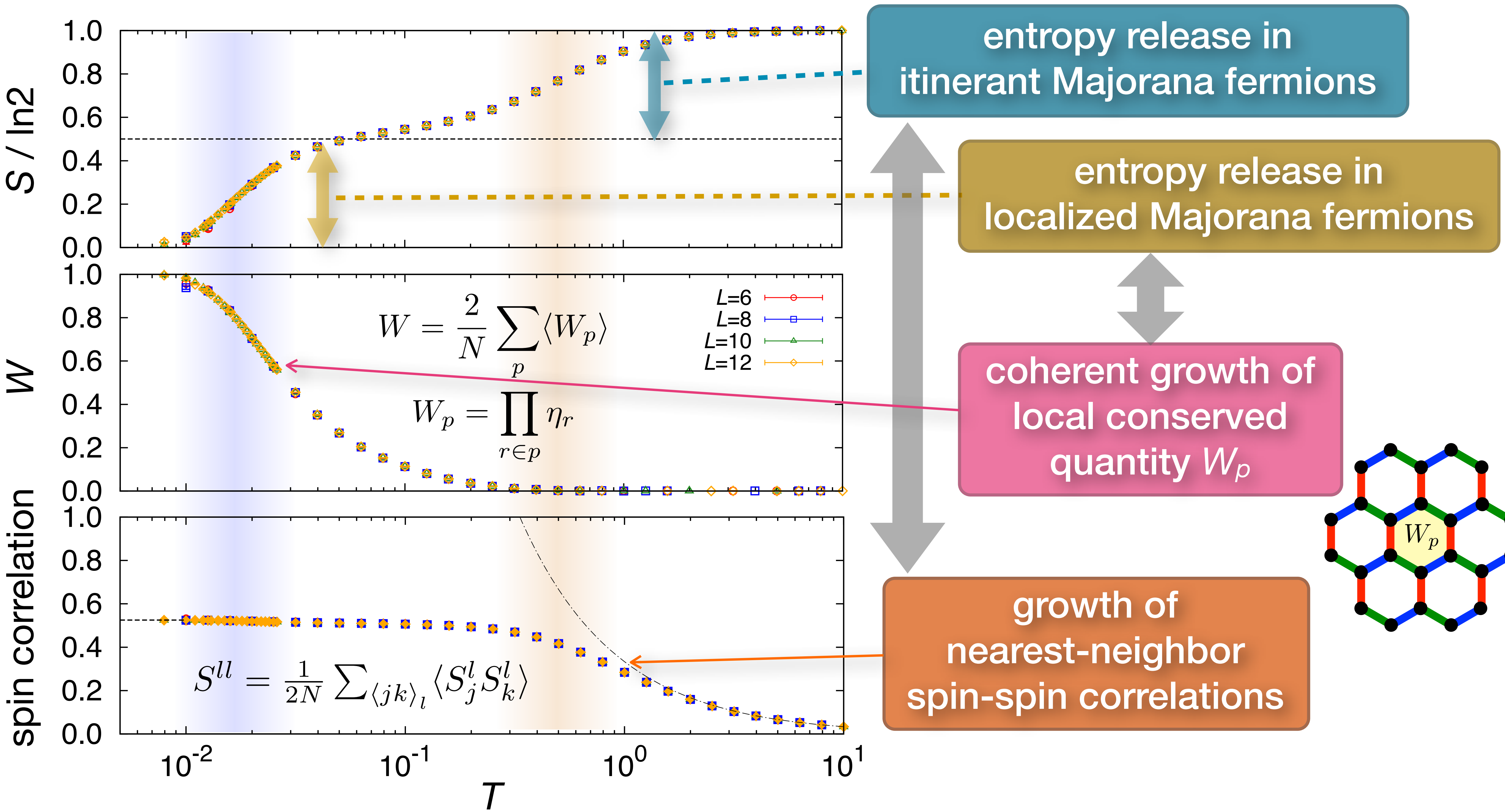
Specific heat and entropy

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



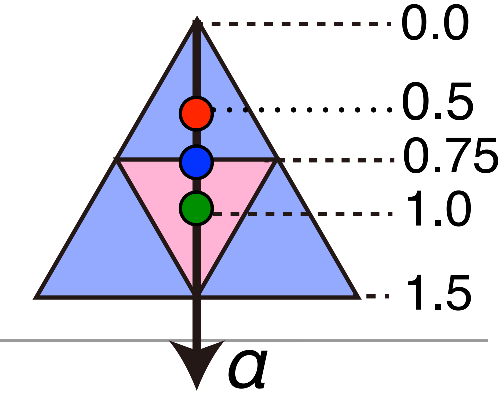


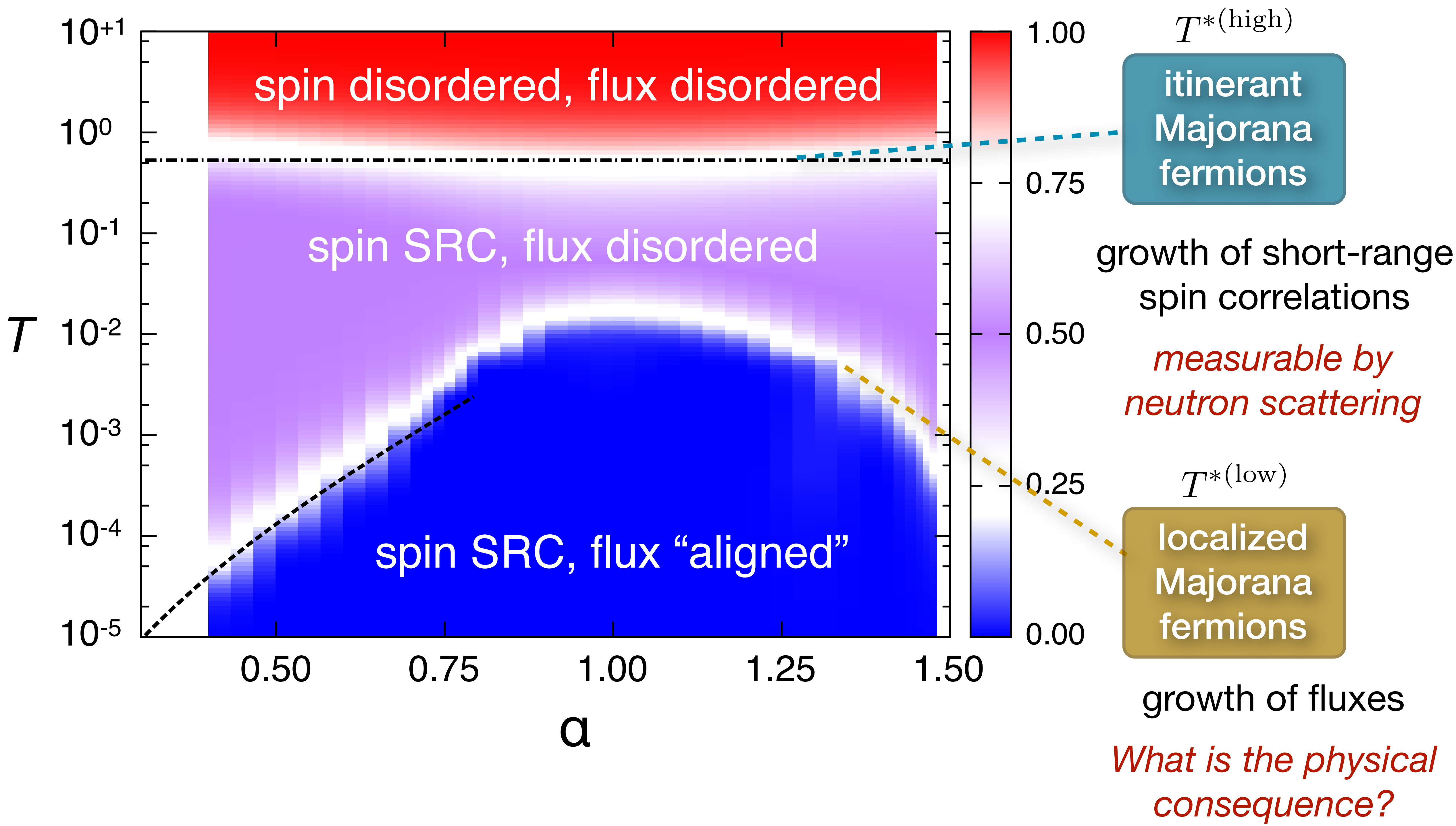
Successive two crossovers



clear signatures of thermal fractionalization of quantum spins

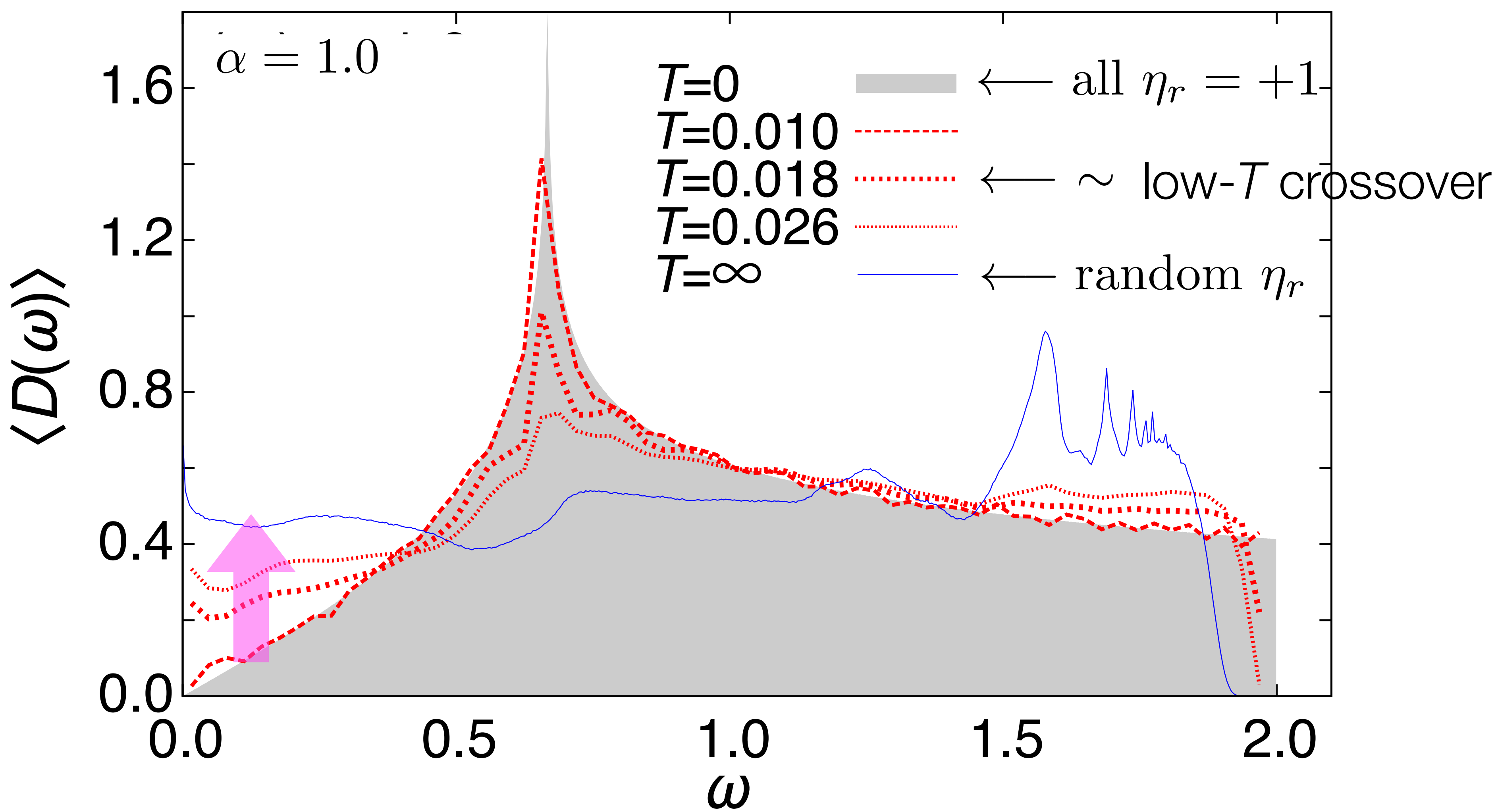
Phase diagram





DOS for itinerant Majorana fermions

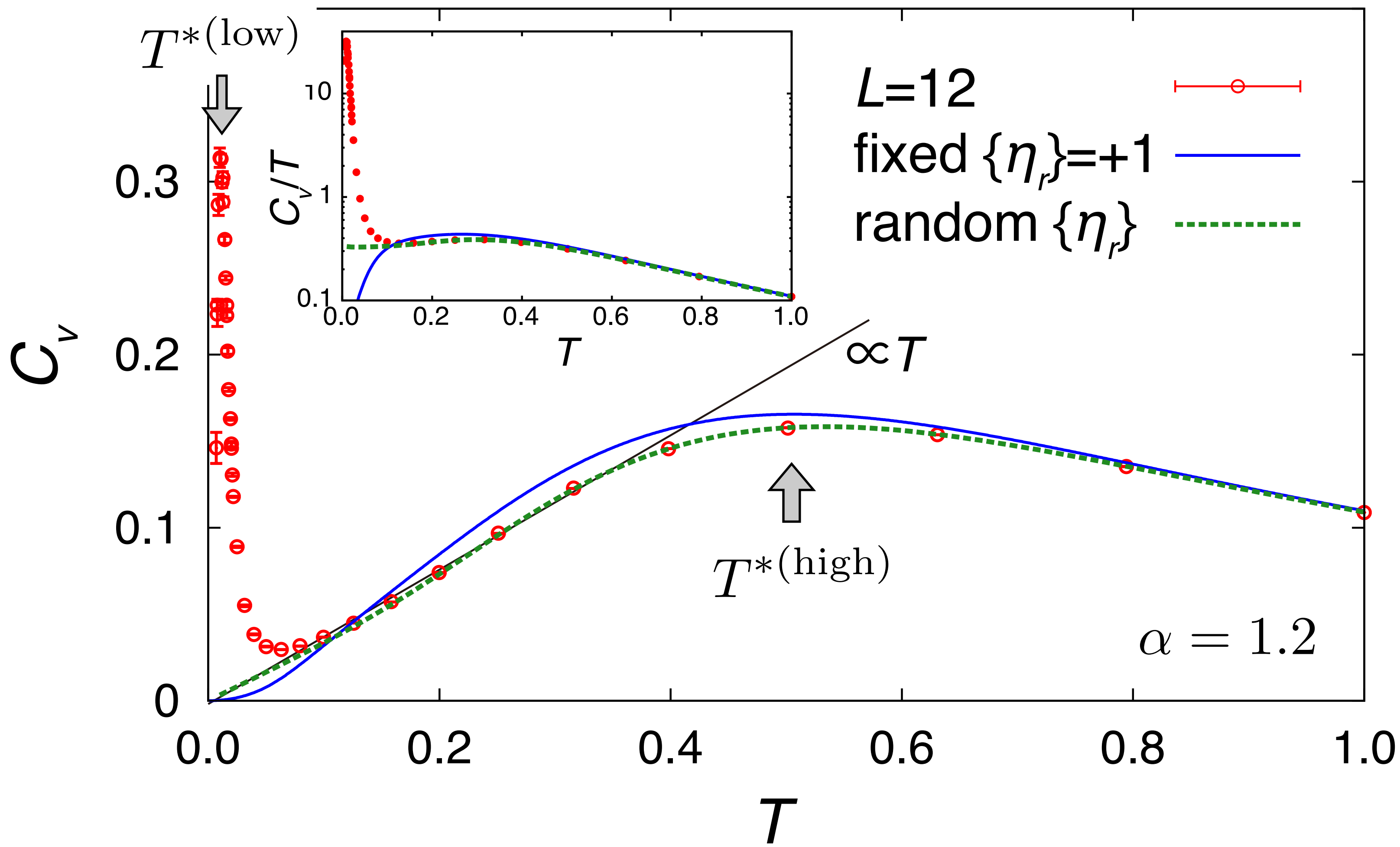
- Thermal fluctuations of the fluxes disturb the Majorana DOS.

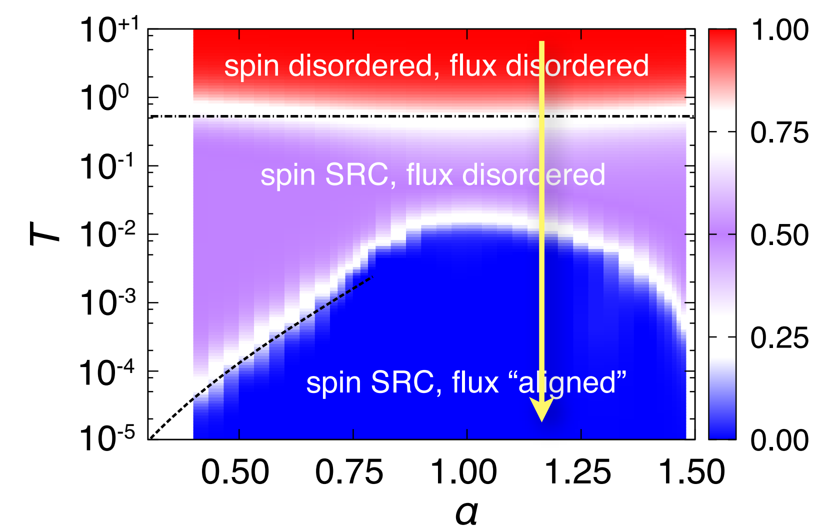


Dirac semimetal → “metal” above the low-T crossover by thermal fluctuations in fluxes (localized Majorana)

Apparent T-linear specific heat

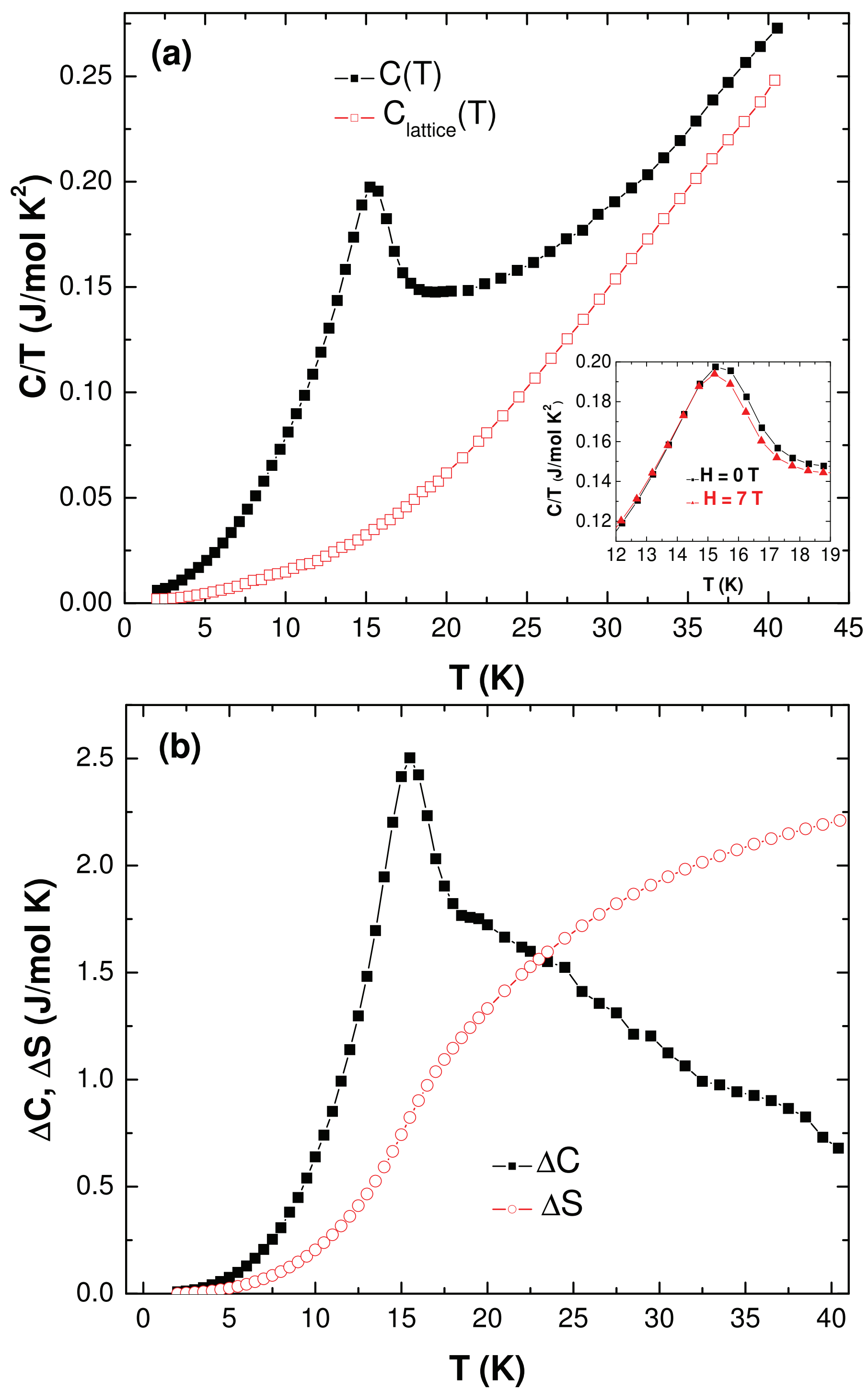
- Above the low-T crossover, the DOS becomes metallic, leading to apparent T-linear behavior in the specific heat, although T^2 behavior is expected for the Dirac semimetallic spectrum at T=0.

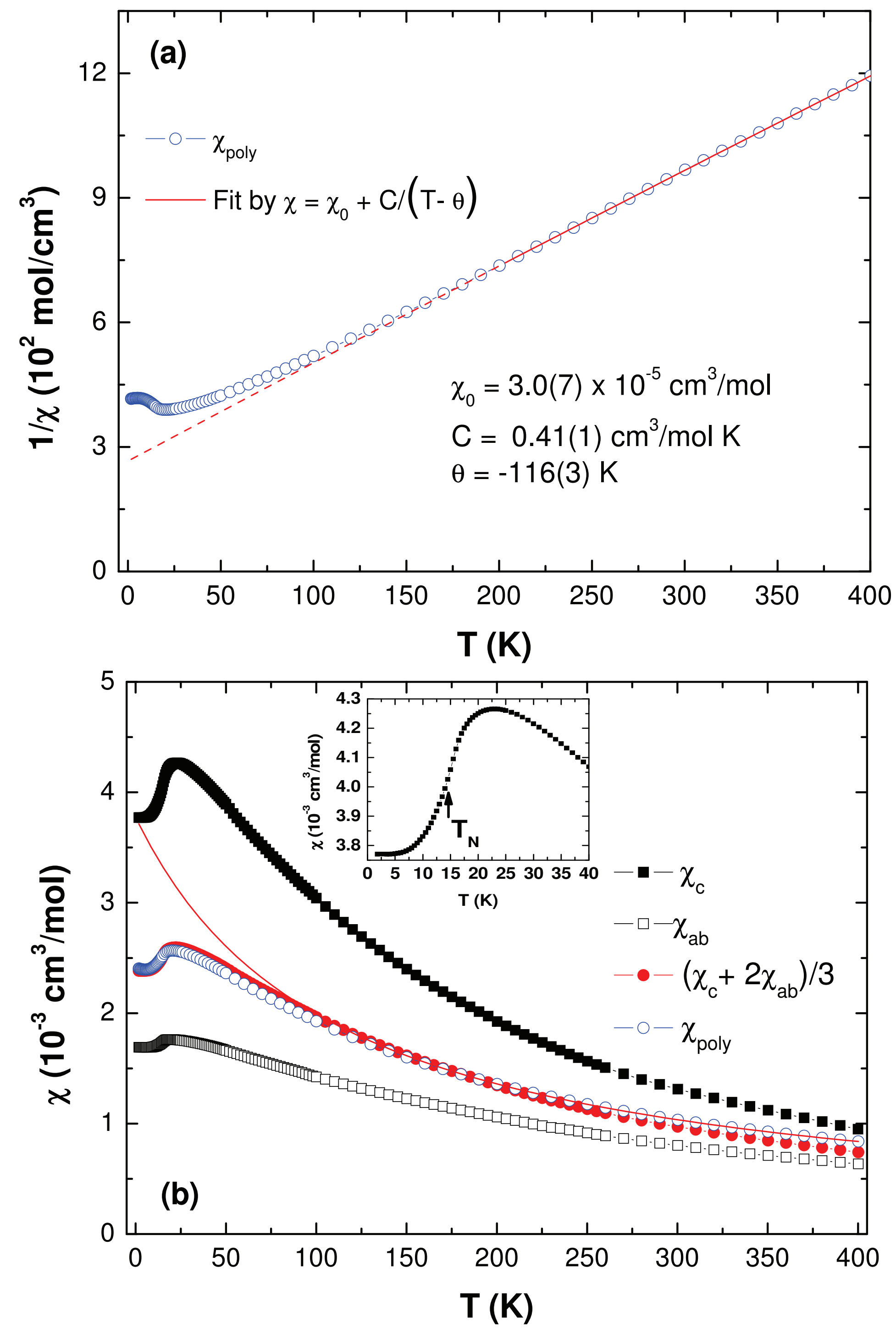




T-linear behavior for the "spin liquid" with well-developed spin correlations

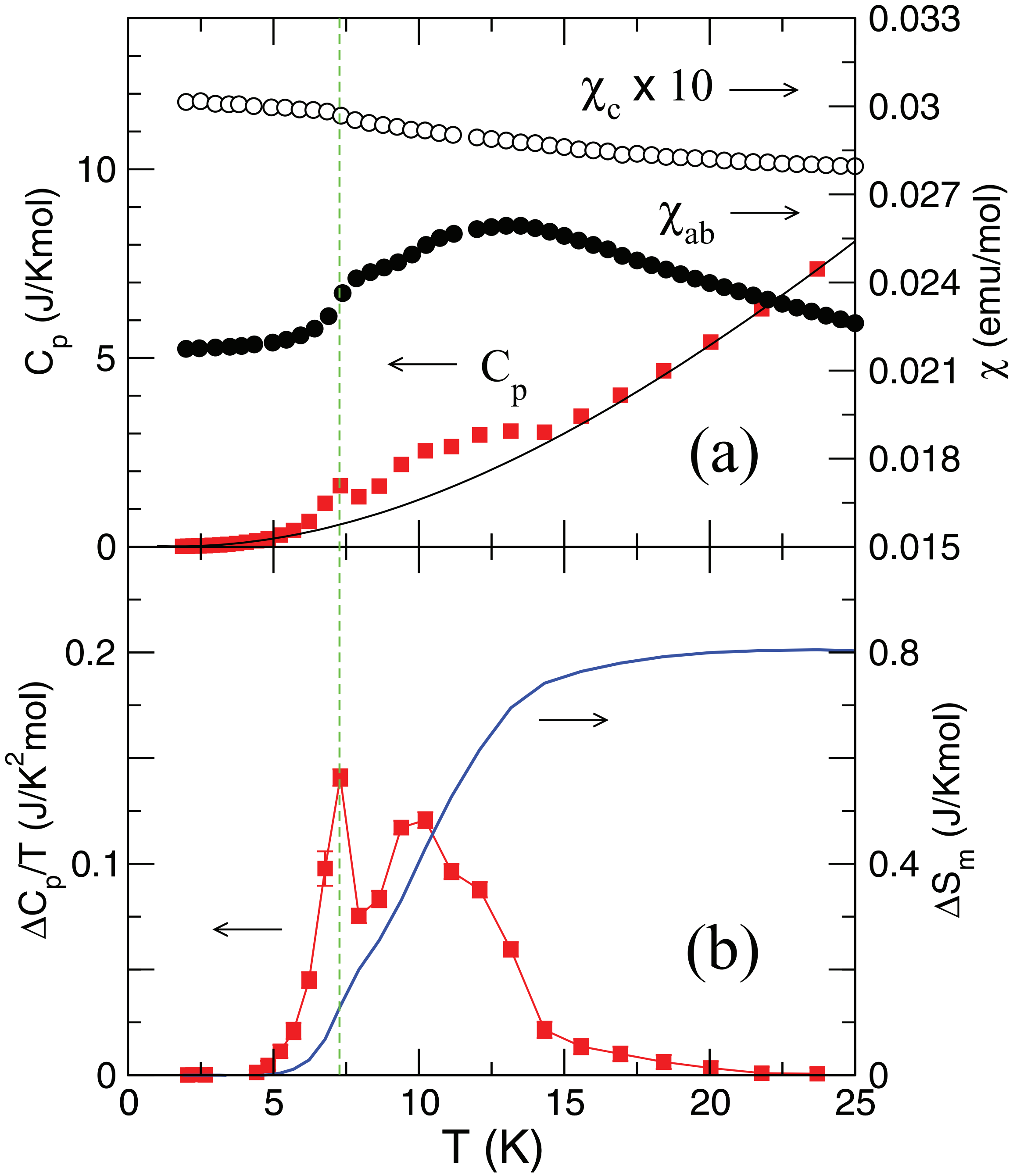
Experiments: Na_2IrO_3



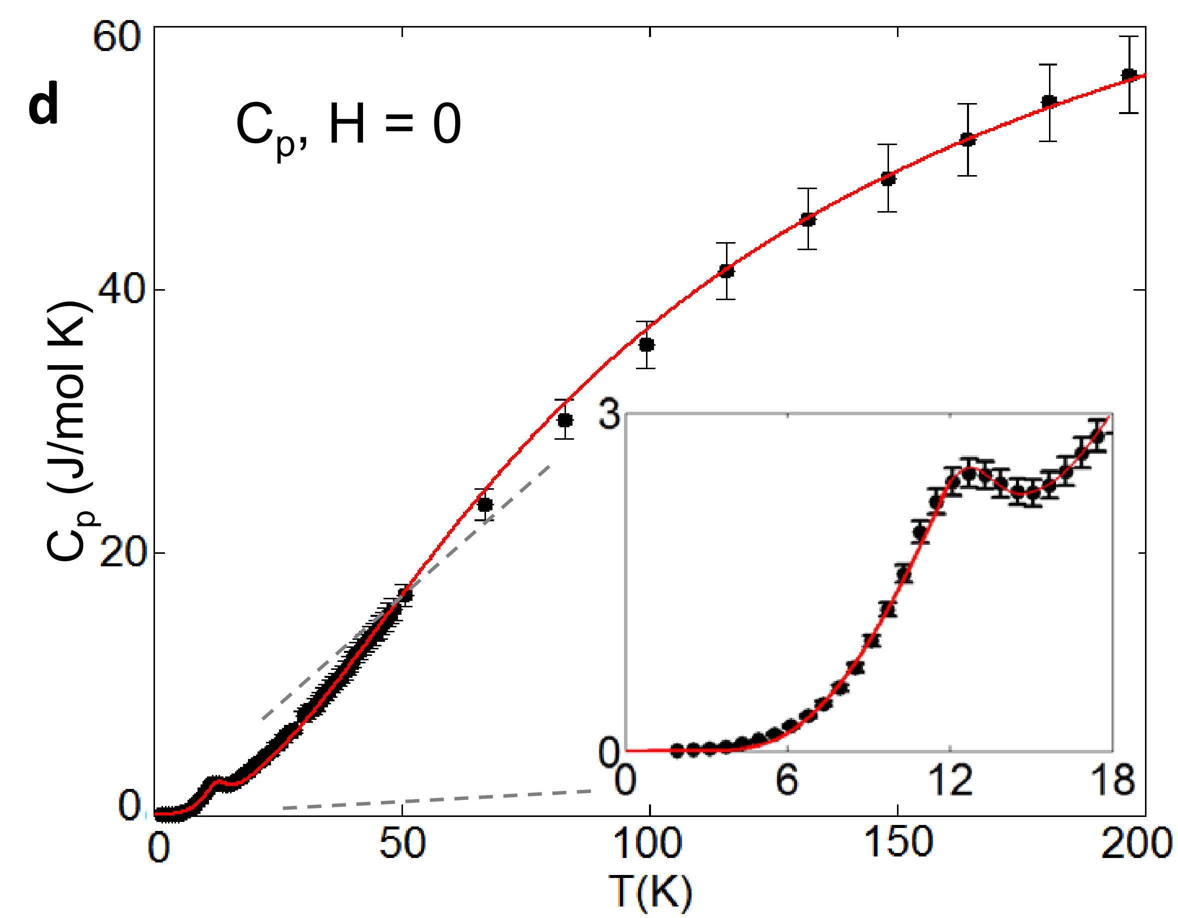


Y. Singh and P. Gegenwart, 2010

Experiments: α-$RuCl_3$

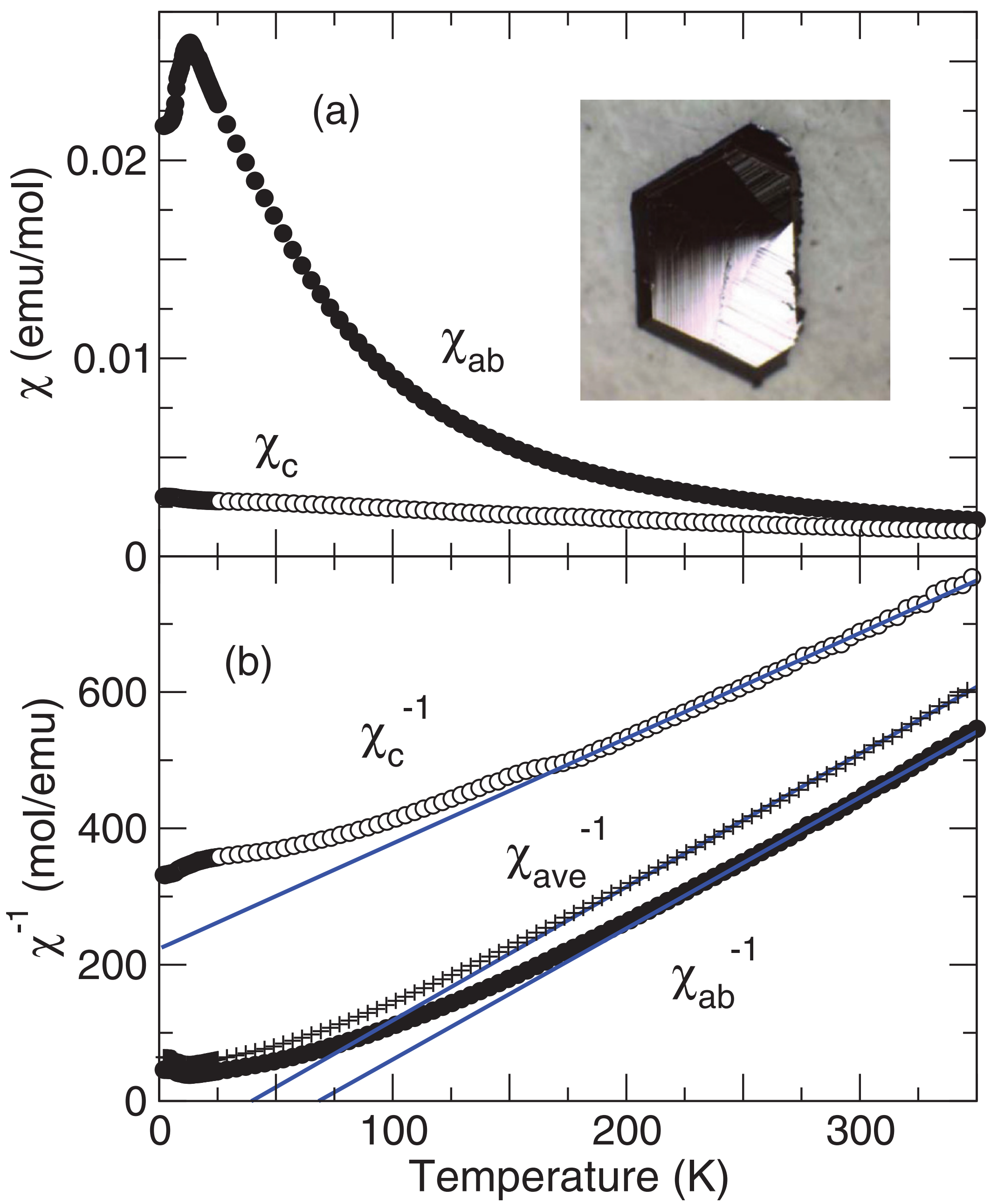


J. A. Sears *et al.*, 2015

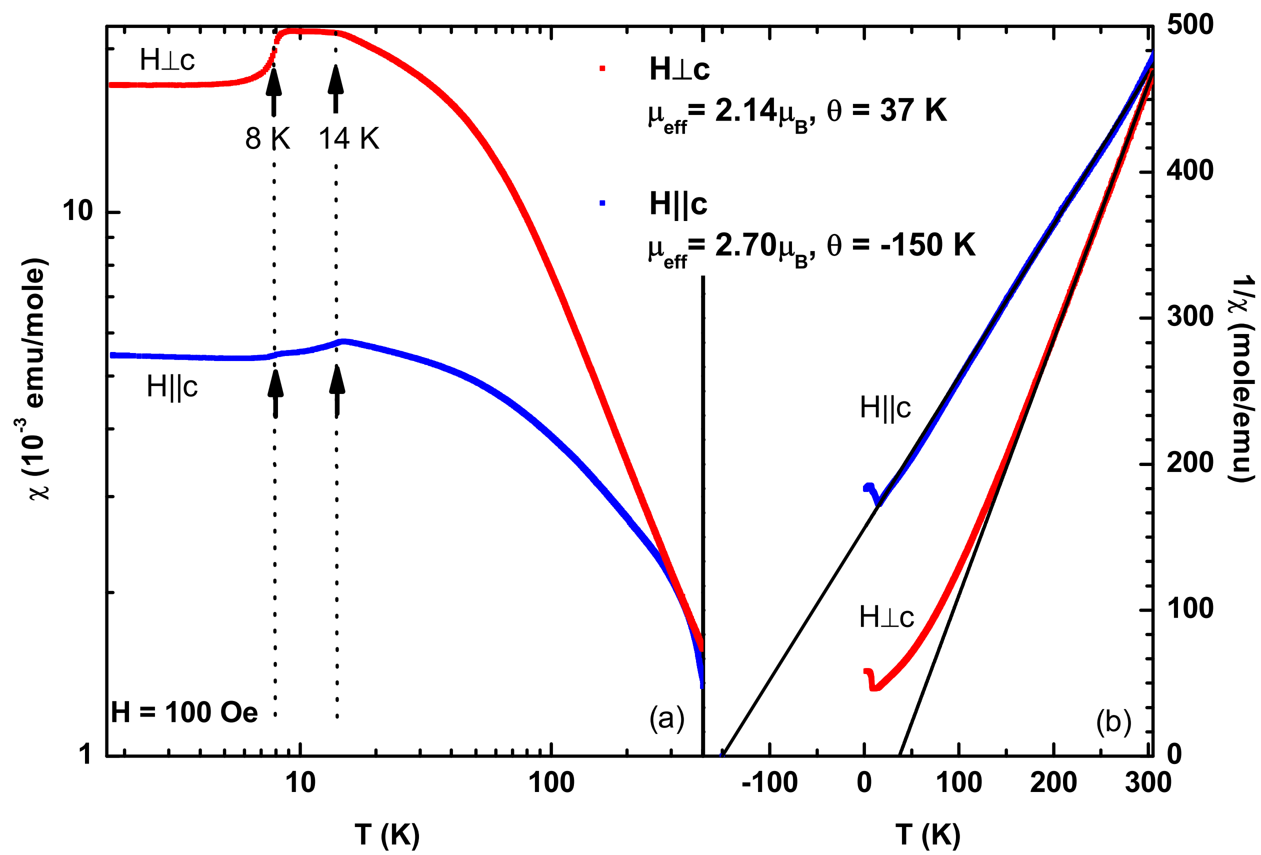


A. Banerjee *et al.*, arXiv:1504:08037

Experiments: α-$RuCl_3$

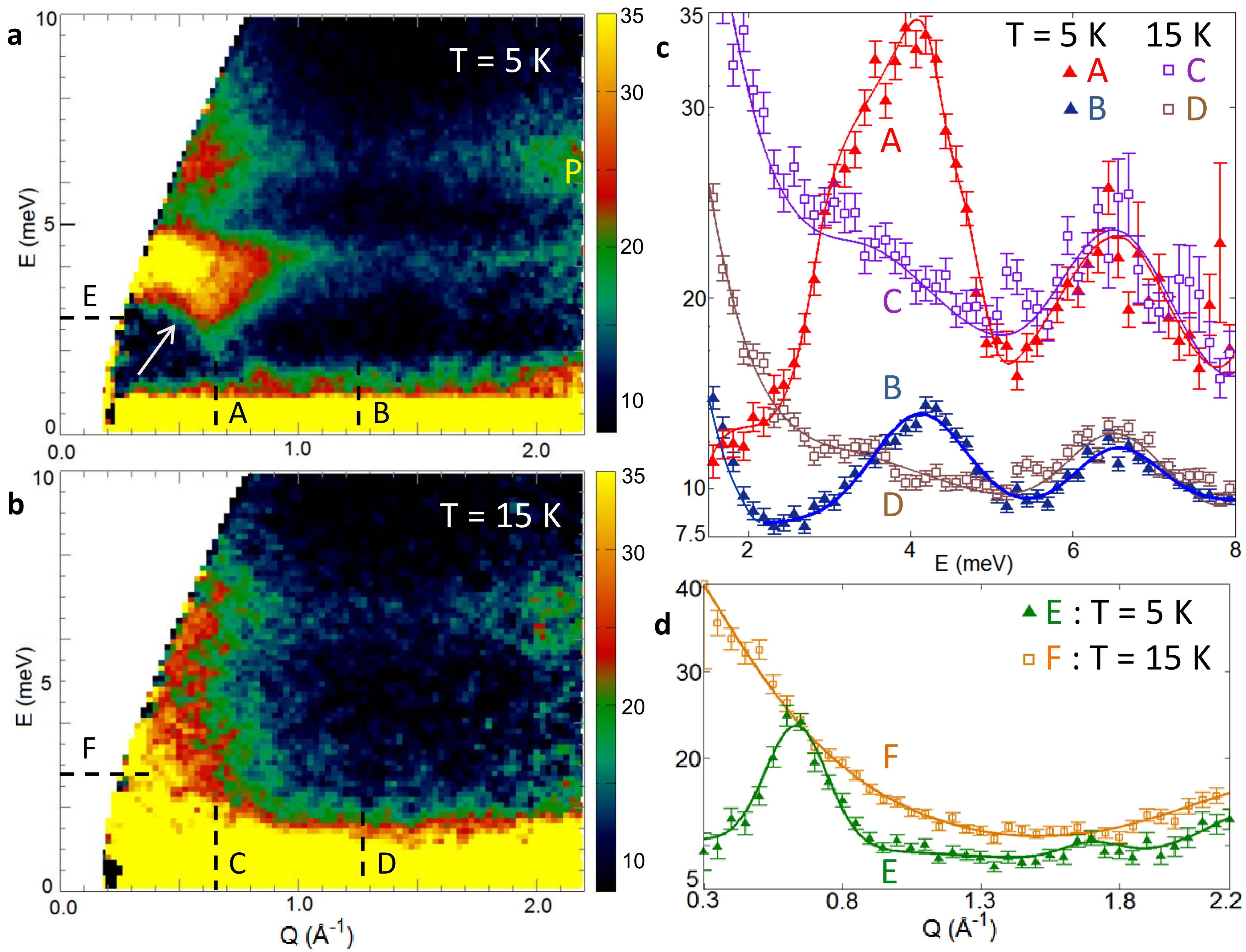


J. A. Sears *et al.*, 2015



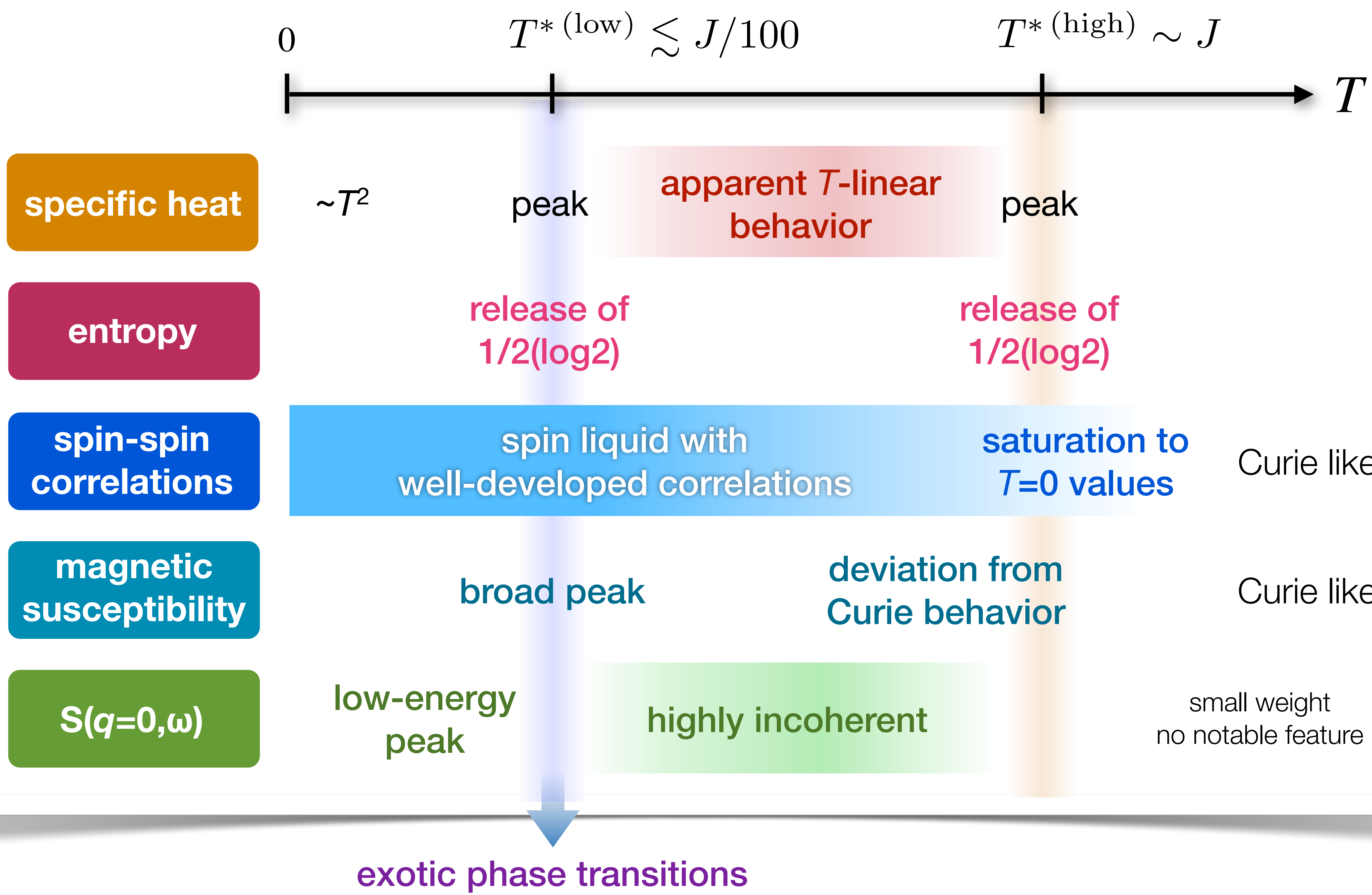
M. Majumder *et al.*, 2015

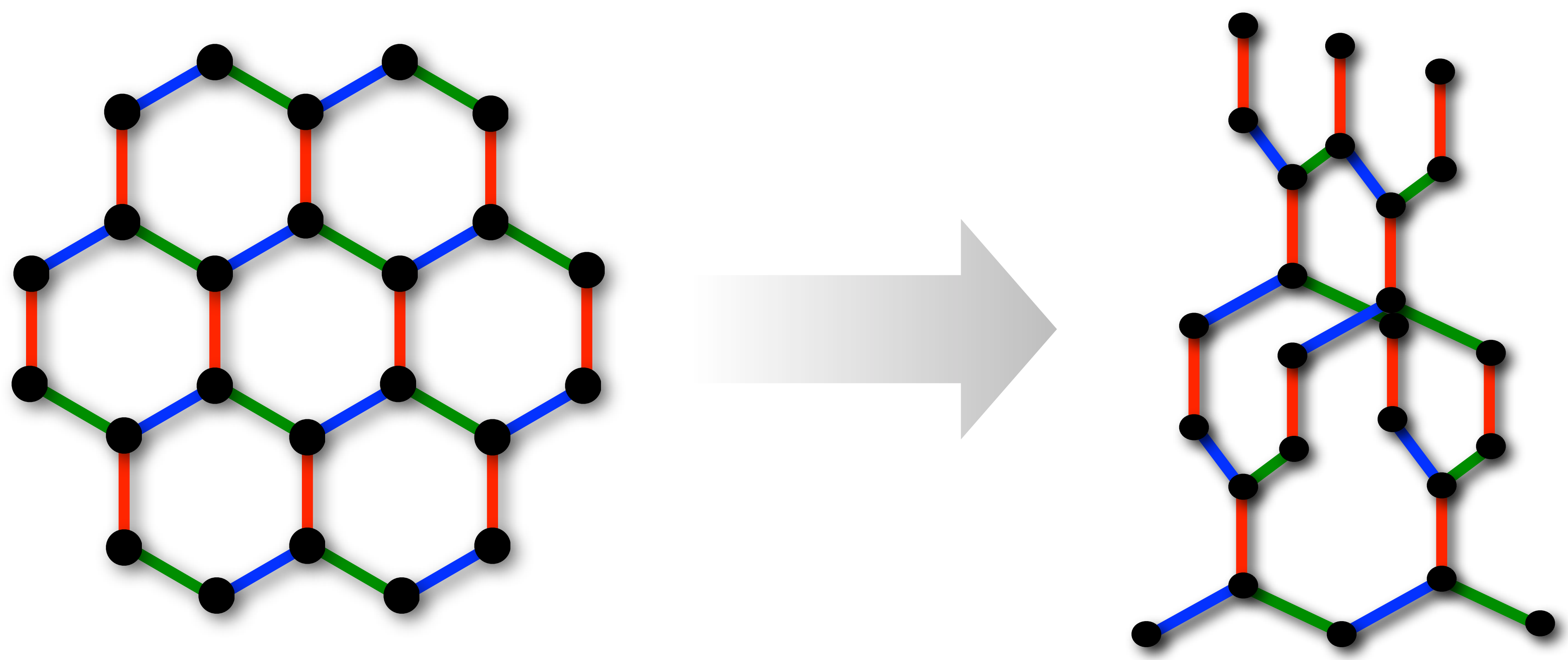
Experiments: α-$RuCl_3$



A. Banerjee *et al.*, arXiv:1504:08037

Diagnostic of Majorana



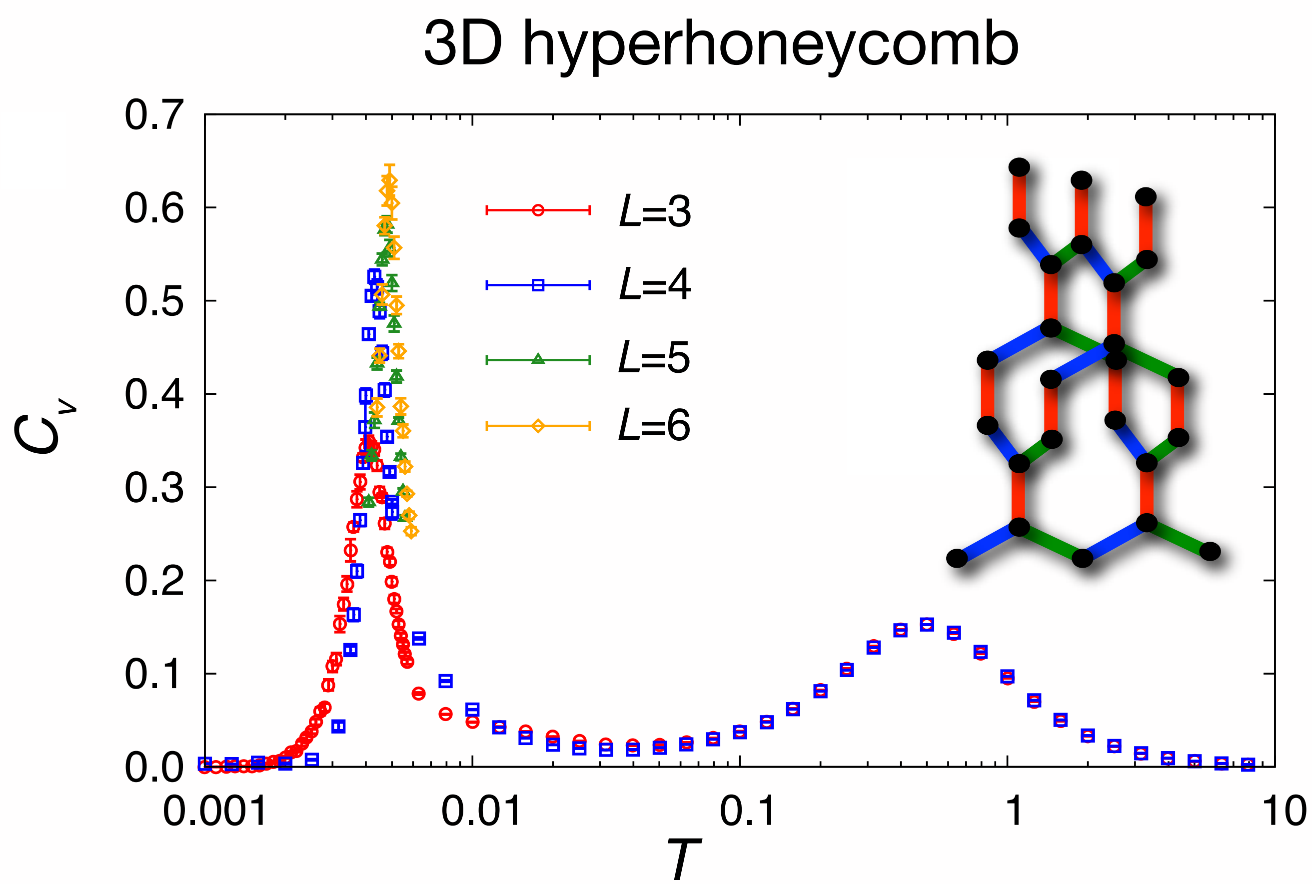


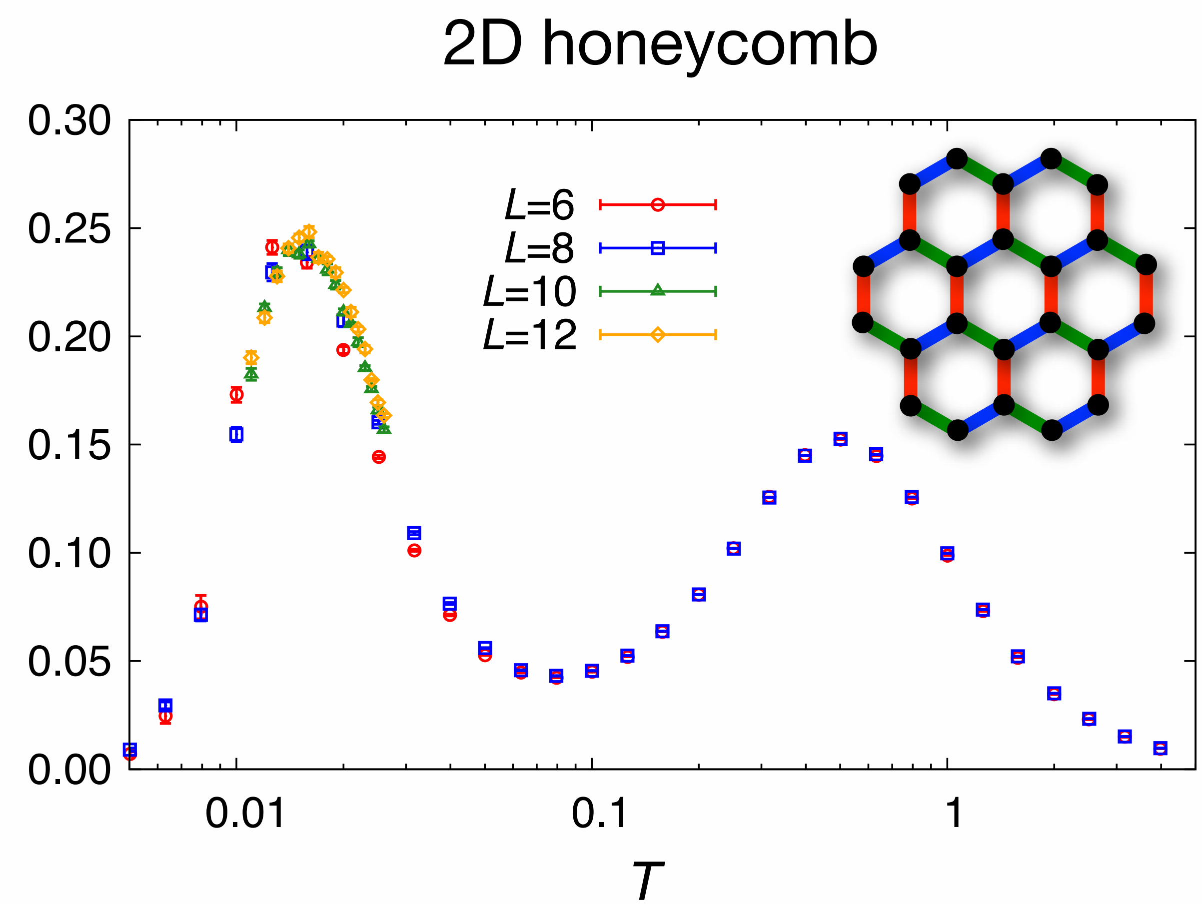
Finite-T phase transition in 3D

Proliferation of flux loops

J. Nasu, M. Udagawa, and Y. Motome, Phys. Rev. Lett. **113**, 197205 (2014)

Comparison between 3D and 2D





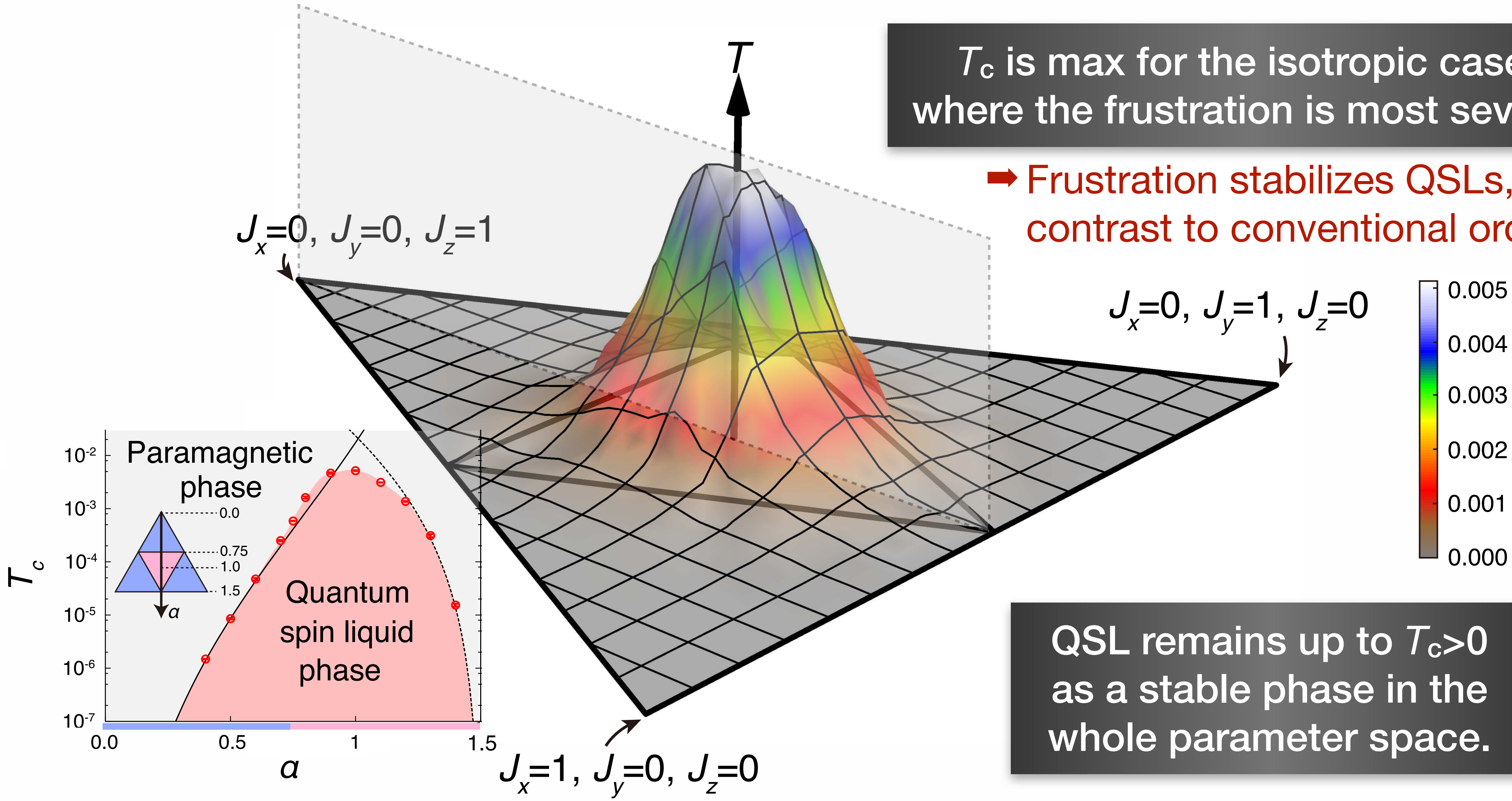
sharp peak growing and becoming narrower as the system size increases

➡ sign of a phase transition

broad peak almost independent of the system sizes

➡ just a crossover

Phase diagram in 3D



T_c is max for the isotropic case, where the frustration is most severe.

➡ Frustration stabilizes QSLs, in contrast to conventional orders.

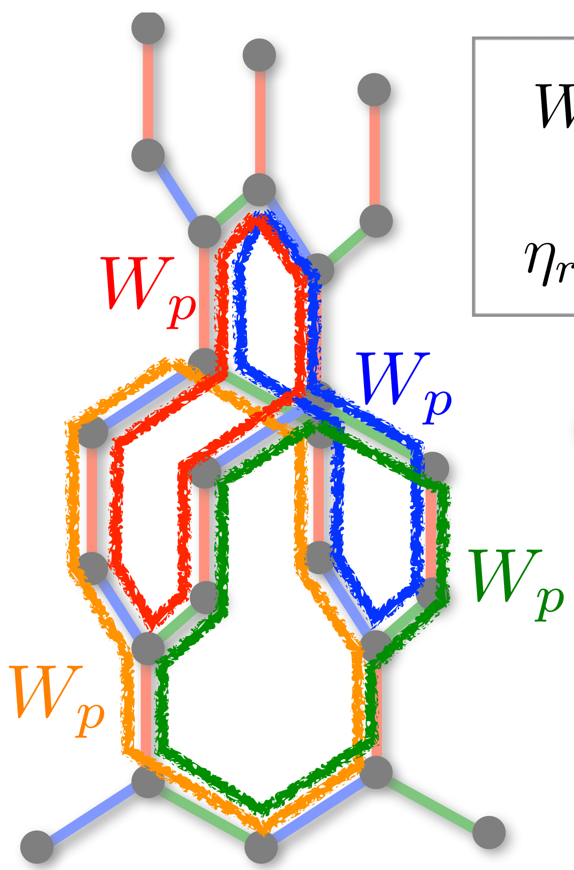
QSL remains up to $T_c>0$ as a stable phase in the whole parameter space.

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

➡ no adiabatic connection, qualitatively different from conventional fluids

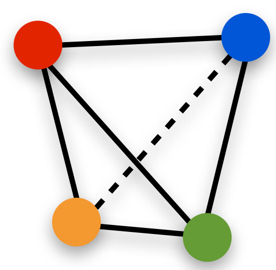
What is this phase transition?

- *difference from 2D*: local conserved quantities W_p form closed objects

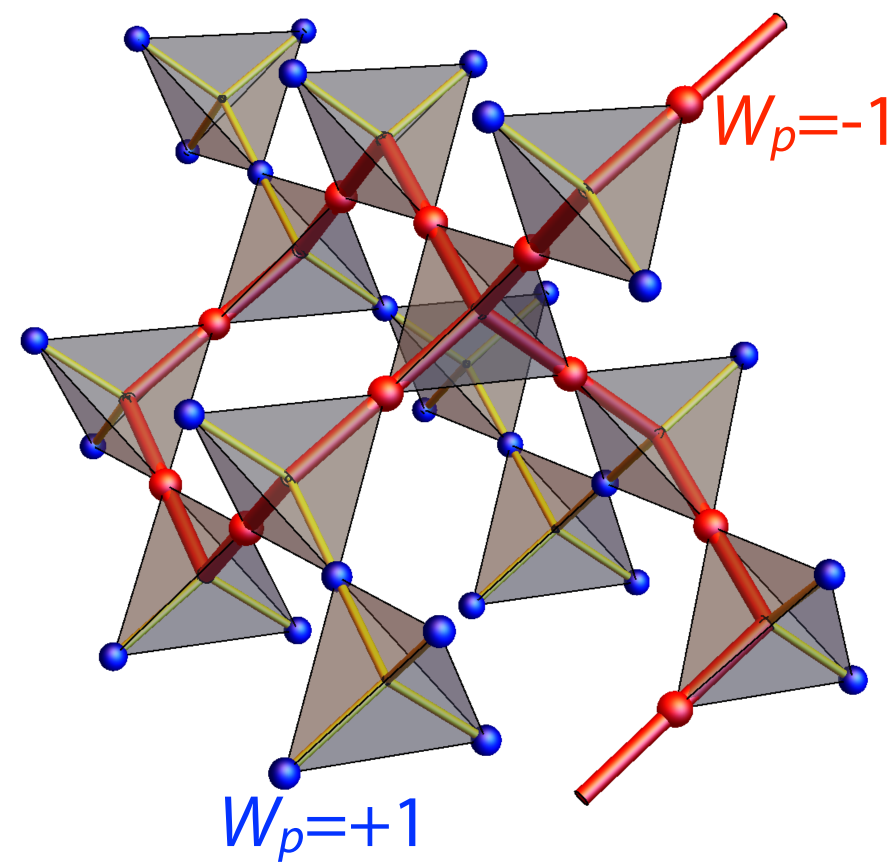


$$W_p = \prod_{r \in p} \eta_r$$

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



$$W_p W_p W_p W_p = 1$$



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

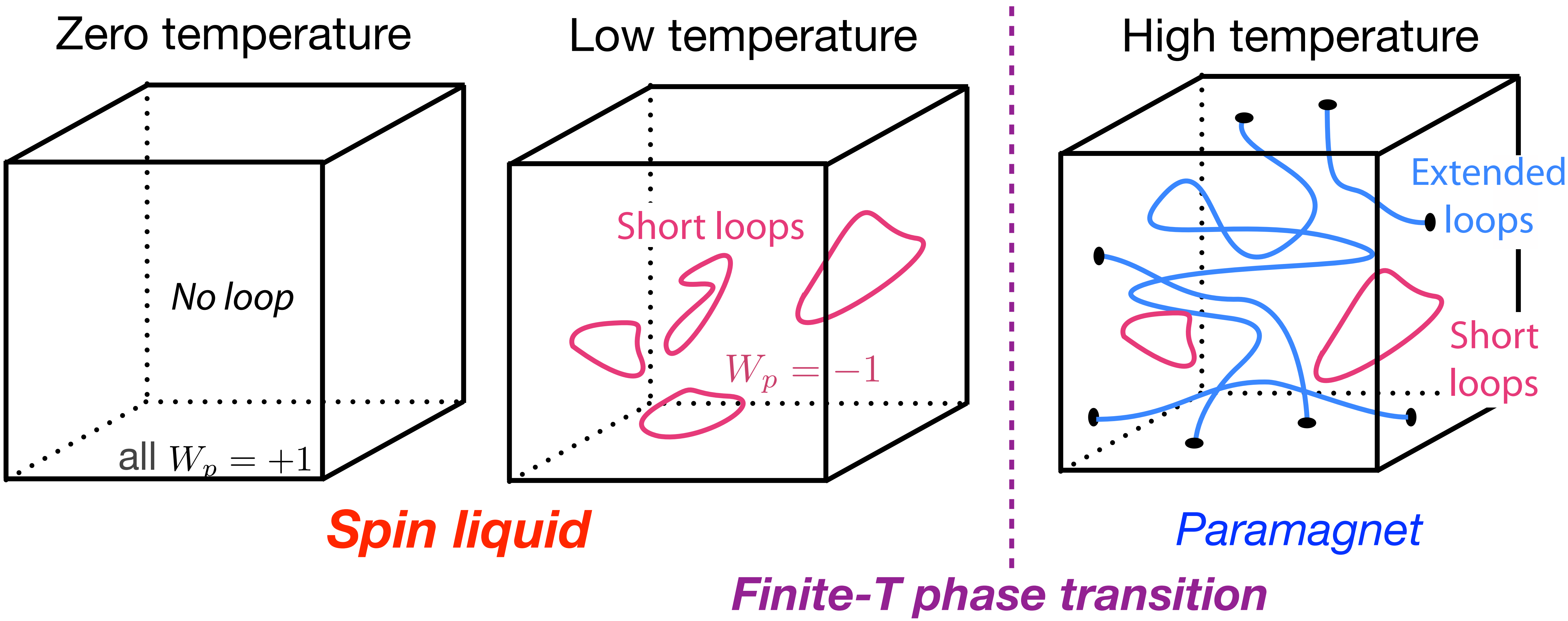
cf.) spin ice: soft constraint, only "2-in 2-out", no intersection

local constraint
(hard constraint by *S*=1/2 algebra)

excited states are given by emergent loops of flipped W_p

Proliferation of excited loops

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

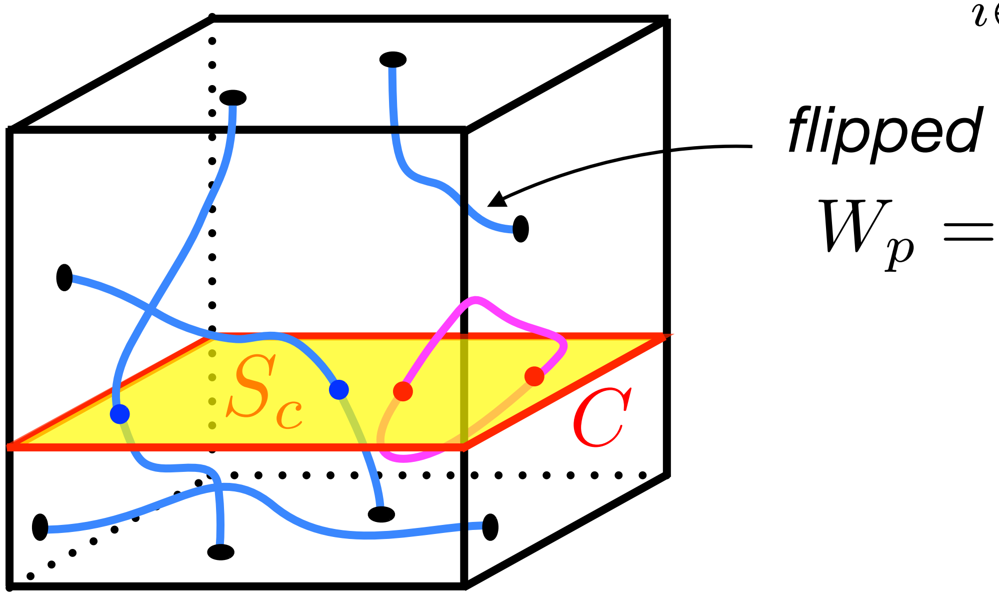


"confinement-deconfinement" type phase transition?

cf. 3D Z_2 lattice gauge theory

Characterization by Wilson loop

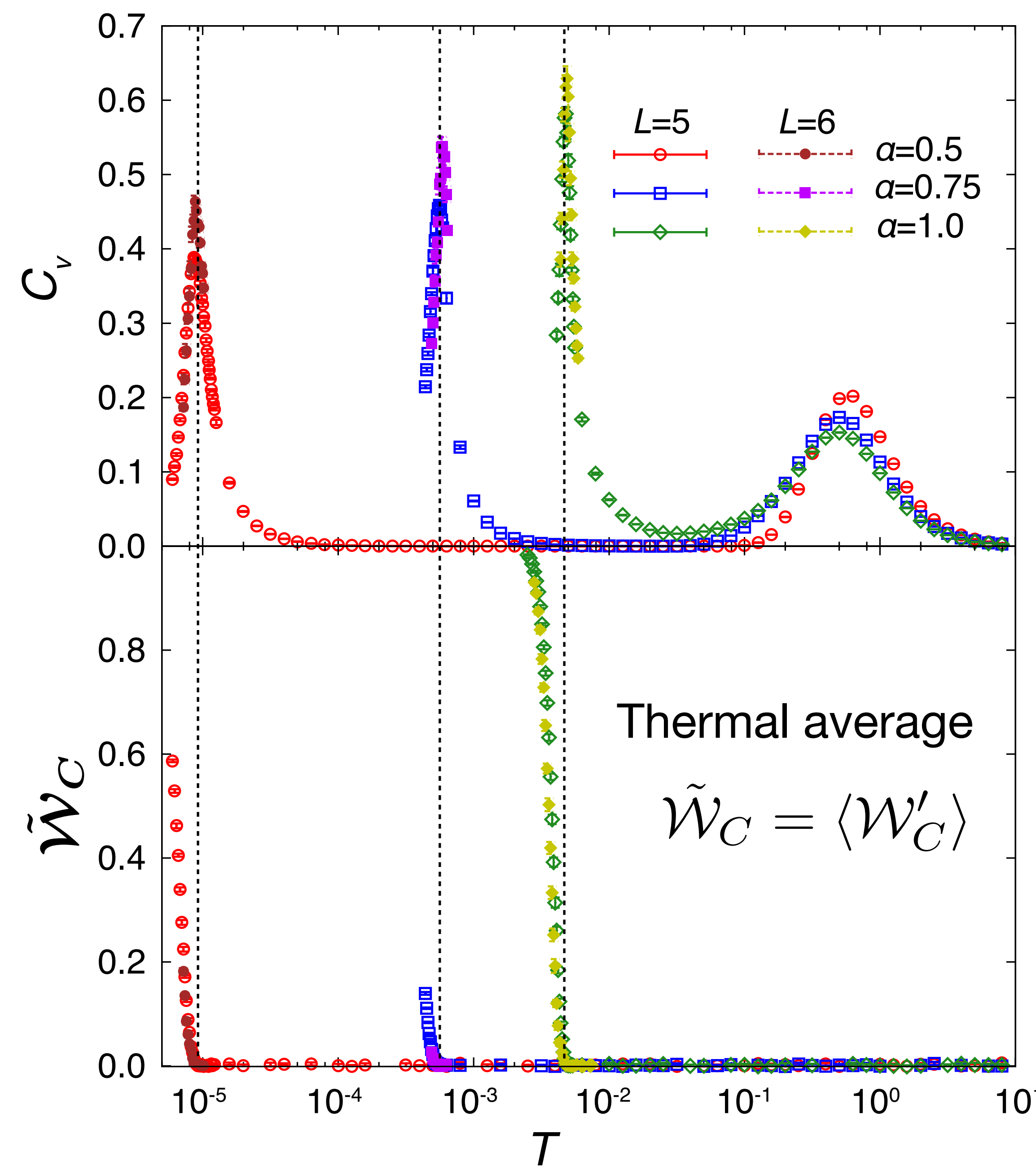
Loop operator (Wilson loop): $\mathcal{W}_C = \prod_{i \in C} \sigma_i^{l_i}$



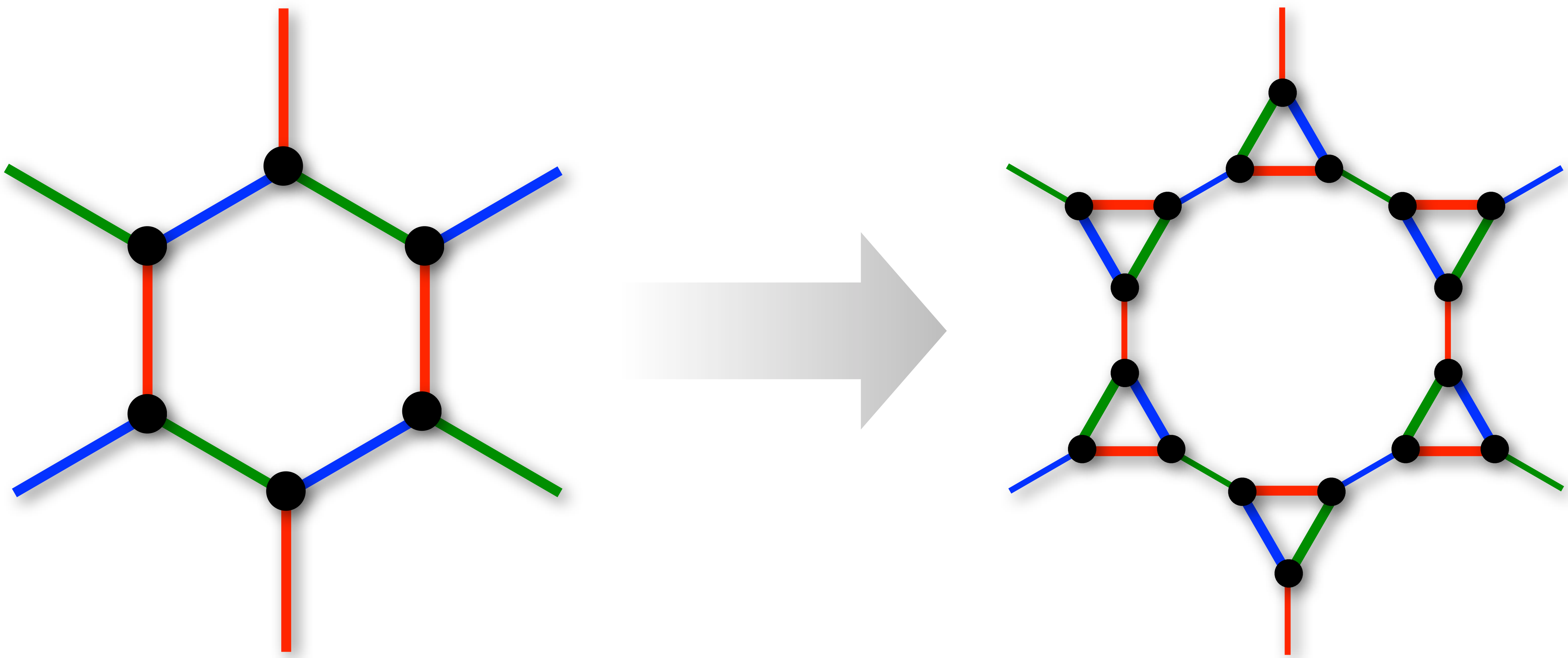
$$\mathcal{W}_C = -\prod_{p \in S_C} W_p = -\prod_{r \in C} \eta_r \equiv -\mathcal{W}'_C$$

Extended loops : $\mathcal{W}_C = +1$ or -1 ➡ $\tilde{\mathcal{W}}_C = \langle \mathcal{W}'_C \rangle = 0$

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



Wilson loop acts as an order parameter in both gapped and gapless regions.

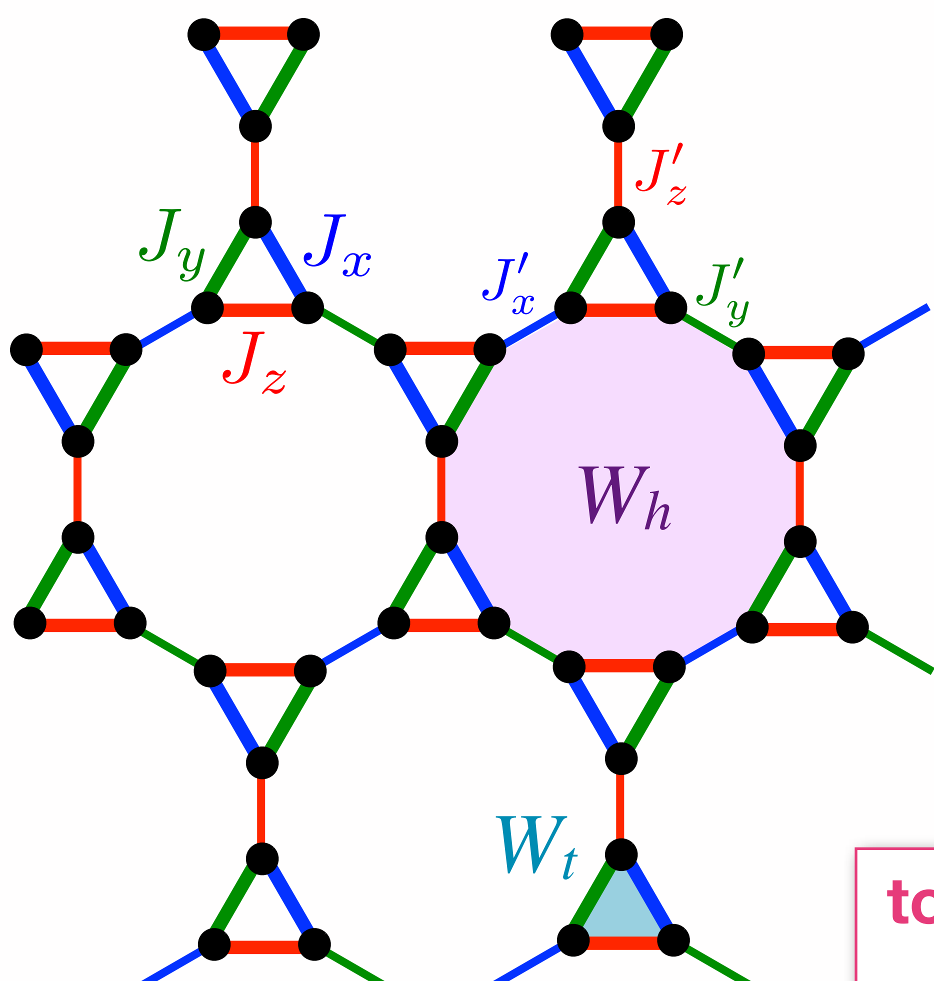


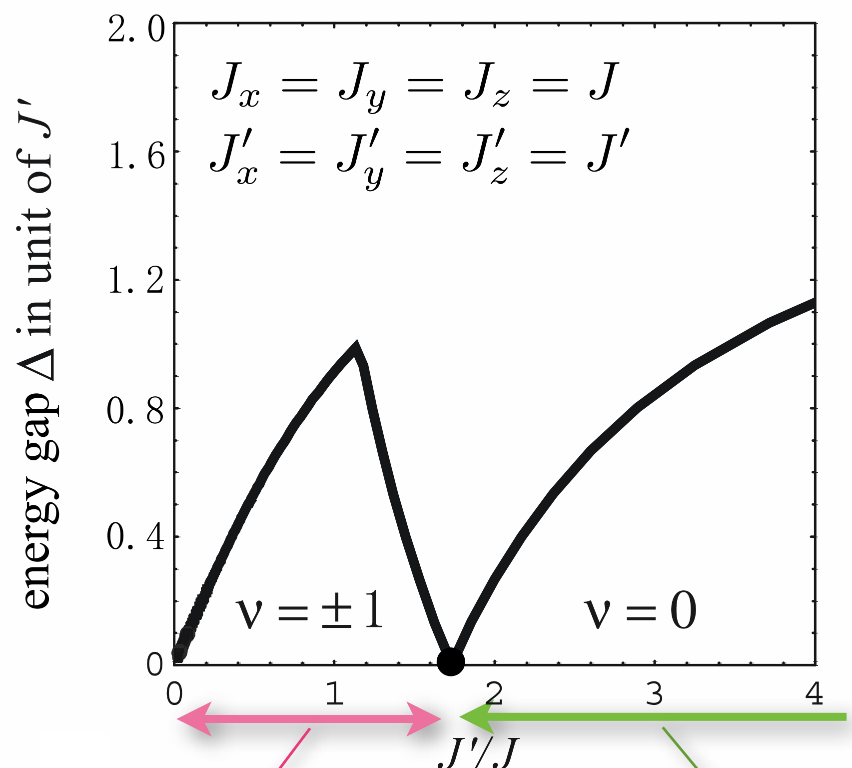
Finite-*T* phase transition in chiral spin liquids

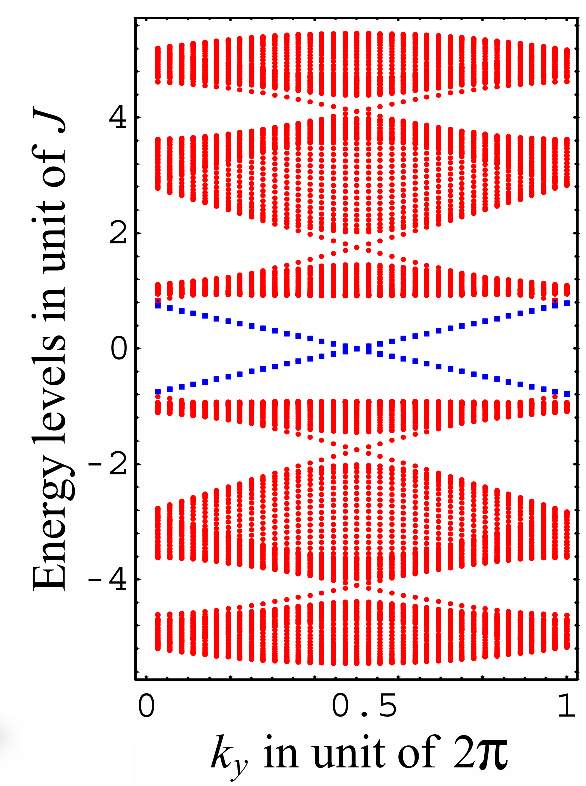
J. Nasu and Y. Motome, preprint (arXiv:1506.01514), accepted by Phys. Rev. Lett.

Chiral spin liquid in Kitaev-type models

- Kitaev-type model with odd-sites plaquettes will possess a chiral spin liquid ground state with time-reversal symmetry breaking (A. Kitaev, 2006)
- exact solution for a variant of the Kitaev model on a decorated honeycomb lattice (3-12 star lattice) (H. Yao and S. A. Kivelson, 2007)



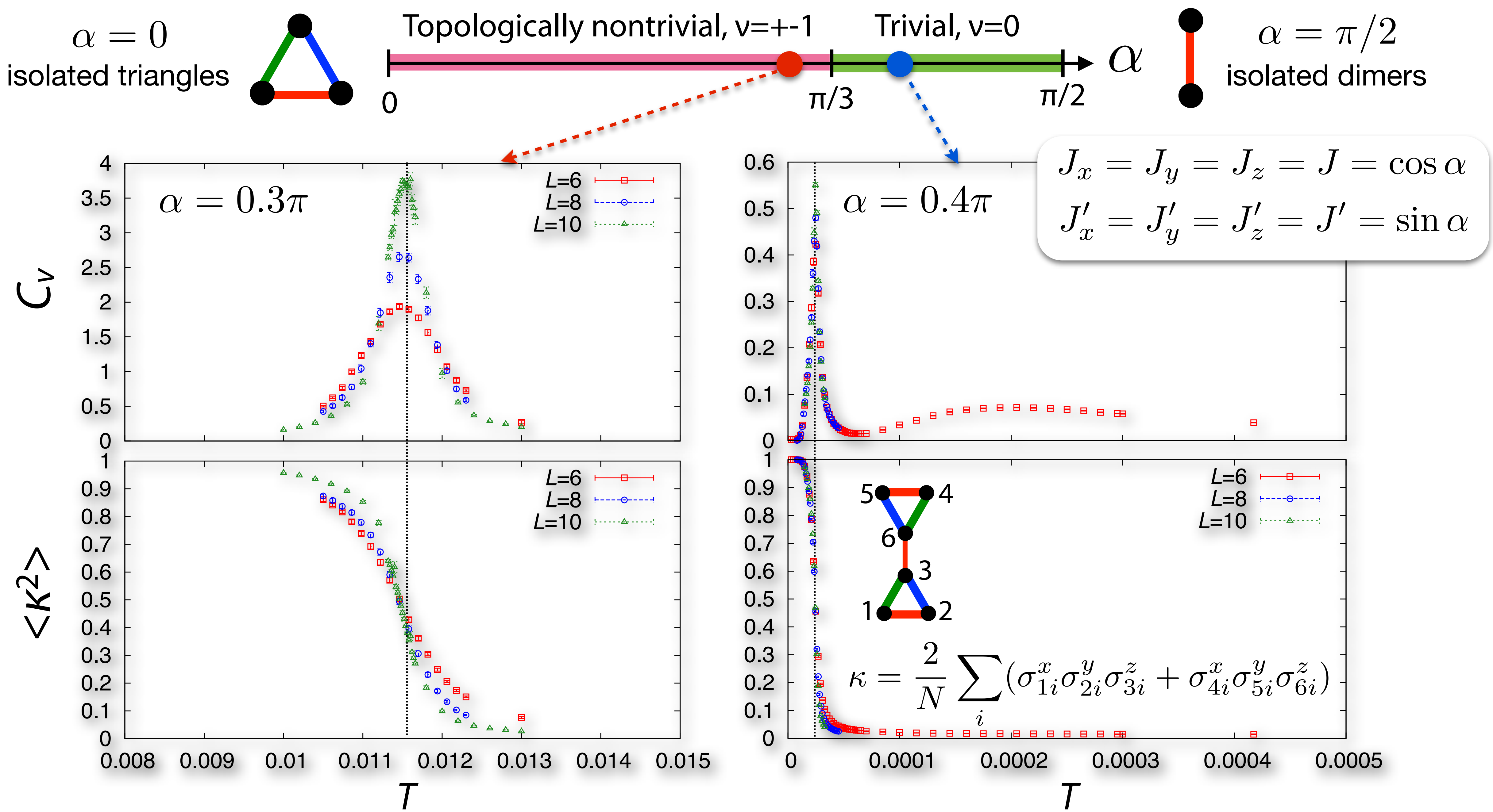




topologically nontrivial
(non-Abelian anyons)

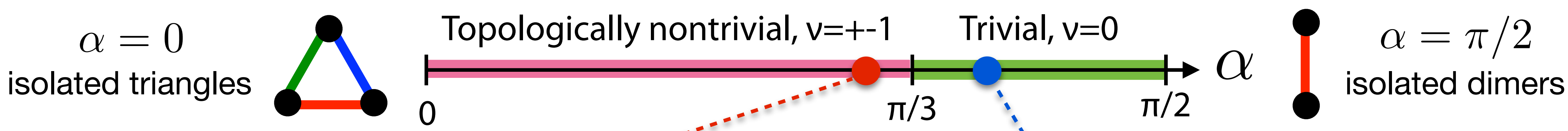
topologically trivial
(Abelian anyons)

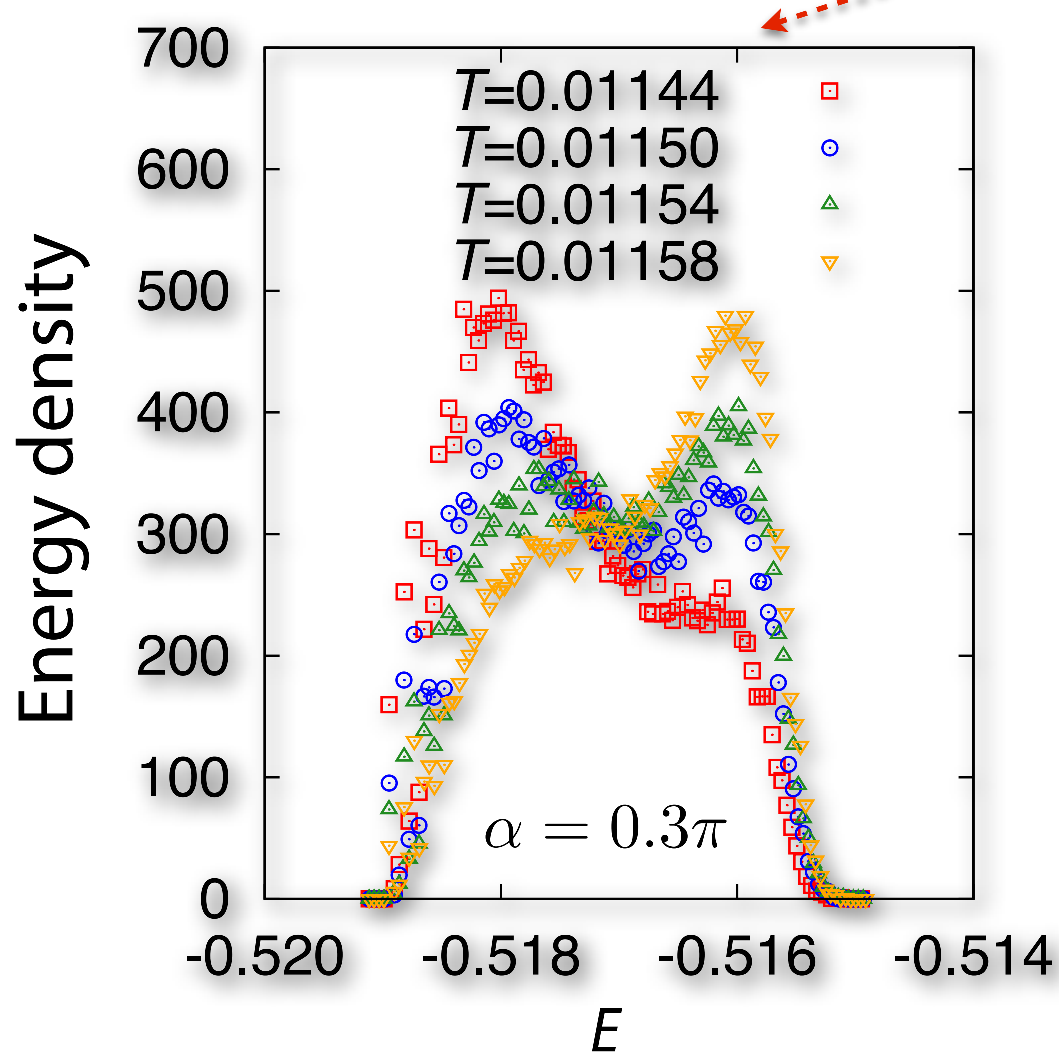
Specific heat and chirality



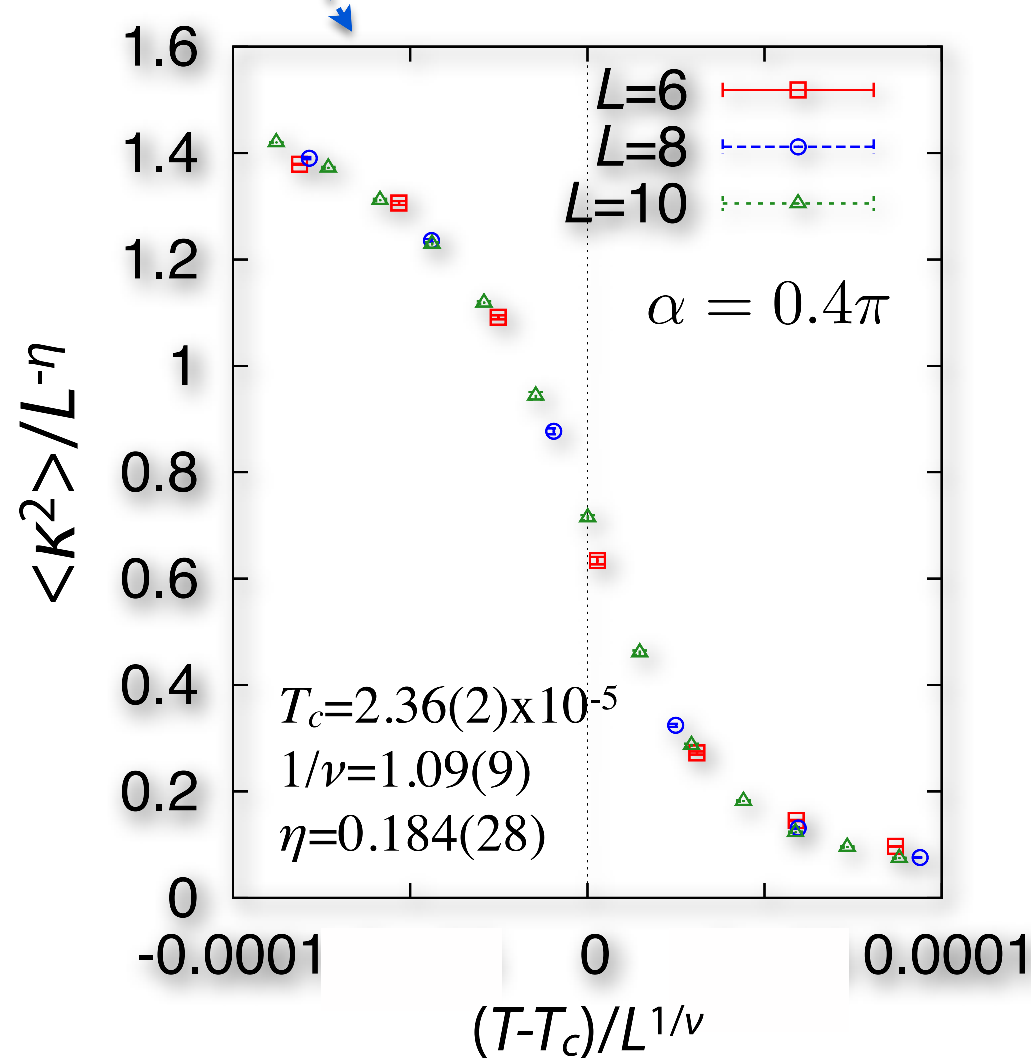
phase transition at a finite temperature associated with chiral ordering

Nature of phase transitions





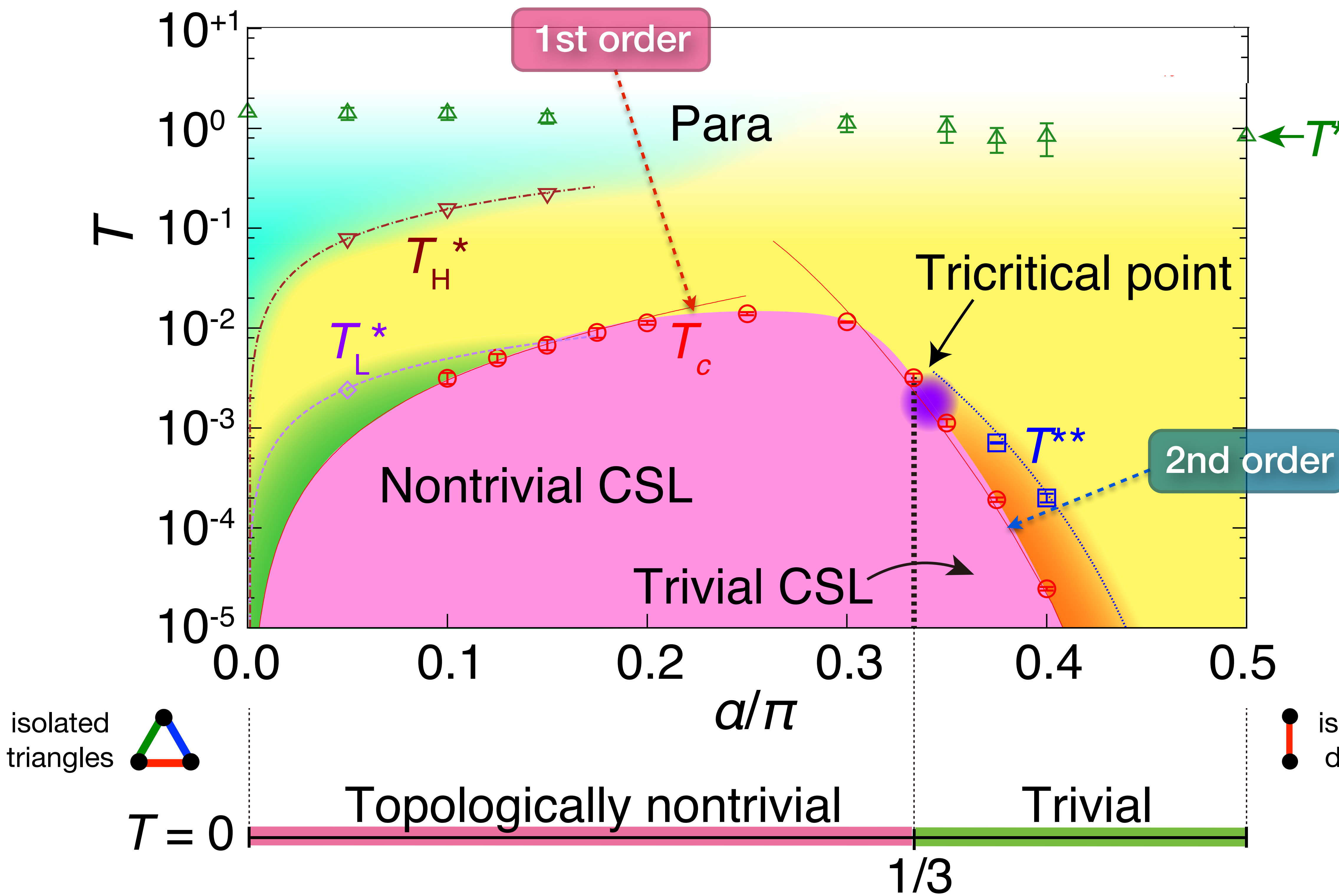
first-order transition



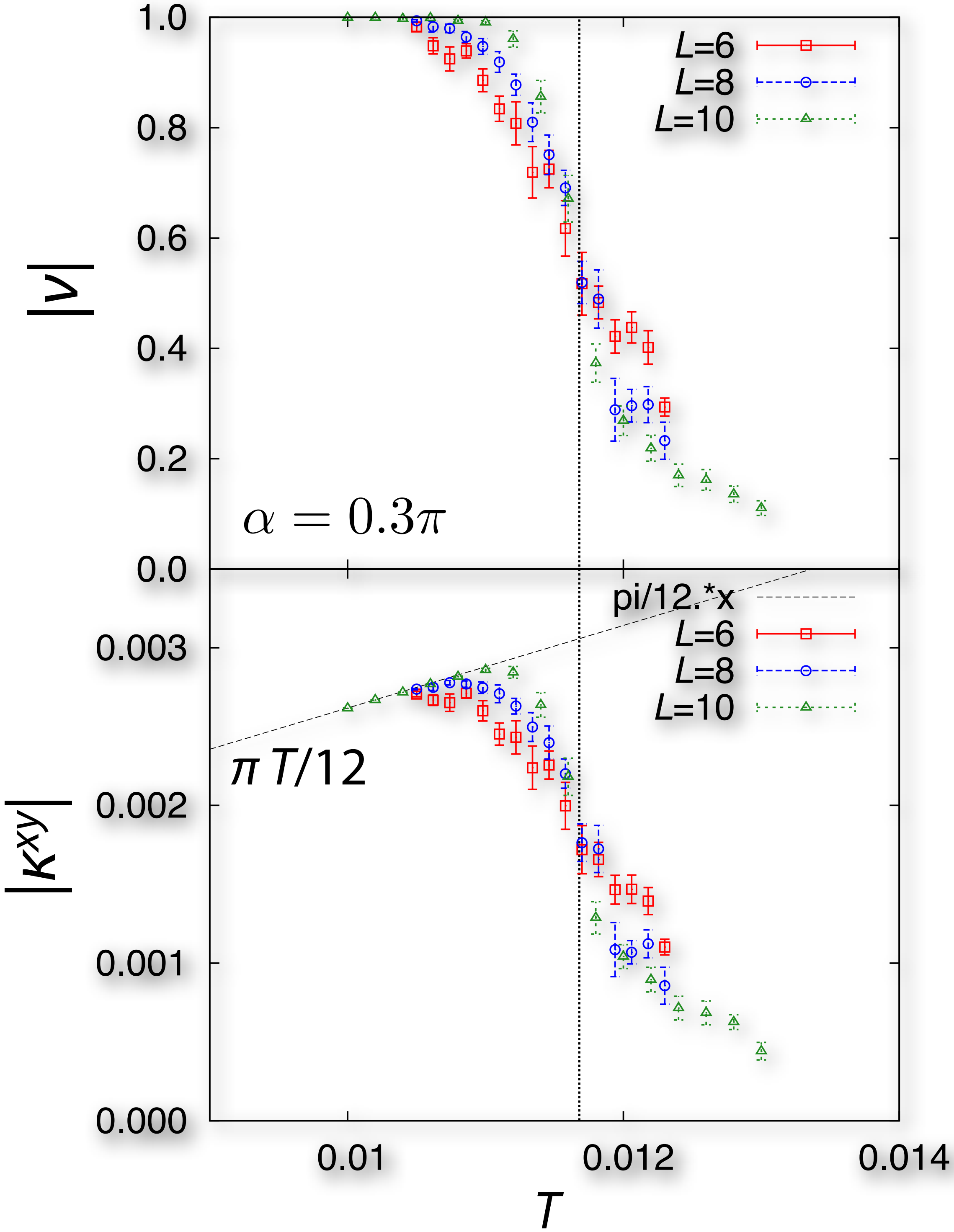
second-order transition

2D Ising universality class

Phase diagram



Topological quantities



- "Chern number"

$$\nu(T) = \frac{4\pi}{V} \sum_{n,\boldsymbol{k}} f(E_{n\boldsymbol{k}}) \sum_{m \neq n} \mathrm{Im} \frac{\langle u_{n\boldsymbol{k}}|v_x|u_{m\boldsymbol{k}}\rangle \langle u_{m\boldsymbol{k}}|v_y|u_{n\boldsymbol{k}}\rangle}{(\varepsilon_{n\boldsymbol{k}} - \varepsilon_{m\boldsymbol{k}})^2 + \gamma^2}$$

$|u_{n\boldsymbol{k}}\rangle$: eigenstate of the Bloch Hamiltonian

$$\mathcal{H} = \sum_{\boldsymbol{k}} \boldsymbol{c}_{\boldsymbol{k}}^{\dagger} H_{\boldsymbol{k}} \boldsymbol{c}_{\boldsymbol{k}} = \sum_{n:\mathrm{half}} \sum_{\boldsymbol{k}} |\varepsilon_{n\boldsymbol{k}}| (2 f_{n\boldsymbol{k}}^{\dagger} f_{n\boldsymbol{k}} - 1)$$

10x10 supercell and γ=0.01

- thermal Hall conductance

$J_{\mathrm{Q}}^{x} = -\kappa^{xy} \partial_y T$: thermal current

$$\kappa^{xy}(T) = \frac{T}{V} \sum_{n,\boldsymbol{k}} c_2(E_{n\boldsymbol{k}}) \sum_{m \neq n} \mathrm{Im} \frac{\langle u_{n\boldsymbol{k}}|v_x|u_{m\boldsymbol{k}}\rangle \langle u_{m\boldsymbol{k}}|v_y|u_{n\boldsymbol{k}}\rangle}{(\varepsilon_{n\boldsymbol{k}} - \varepsilon_{m\boldsymbol{k}})^2 + \gamma^2}$$

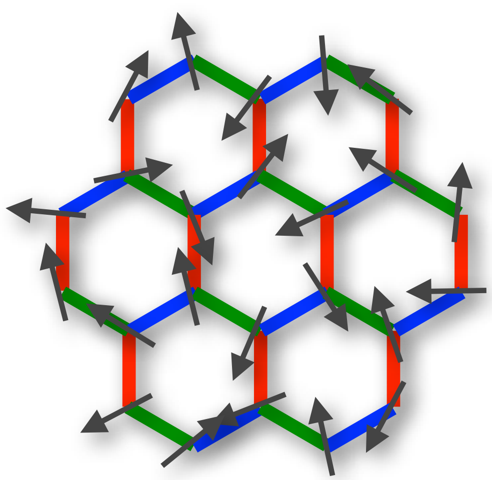
$$c_2(E_{n\boldsymbol{k}}) = \int_{E_{n\boldsymbol{k}}}^{\infty} dE (\beta E)^2 (-f'(E))$$

J. M. Luttinger, 1964; C. L. Kane and M. P. A. Fisher, 1996;
A. Cappelli et al., 2001; T. Qin et al., 2011;
H. Sumiyoshi and S. Fujimoto, 2013

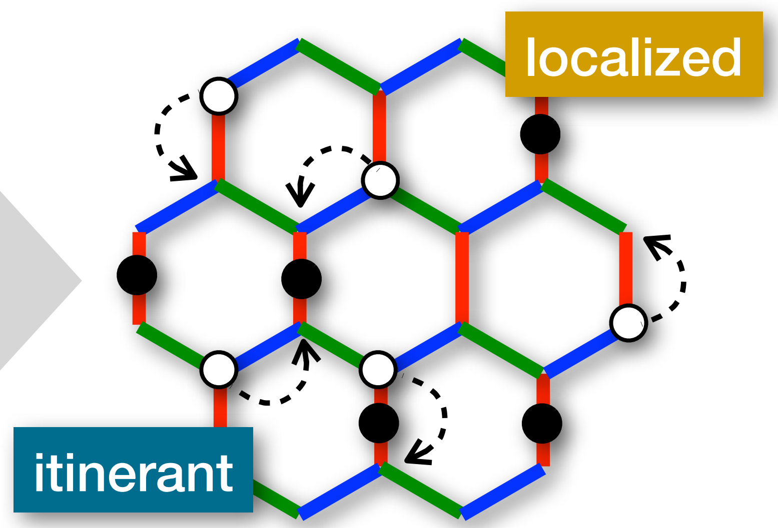
Summary

Kitaev-type localized spin systems may offer a good hunting place for Majorana fermions!

quantum spins

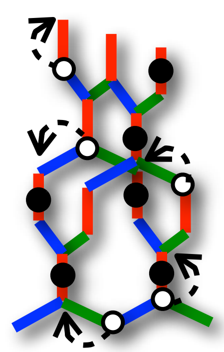


Majorana fermions



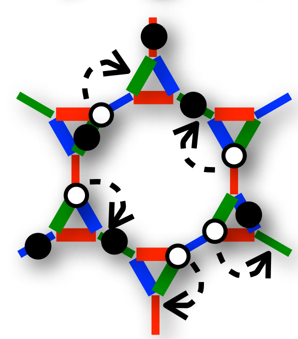
Diagnostic of Majorana

	0	$T^{*\,(\mathrm{low})} \lesssim J/100$		$T^{*\,(\mathrm{high})} \sim J$	T
specific heat	$\sim T^2$	peak	apparent T-linear behavior	peak	
entropy		release of 1/2(log2)		release of 1/2(log2)	
spin-spin correlations	spin liquid with well-developed correlations			saturation to T=0 values	Curie like
magnetic susceptibility		broad peak	deviation from Curie behavior		Curie like
$S(q=0,\omega)$	low-energy peak		highly incoherent		small weight no notable feature



emergent loops

transition by loop proliferation



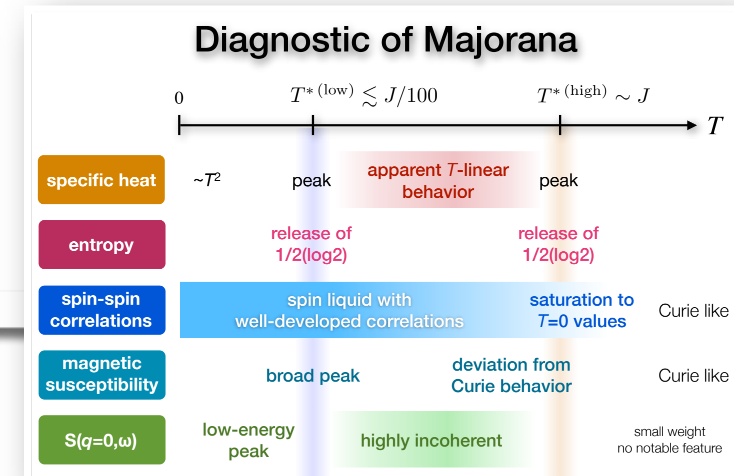
chirality degree of freedom

1st- and 2nd-order transitions

Perspectives

further exploration of Majorana physics in quantum magnets!

- more inputs for/from experiments
- How universal are our findings?
- Any other smoking gun of "Majorana-ness"?



extension to other Kitaev-type QSLs with different topology

- Majorana Fermi surfaces/nodes/Weyl points, ...

M. Hermanns and S. Trebst, 2014
M. Hermanns, K. O'Brien, and S. Trebst, 2015

Methodology: further development of new numerical methods for quantum spin systems by using Majorana fermion representations

- Majorana representation is not unique: many possibilities for each
- exchange interactions beyond Kitaev lead to many-body interactions between Majoranas → many-body techniques for Majorana fermions?