

Gauge-frustrated Kitaev Spin Liquid

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[arXiv:1901.05283](https://arxiv.org/abs/1901.05283)

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NORDITA



Vetenskapsrådet

Outline

Frustration

Kitaev interactions in materials

‘Conventional’ Kitaev spin liquids

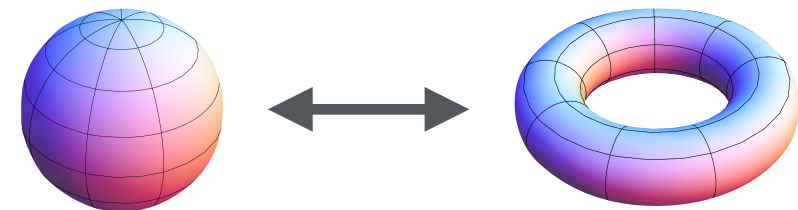
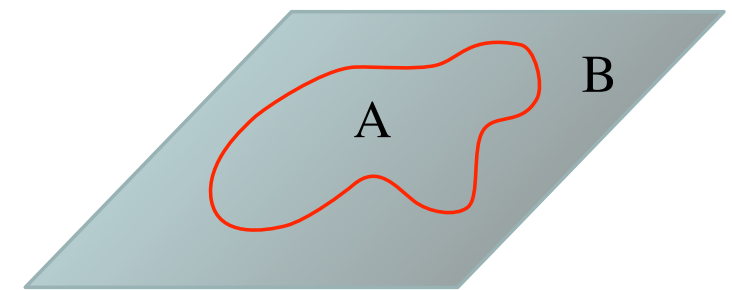
- Solving the Kitaev model
- Majorana metals
- Thermodynamic signatures

‘Gauge frustration’ – geometric frustration in the gauge sector

Thermodynamics

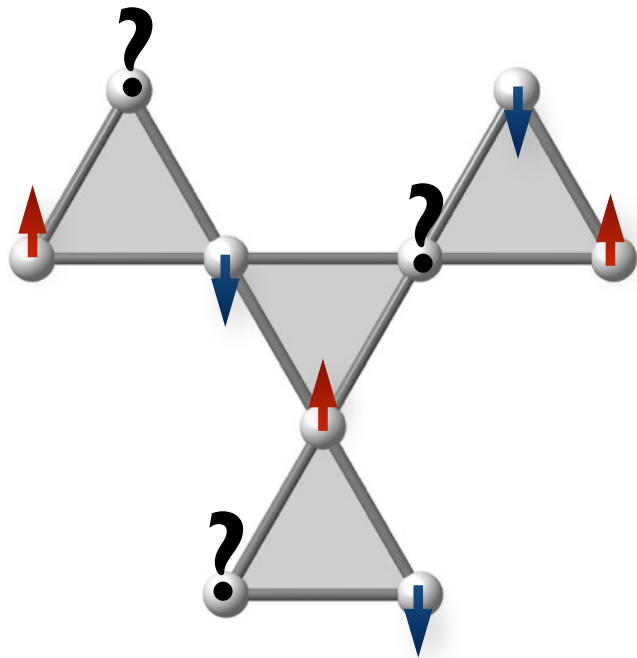
Quantum spin liquids

- ▶ no magnetic order
- ▶ strongly fluctuating spins down to zero temperature
- ▶ no long-range correlations, but long-range entanglement
- ▶ topological ground state degeneracy
- ▶ spin fractionalization
- ▶ **elusive**
 - no experimentally verified candidates (no smoking gun signature)
 - very few theoretical models, where QSL ground state is rigorously established – **Kitaev spin liquids**



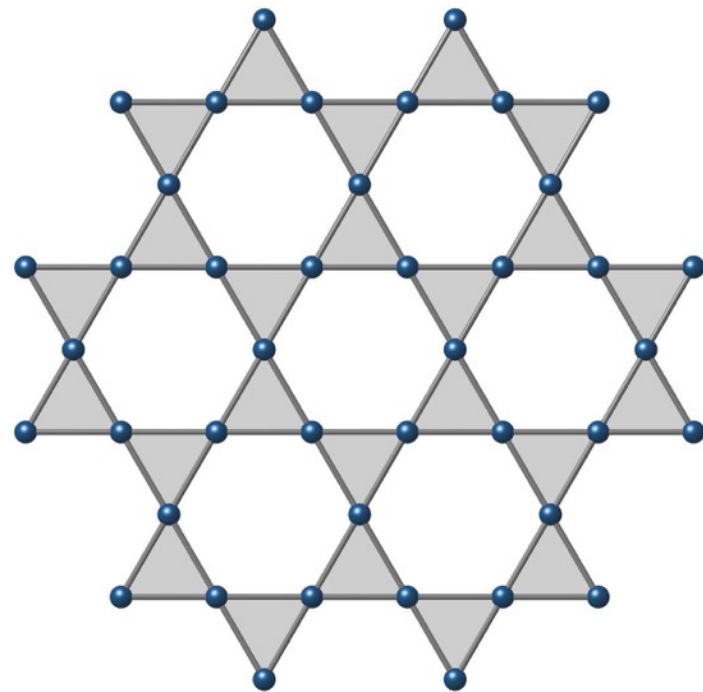
Towards quantum spin liquids – frustration

geometric frustration



Towards quantum spin liquids – frustration

geometric frustration

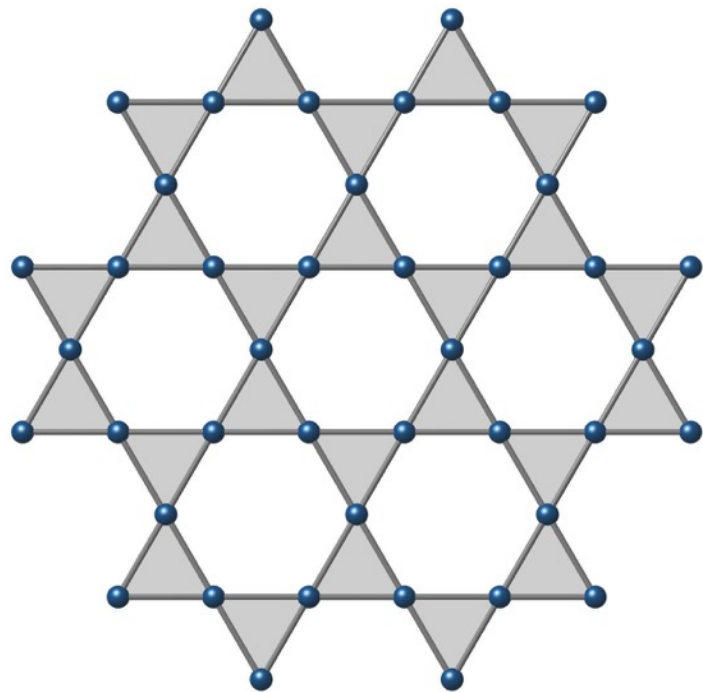


Herbertsmithite
 $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$

Han et al., Nature (2012)

Towards quantum spin liquids – frustration

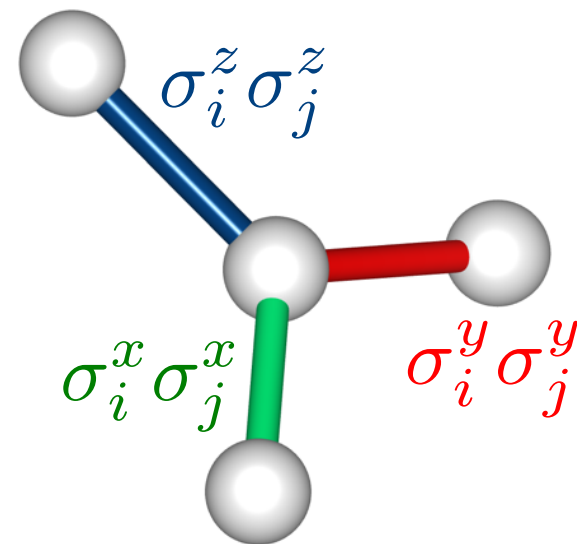
geometric frustration



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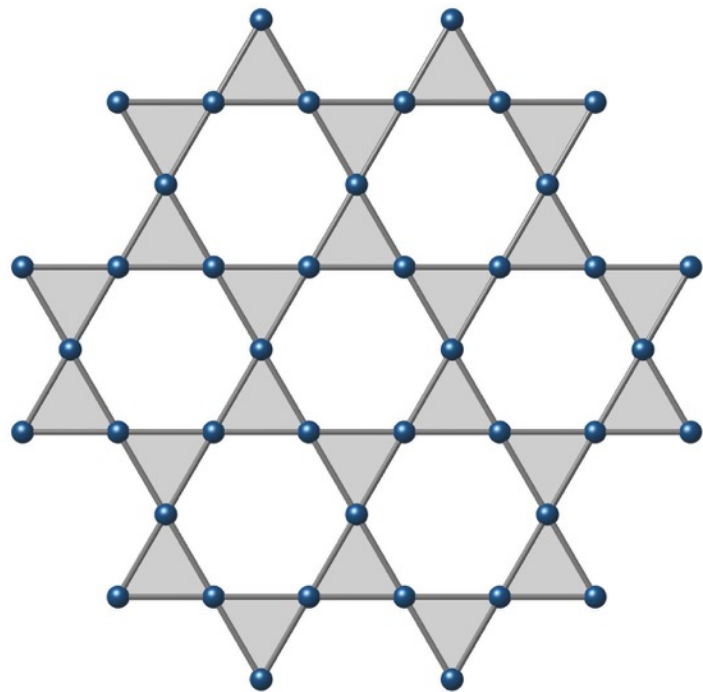
Han et al., Nature (2012)

exchange frustration



Towards quantum spin liquids – frustration

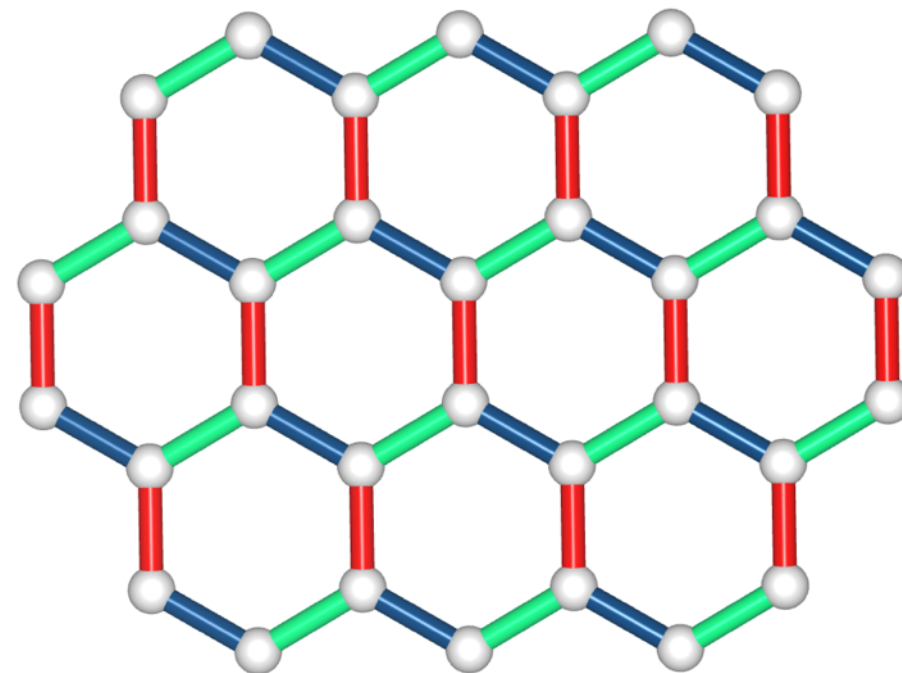
geometric frustration



Herbertsmithite
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Han et al., Nature (2012)

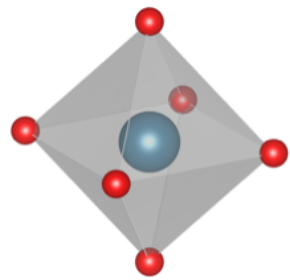
exchange frustration



Kitaev honeycomb model
Iridates

Exchange Frustration in Iridates

G. Jackeli and G. Khaliullin, PRL 102, 017205 (2009)



IrO₆

- Interplay of
- octahedral crystal field
 - spin-orbit coupling
 - e⁻-e⁻ correlations

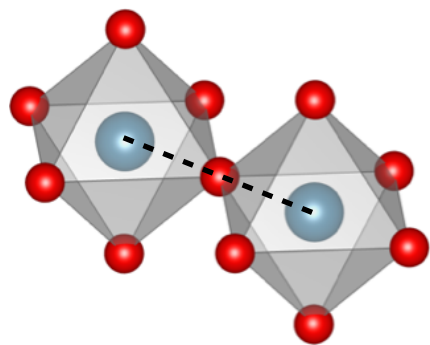


Mott insulator with spin-orbit-entangled spin-1/2 on Ir atom

Heisenberg exchange

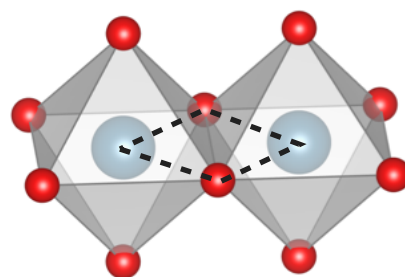
dominant Kitaev exchange

corner-sharing



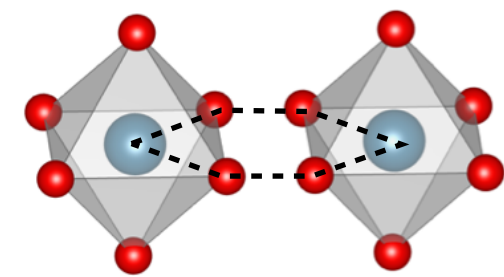
Sr₂IrO₄

edge-sharing



Na₂IrO₃ / Li₂IrO₃

parallel edge-sharing

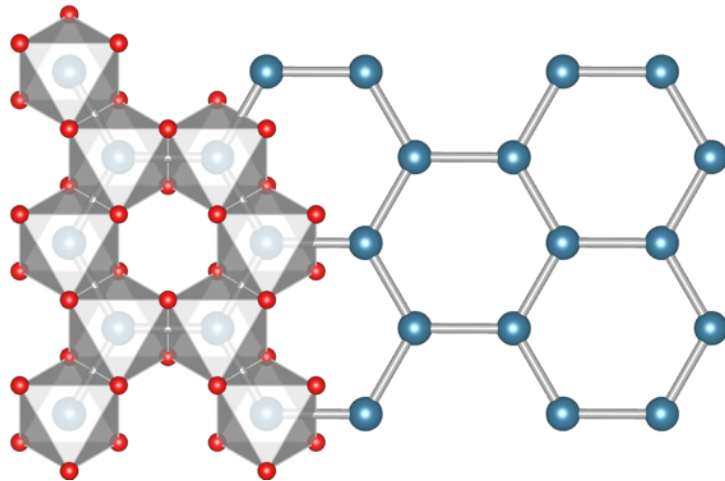


Ba₃IrTi₂O₉

$$H = J_K \sum_{\langle i,j \rangle \in \gamma} \sigma_i^\gamma \sigma_j^\gamma + J_H \sum_{\langle i,j \rangle \in \gamma} \vec{\sigma}_i \vec{\sigma}_j + \Gamma \sum_{\langle i,j \rangle \in \gamma} (\sigma_i^\alpha \sigma_j^\beta + \sigma_i^\beta \sigma_j^\alpha)$$

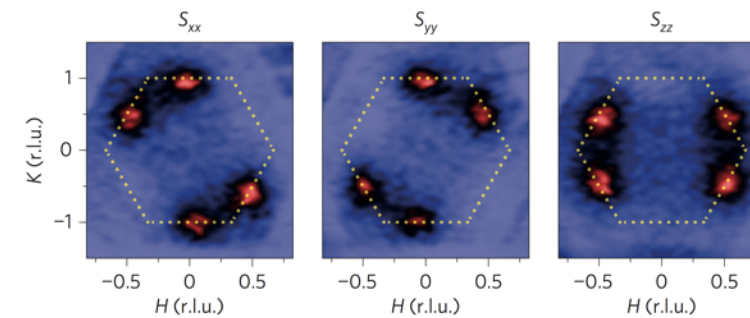
Materials – 2D

honeycomb



Kitaev interaction **dominant**

Chun et al., Nature Physics (2015)



α -Li₂IrO₃,
Na₂IrO₃

Singh et al. PRL (2012)

RuCl₃

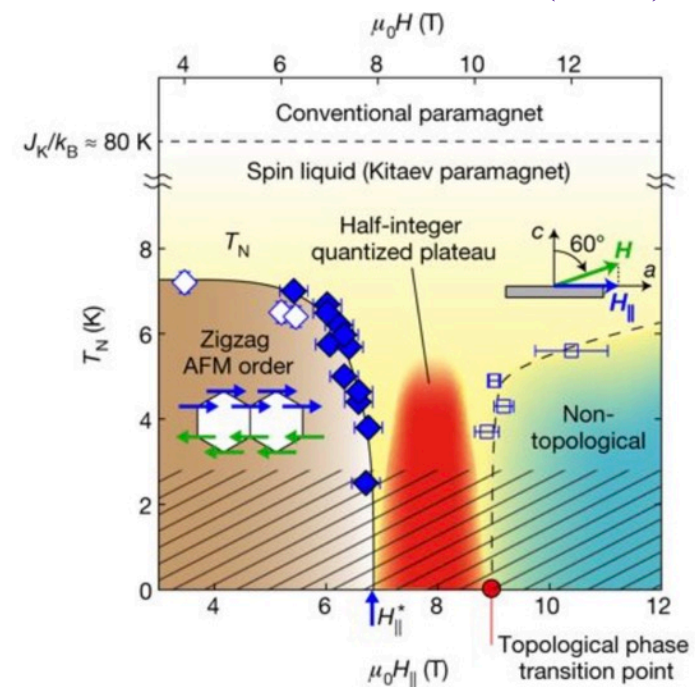
Banerjee et al., Nat. Mat. (2016)

H₃LiIr₂O₆

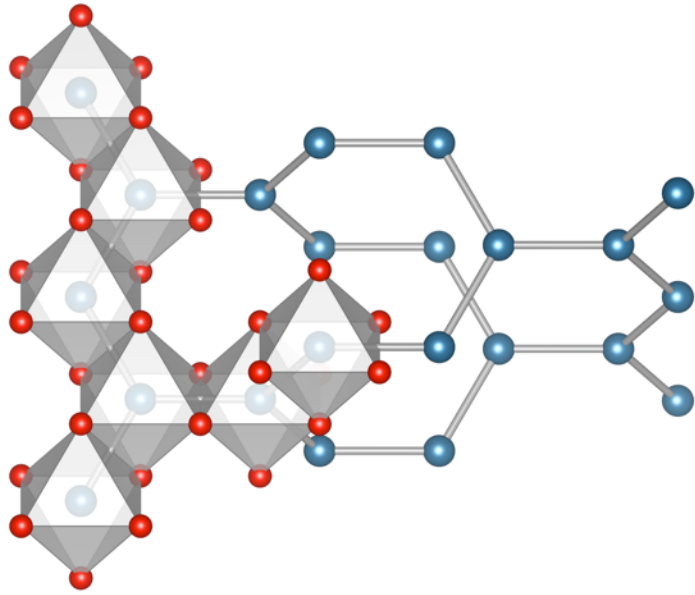
Kitagawa et al. Nature (2018)

quantized thermal Hall conductance

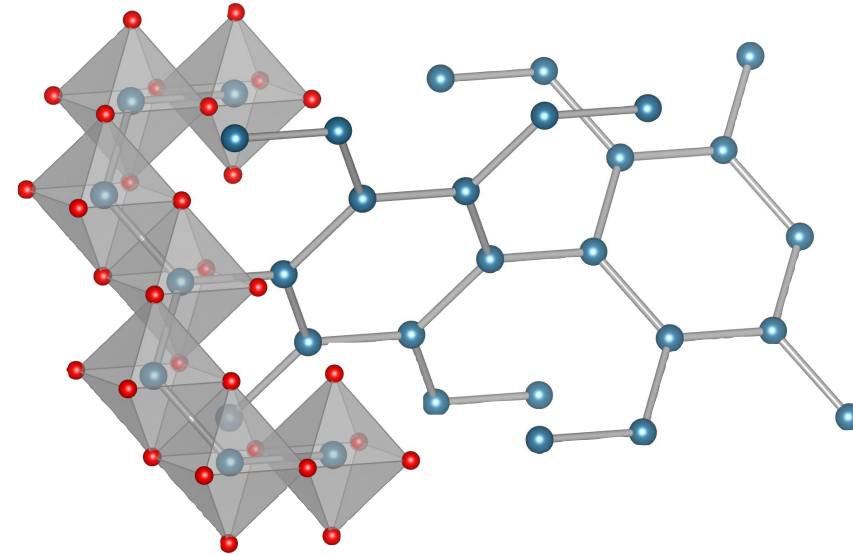
Kasahara et al. Nature (2018)



Materials – 3D



β -Li₂IrO₃ Takayama et al., PRL (2015)



γ -Li₂IrO₃ Modic et al., Nat. Comm. (2014)

Copper-Oxalate Framework

Zhang, J. Am. Chem. Soc. (2018)

→ learn more about **quantum spin liquids in 3D**

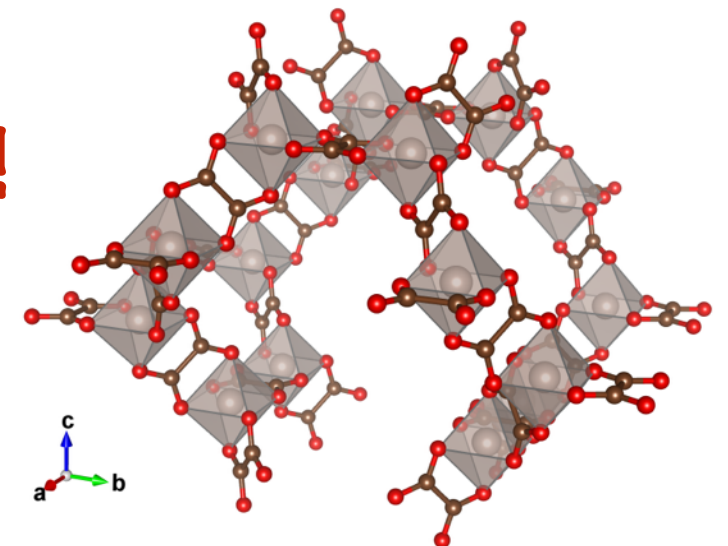
Can we realize many more 3D tri-coordinated lattice structures?

yes!

potential materials: *metal-organic-frameworks*

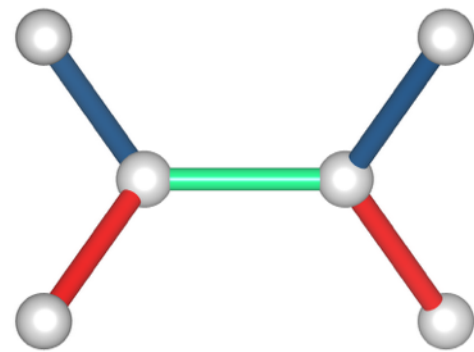
Yamada et al. PRL (2016)

Dwivedi et al. PRB (2017)

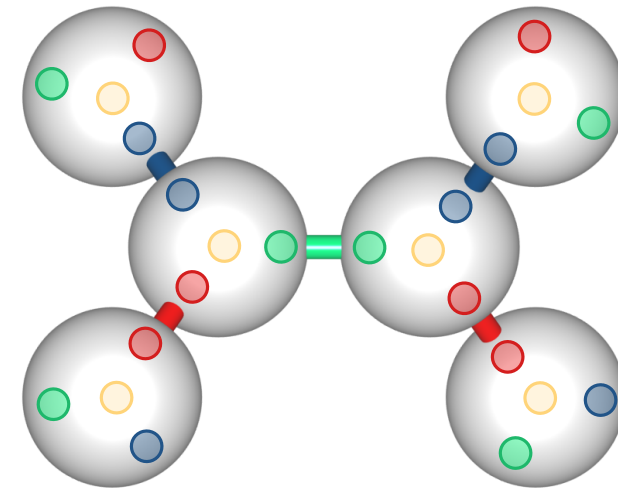


Spin fractionalization and Majorana fermions

A. Kitaev, Annals of Physics (2006)



splitting spins
 $\sigma^\alpha = ia^\alpha c$

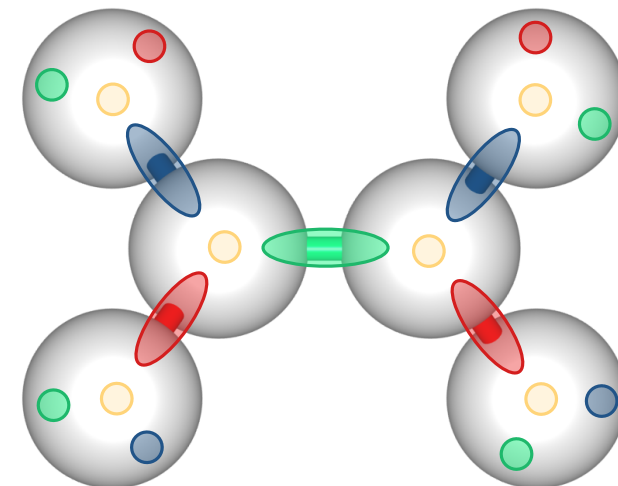


● a^x
● a^y
● a^z
● c

$$H = - \sum_{\gamma\text{-bond}} J_\gamma \sigma_j^\gamma \sigma_k^\gamma$$

joining Majoranas

$$\hat{u}_{jk} = ia_j^\alpha a_k^\alpha$$



◻ $ia^x a^x$
◻ $ia^y a^y$
◻ $ia^z a^z$
● c

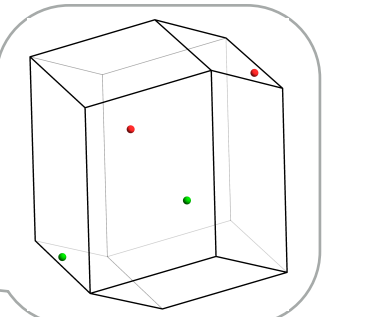
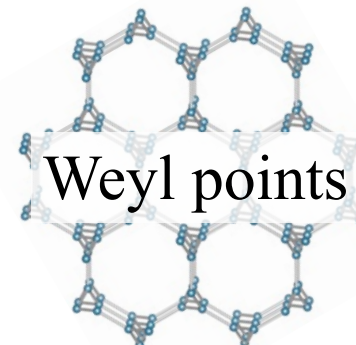
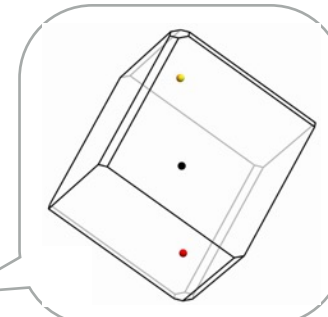
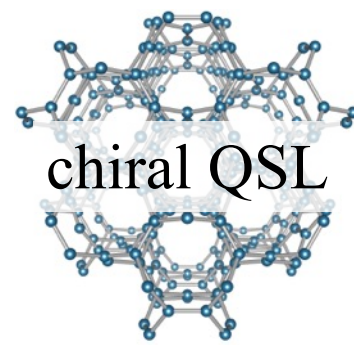
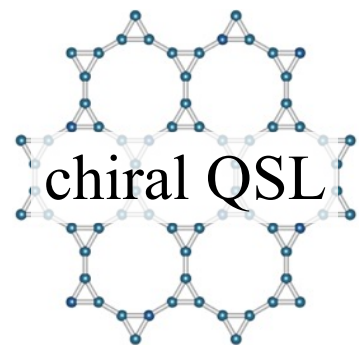
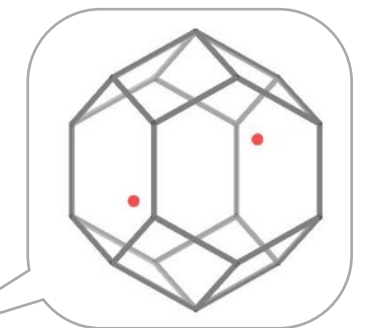
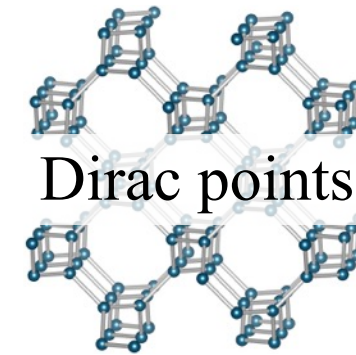
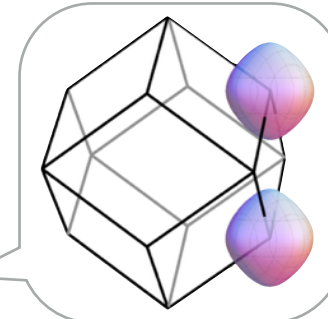
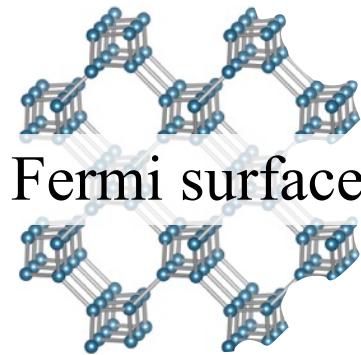
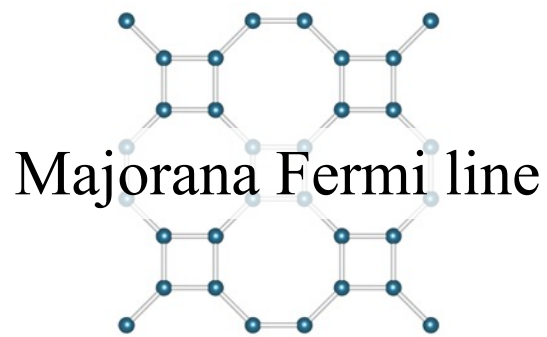
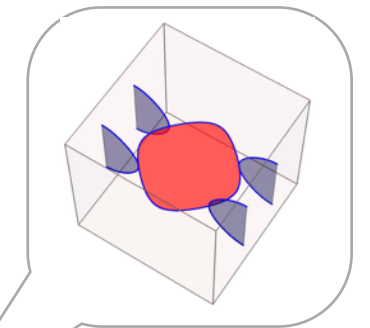
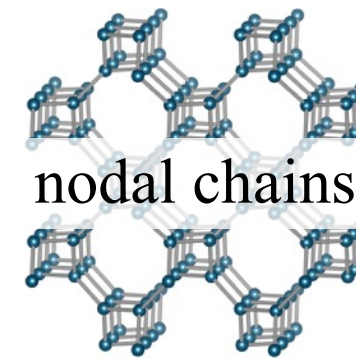
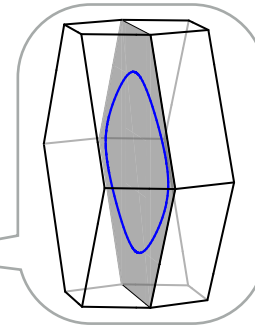
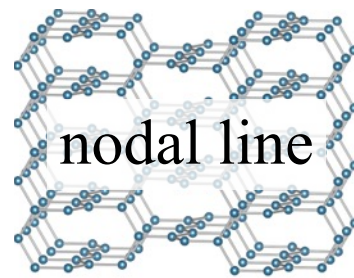
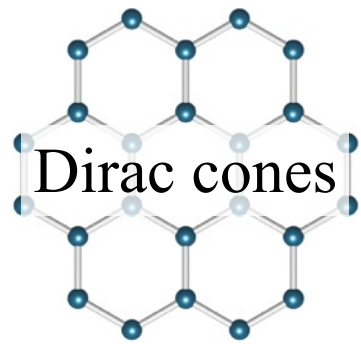
- represent spins by four **Majorana fermions**
- emergent **\mathbf{Z}_2 gauge field** on bonds

- Hilbert space split into two separate sectors: $2^N = 2^{N/2} \times 2^{N/2}$

Majorana fermions c_j
 “spinons”

flux loops “visons”
 (static and gapped)

Zoo of gapless Kitaev Spin Liquids

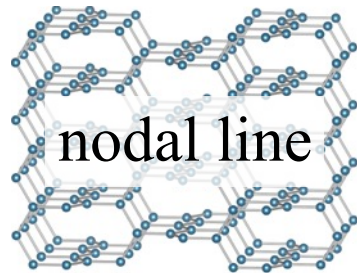
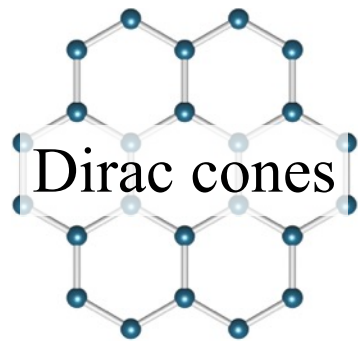


Kitaev, Annals of Physics (2006)
Yang et al. PRB (2007)
Yao and Kivelson, PRL (2007)

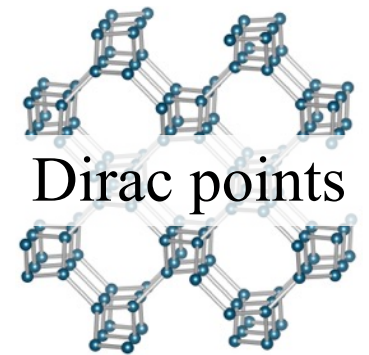
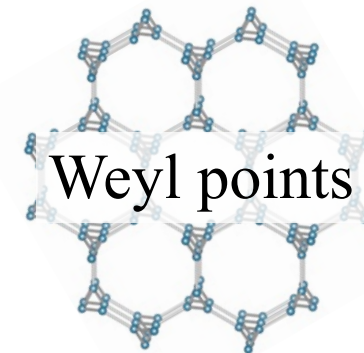
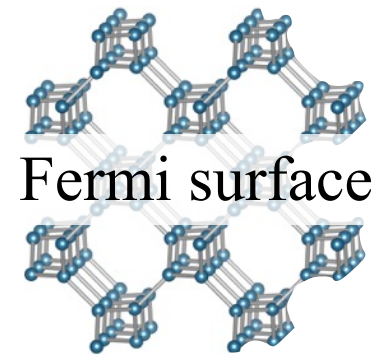
O'Brien, Hermanns, Trebst, PRB (2016)
Yamada, Dwivedi, Hermanns, PRB (2017)

Zoo of gapless Kitaev Spin Liquids

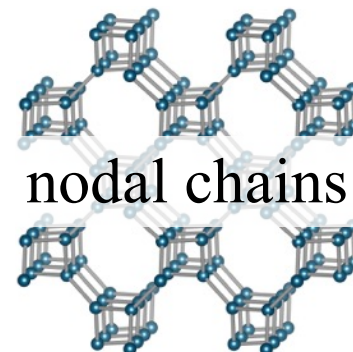
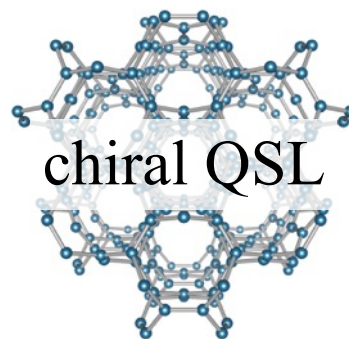
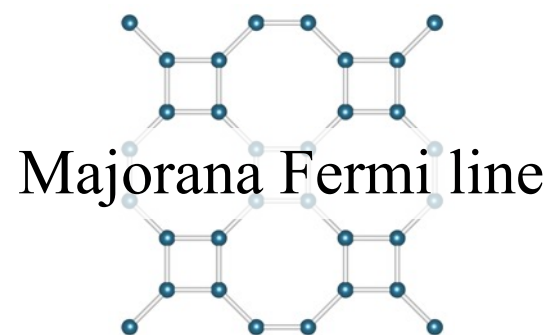
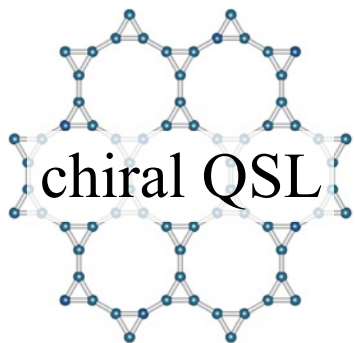
real



complex

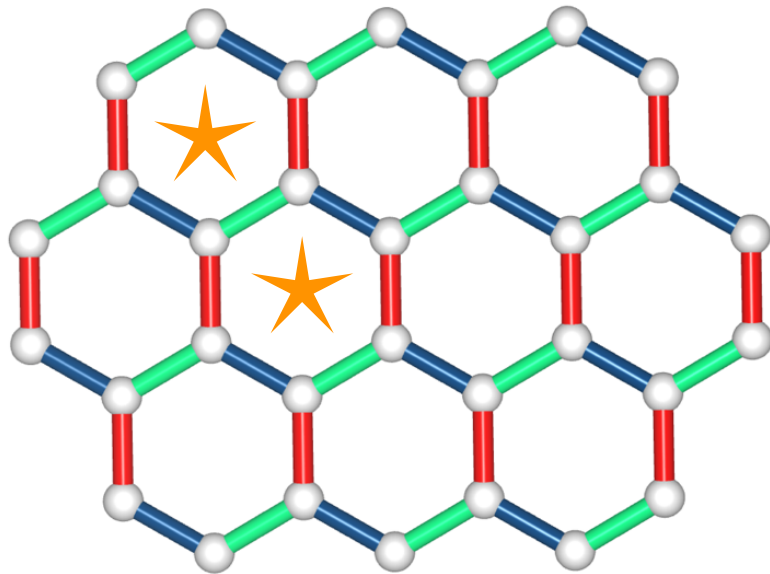


imaginary



Z_2 gauge field – vison excitations

2D



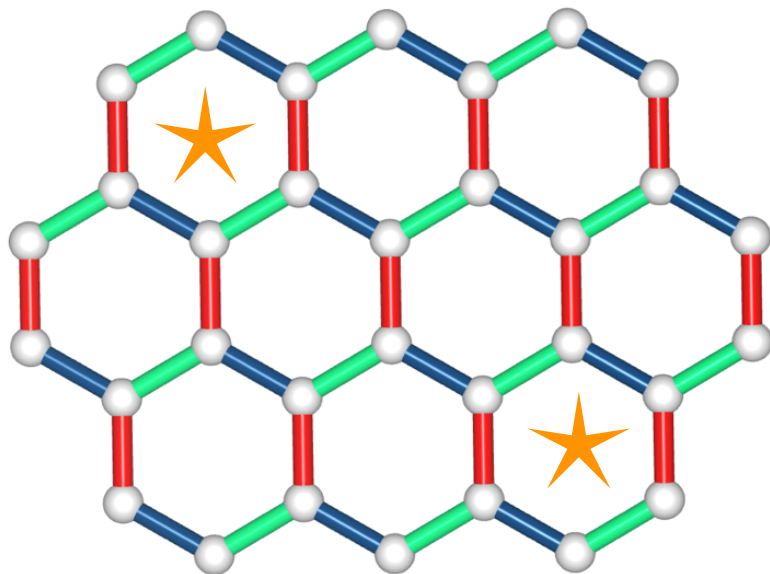
fluxes are point particles

deconfined

any finite temperature destroys
the spin liquid

Z_2 gauge field – vison excitations

2D



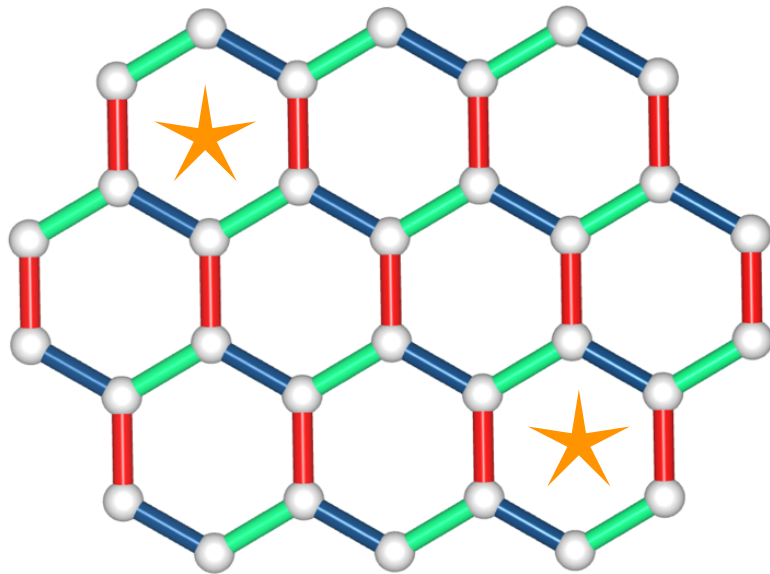
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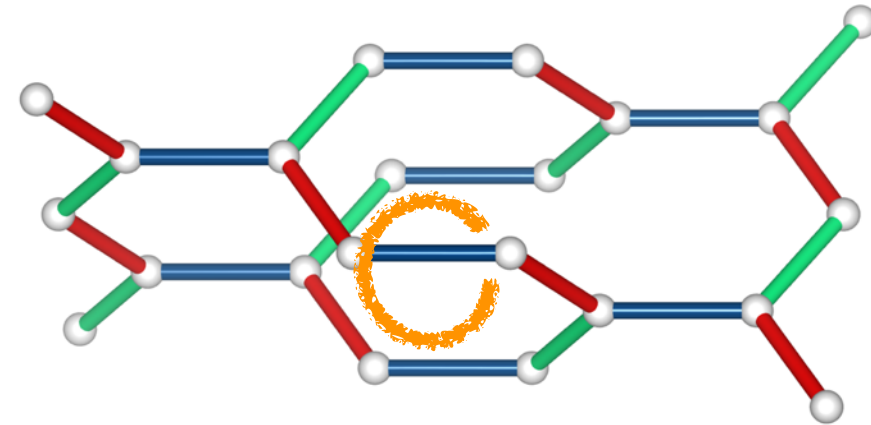
Z_2 gauge field – vison excitations

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fluxes are point particles
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any finite temperature destroys
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3D

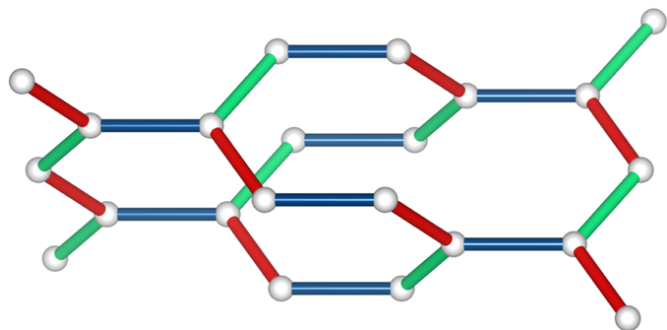


fluxes form loops
finite loop tension \rightarrow confined at
low temperatures
finite temperature transition

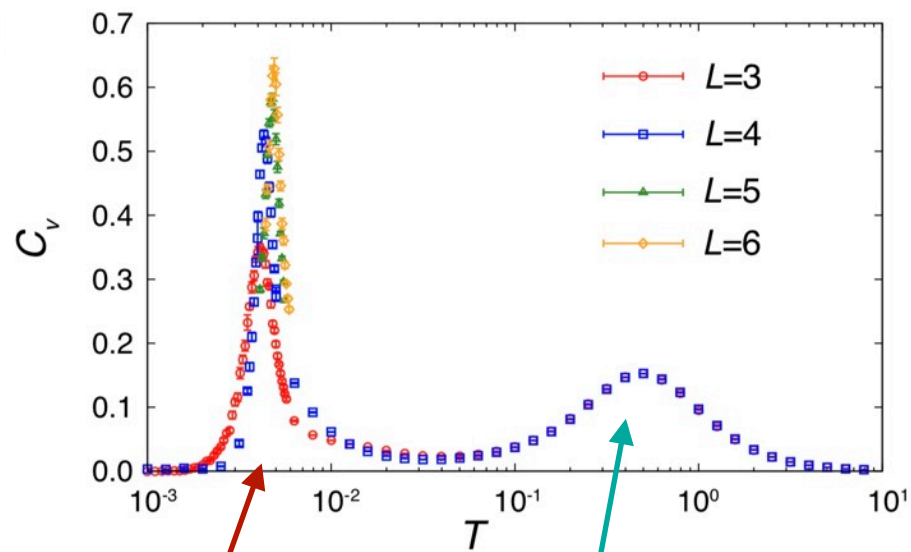
Thermodynamic Signatures

Nasu, Udagawa, Motome, PRL (2014)

(10,3)b 'hyperhoneycomb'



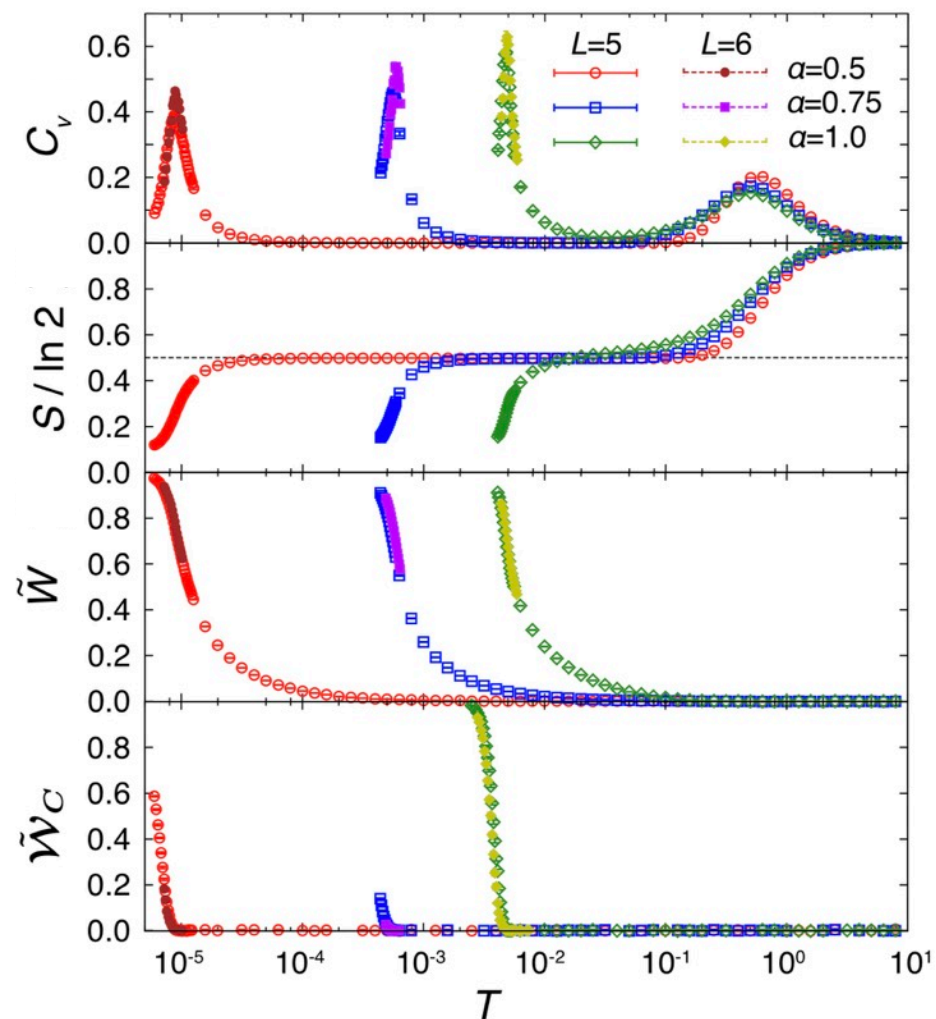
specific heat



local correlations build up

fluxes order

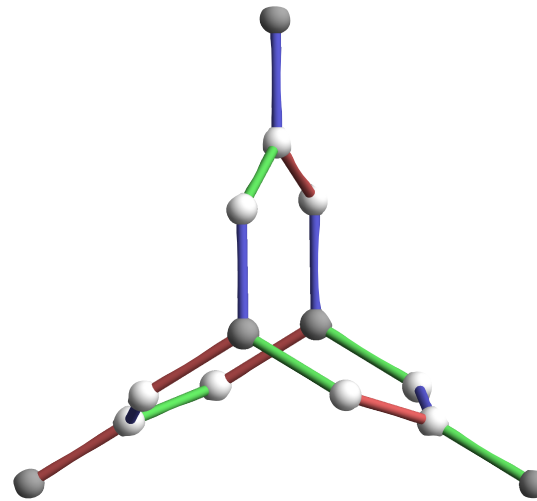
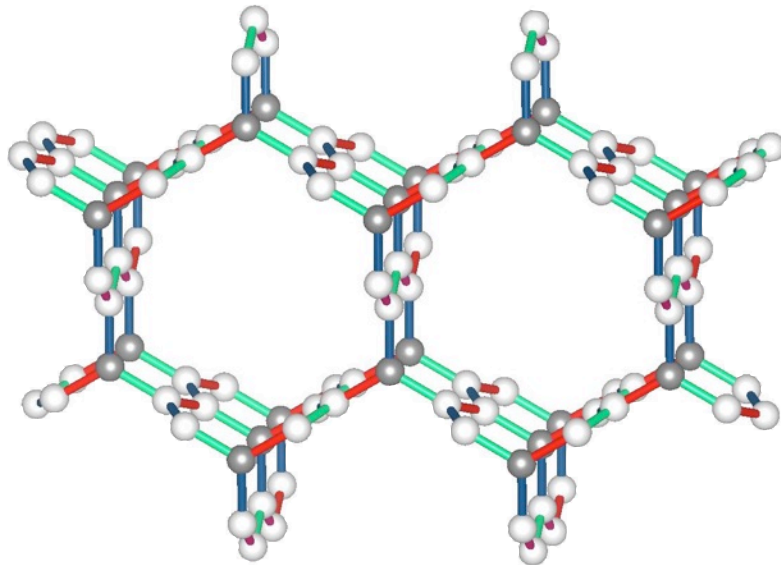
T_c set by vison gap



'Gauge-frustration'

no Z_2 monopoles
(vison excitations form closed loops in 3D)

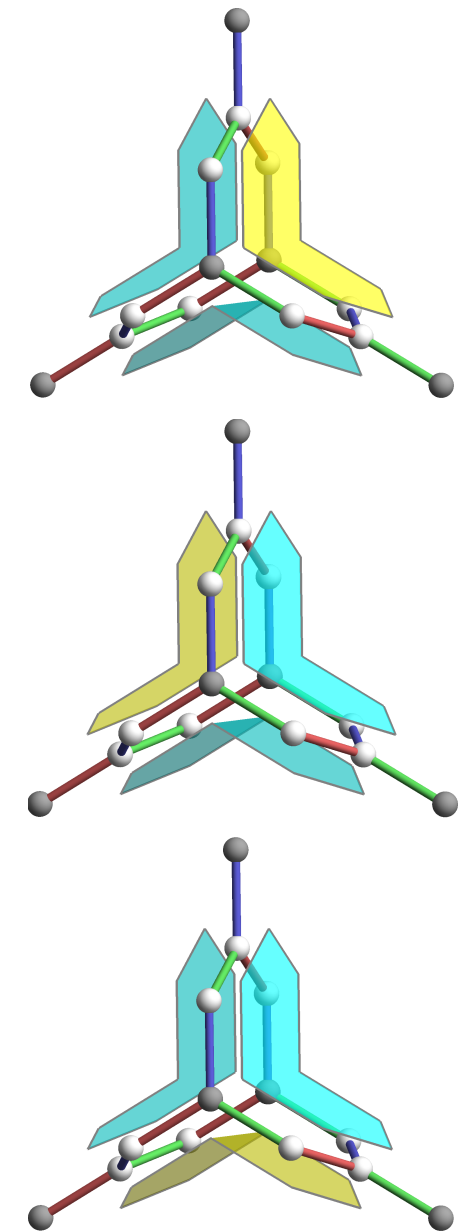
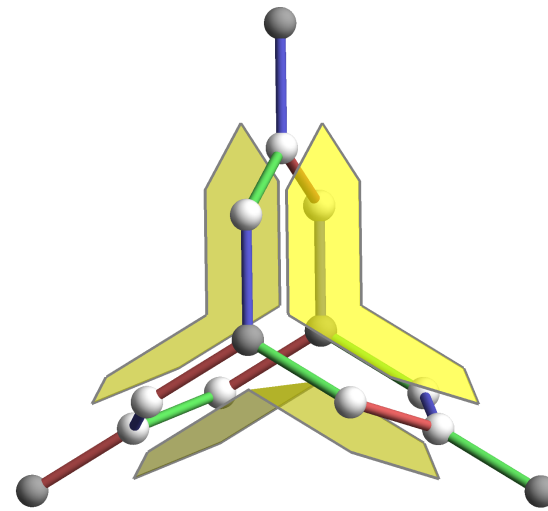
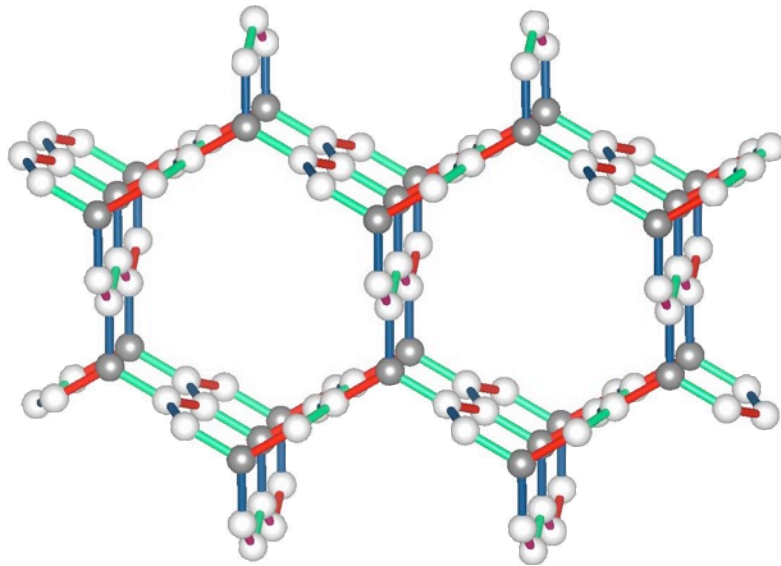
(8,3)c lattice



'Gauge-frustration'

no Z_2 monopoles
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(8,3)c lattice



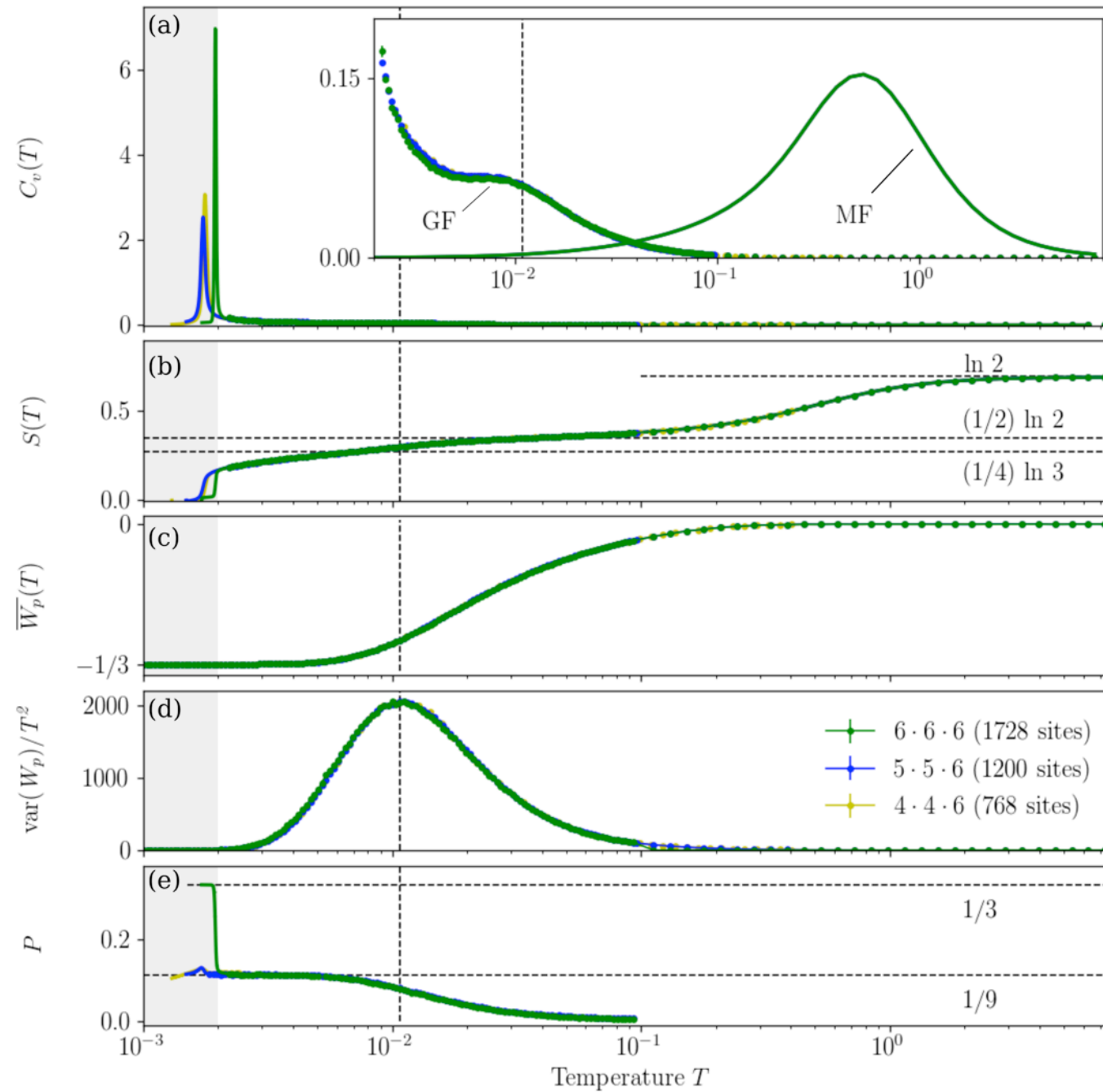
Lieb theorem $\rightarrow \pi$ flux per plaquette

local constraints

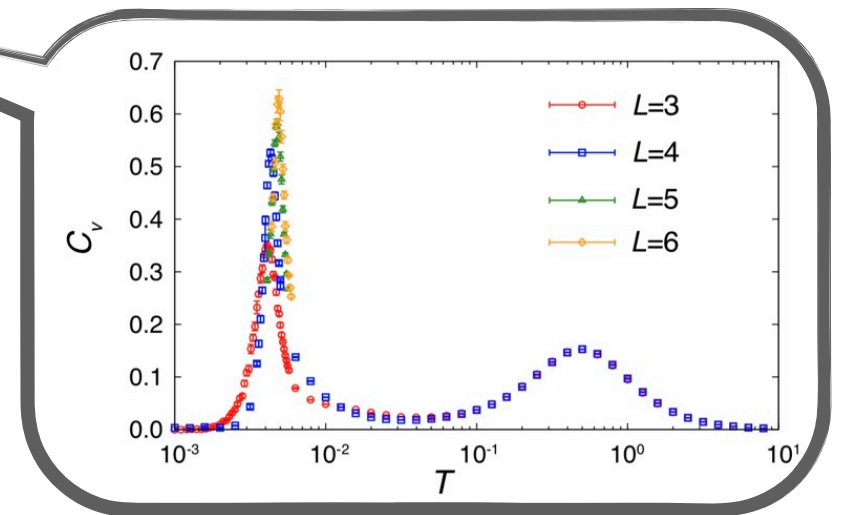
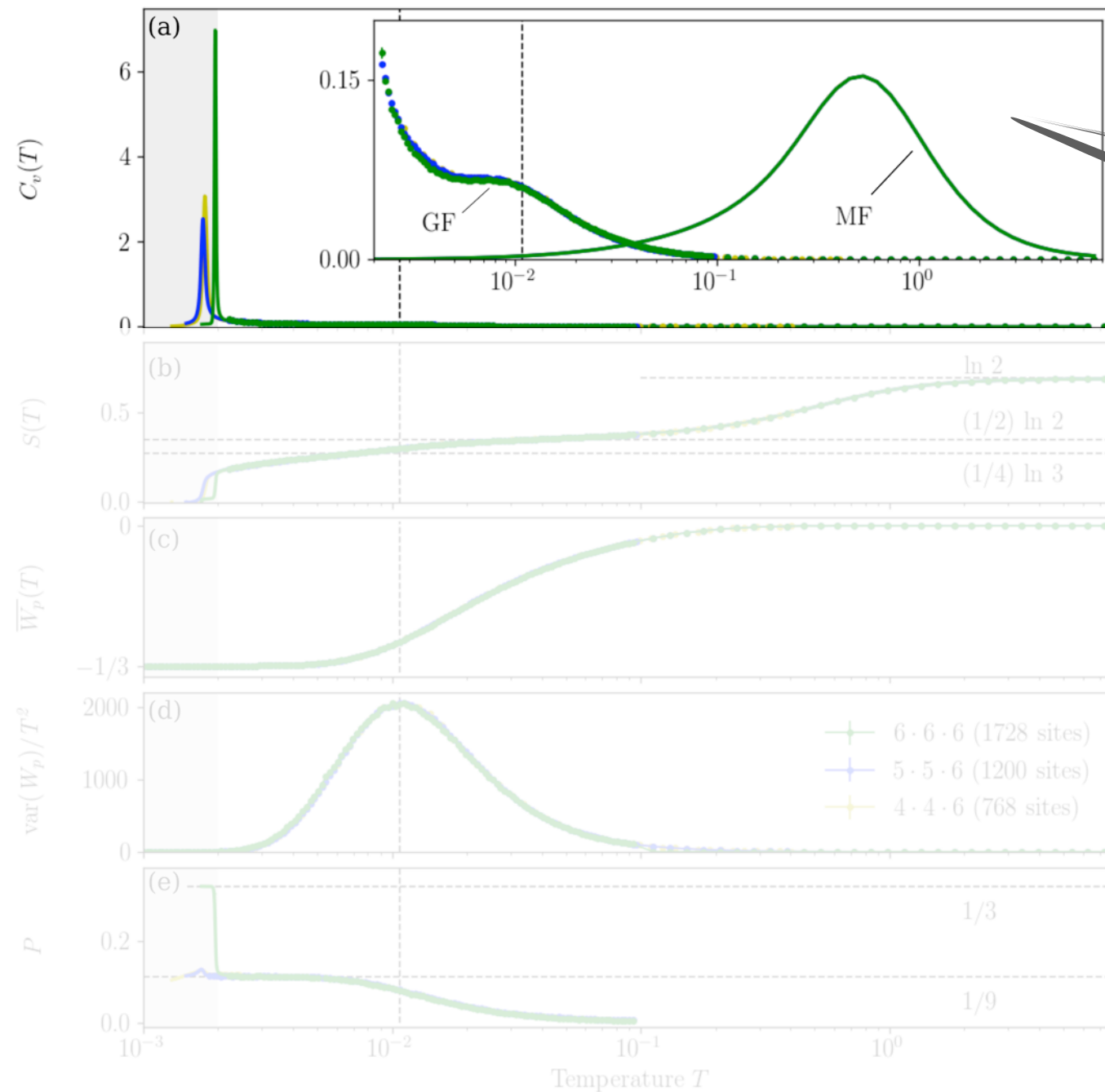
extensive degeneracy

(partially) lift degeneracy by altering the coupling strengths

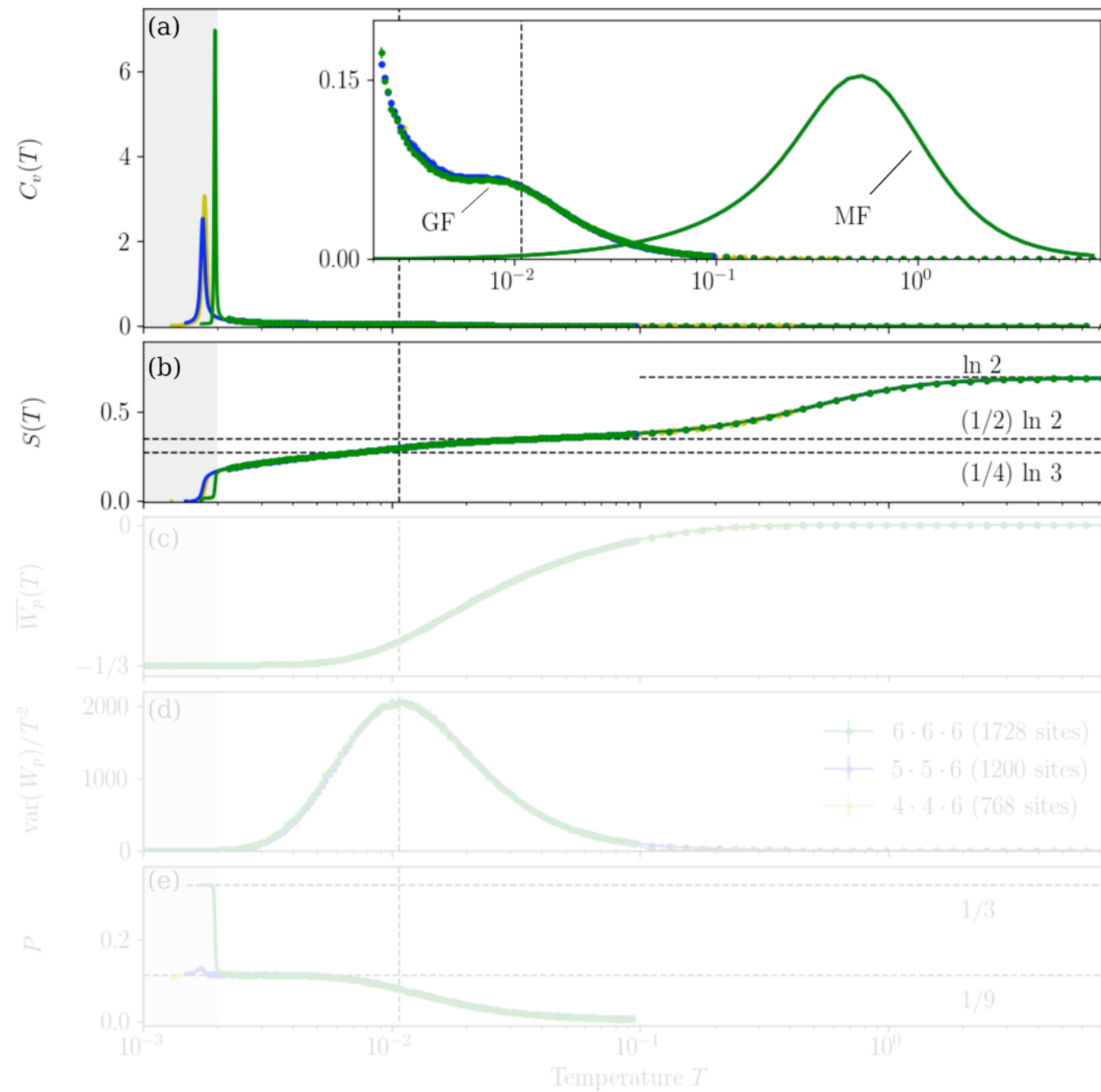
Thermodynamics of gauge-frustrated KSL



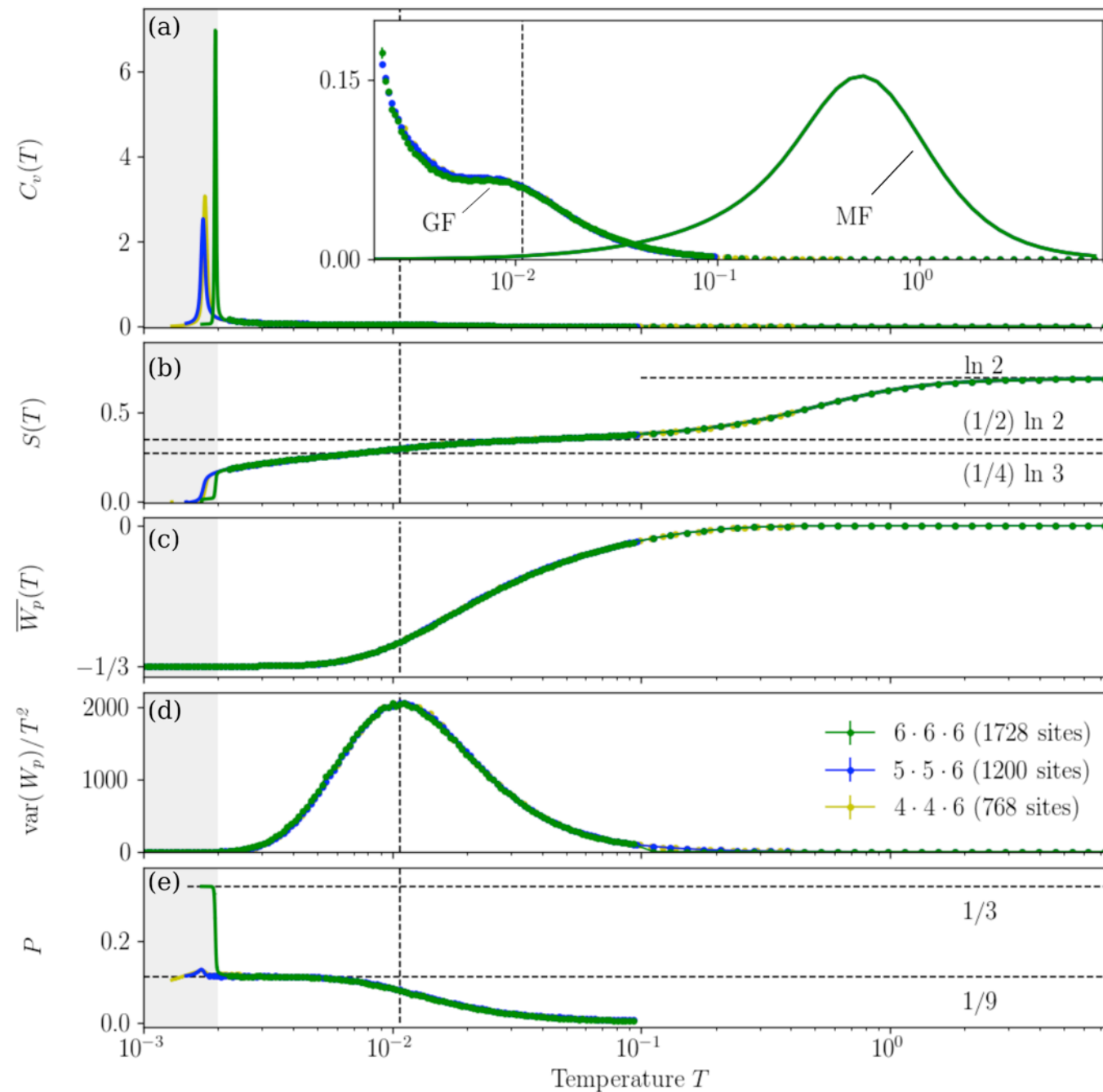
Thermodynamics of gauge-frustrated KSL



Thermodynamics of gauge-frustrated KSL

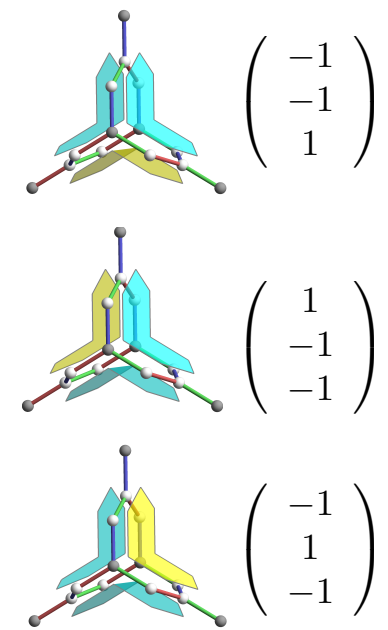


Thermodynamics of gauge-frustrated KSL



$$P = \frac{4}{3N} \sum_j \langle \mathbf{w}_0 \cdot \mathbf{w}_j \rangle$$

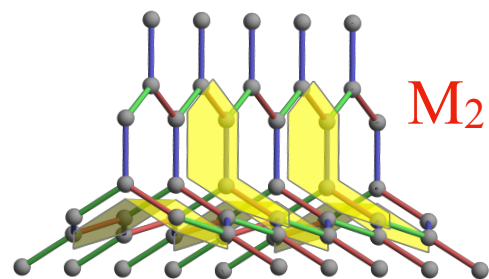
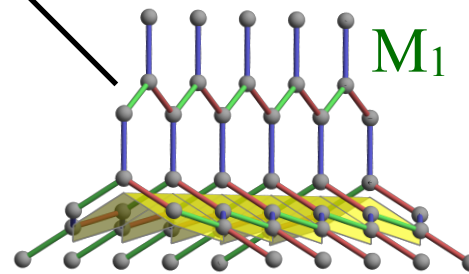
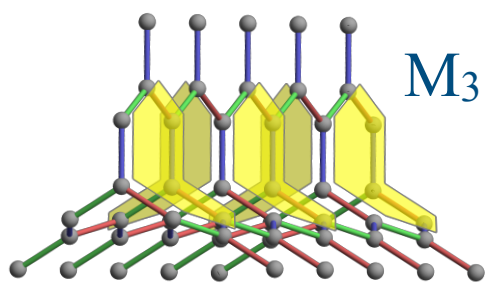
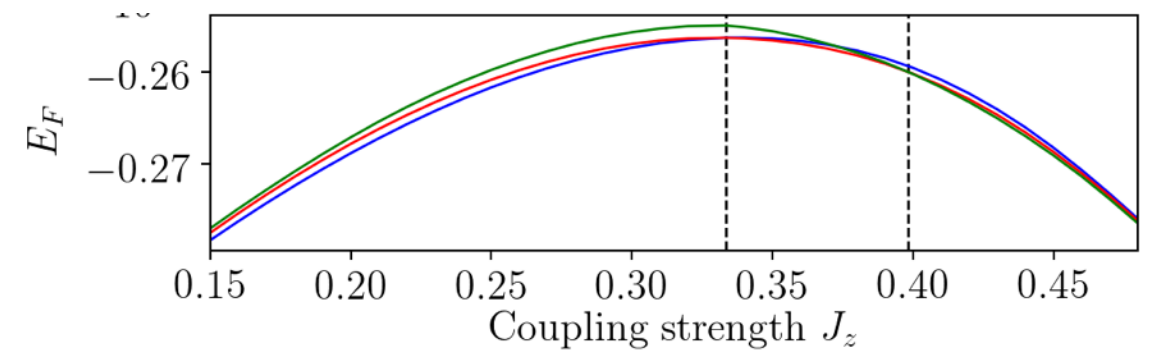
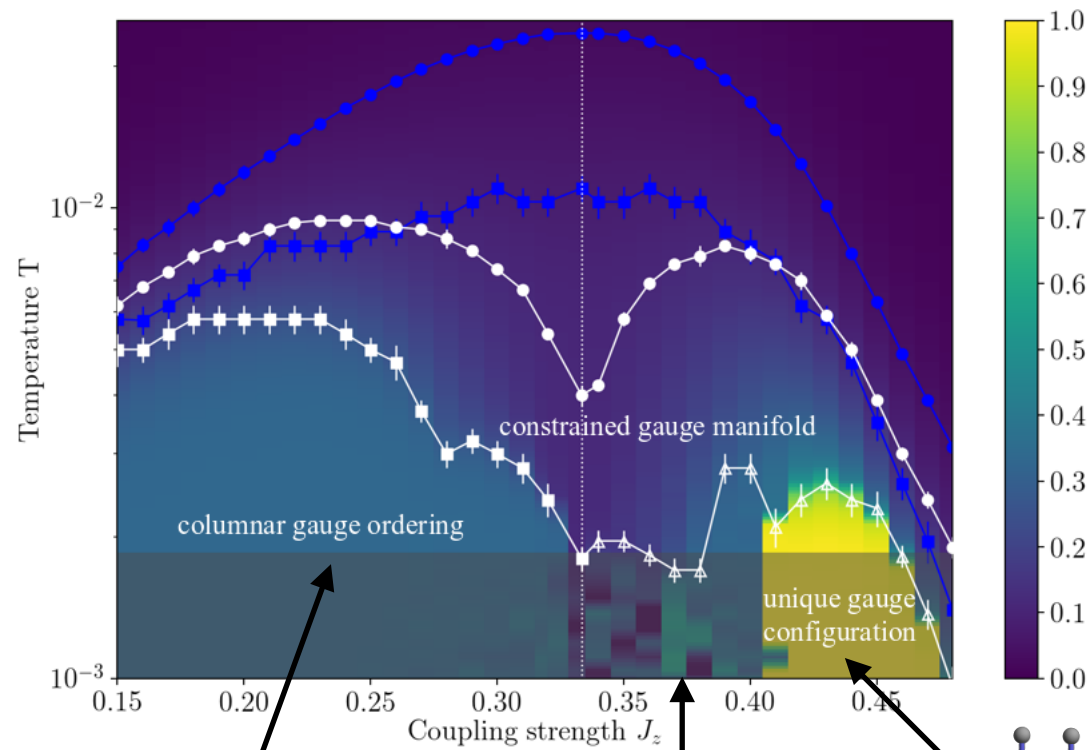
← pseudospin vector of fluxes around 'star'



Interplay of Majoranas and fluxes

Ordering the Z_2 fluxes

phase diagram for $J_x=J_y$



Conclusions

Kitaev spin liquids and materials

‘Gauge-frustration’

extensive residual entropy arising in the gauge sector

interplay of Majoranas and gauge field leads to ordering of the fluxes and formation of a Majorana metal