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Quantum Spin Liquids: Signatures of Fractionalization

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Université Paris-Saclay, Zoom Seminar, July 1, 2020

Center of Emergent Materials
NSF MRSEC – DMR

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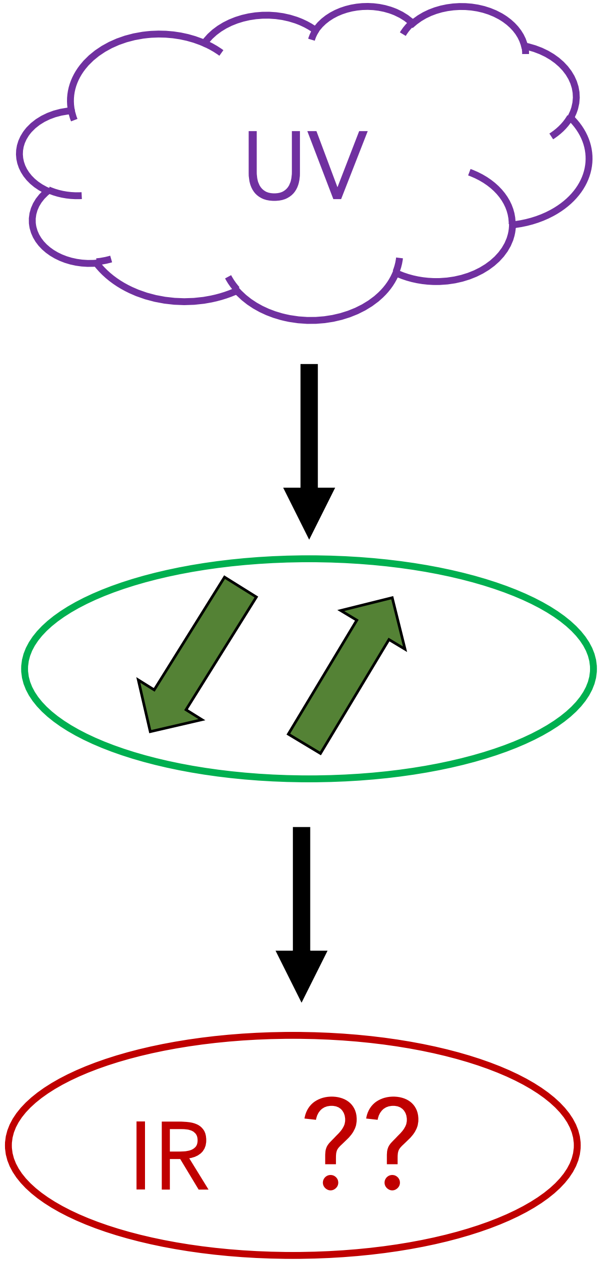
Roadmap

- Big picture
- 2D: Kitaev Model
  - Discovery of a new gapless QSL with a spinon Fermi surface
  - Spectrum of 1 spin flip and 2 spin flip excitations
- QSL Materials
- How do you detect a QSL?
- Going forward….

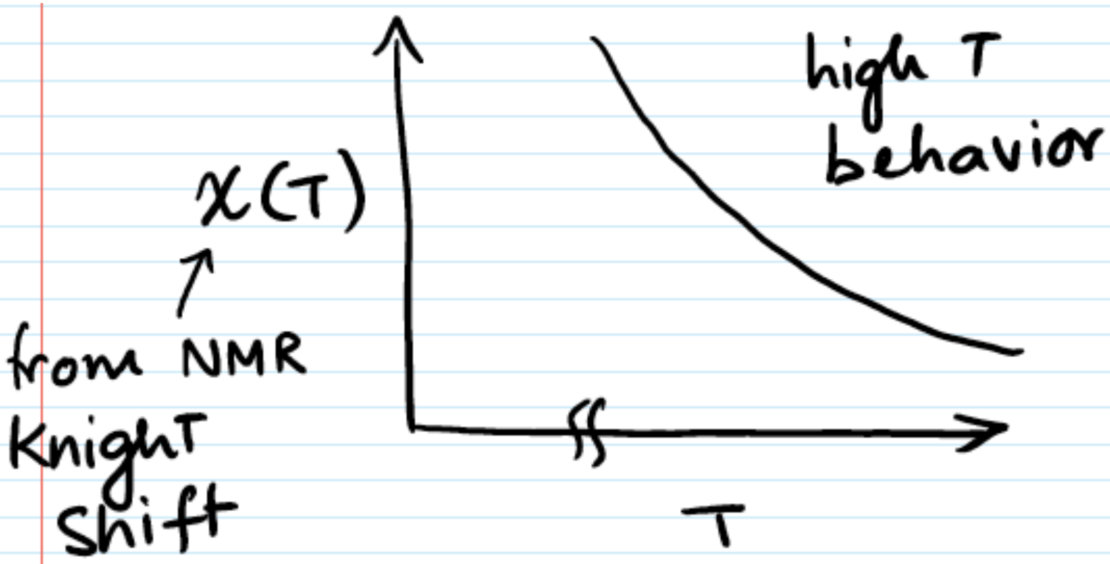
Big Picture

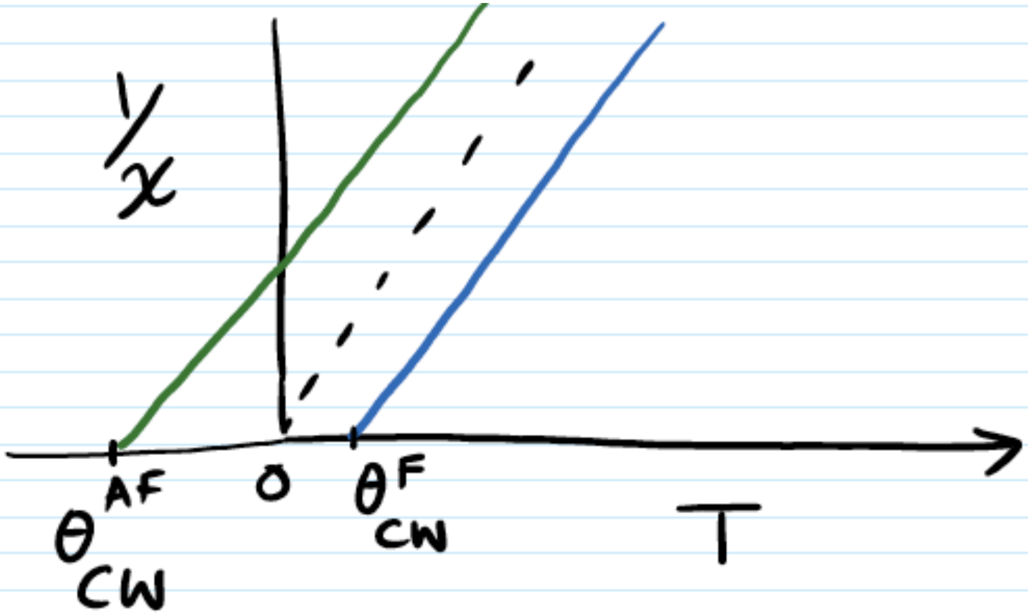
What is a QSL?
Why is it interesting? Important?

First Signatures of a QSL



First signatures of a QSL: large frustration parameter



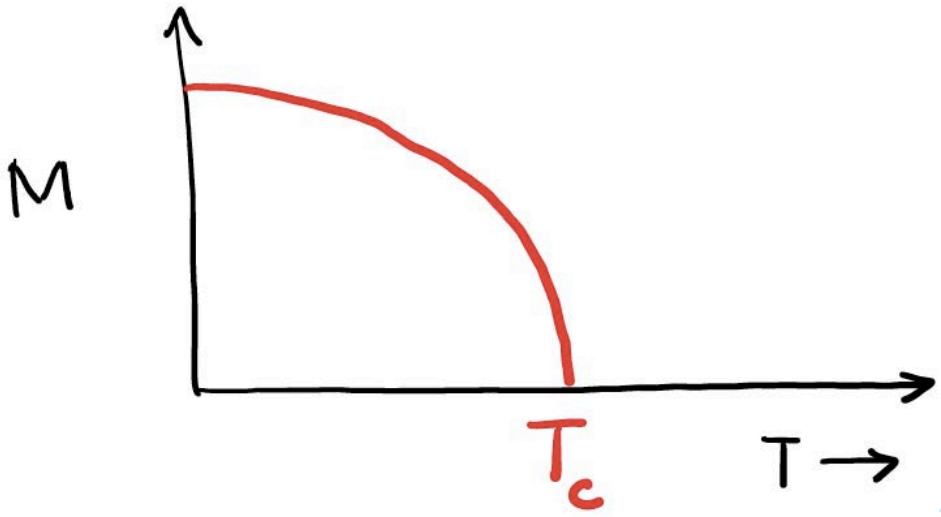


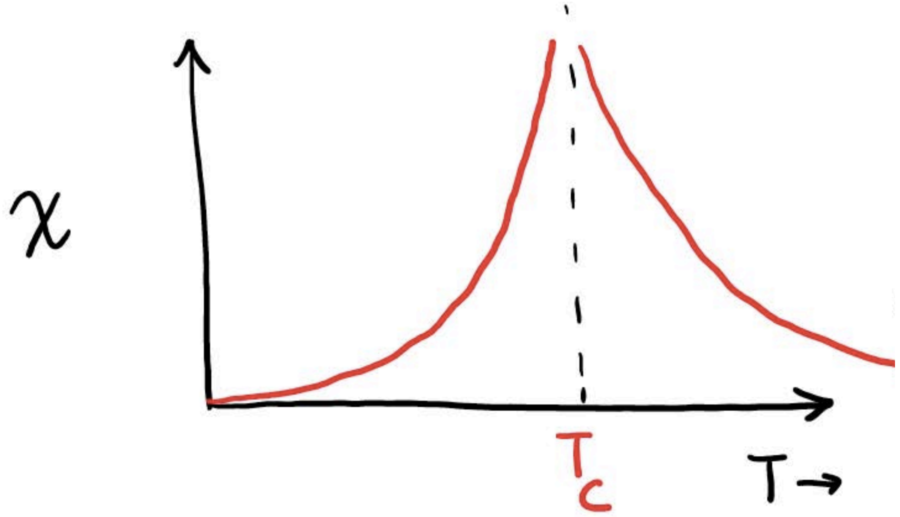
$$\chi(T) = \frac{C}{T - \theta_{CW}}$$

Spontaneously broken time reversal symmetry

$$\mathcal{H} = J \sum_{\langle ij \rangle} S_i^z S_j^z \qquad S_i = \pm \frac{1}{2}$$

$$M = \langle S_i^z \rangle$$

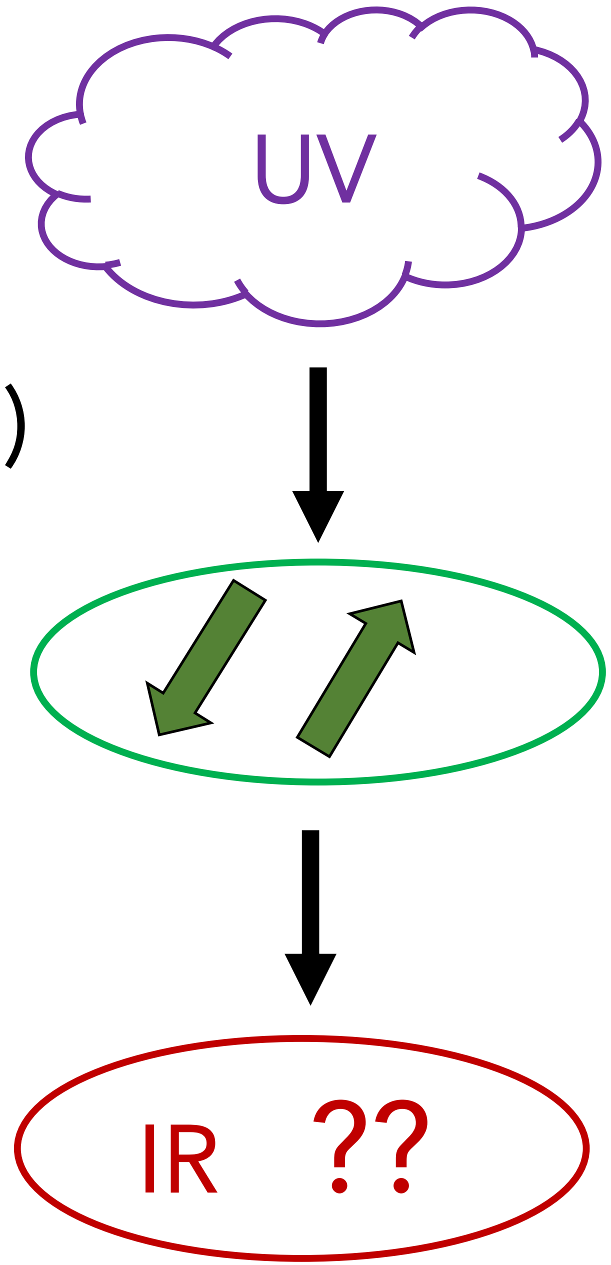




$$f = \frac{|\theta_{cw}|}{T_c}$$

First Signatures of a QSL

- **Mott insulator**
  (odd number of electrons in unit cell)
- **Local moments**
  (typically $S=1/2$ or $J_{eff}=1/2$)
- **Strongly interacting moments**
  $\theta_{CW} \sim 100$ K
- **No magnetic ordering**
  $f = \theta / T_c \sim 10^4$



First Signatures of a QSL

So why is a paramagnet interesting?

- Mott insulator
  (odd number of electrons in unit cell)
- Local moments
  (typically S=1/2 or J_{eff}=1/2)
- Strongly interacting moments
  θ~100 K
- No magnetic ordering
  $f = \theta / T_c \sim 10^4$

Quantum Matter

- ❑ Landau paradigm: spontaneously broken symmetry→
  local order parameter m
  bosonic excitations: magnons (for continuous spins)

- ❑ Topological Paradigm

"IQHE"
Topological Insulators
Topological Superconductors
Topological Weyl and Dirac Semimetals
Topological magnons

"FQHE"
Quantum Spin Liquids
Possess Topological Order

- Ground state degeneracy
- Long range entanglement
- Fractionalized Excitations

Review: Savary and Balents, Repts. on Progress in Physics 80, 016502 (2017)

Wen, X.-G. (1989) PRB 40, 7387
Wen, X.-G. and Niu, Q. (1990) PRB 41, 9377

Quantum Matter

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- Long range entanglement
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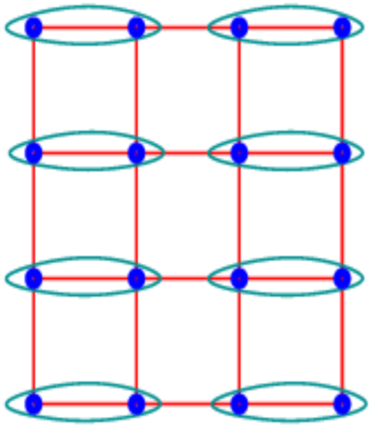
Important for storing information non-locally; robust against decoherence

Picture of a QSL

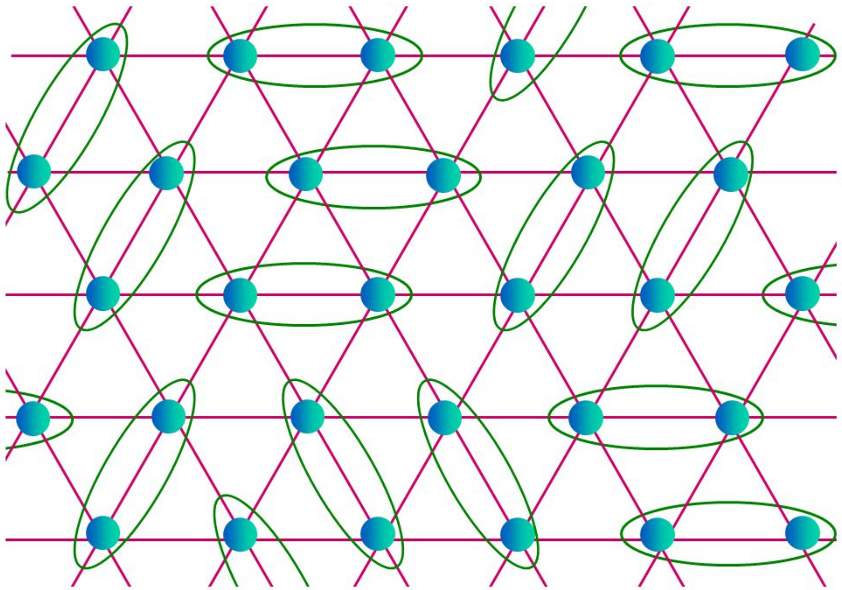
Singlet
or valence bond

$$= \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

valence
bond solid



Resonating valence bond
-- candidate quantum spin liquid



Anderson 1973

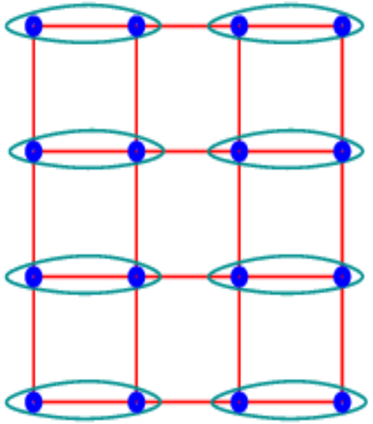
Excitations of a QSL

Singlet
or valence bond

$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Contrast with
ordered magnet:
Magnons: S=1 (bosons)

valence
bond solid



Resonating valence bond
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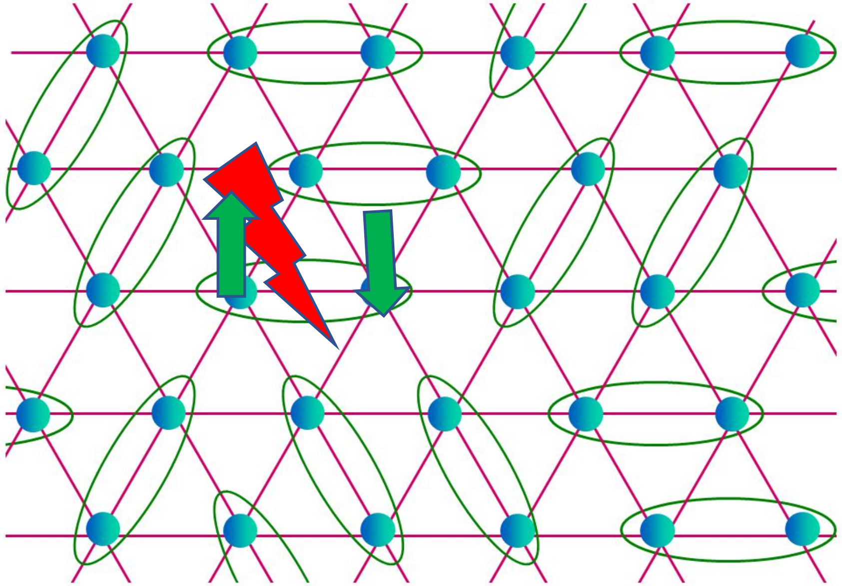
Anderson 1973



deconfined
S=1/2
spinons

Fermionic
excitations

Why would a bunch of interacting spins not order at T=0 ?

(1) Low spin

(2) Low dimensionality

(3) Frustration
[Geometric, Interactions, …]

→ Quantum Fluctuations

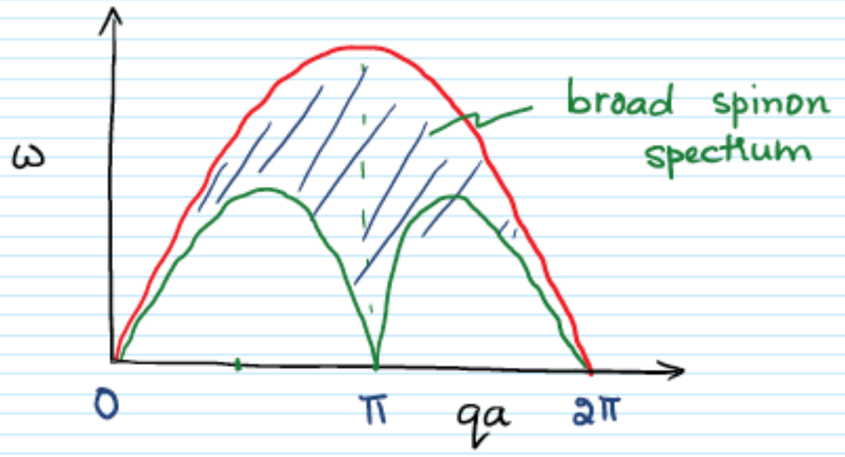
Fractionalization of excitations in quantum spin liquids

1d Quantum Spin Liquid

Fractionalized S=1 magnons (bosons) into two S=1/2 neutral spinons (fermions)

$|RVB\rangle = \{ |\bullet\!-\!\bullet \quad \bullet\!-\!\bullet\!-\!\bullet\!-\!\bullet\rangle + |\bullet\!-\!\bullet \quad \bullet\!-\!\bullet \quad \bullet\!-\!\bullet\rangle + \dots \}$

linear superposition of all possible singlet coverings → Spin liquid

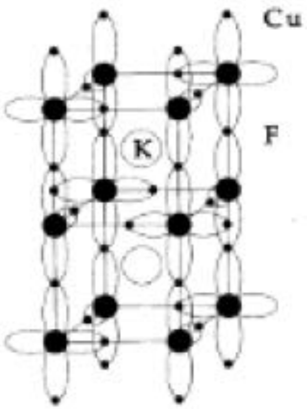


$$\omega_l(q) = \pi \frac{J}{2} |\sin qa|$$

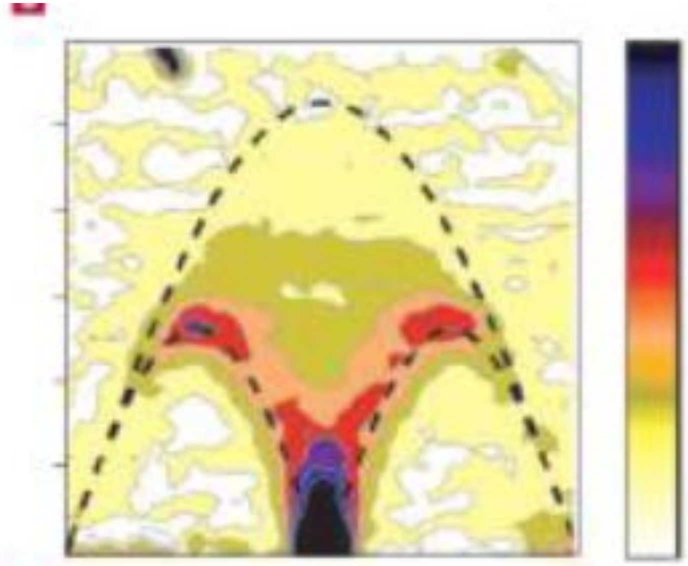
$$\omega_u(q) = \pi J \left| \sin \frac{qa}{2} \right|$$

compare with $\omega_{cl}(q) = 2J|\sin qa|$

$KCuF_3$



Inelastic neutron scattering S(q,w)



Lake et al Nat. Mat. 4, 329 (2005)

Broad spectrum indicates fractionalization of magnons

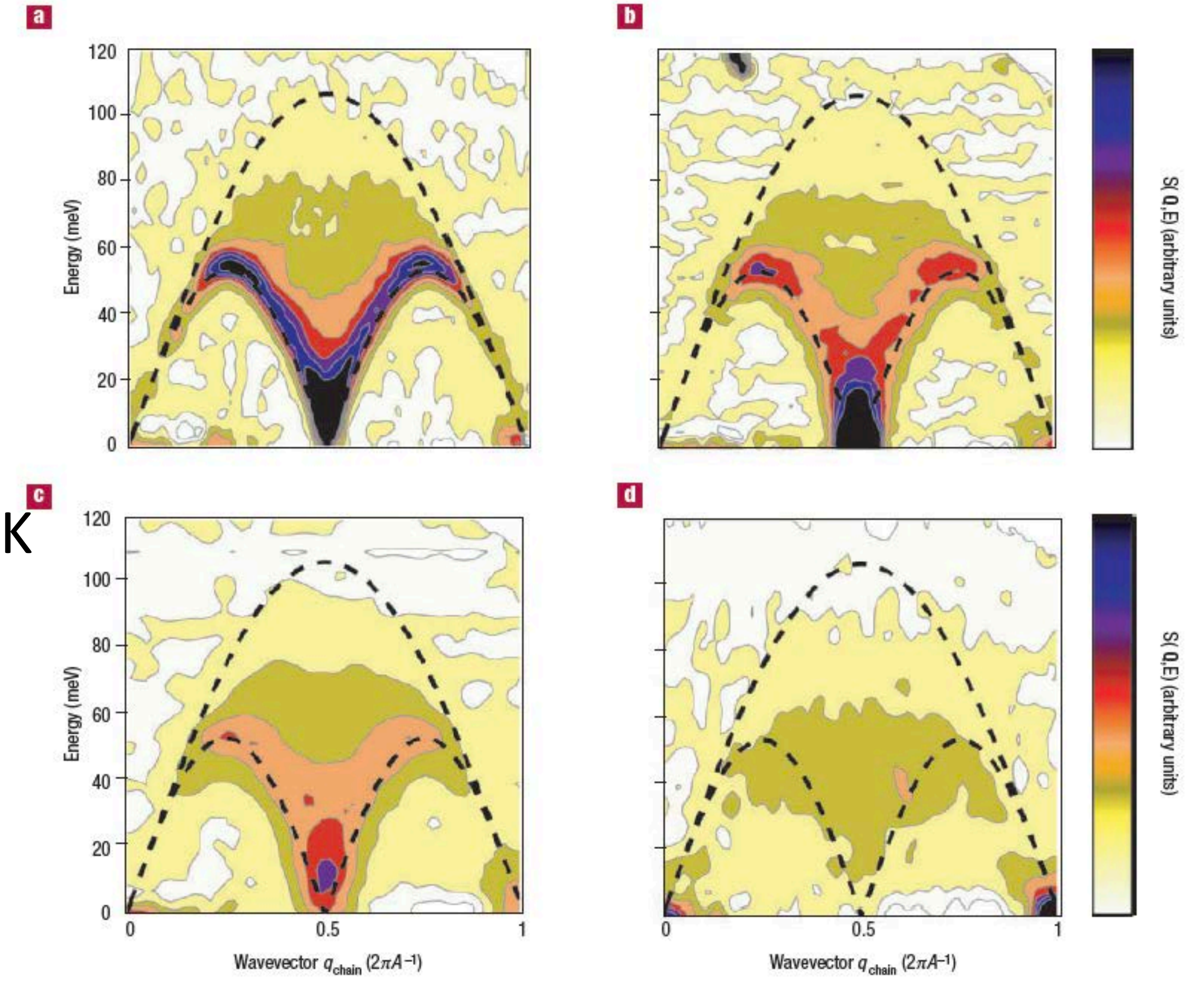
Ordering~ 10K

T=6K

T=50 K

T=150 K

T=300 K



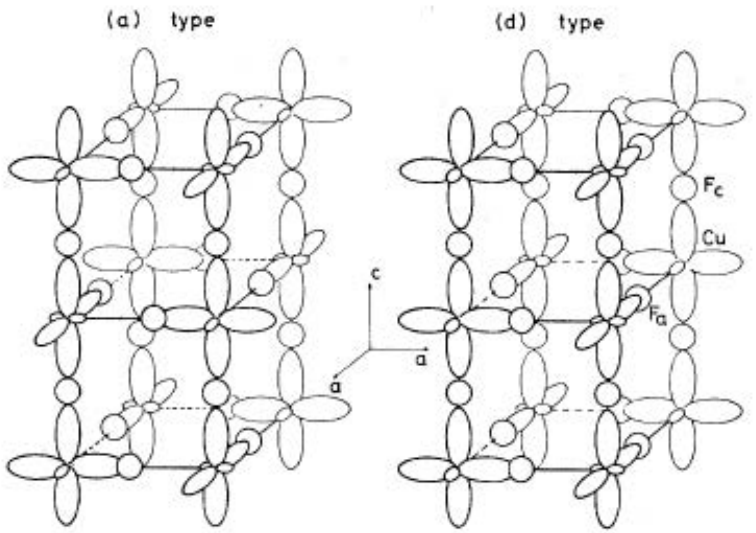


FIG. 1. Schematics of type (a) and (d) structures observed in $KCuF_3$.

$J \sim 340\,K$ $\quad J_\perp = -16\,K$

Black dotted: multi-spinon continuum predicted at T=0 (Muller ansatz equation)

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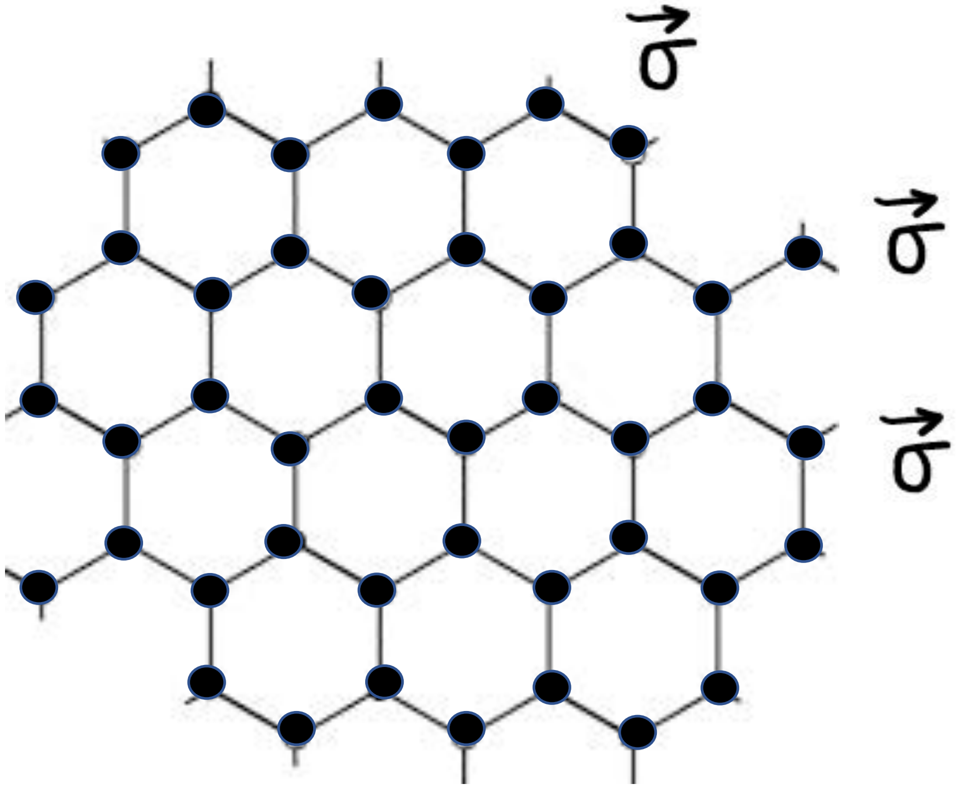
- ➢ How do you detect a QSL?
- ➢ Going forward….

Kitaev Model



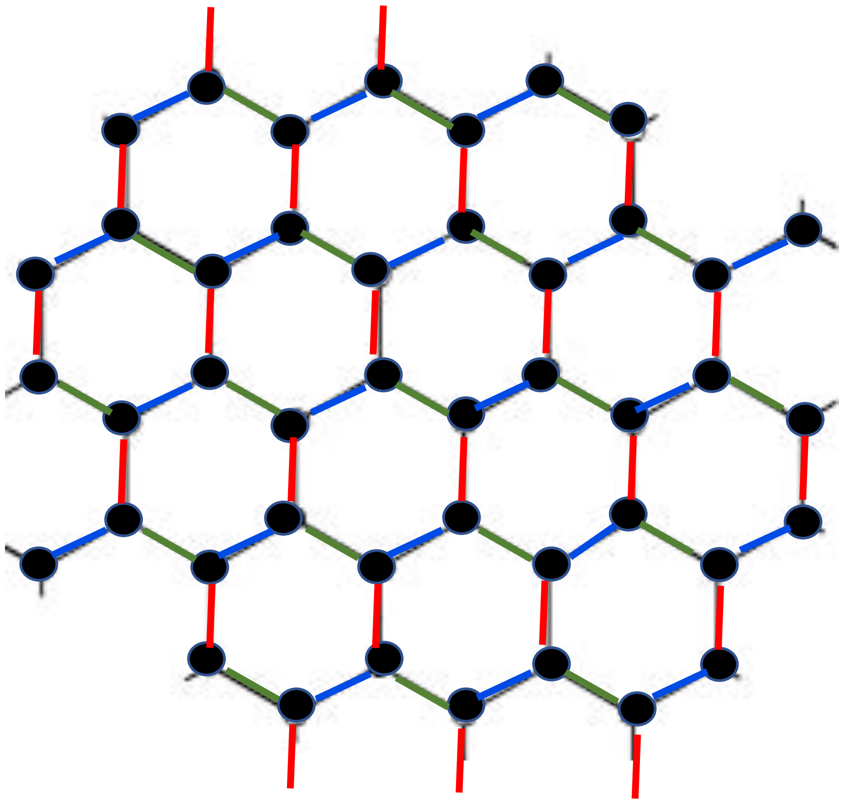
A. Kitaev, Annals of Physics 321, 2-111 (2006)

put qubit on each site

Honey comb lattice

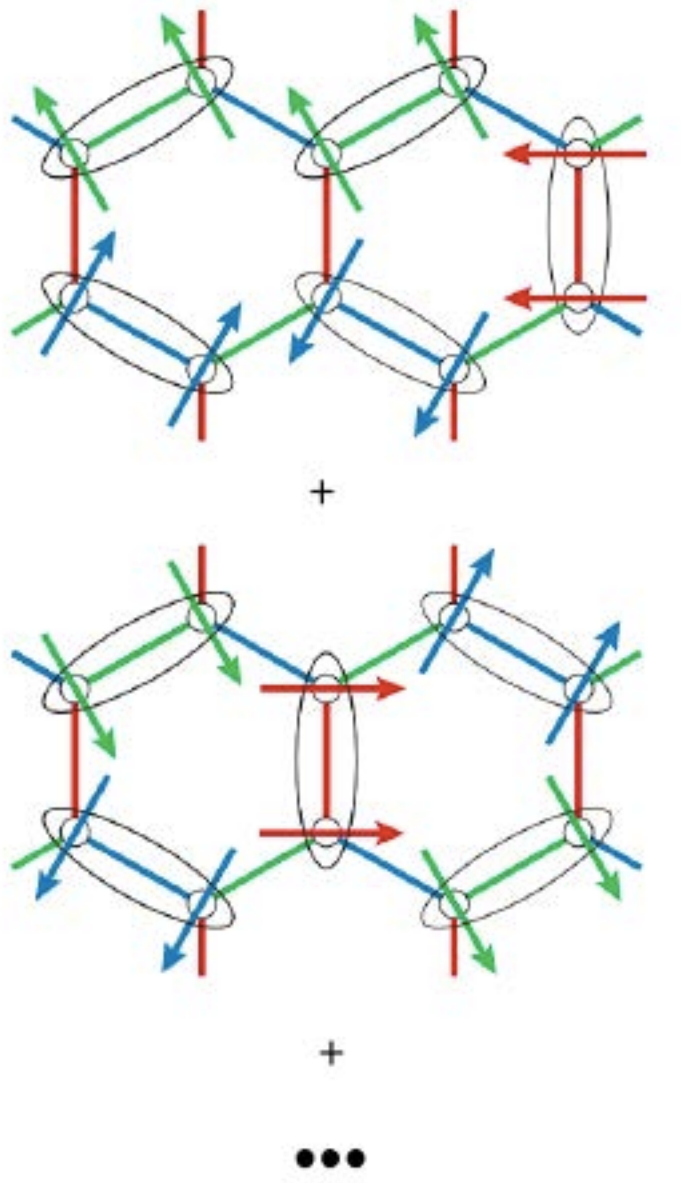
Bipartite lattice; no geometric frustration

Kitaev Model: bond-dependent interactions

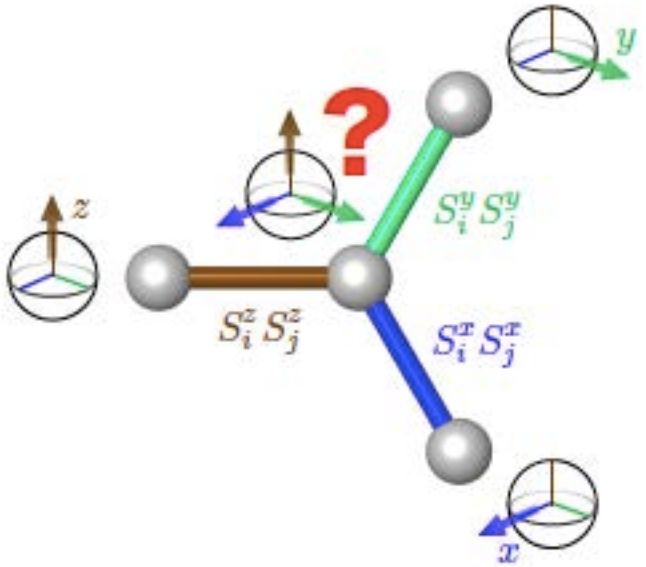


$$\mathcal{H} = K\left[\sum_{\langle ij\rangle \in x} \sigma_i^x \sigma_j^x + \sum_{\langle ij\rangle \in y} \sigma_i^y \sigma_j^y + \sum_{\langle ij\rangle \in z} \sigma_i^z \sigma_j^z\right]$$

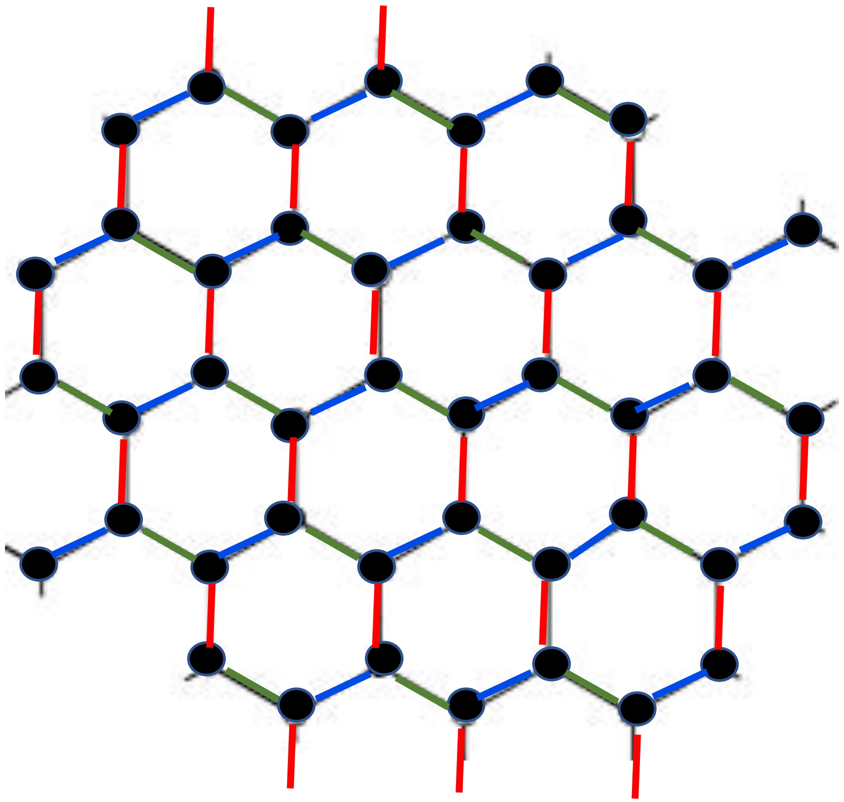
Kitaev Model: bond-dependent interactions



$$\mathcal{H} = K\left[\sum_{\langle ij\rangle\in x}\sigma_i^x\sigma_j^x + \sum_{\langle ij\rangle\in y}\sigma_i^y\sigma_j^y + \sum_{\langle ij\rangle\in z}\sigma_i^z\sigma_j^z\right]$$



Kitaev Model: bond-dependent interactions



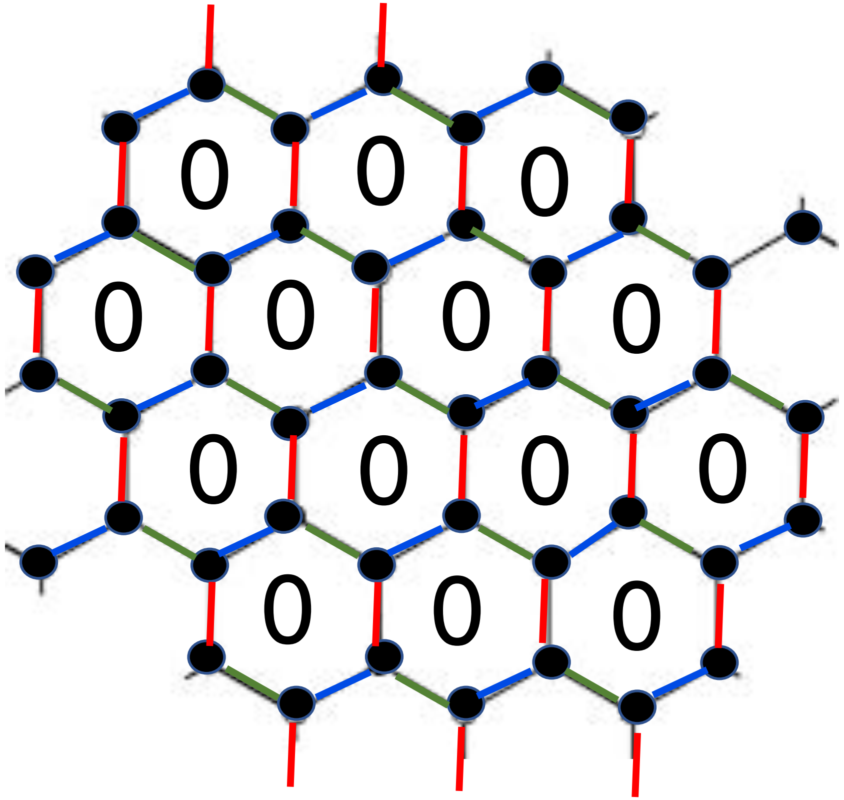
$$\mathcal{H} = K\left[\sum_{\langle ij\rangle \in x} \sigma_i^x \sigma_j^x + \sum_{\langle ij\rangle \in y} \sigma_i^y \sigma_j^y + \sum_{\langle ij\rangle \in z} \sigma_i^z \sigma_j^z\right]$$

Parton construction:

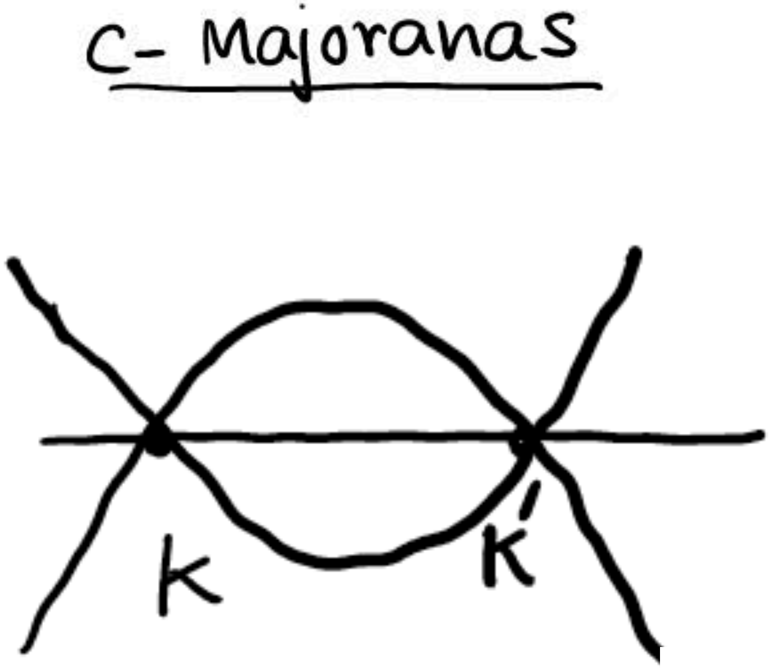
$$\sigma^\alpha = i\, b^\alpha c$$

$$\mathcal{H} = K\,\frac{i}{2}\sum_{\langle ij\rangle} \hat{u}_{ij}\, c_i c_j$$

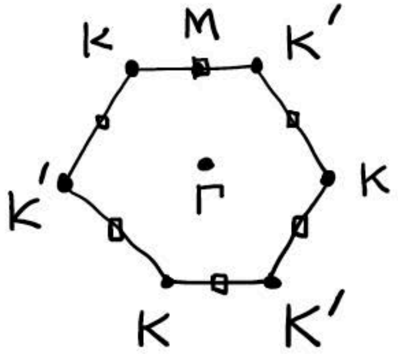
Ground State:



All plaquettes have zero flux

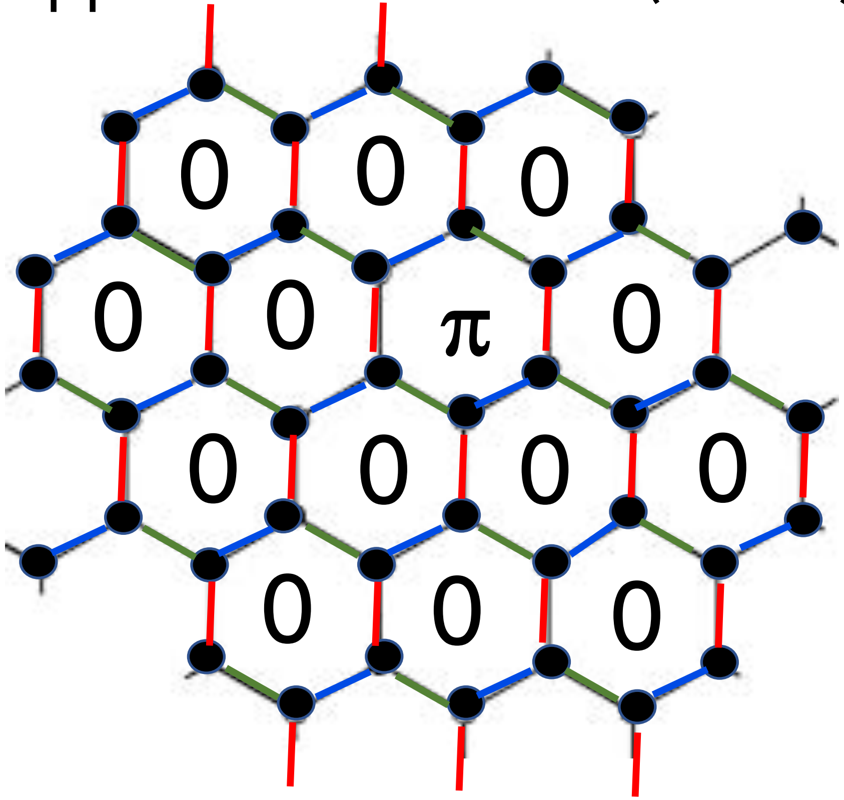


c-majorana fermions have a Dirac dispersion

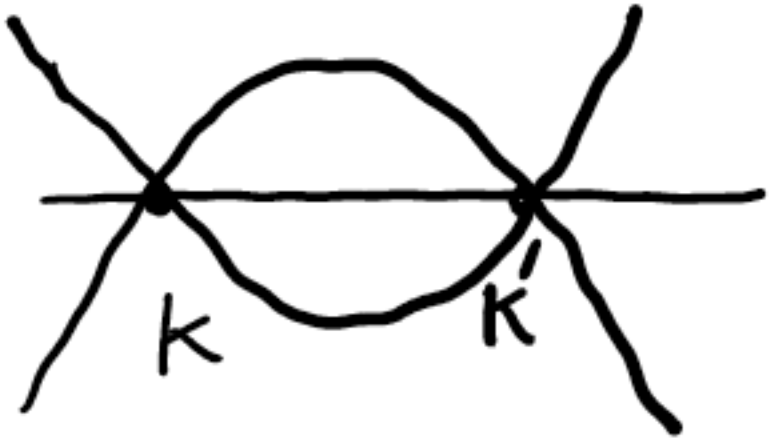


Excitations:

(1)Gapped flux excitation (visons)



(2) Gapless majorana fermions



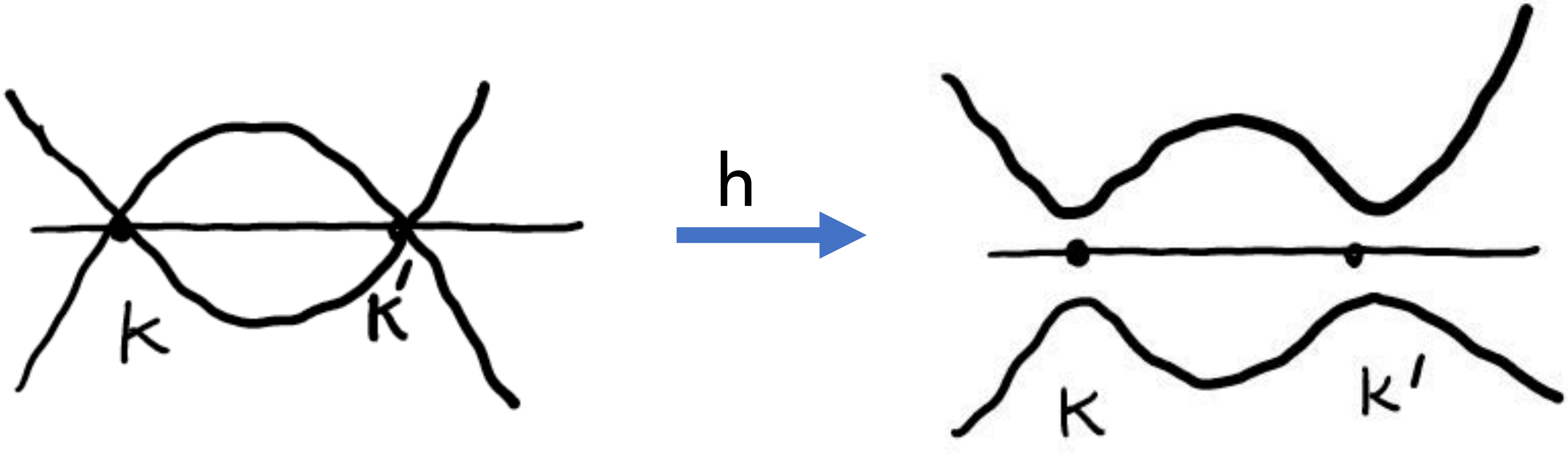
Gapless Z_2 Quantum Spin Liquid

Now add a magnetic field…

$$H = H_K + h \sum_{i\alpha} S_i^\alpha$$

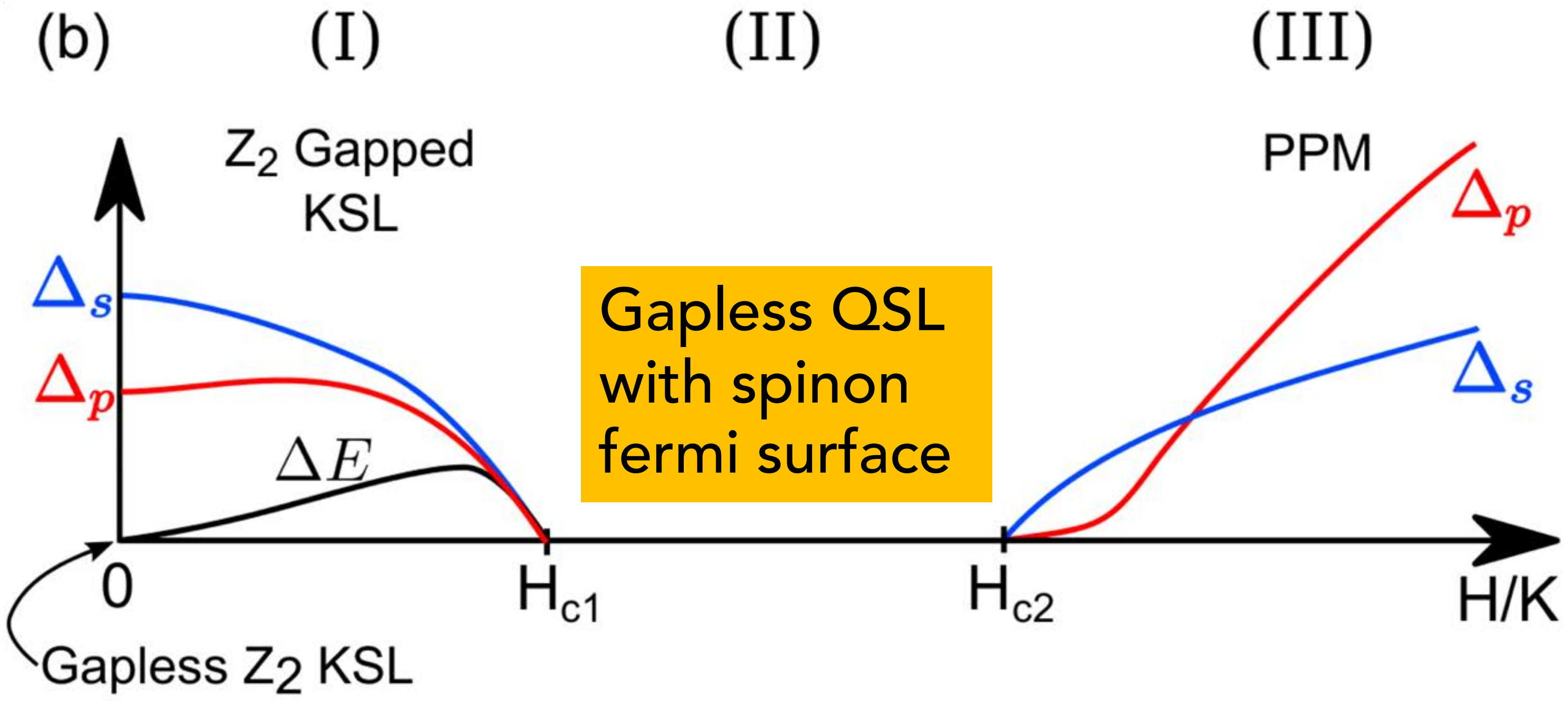
Focus on here:
AF Kitaev interactions and field along $h||[111]$

Non-abelian gapped Kitaev spin liquid:



- Majorana fermions get gapped

Our Main Results: Kitaev Model in a Magnetic Field



Δ_s: single spin flip energy
Δ_p: 2-spin flip energy

Results based on exact diagonalization ED and Density matrix renormalization group (DMRG)

David Ronquillo   Adu Vengal   Nirav Patel   Subhasree Pradhan

Field-orientation-dependent spin dynamics of the Kitaev honeycomb model
Phys. Rev. B 99, 140413 (2019)

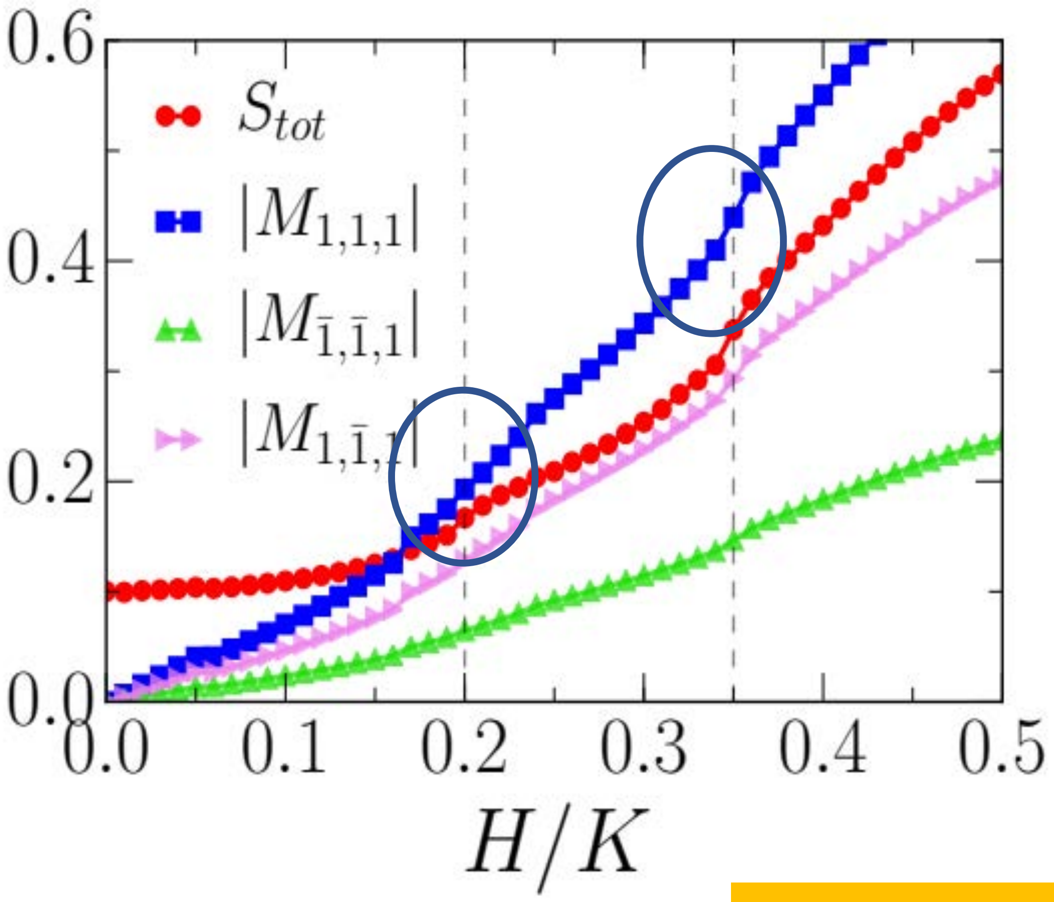
Magnetic field induced intermediate gapless spin-liquid phase with a spinon Fermi surface
PNAS 201821406 (2019)

Two-Magnon Bound States in the Kitaev Model in a [111]-Field
PRB 101, 180401 (2020)

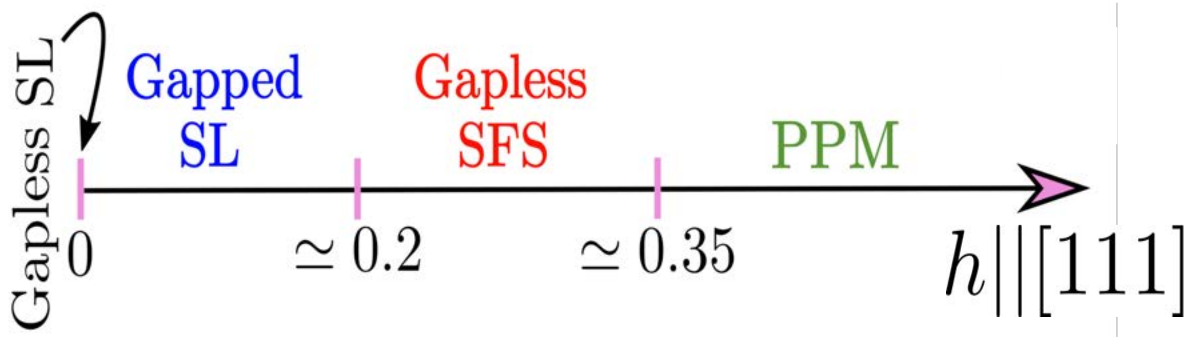
Related work:
Z. Zhu, et al., Phys. Rev. B 97, 241110 (2018)
M. Gohlke, et al., Phys. Rev. B 98, 014418 (2018)
C. Hickey and S. Trebst, Nat. Comm. 10, 530 (2019)
H.C. Jiang et al. arXiv 1809.08247
Y. Motome and J. Nasu, JPSJ 89, 012002 (2020)

Evidence for TWO phase transitions

Kitaev Model + Magnetic field: magnetization $h||[111]$

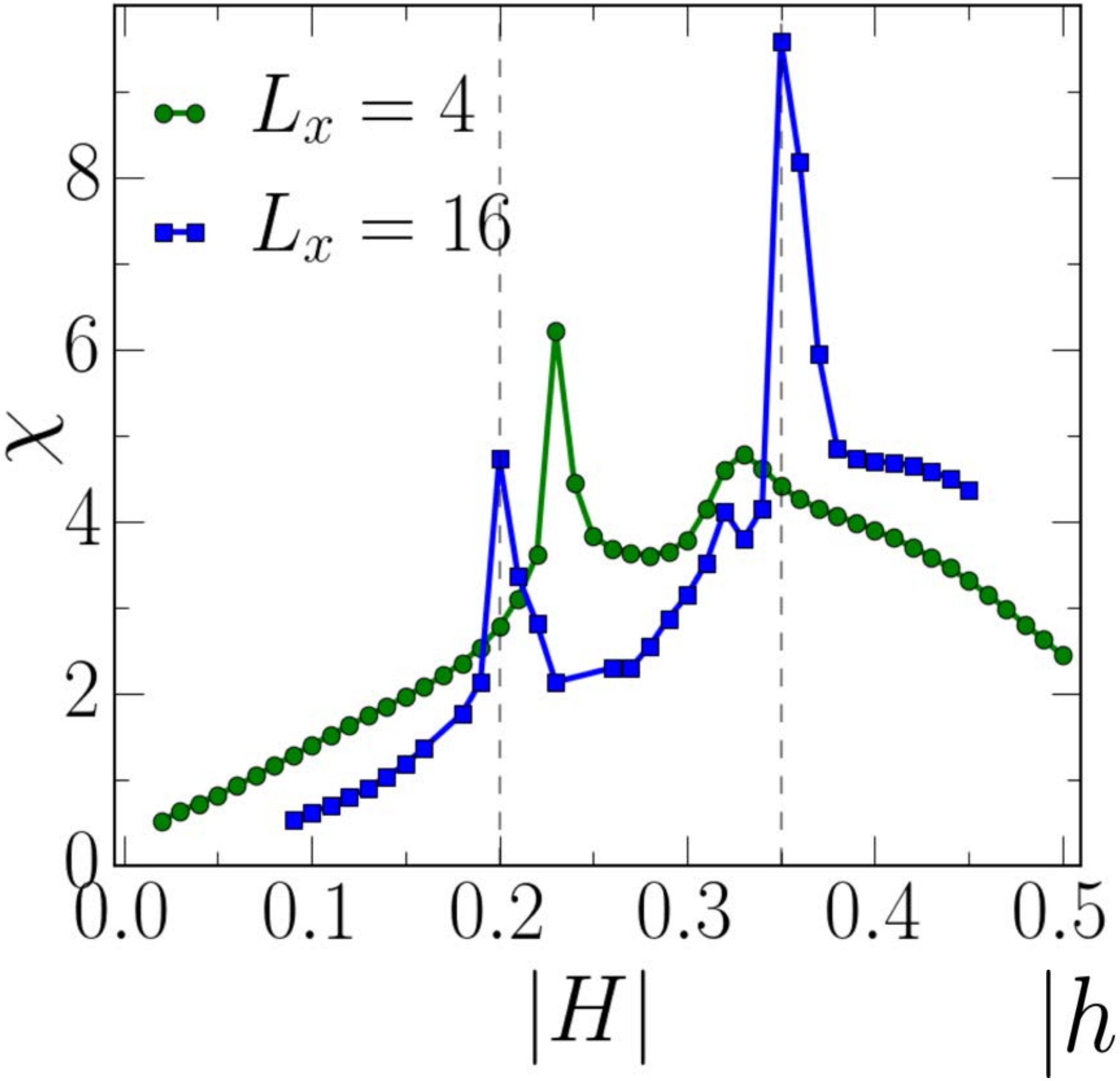


$$H = H_K + h \sum_{i\alpha} S_i^\alpha$$



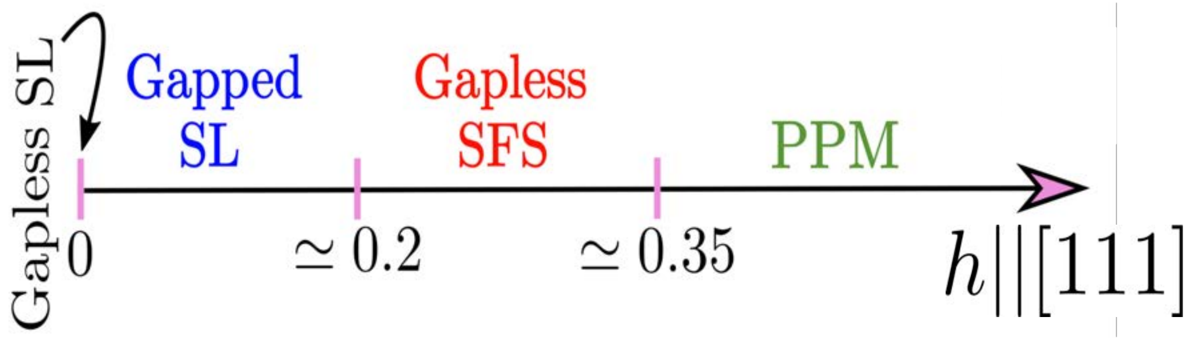
Density Matrix Renormalization Group calculations with 160 spins

Kitaev Model + Magnetic field: susceptibility $h||[111]$



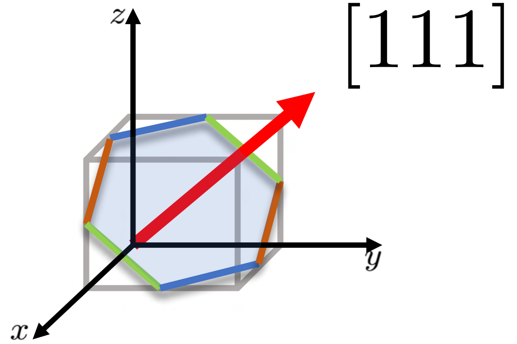
$|h|/K$

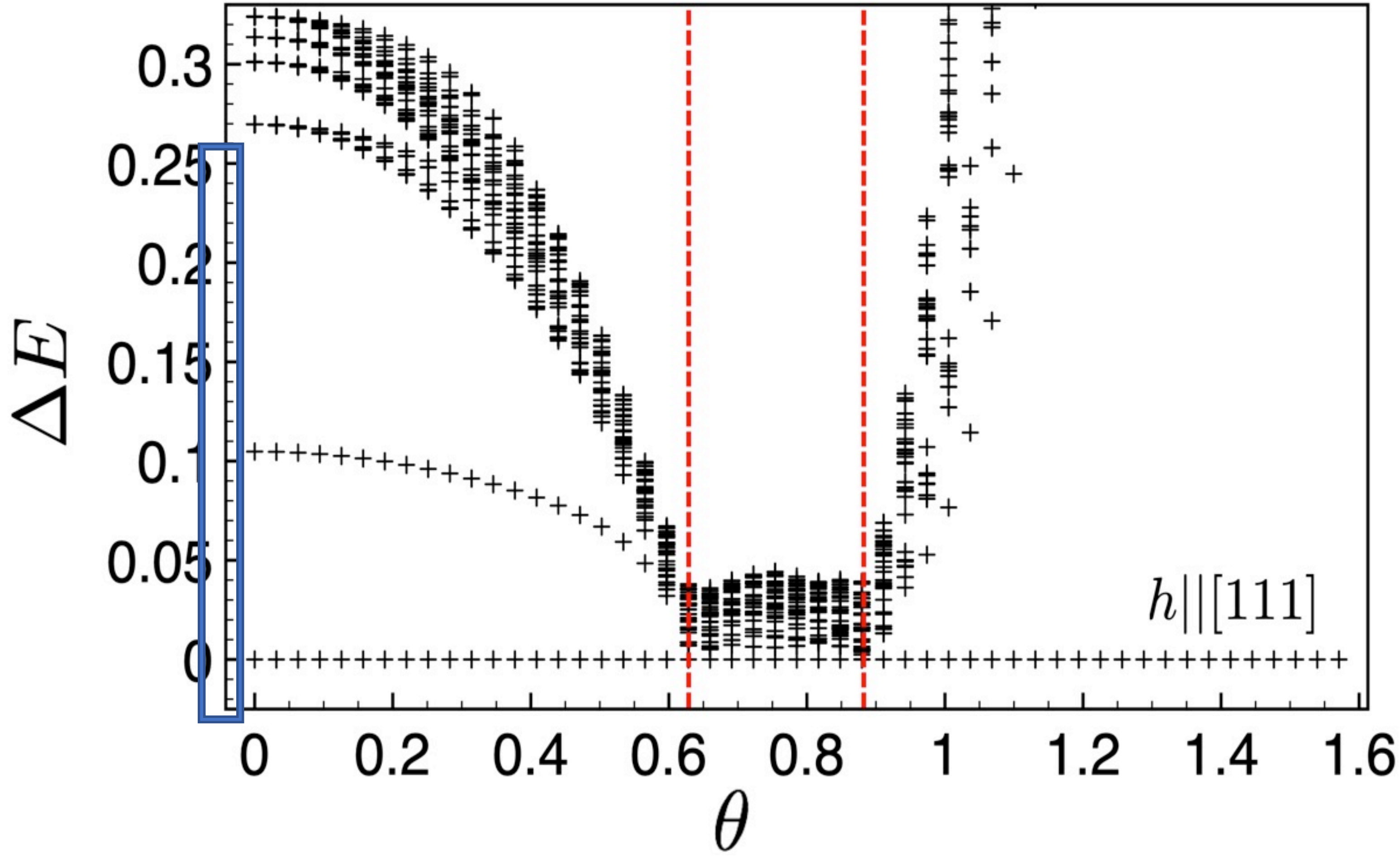
$$H = H_K + h \sum_{i\alpha} S_i^\alpha$$



Evidence for gapless intermediate phase

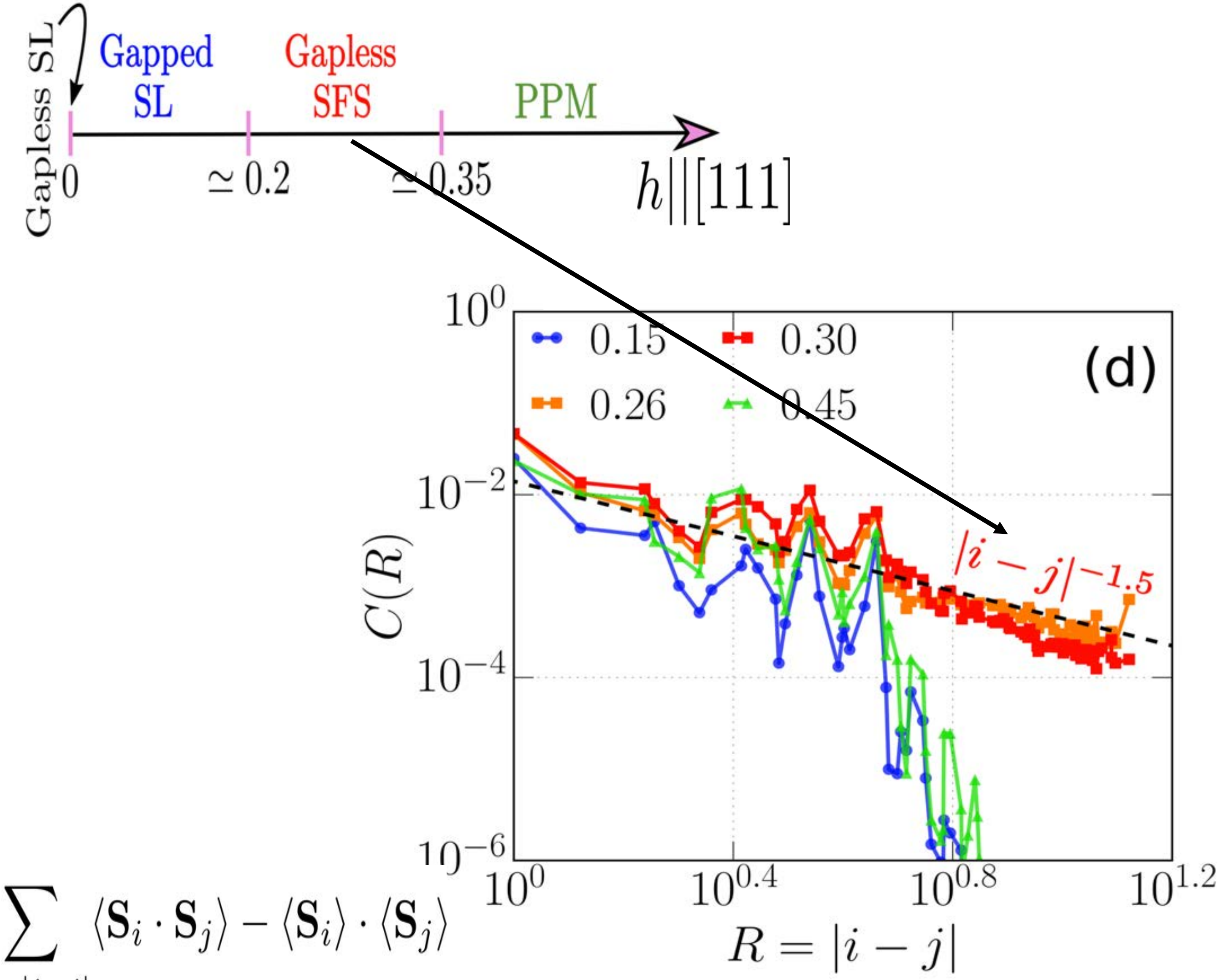
Energy Spectra in a field





$$\theta \sim |\vec{h}|/K$$

Spin-Spin Correlations in Intermediate phase



$$C(R) = \frac{1}{N_R} \sum_{R=|i-j|} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle - \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle$$

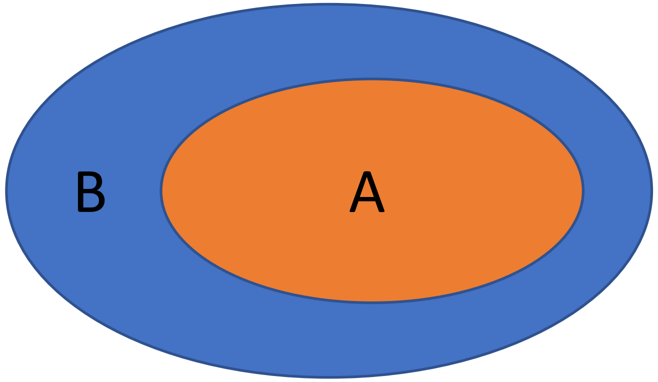
Distinct power law decay of real-space spin-spin correlations!

Evidence for QSL

Entanglement Entropy for a Gapped QSL

$$\rho_A \equiv \mathrm{Tr}_B(\rho)$$

$$S_A = -\mathrm{Tr}\rho_A \log \rho_A$$



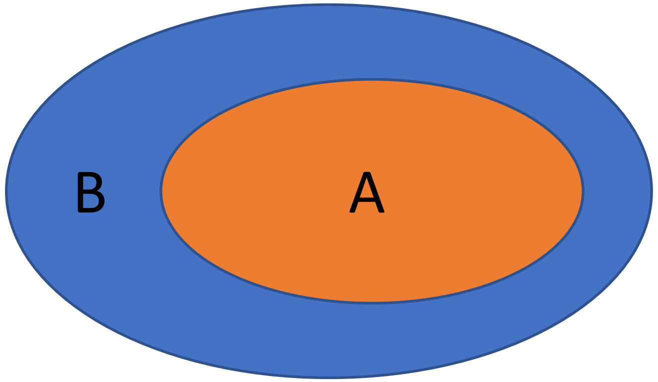
$$S_A \sim \alpha L$$

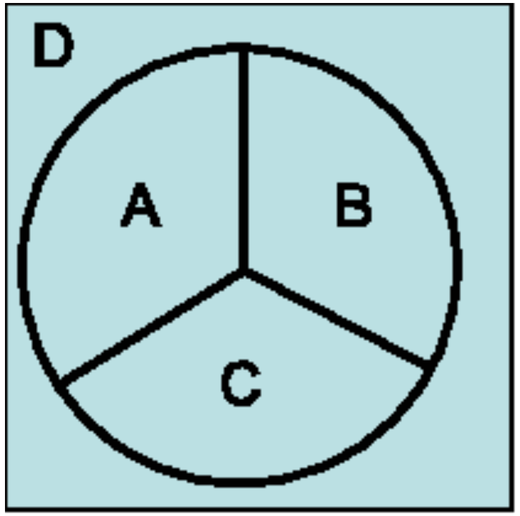
"Area Law" Entanglement in a gapped system

Topological Entanglement Entropy γ

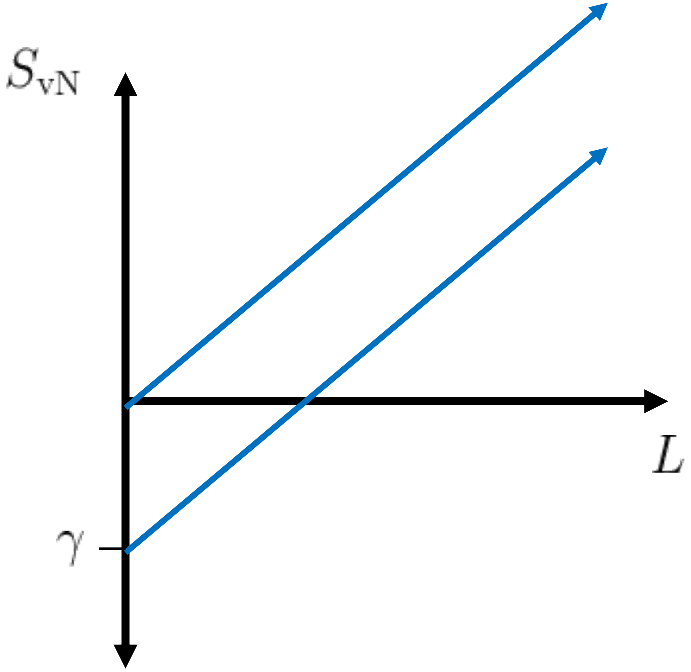
$$S_A \sim \alpha L - \gamma$$

with $\gamma > 0$.



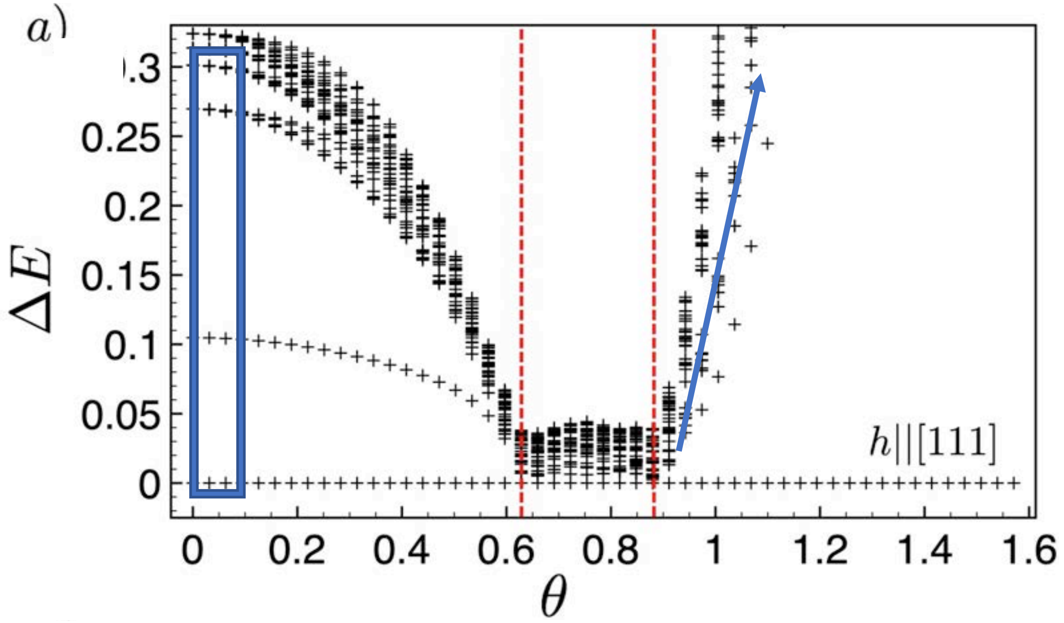


Kitaev-Preskill Construction
to extract γ

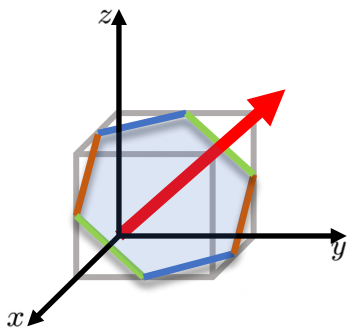


$$S_{\text{topo}} = S_A + S_B + S_C - S_{AB} - S_{BC} - S_{CA} + S_{ABC}$$

Energy
Spectra

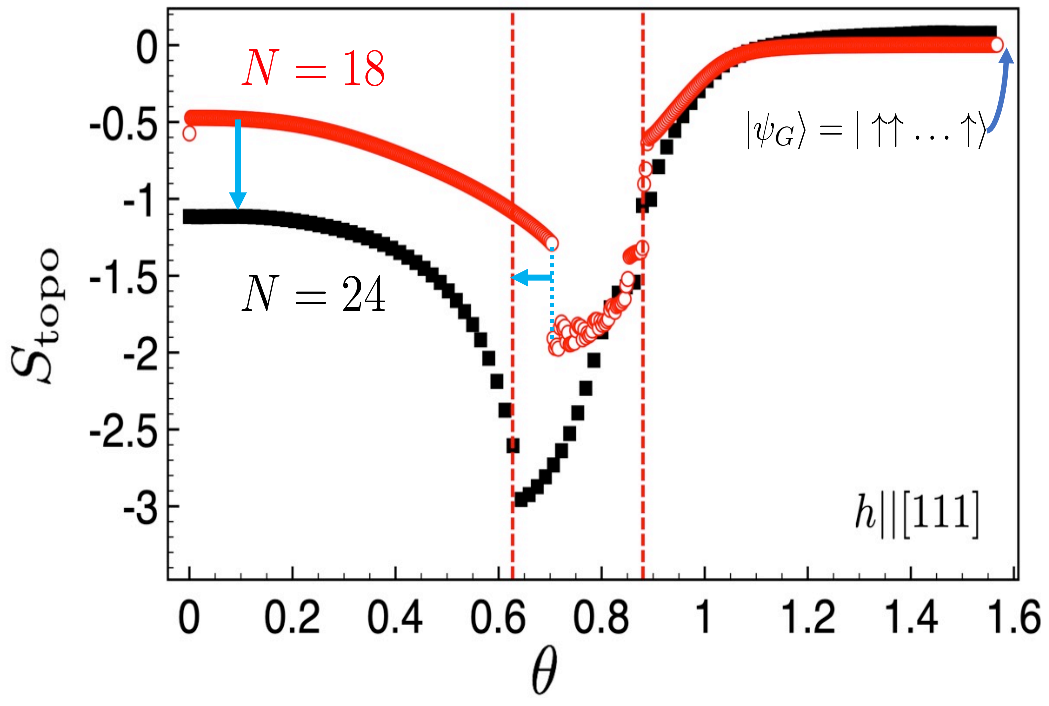


[111]

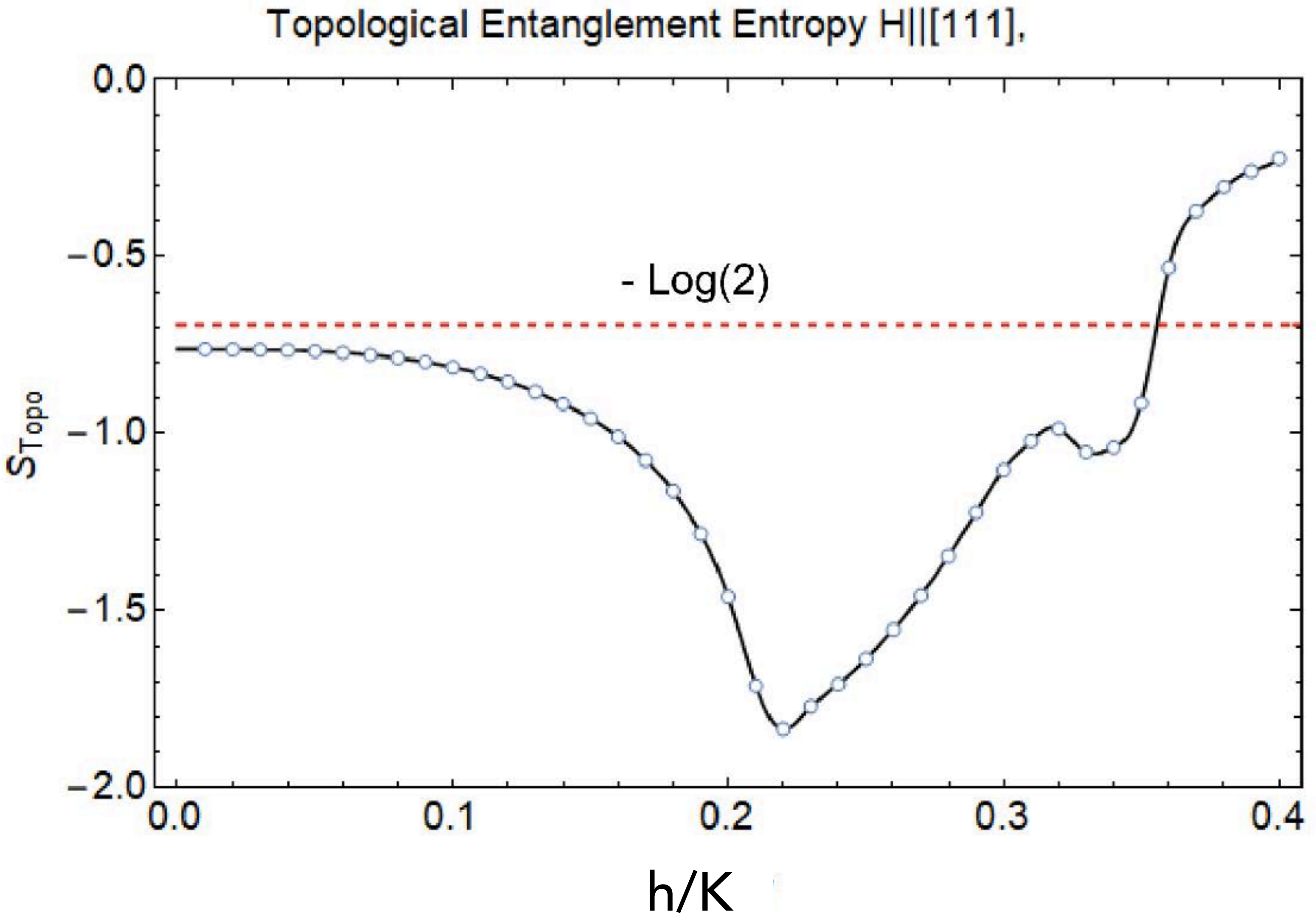


$$\theta \sim |\vec{h}|/K$$

TEE



Ronquillo, Vengal, Trivedi,
PRB 99, 140413(R) (2019)



Topological entanglement entropy: Information resource

Ian Osbourne

Finite γ implies the existence of topological order

→ long range entanglement structure
→ Quantum dimension of excitations

Gapped Non abelian KSL

Vacuum $1 \sim d_1 = 1$

Fermion $\epsilon \sim d_\epsilon = 1$

} abelian

Vortex $v \sim d_v = \sqrt{2} > 1$ } Non abelian

$$\rightarrow D = \sqrt{d_1^2 + d_\epsilon^2 + d_v^2}$$

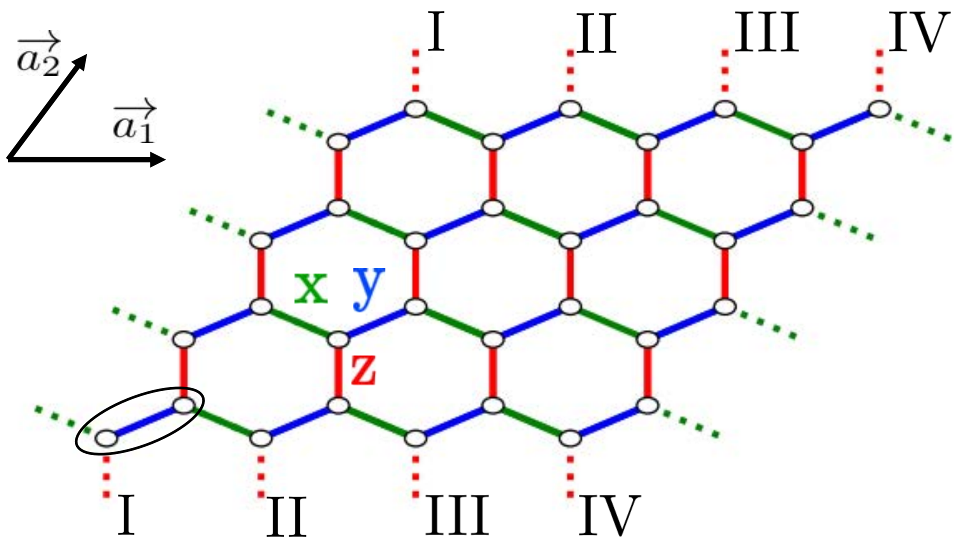
$$= \sqrt{1+1+2}$$

$$= 2$$

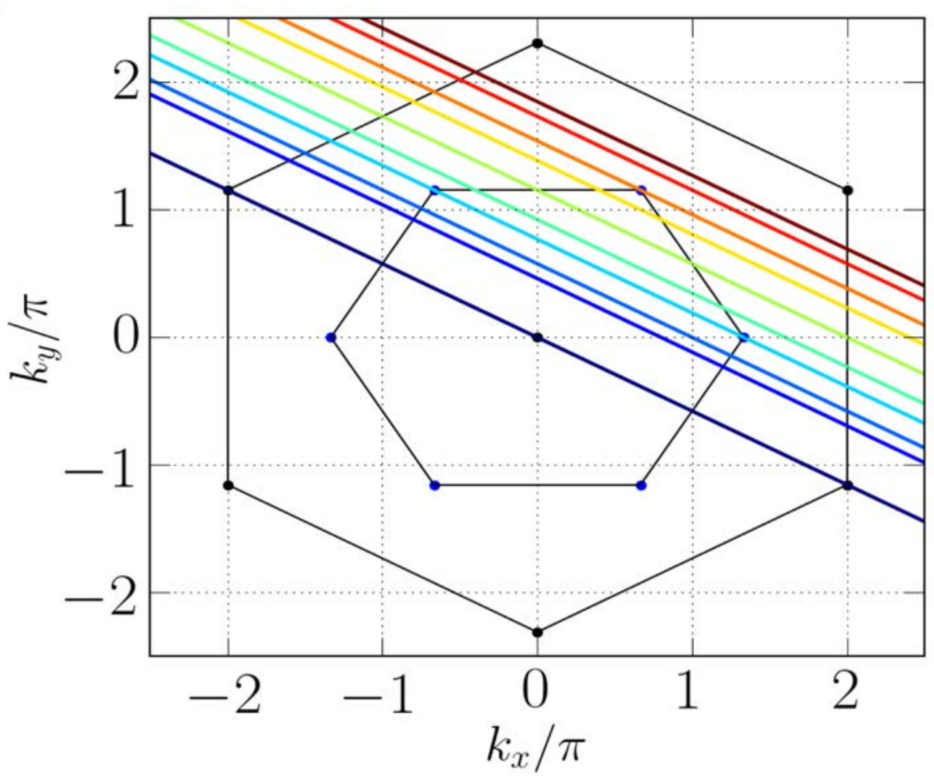
$$\rightarrow \gamma = \log D = \log 2$$

Evidence for spinon Fermi surface

Kitaev Model: spin structure factor



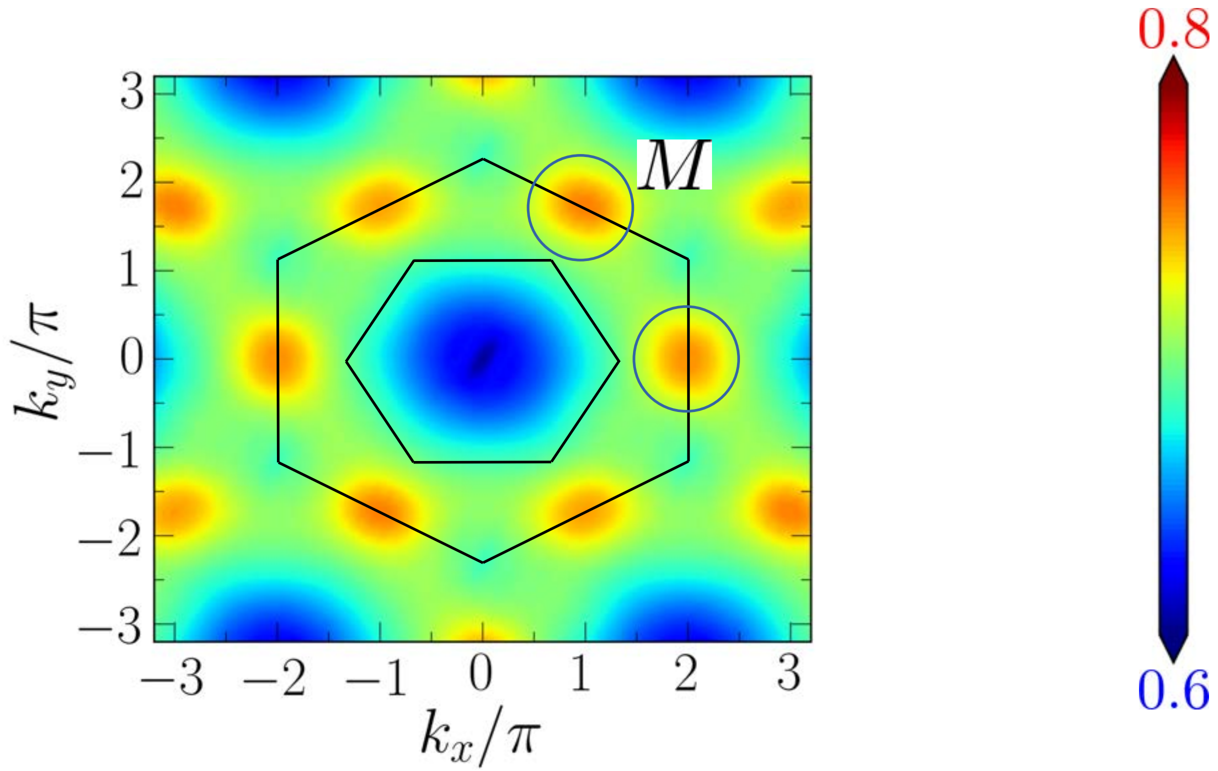
Brillouin Zone: Momenta cuts

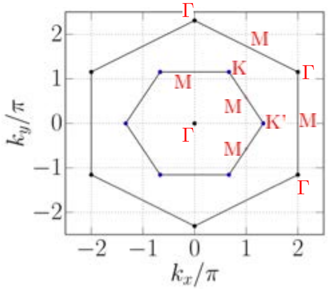


$$H_K = K \sum_{\langle ij \rangle} S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z$$

DMRG++ Open Source:
https://web.ornl.gov/~gz1/dmrgPlusPlus/

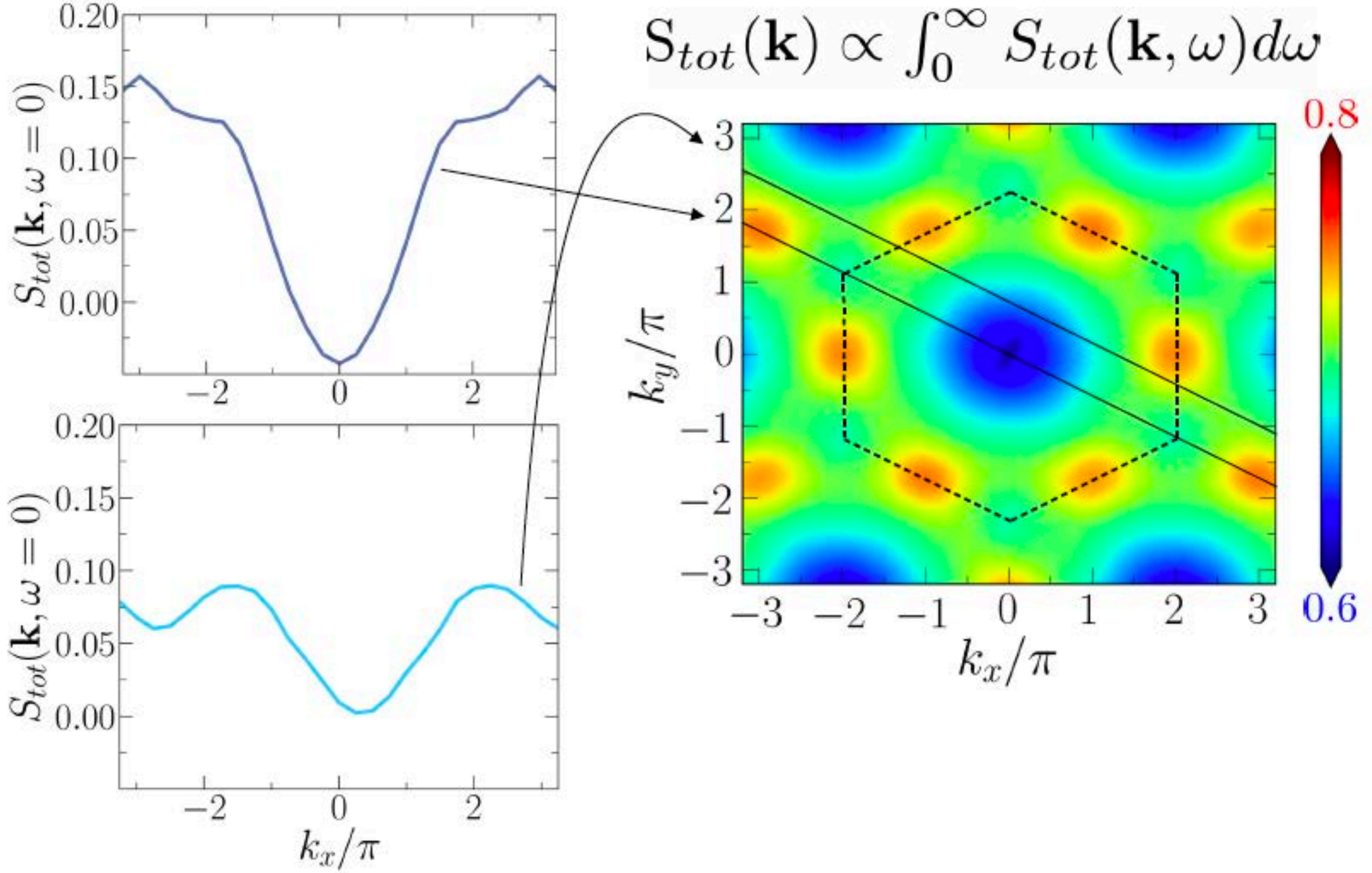
Structure Factor S(k) – Intermediate phase





$$S_{\gamma\gamma'}(\mathbf{k}) = \frac{1}{L^2} \sum_{i\in\gamma, j\in\gamma'} e^{-i\mathbf{k}\cdot\mathbf{r_{ij}}} \left[\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle - \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle\right]$$

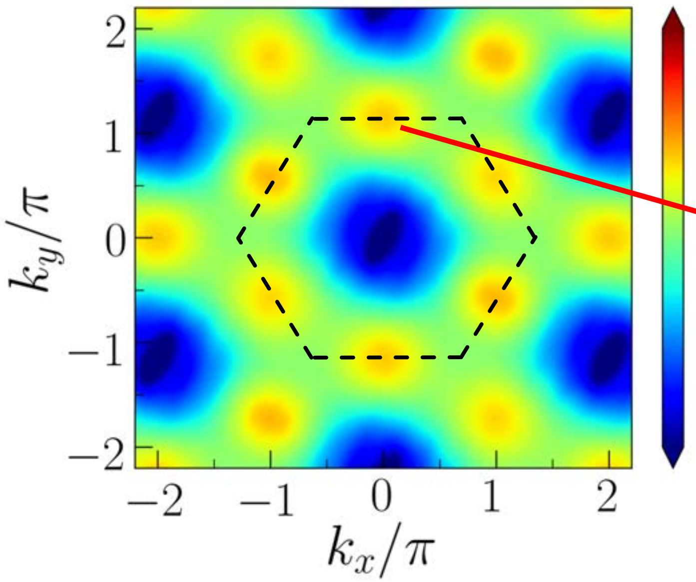
$$\mathrm{S}_{tot} = \sum_{\gamma\gamma'} S_{\gamma\gamma'} \qquad \mathrm{S(k)} = \begin{bmatrix} S_{AA} & S_{AB} \\ S_{BA} & S_{BB} \end{bmatrix}$$

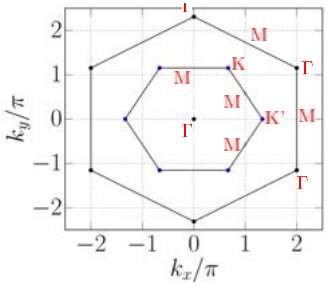


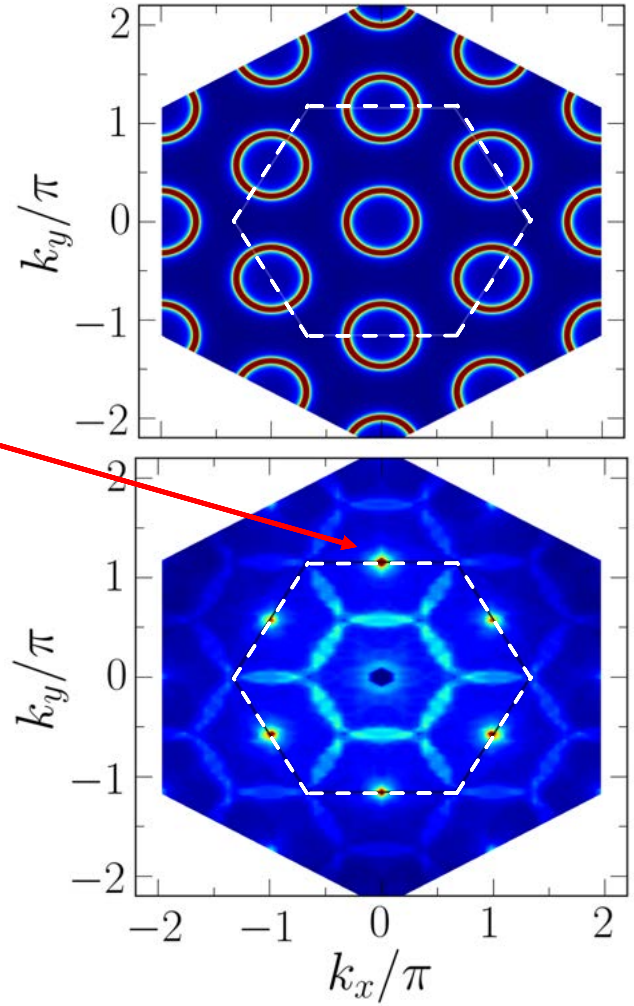
$S_{tot}(\mathbf{k}) \propto \int_0^\infty S_{tot}(\mathbf{k},\omega)d\omega$
$S_{tot}(\mathbf{k},\omega=0)$
k_x/π
k_y/π
0.8
0.6

S(k) → spinon Fermi surface

DMRG Results







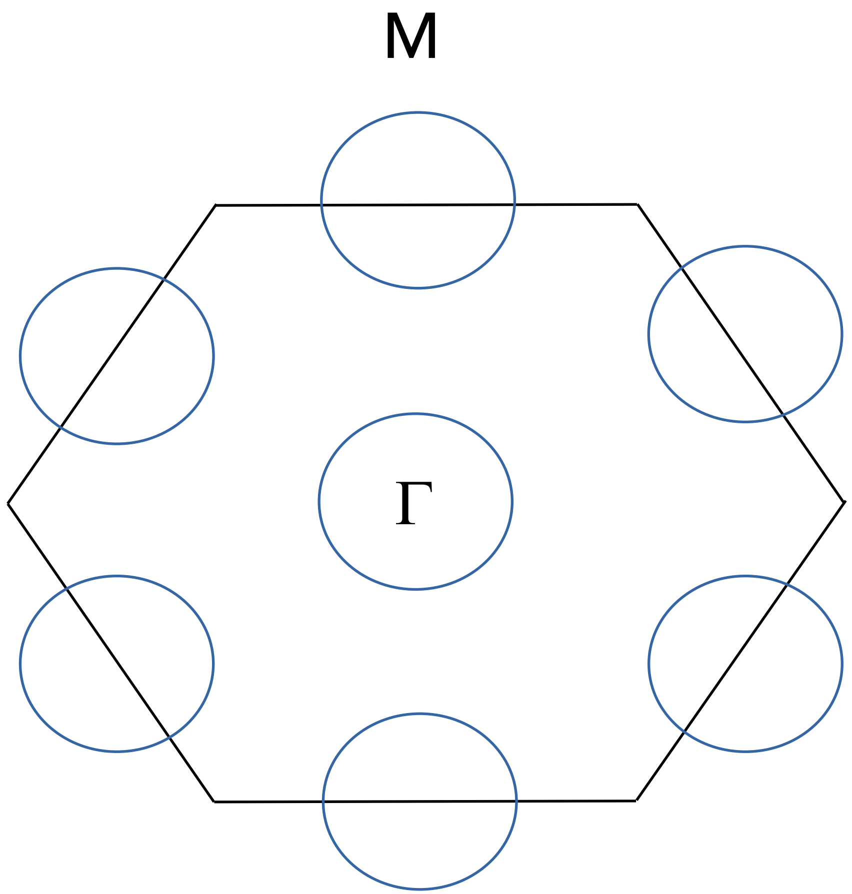
$A(\mathbf{k}, \omega = 0)$

Conjectured Fermi surface

$\omega = 0$

$$\Im(\mathbf{k}) = \sum_q A(\mathbf{k}+\mathbf{q})A(\mathbf{q})$$

“Fermi Surface” of spinons in a Mott insulator!



Singularities at all the M points related by C3 Rotations and Translations

Test using VMC on projected wave function

Roadmap

- ➢ Big picture
- ➢ 2D: Kitaev Model
- ❖ Discovery of a new gapless QSL with a spinon Fermi surface
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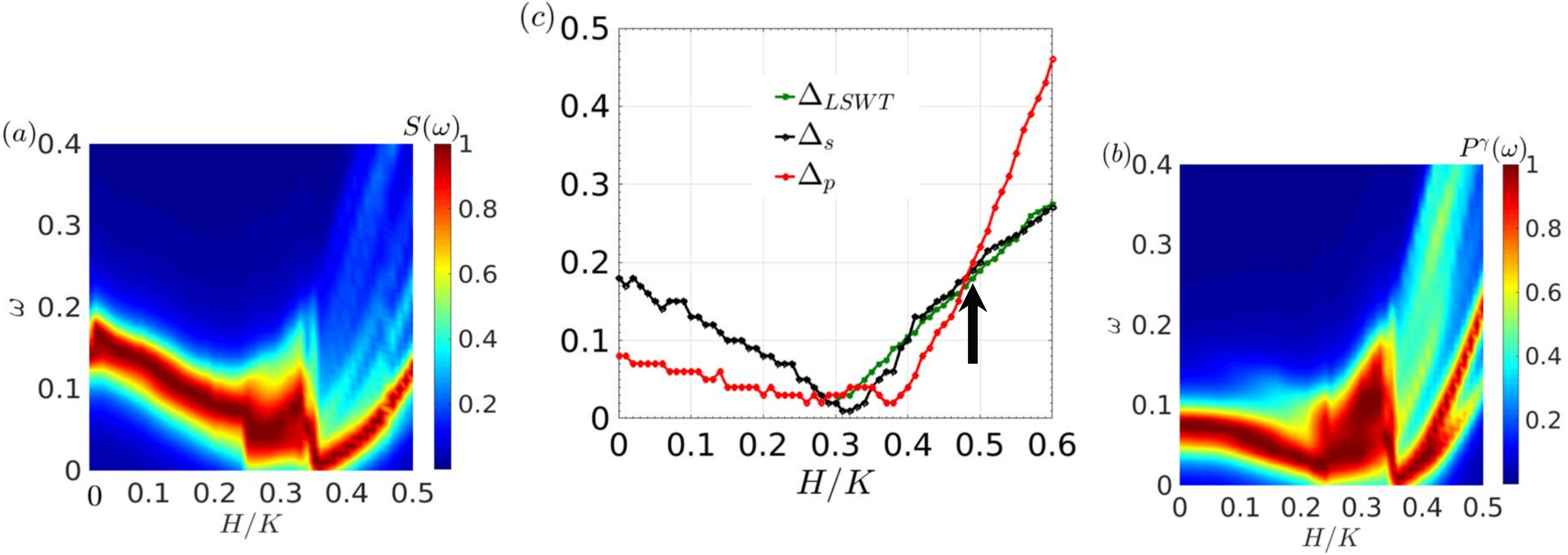
- ➢ QSL Materials
- ➢ How do you detect a QSL?
- ➢ Going forward....

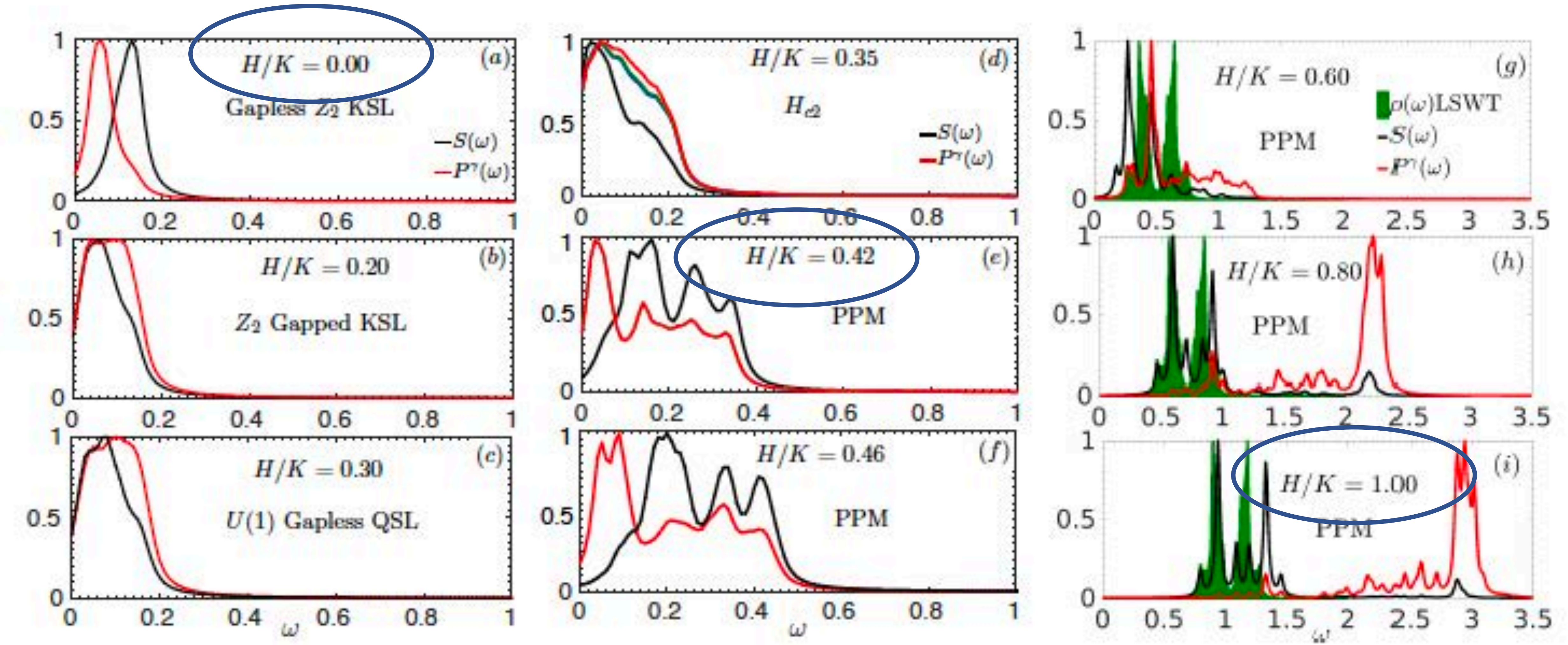
1-spin flip spectral functions

1-spin flip and 2 spin-flip spectral functions

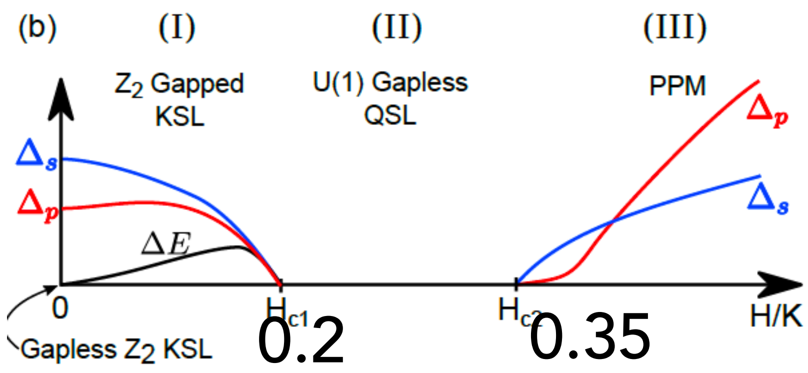


$$S(\omega) = \frac{-1}{N\pi}\,\mathrm{Im}\left[\sum_{\substack{m\neq 0,i\\ \alpha=+,-,z}} \frac{|\langle 0|S_i^\alpha|m\rangle|^2}{\omega + E_0 - E_m + i\eta}\right]$$

$$P^\gamma(\omega) = \frac{-1}{N\pi}\,\mathrm{Im}\left[\sum_{\substack{m\neq 0,i\\ \alpha=+,-,z}} \frac{|\langle 0|S_i^\alpha S_{i+\gamma}^\alpha|m\rangle|^2}{\omega + E_0 - E_m + i\eta}\right]$$



H/K = 0.00
Gapless Z2 KSL
(a)
S(ω)
P^γ(ω)
H/K = 0.20
Z2 Gapped KSL
(b)
H/K = 0.30
U(1) Gapless QSL
(c)
H/K = 0.35
H_c2
(d)
H/K = 0.42
PPM
(e)
H/K = 0.46
PPM
(f)
H/K = 0.60
PPM
(g)
ρ(ω)LSWT
H/K = 0.80
PPM
(h)
H/K = 1.00
PPM
(i)
ω



(b)
(I)
(II)
(III)
Z2 Gapped KSL
U(1) Gapless QSL
PPM
Δs
Δp
ΔE
0
Hc1
Hc2
H/K
Gapless Z2 KSL
0.2
0.35

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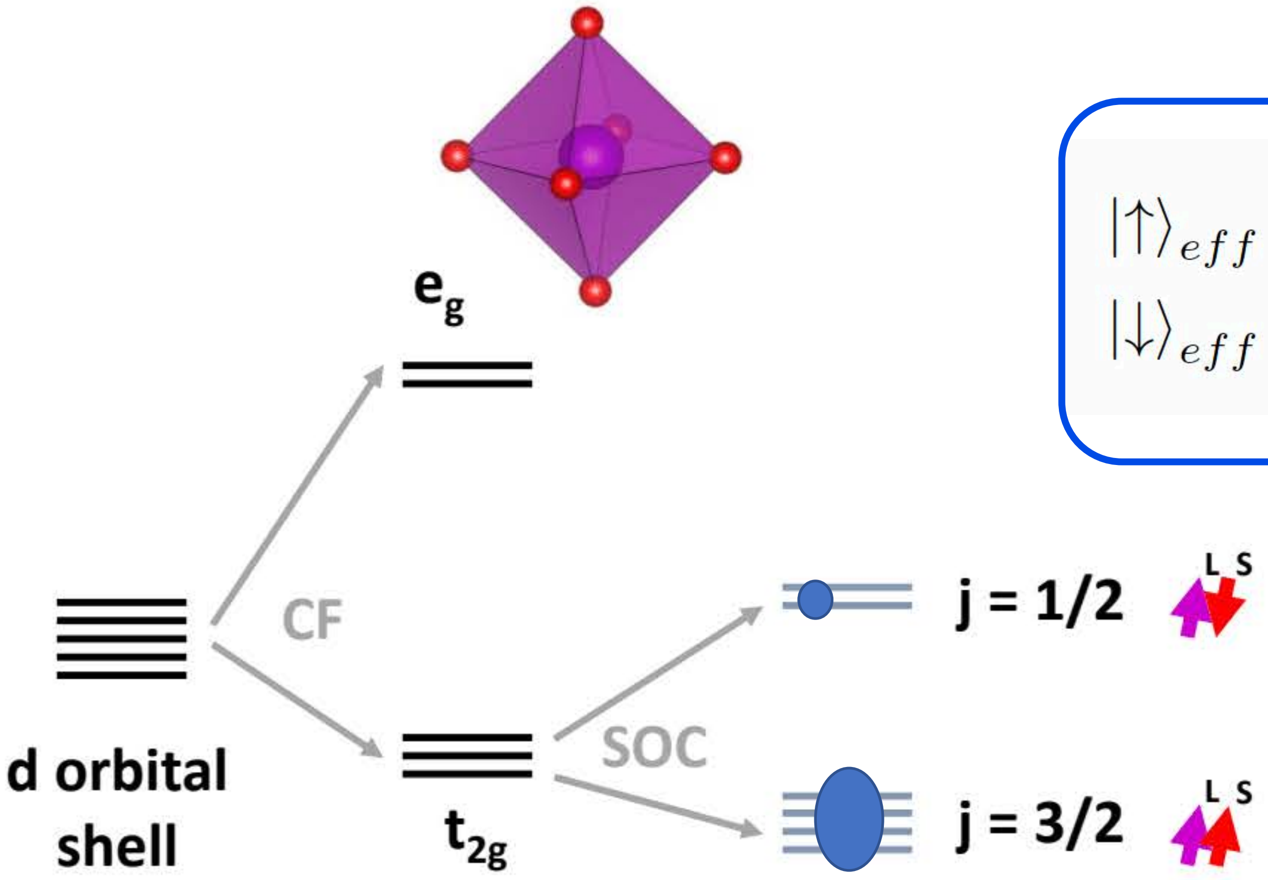
Main ingredients for Kitaev materials

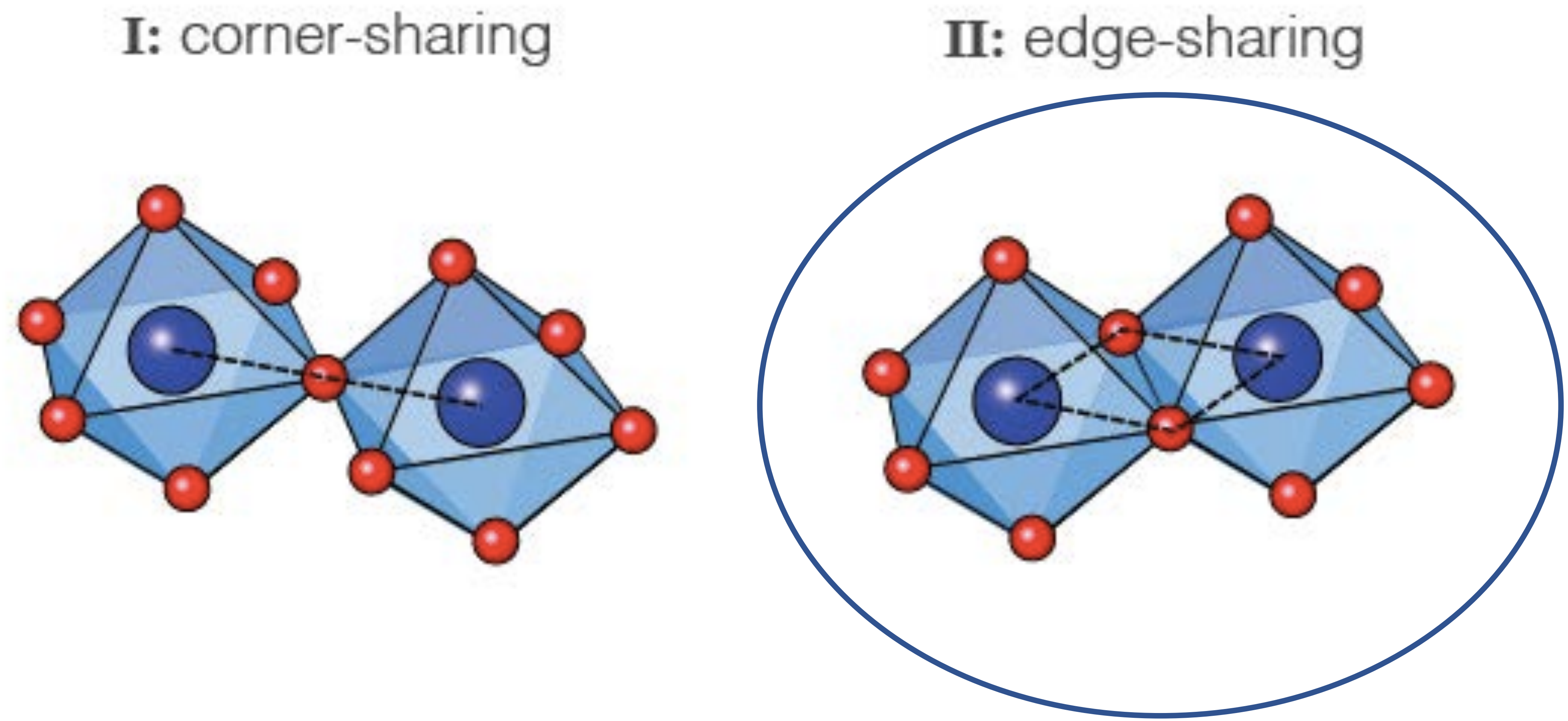
Spin-Orbit coupled Mott Insulators

Mo	Tc	**Ru**	Rh
W	**Re**	**Os**	**Ir**



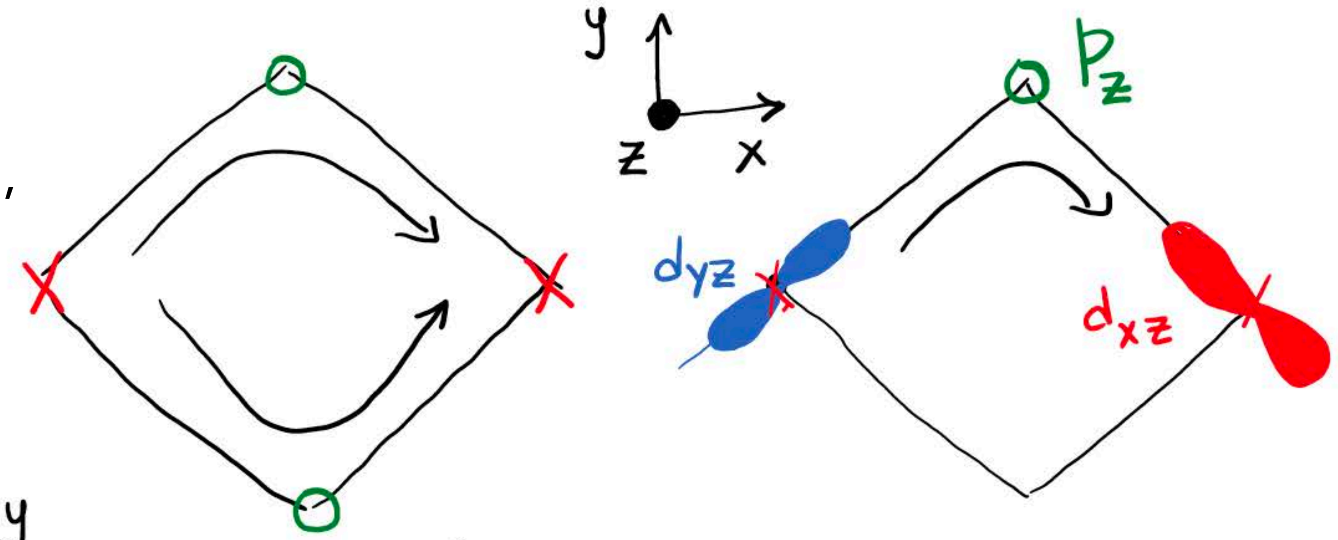
$$|\uparrow\rangle_{eff} \sim i\,|zx,\downarrow\rangle + |yz,\downarrow\rangle + |xy,\uparrow\rangle$$

$$|\downarrow\rangle_{eff} \sim -i\,|zx,\uparrow\rangle + |yz,\uparrow\rangle - |xy,\downarrow\rangle$$

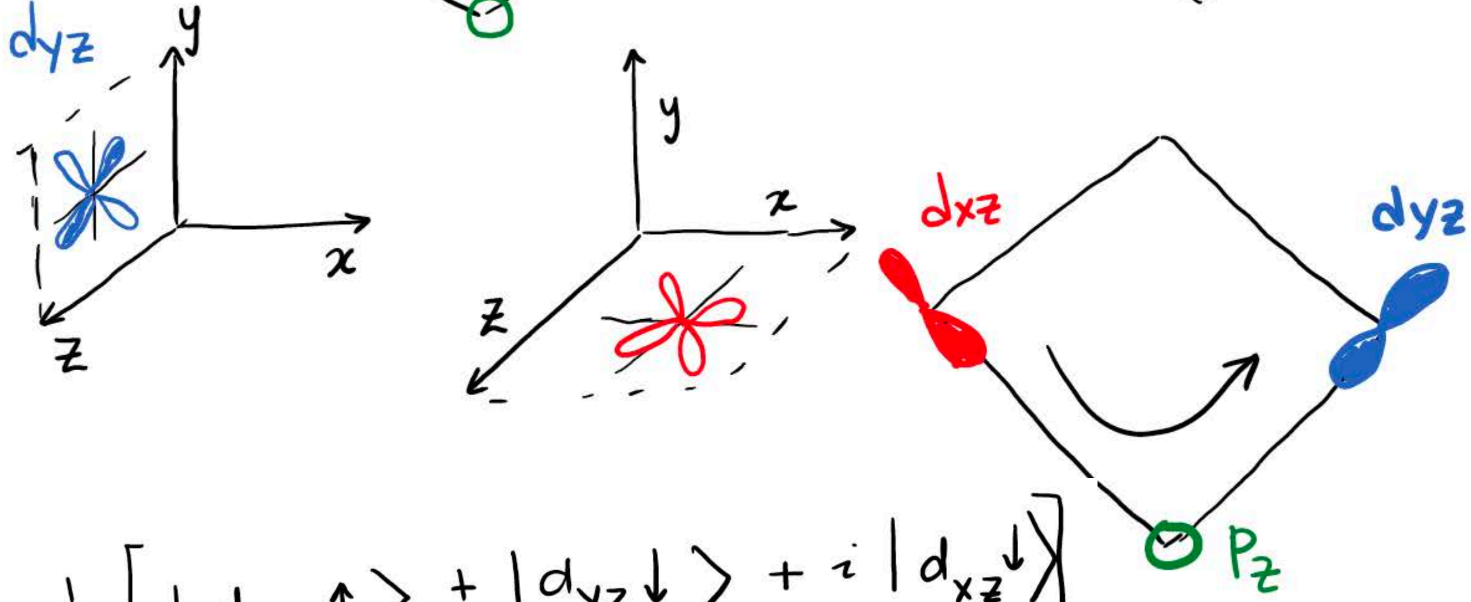


Destructive interference between the two pathways generates bond-dependent interactions


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



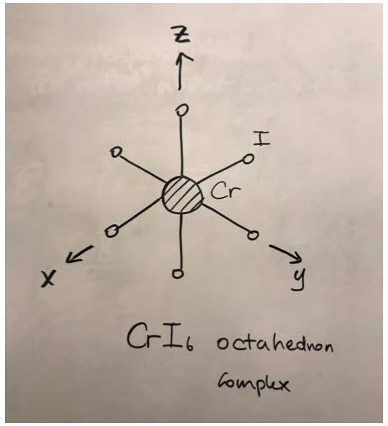
hopping via p_z orbital on ligand changes $d_{yz} \to d_{xz}$

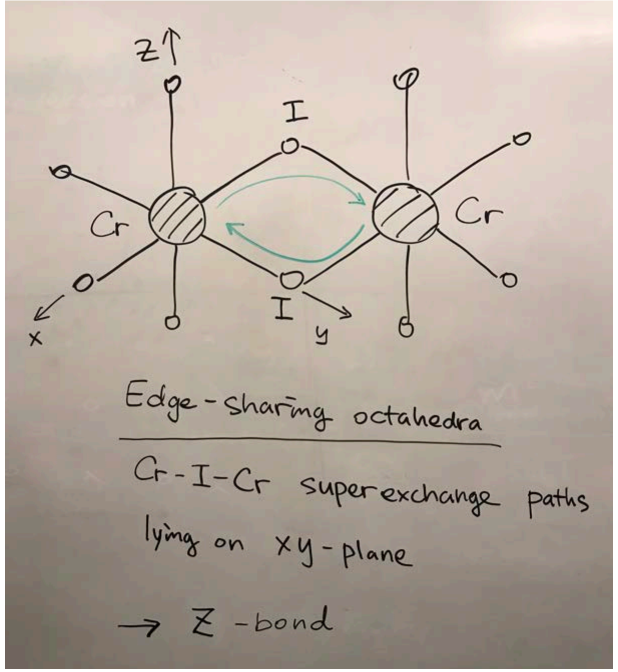


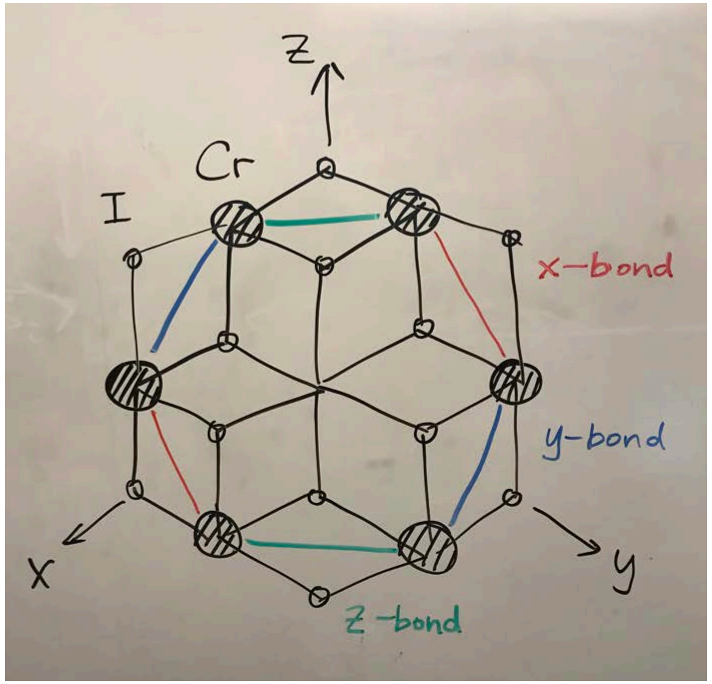
$d_{xz} \longrightarrow d_{yz}$

$$|J_z = +\tfrac{1}{2}\rangle = \frac{1}{\sqrt{3}}\left[\,|d_{xy}\uparrow\rangle + |d_{yz}\downarrow\rangle + i\,|d_{xz}\downarrow\rangle\right]$$

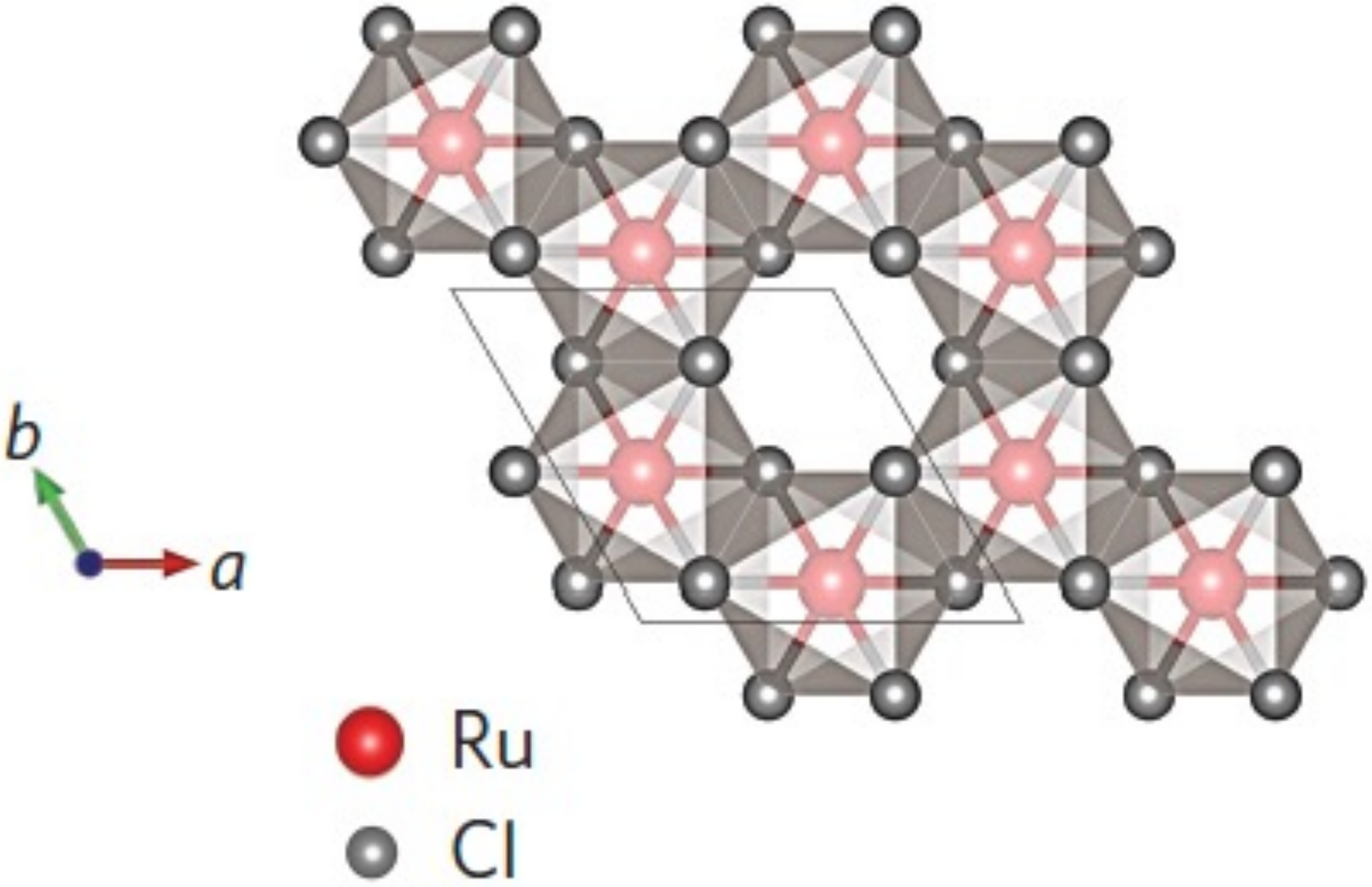
Crystal structure of α-$RuCl_3$
→ candidate Kitaev material

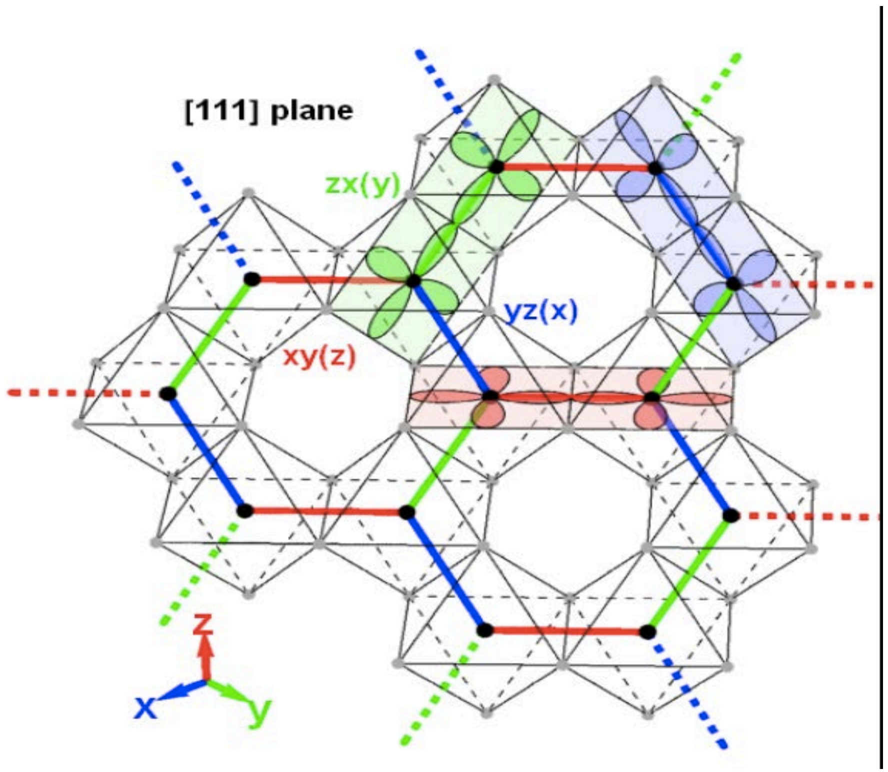






α-$RuCl_3$





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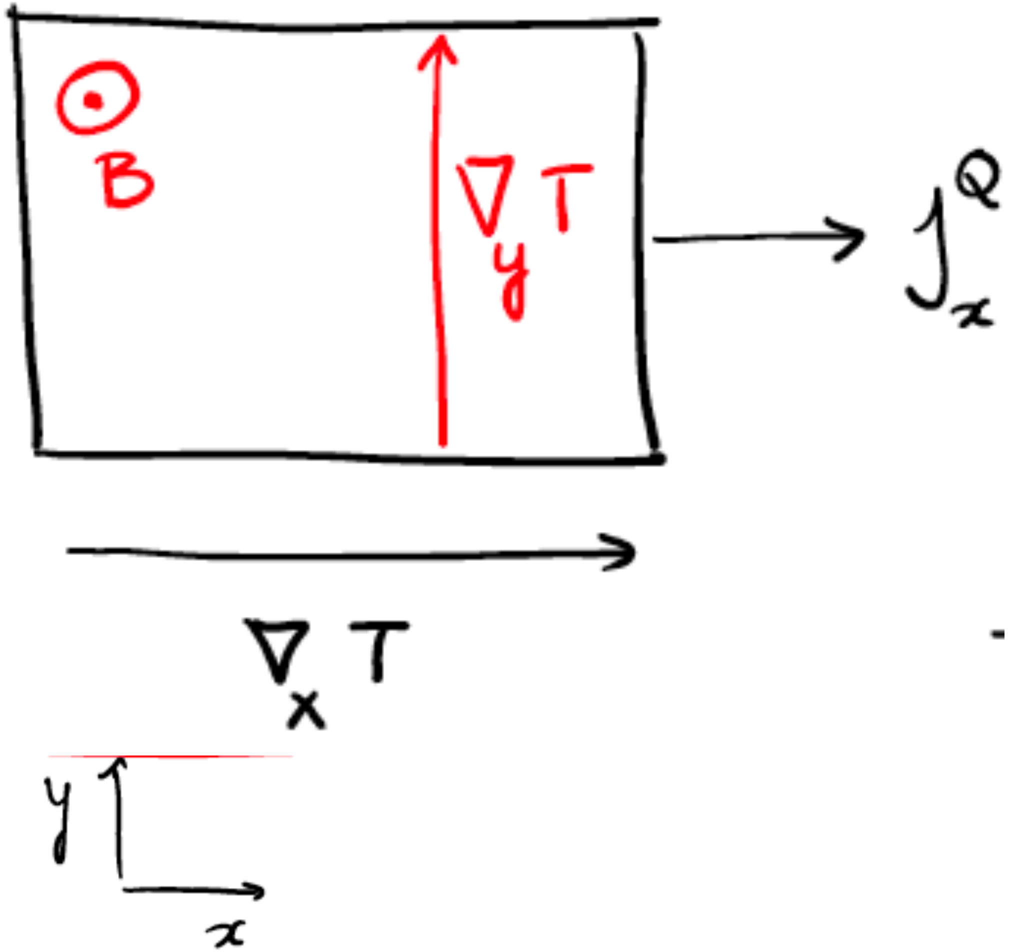
Thermal Hall Conductivity



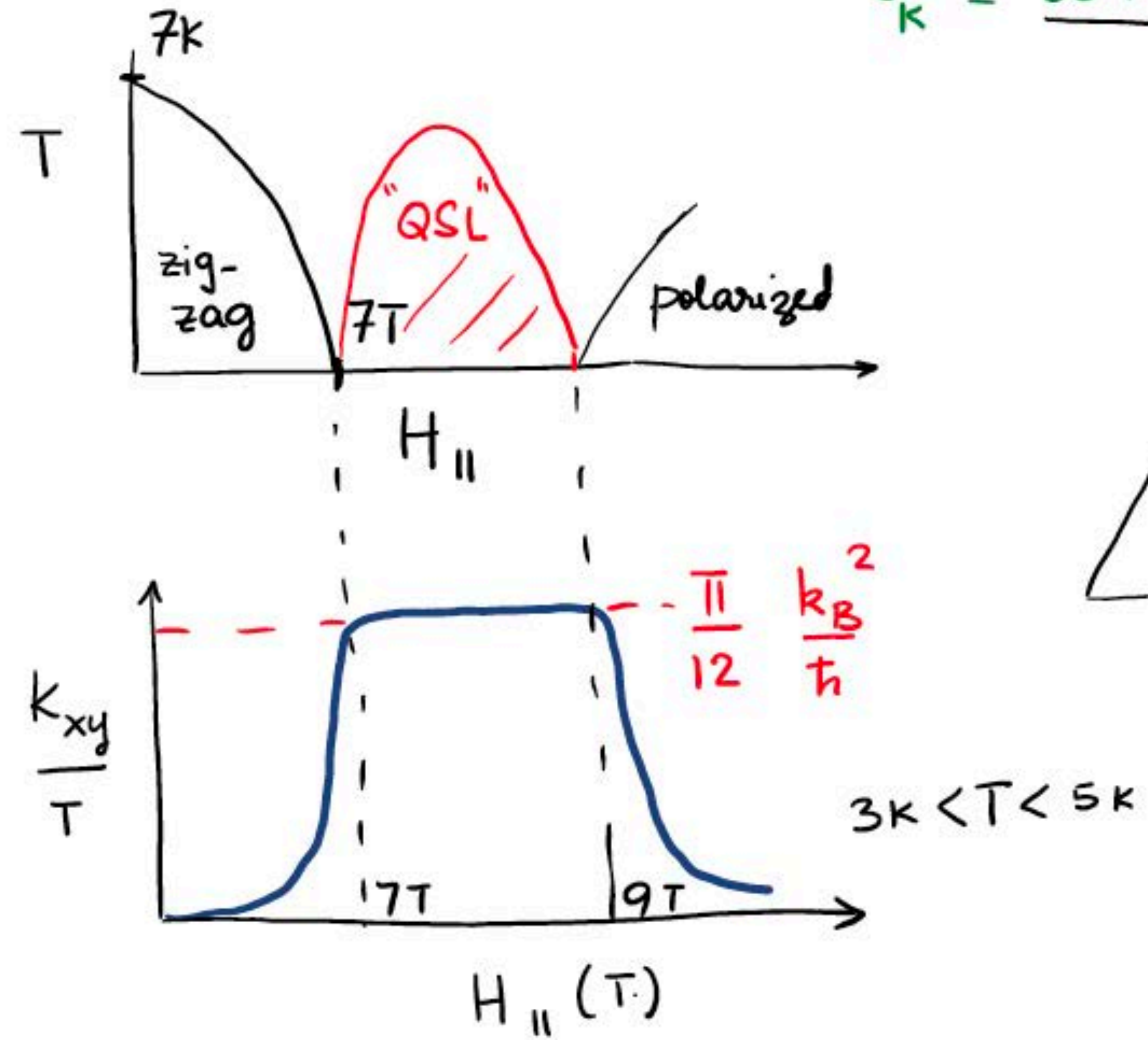
$$\vec{J}^Q = \overleftrightarrow{K}\,(-\vec{\nabla} T)$$

$$\overleftrightarrow{K} = \begin{pmatrix} K_{xx} & \boxed{K_{xy}} \\ -K_{xy} & K_{xx} \end{pmatrix}$$

$J_y^Q = 0$ (impose condition)

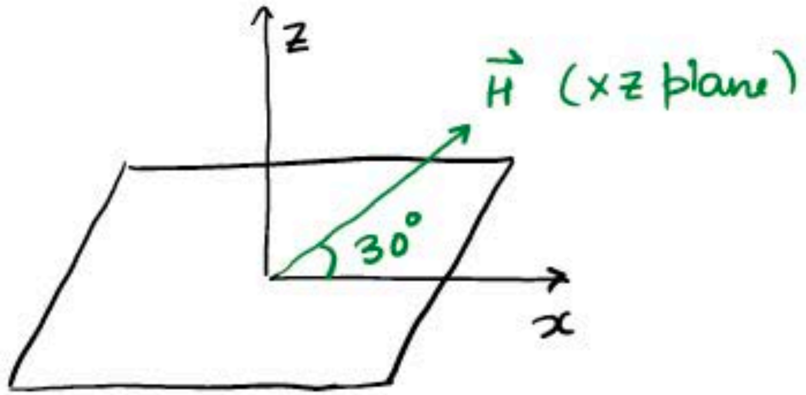
Material : α - $RuCl_3$ $\simeq$ Kitaev Magnet

$J_K \simeq$ 80 K



For $S = 1/2$

1 Tesla $\simeq$ 1 K

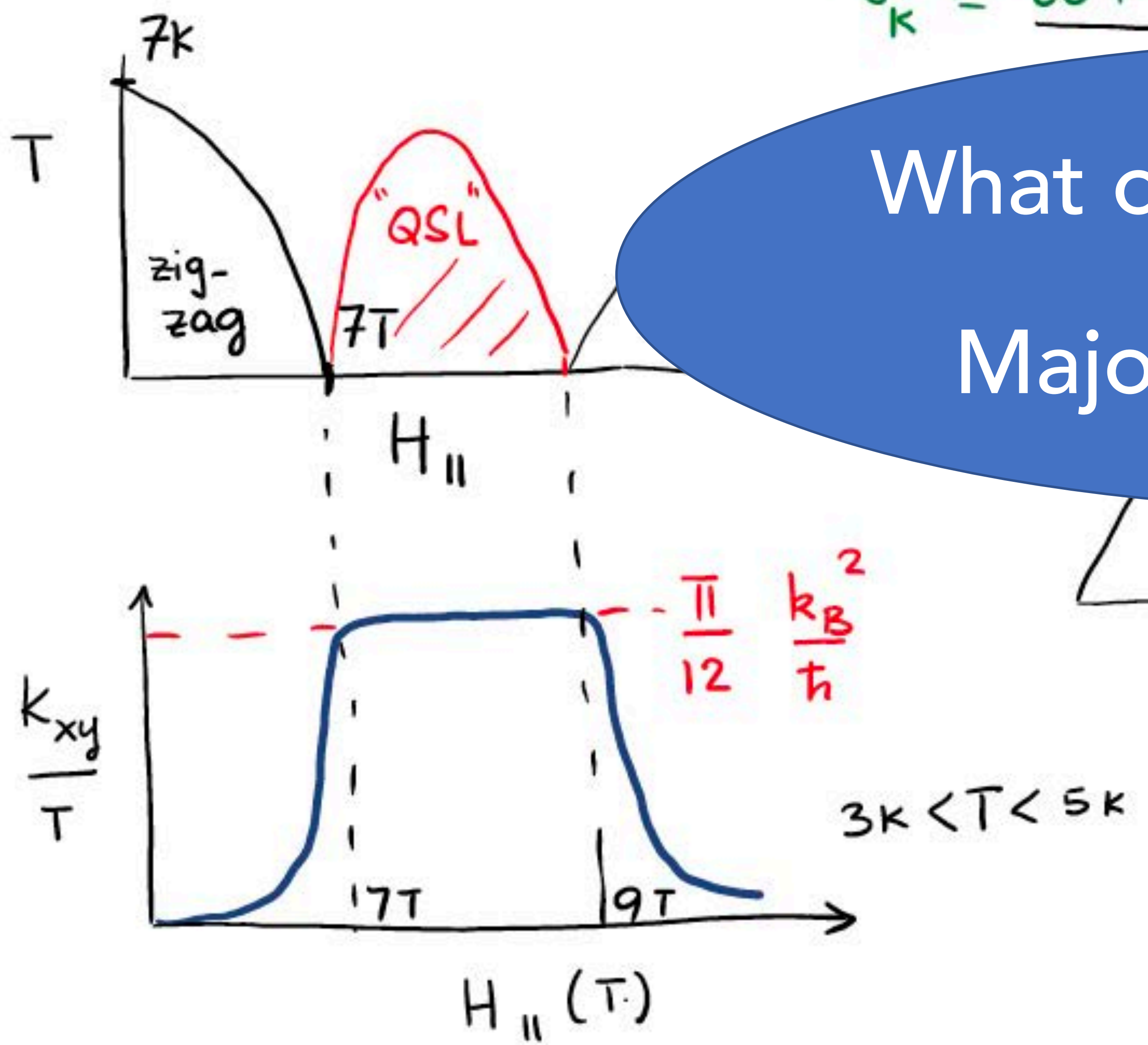


$$K_{xy} = \frac{1}{2} K_Q$$

$$K_Q = \frac{\pi^2}{6} k_B^2/\hbar$$

Material: α-$RuCl_3$ $\simeq$ Kitaev Magnet

$J_K \simeq 80\,K$



What object carries heat?

Electron? Spin?

Majorana edge mode

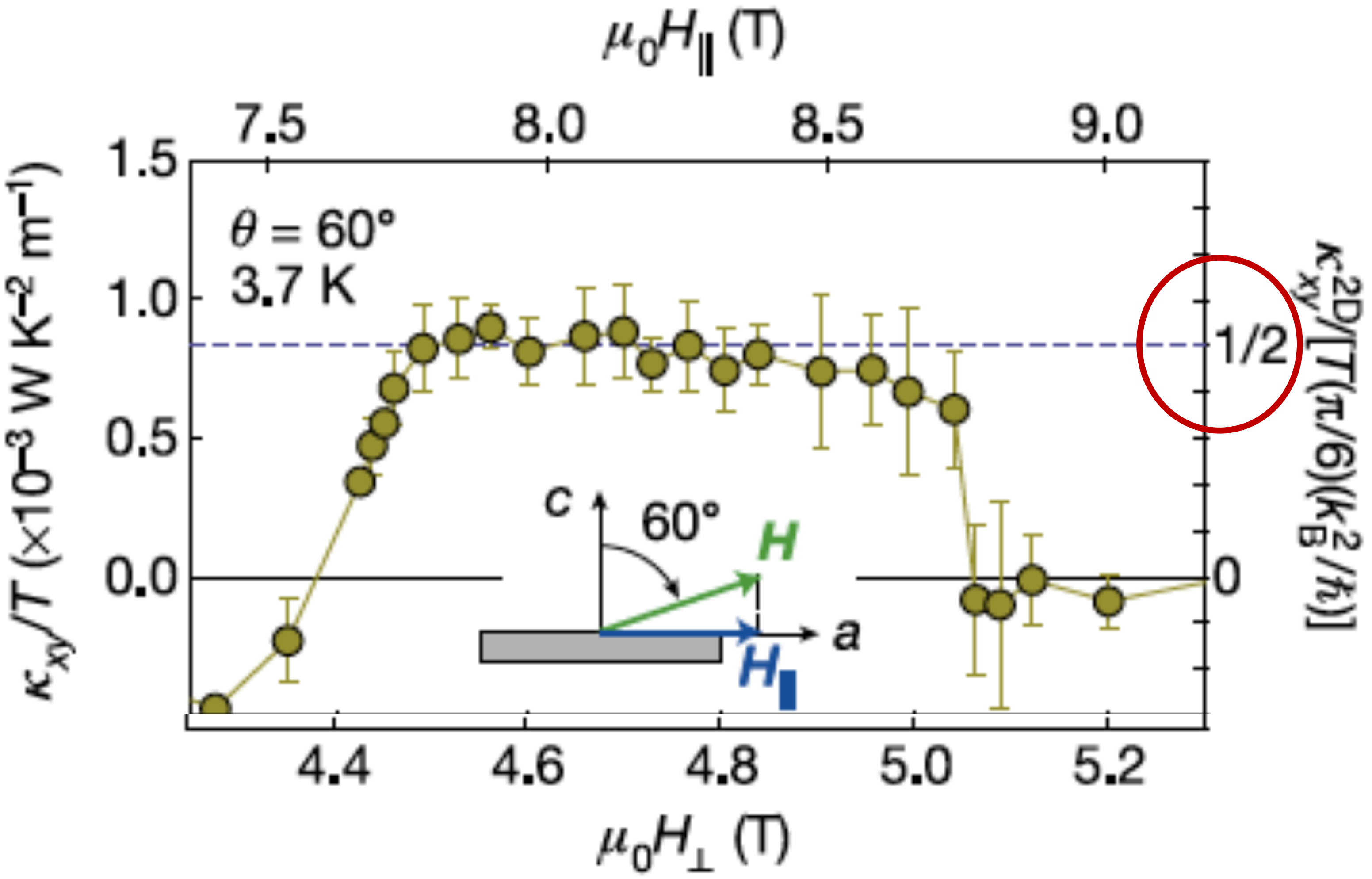
$$\kappa_{xy} = \frac{1}{2}\kappa_Q$$

$$\kappa_Q = \frac{\pi^2}{6} k_B^2/\hbar$$

Signatures of a QSL: ***quantized*** thermal Hall conductance

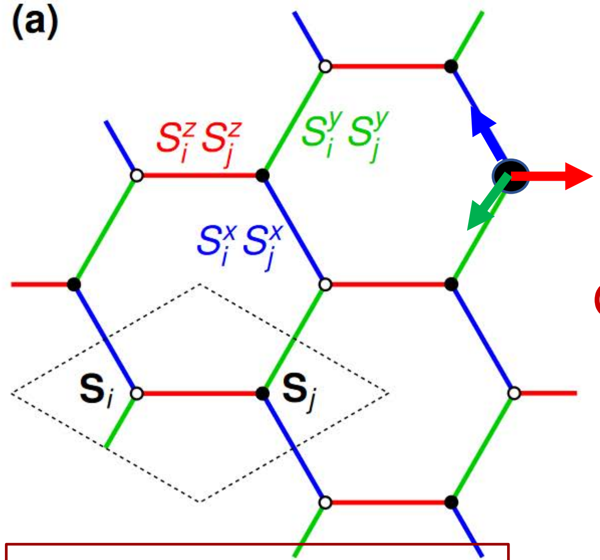
$$\kappa_{xy}^{2D} = \left[\frac{1}{2}\right] \frac{\pi}{6} \frac{k_B^2}{\hbar} T$$

$$\kappa_{xy}^{2D} = \kappa_{xy} d$$



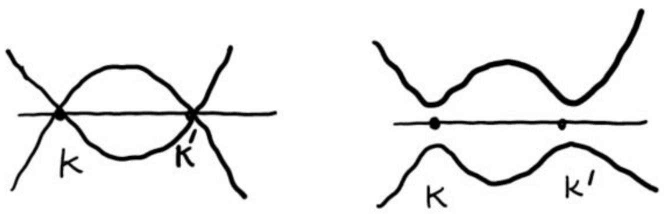
Y. Kasahara, T. Ohnishi, Y. Mizukami, O. Tanaka, Sixiao Ma, K. Sugii, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibauchi & Y. Matsuda, Nature 559, 227 (2018).

Predictions for Kitaev magnets



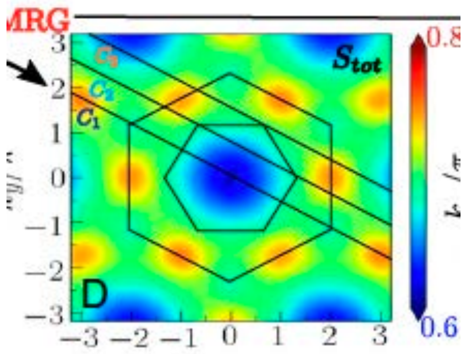
Frustration from bond-dependent interactions

Kitaev (2006)
Jackeli, Khaliullin (2009)



Gapless Z_2 QSL

Gapped Z_2 QSL



Gapless U(1) QSL

Magnon bound states

h=0 — h_{c1} — h_{c2} — h/K (field)

$$\kappa_{xy}^{2D} = \left[\frac{1}{2}\right]\frac{\pi}{6}\frac{k_B^2}{\hbar}T$$

cf: FQHE $\sigma_{xy} = \frac{1}{3}\frac{e^2}{h}$

Fermi surface of neutral, gapless spinons in an insulator!

$$\kappa_{xx} \sim T$$

Chiral spinon edge mode → Quantized thermal Hall conductance

Ronquillo, Vengal, Trivedi, PRB **99**, 140413 (2019)
Patel & Trivedi, *PNAS* **116**,12199 (2019)
Pradhan, Patel, Trivedi, PRB 101, 180401 (2020)

Going forward…..

1. Predictions for Raman scattering to observe magnon bound states

2. Spin and heat transport

3. Observation of neutral spinon Fermi surfaces

4. Doped QSLs → ??