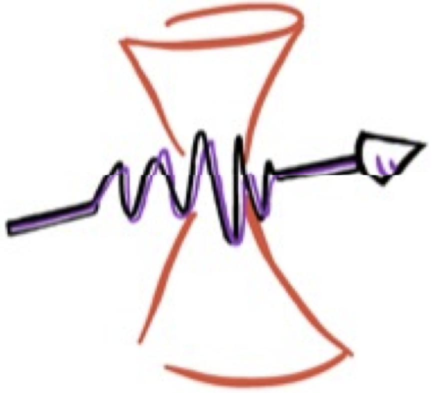
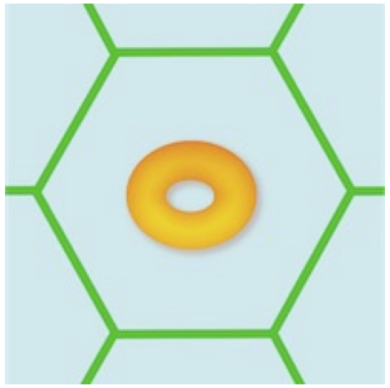


Quantum Spin Liquids: Signatures of Fractionalization

Nandini Trivedi
Physics Department
The Ohio State University

trivedi.15@osu.edu

http://trivedireseach.org.ohio-state.edu/



Center of Emergent Materials
NSF MRSEC – DMR

Spin and Heat Transport in Quantum and Topological Materials
Topological Quantum Matter: Concepts and Realizations
November 11-15, 2019

Gordon Research Conference

Correlated Electron Systems

Topology and Correlations: Long-Range Entanglement in Many-Body Systems

June 28 - July 3, 2020

Mount Holyoke College, South Hadley, MA

https://www.grc.org/correlated-electron-systems-conference/2020/

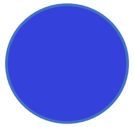
Chairs: Nandini Trivedi and James G. Analytis

Roadmap

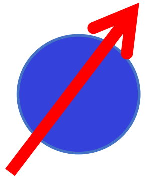
- Big picture
- 2D: Kitaev Model
  - Discovery of a new gapless QSL with a spinon Fermi surface
  - Spectrum of 1 spin flip and 2 spin flip excitations
- QSL Materials
- How do you detect a QSL?
- Going forward….

Big Picture

Quantum Matter: Fractionalization



electron

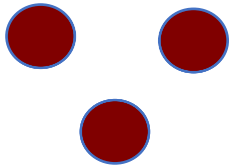


Electron=charge+spin

Spin wave (magnon) S=1

$$\nabla \cdot B = 0$$

No monopoles



fractionalization

Fractional Quantum Hall effect

spin-charge separation

Luttinger Liquids

Fractionalization: S=1/2 spinons: (neutral) spinon Fermi surface

Monopoles in spin ice

Quantum Spin Liquid

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

- ❑ Topological Paradigm

"IQHE"

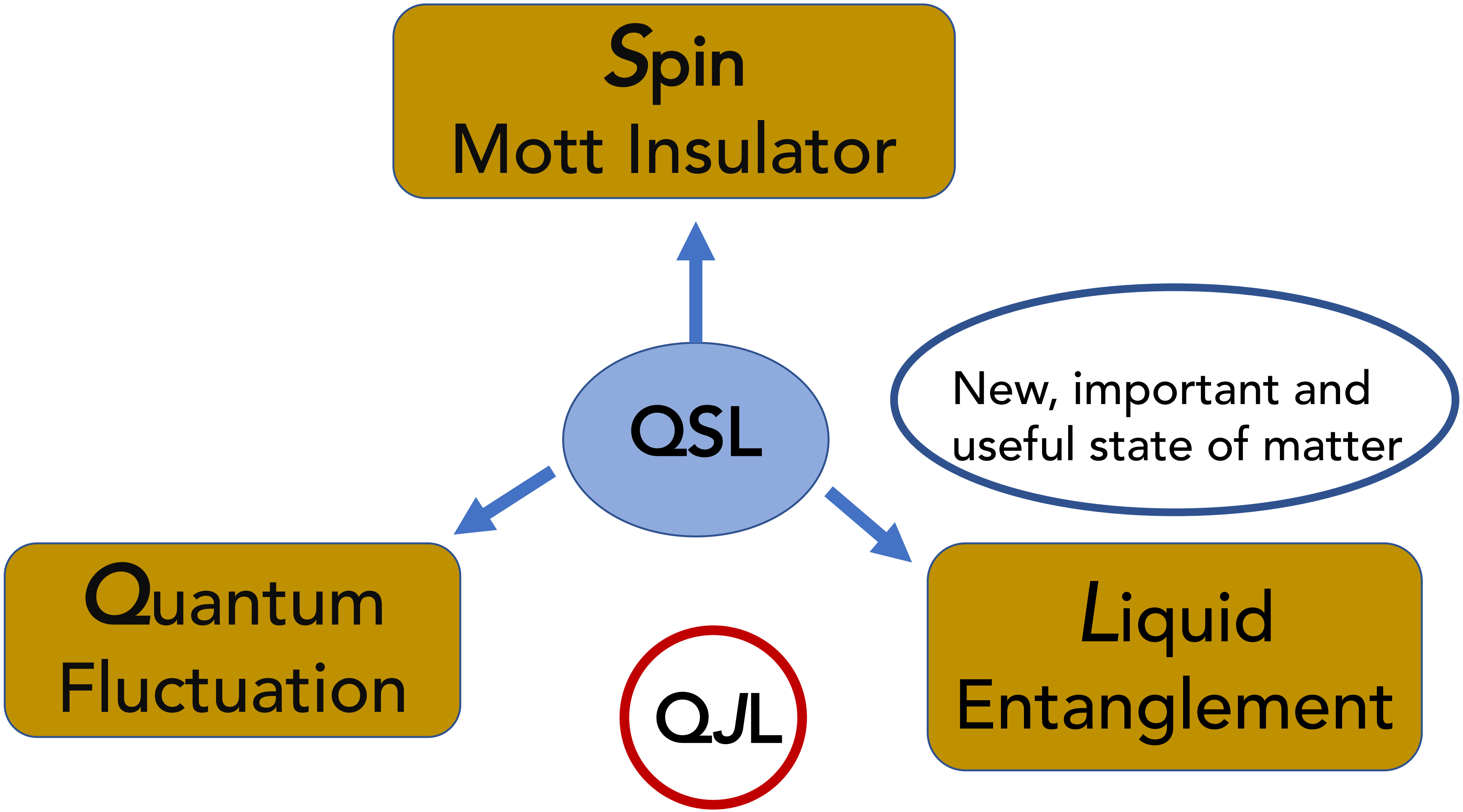
Topological Insulators
Topological Superconductors
Topological Weyl and Dirac Semimetals
Topological magnons

"FQHE"

- Ground state degeneracy
- Long range entanglement
- Fractionalized Excitations
- Topological Order

Important for storing information non-locally; robust against decoherence

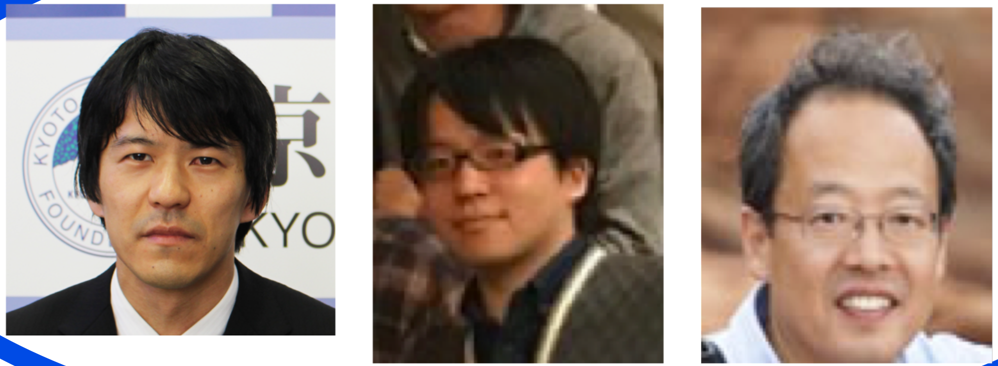
Review: Savary and Balents, Repts. on Progress in Physics 80, 016502 (2017)


Spin
Mott Insulator
QSL
New, important and
useful state of matter
Quantum
Fluctuation
QJL
Liquid
Entanglement

Burning question….
Have we seen a quantum spin liquid?

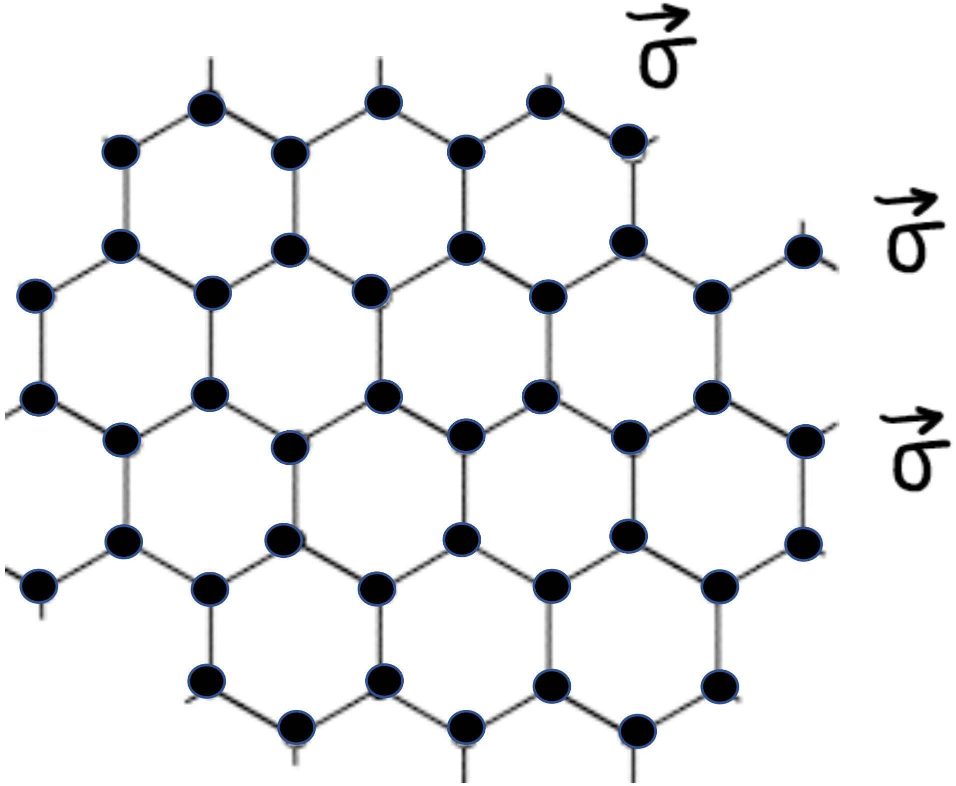
A. Kitaev, Annals of Physics 321, 2-111 (2006)

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



Kasahara, **Ohnishi**, Kurita, Tanaka, Nasu, Motome, Shibauchi, **Matsuda**, Nature 559, 227-231 (2018)

Kitaev Model

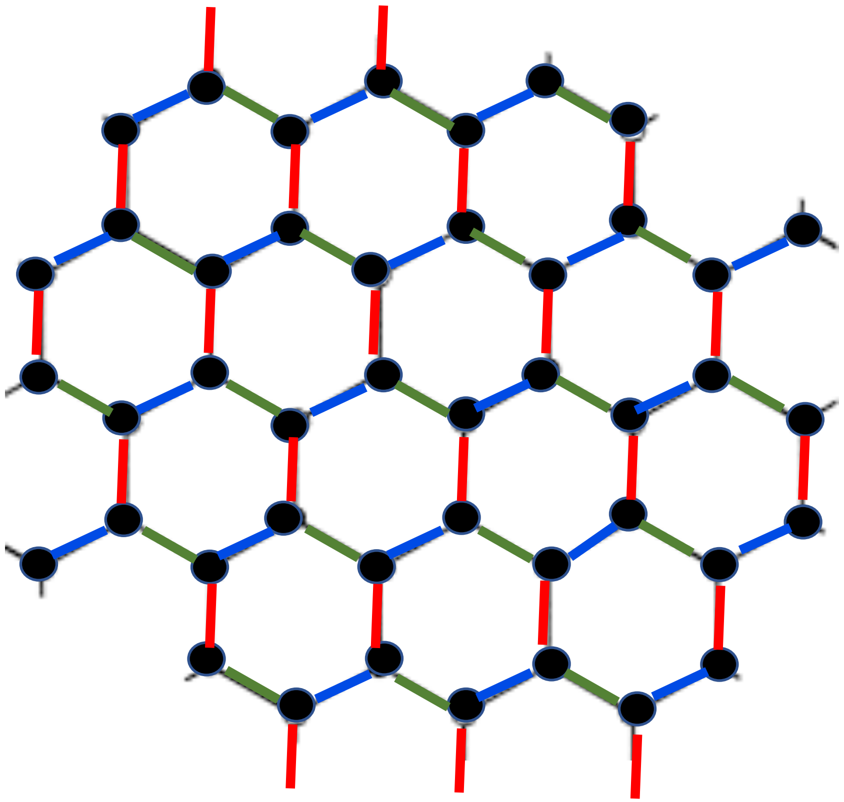


put qubit on each site

Honey comb lattice

Bipartite lattice; no geometric frustration

Kitaev Model: bond-dependent interactions



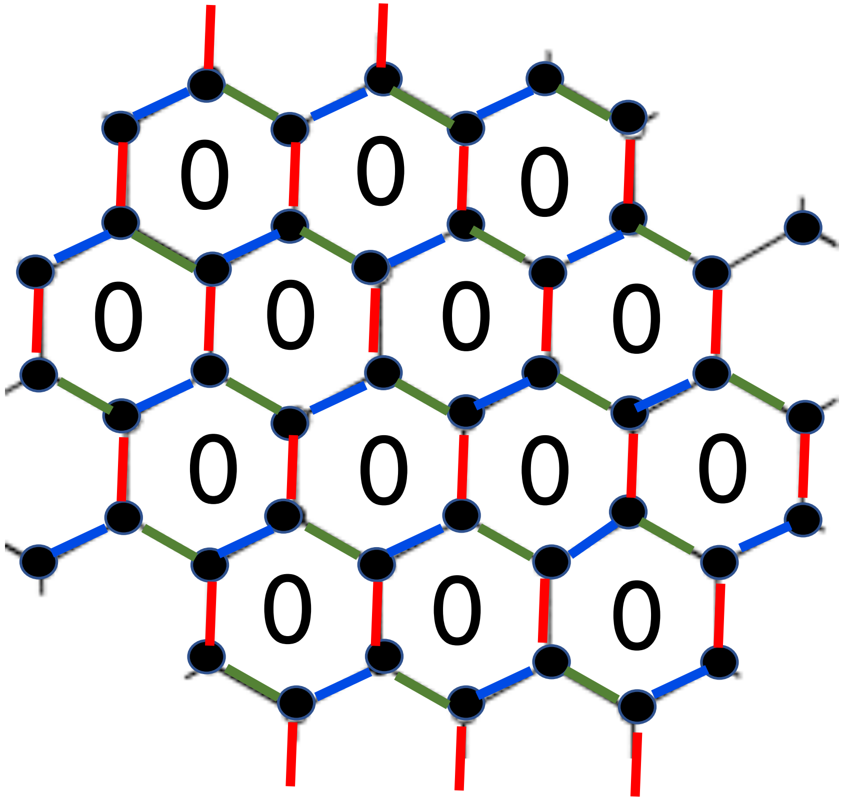
$$\mathcal{H} = K\left[\sum_{\langle ij\rangle \in x} \sigma_i^x \sigma_j^x + \sum_{\langle ij\rangle \in y} \sigma_i^y \sigma_j^y + \sum_{\langle ij\rangle \in z} \sigma_i^z \sigma_j^z\right]$$

Parton construction:

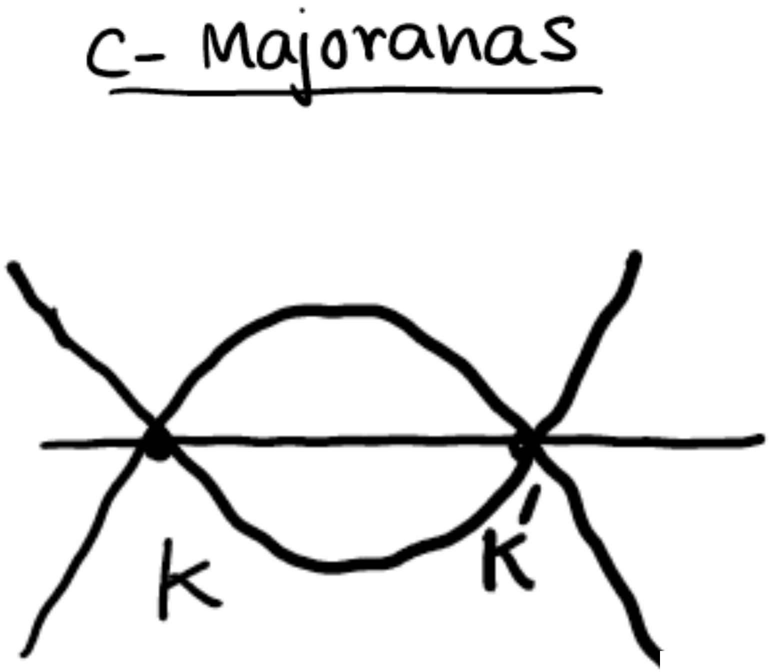
$$\sigma^\alpha = i\, b^\alpha c$$

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

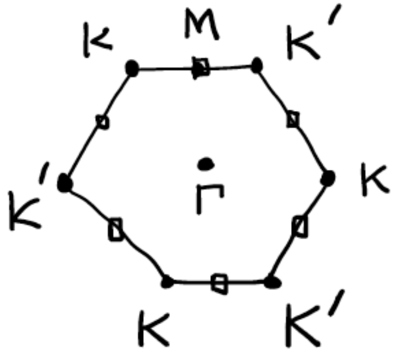
Ground State:



All plaquettes have zero flux

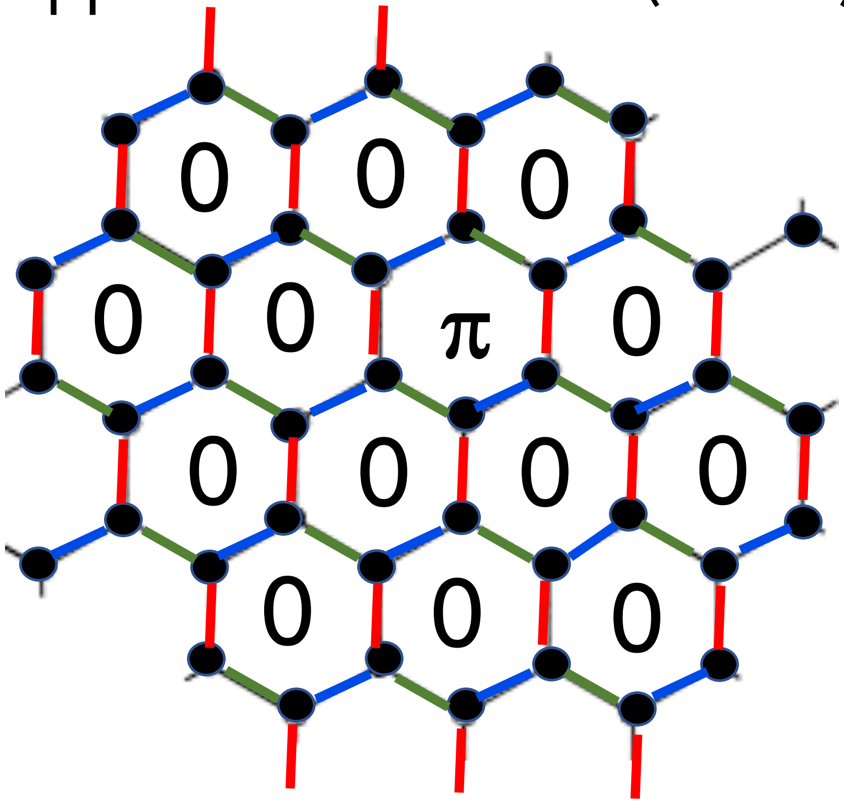


c-majorana fermions have a Dirac dispersion

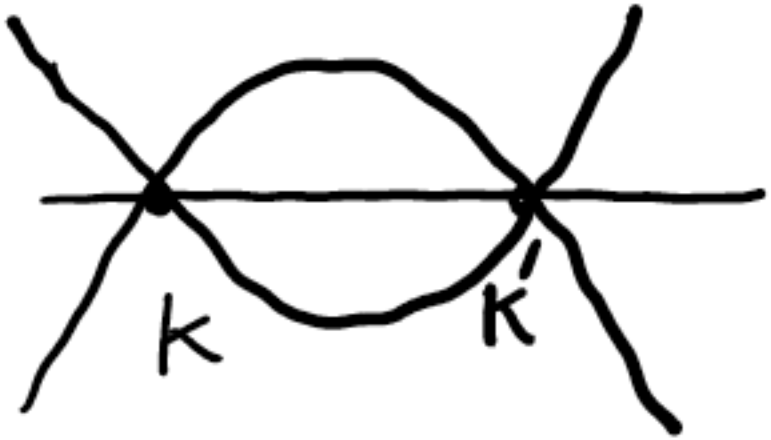


Excitations:

(1)Gapped flux excitation (visons)



(2) Gapless majorana fermions



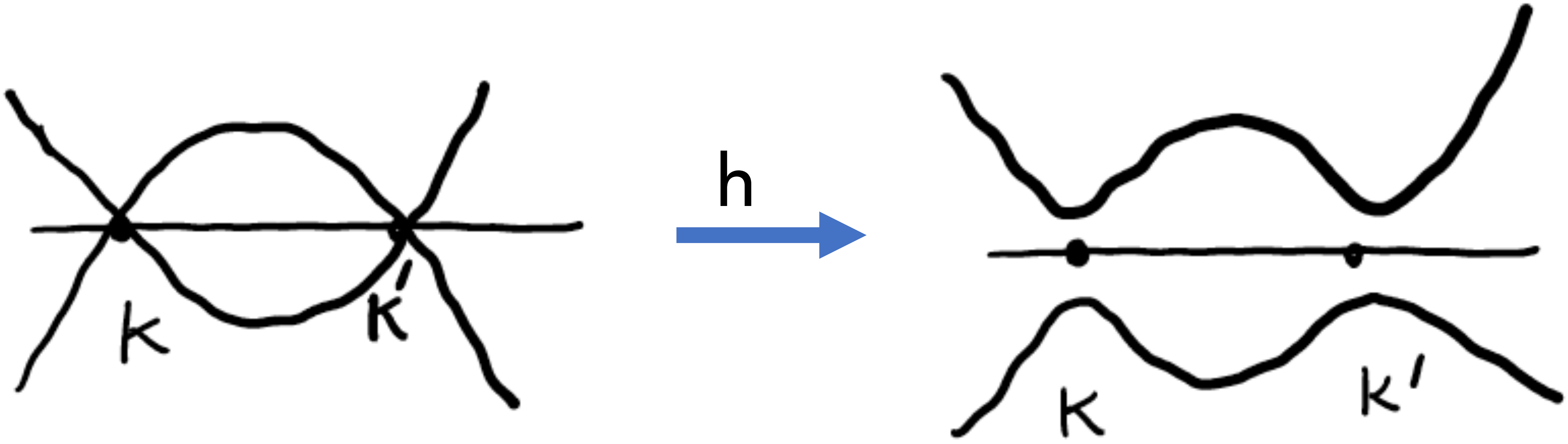
Gapless Z_2 Quantum Spin Liquid

Now add a magnetic field…

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

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

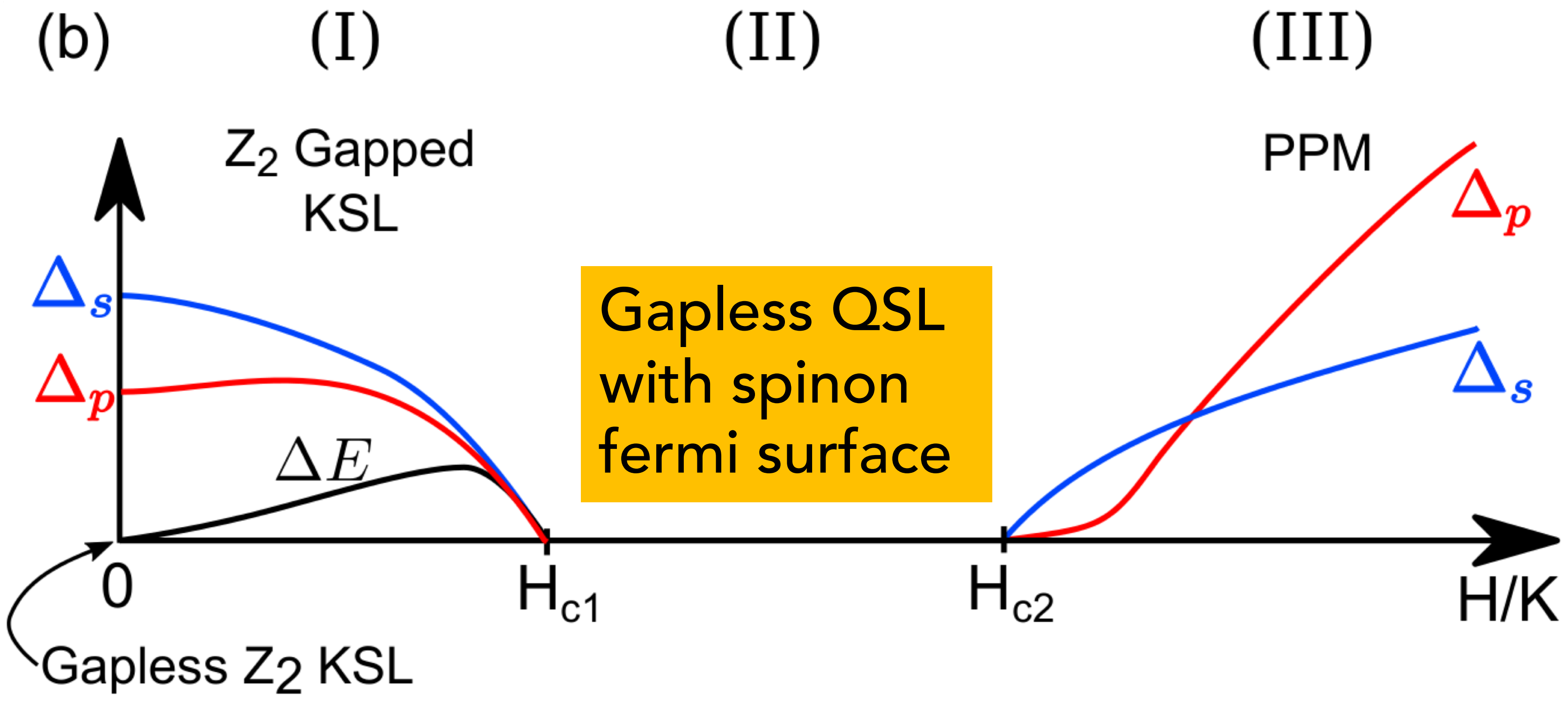
Non-abelian gapped Kitaev spin liquid:



- Majorana fermions get gapped
- Chern insulator
- Chiral edge mode with thermal Hall conductance

$\kappa_{xy}/T=(1/2)\,(\pi/6)(k_B^2/\hbar)$

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

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

Nirav Patel

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

Subhasree Pradhan

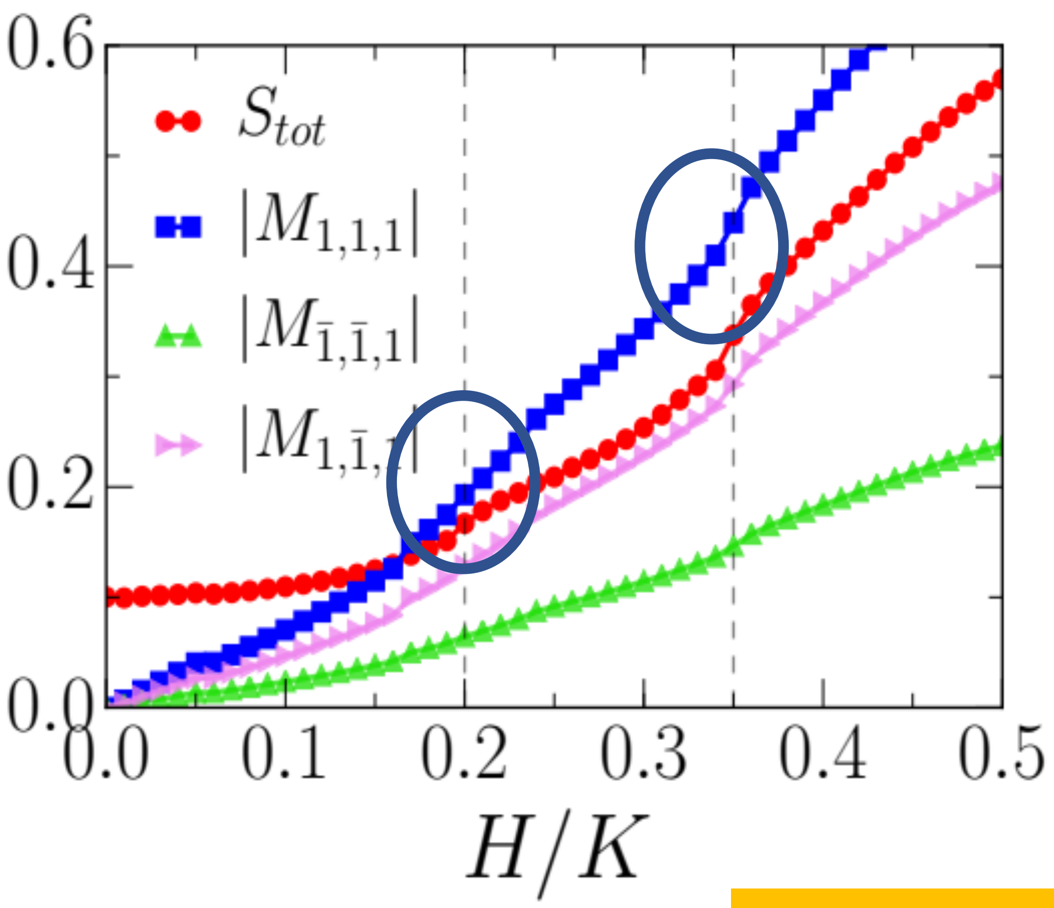
Two-Magnon Bound States in the Kitaev Model in a [111]-Field
arXiv:1908.10877

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, arXiv:1909.02234

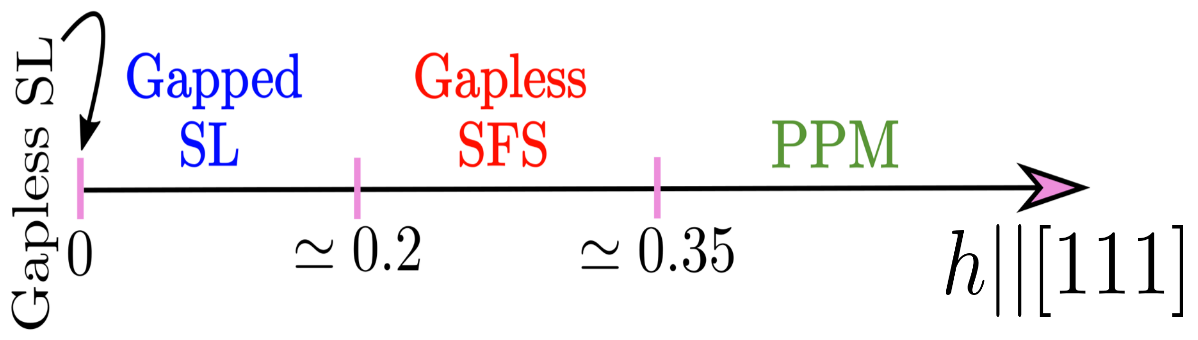
Gonzalo Alvarez
ORNL

Evidence for TWO phase transitions

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

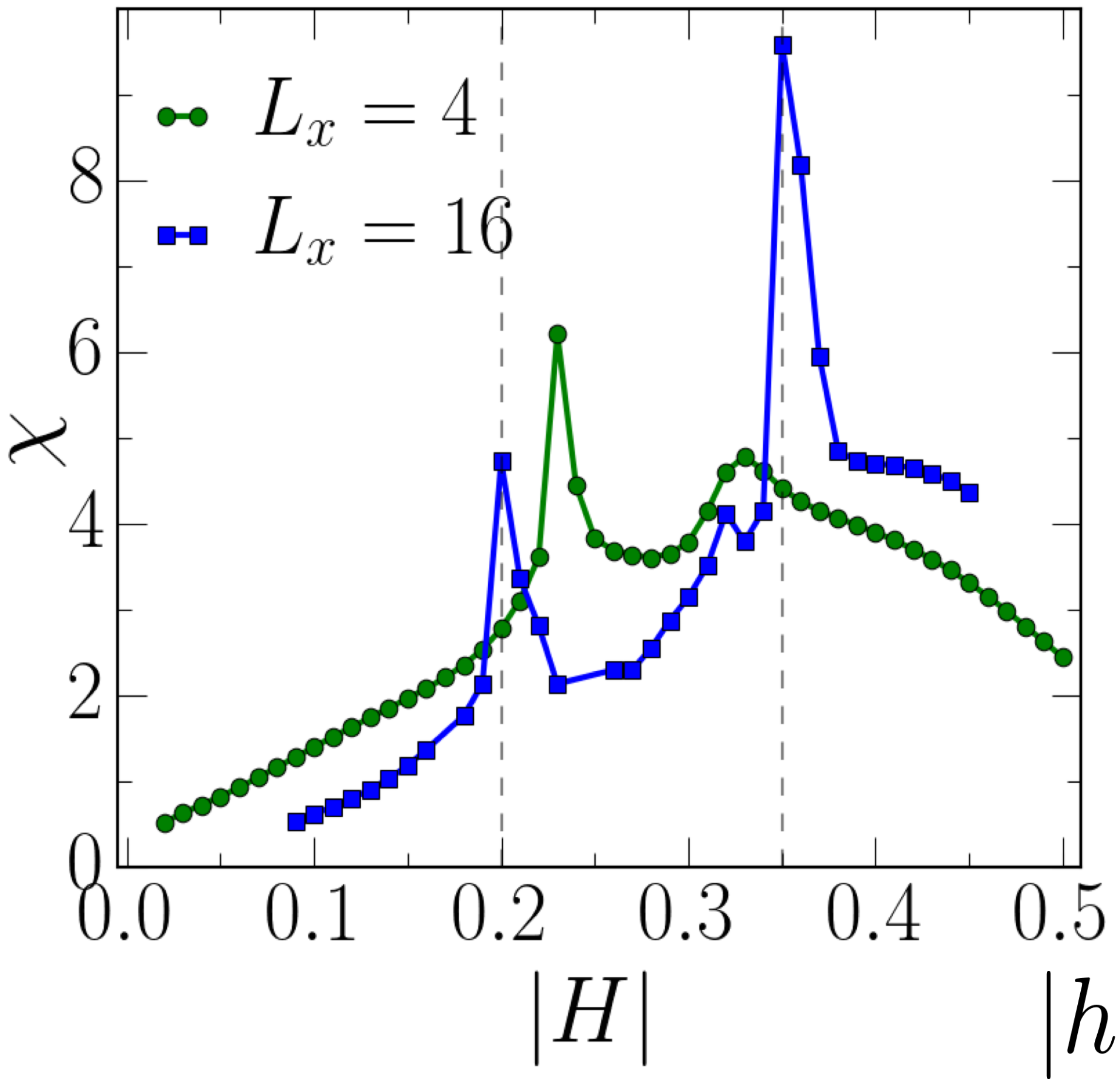


$$H = H_K + h \sum_{i\alpha} S_i^{\alpha}$$



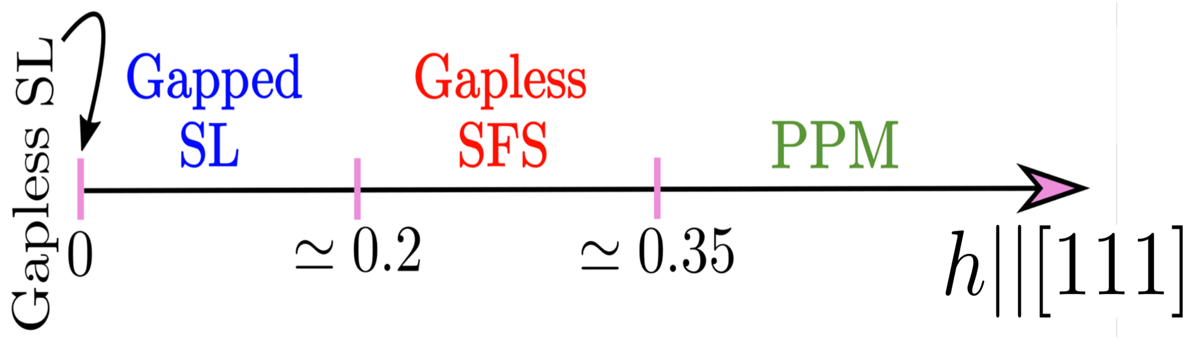
Density Matrix Renormalization Group calculations with 160 spins

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



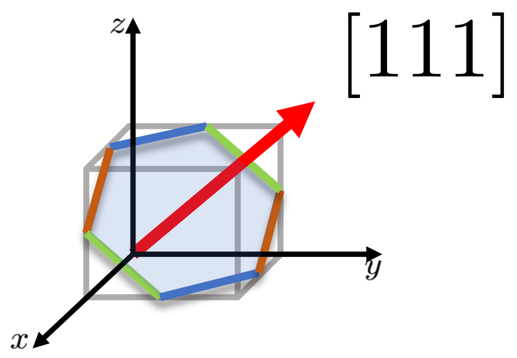
$|h|/K$

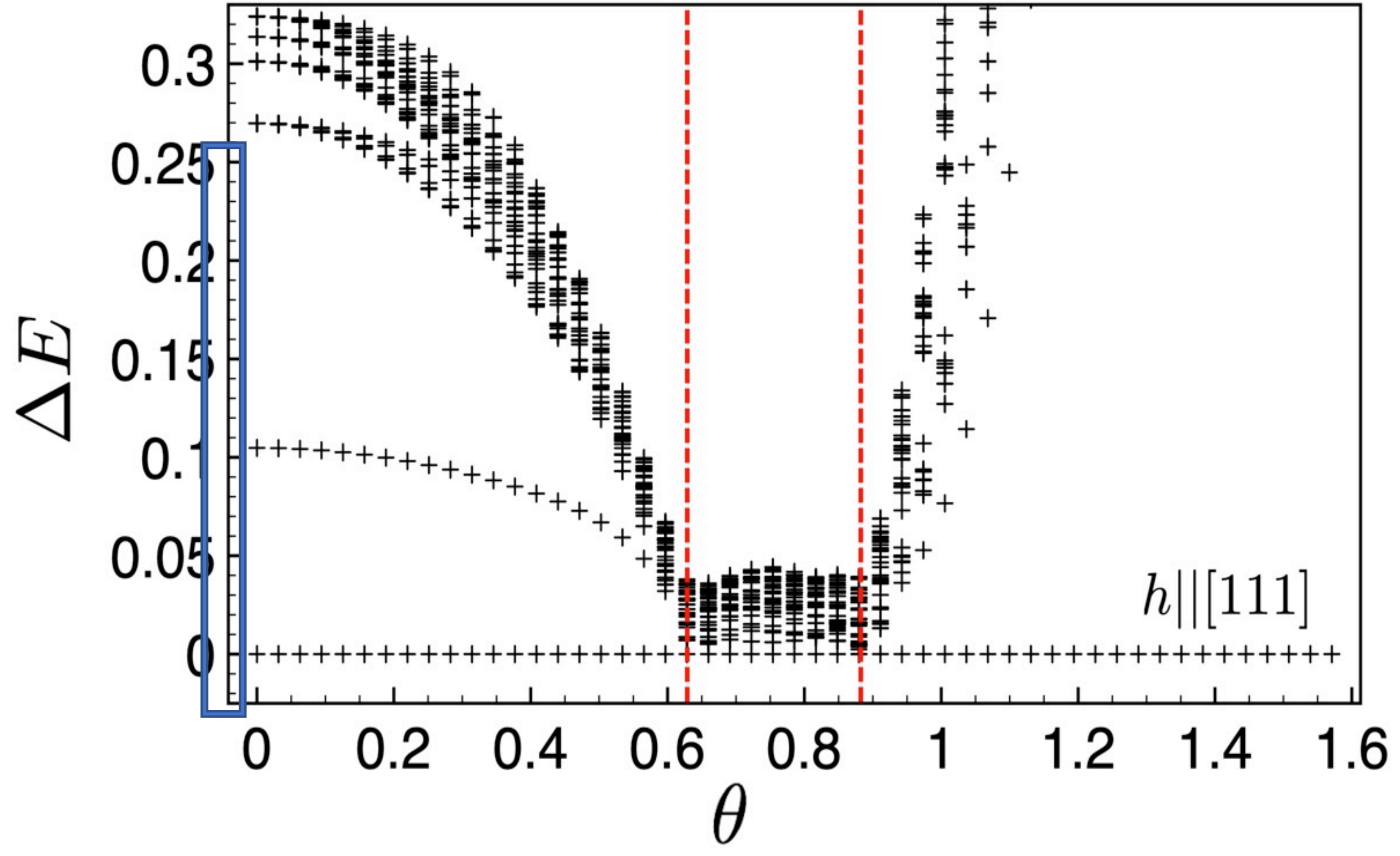
$$H = H_K + h \sum_{i\alpha} S_i^\alpha$$



Evidence for gapless intermediate phase

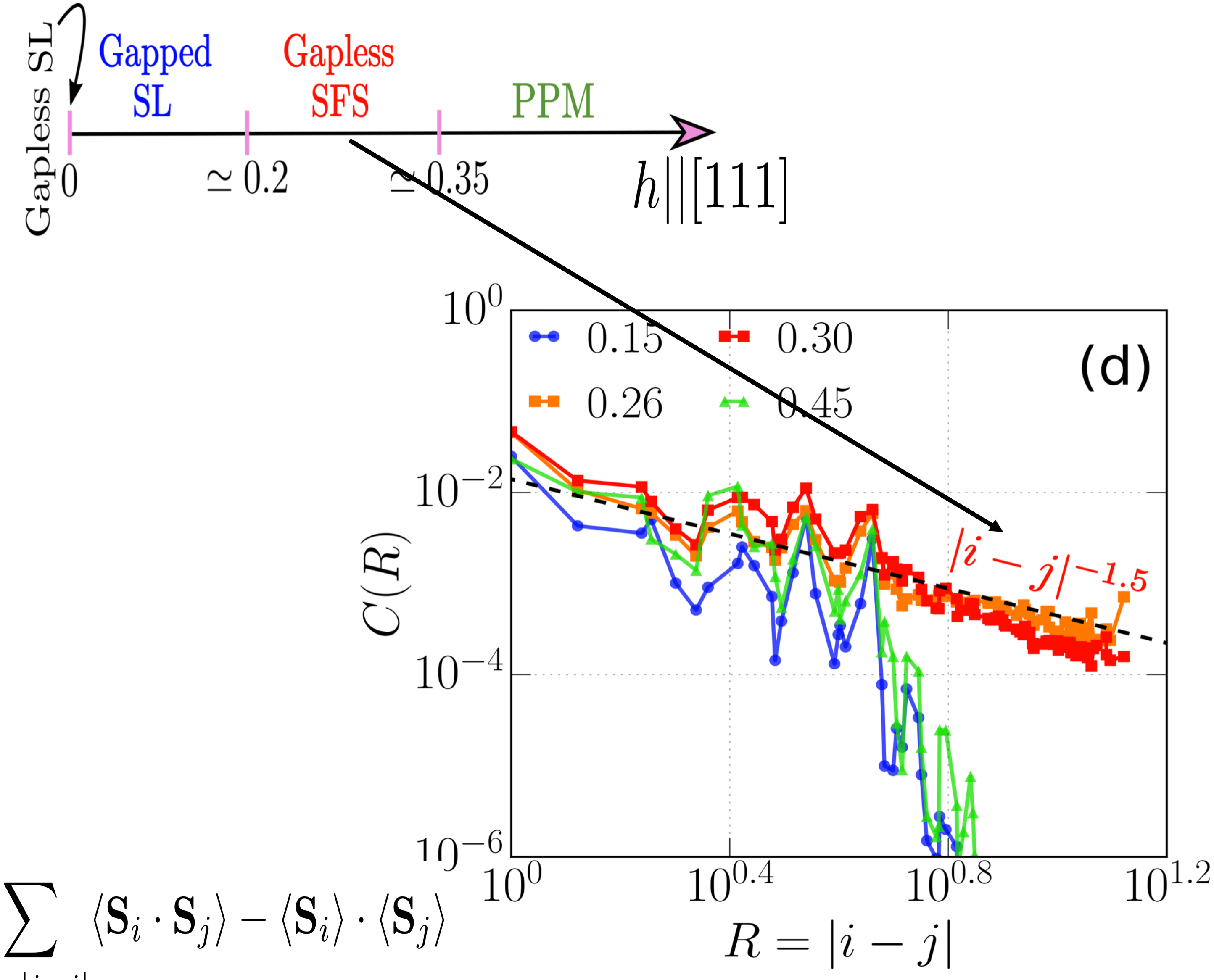
Energy Spectra in a field





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

Spin-Spin Correlations in Intermediate phase



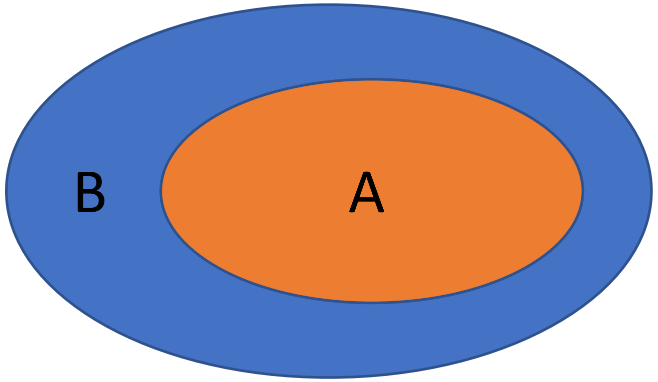
Distinct power law decay of real-space spin-spin correlations!

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

Evidence for QSL

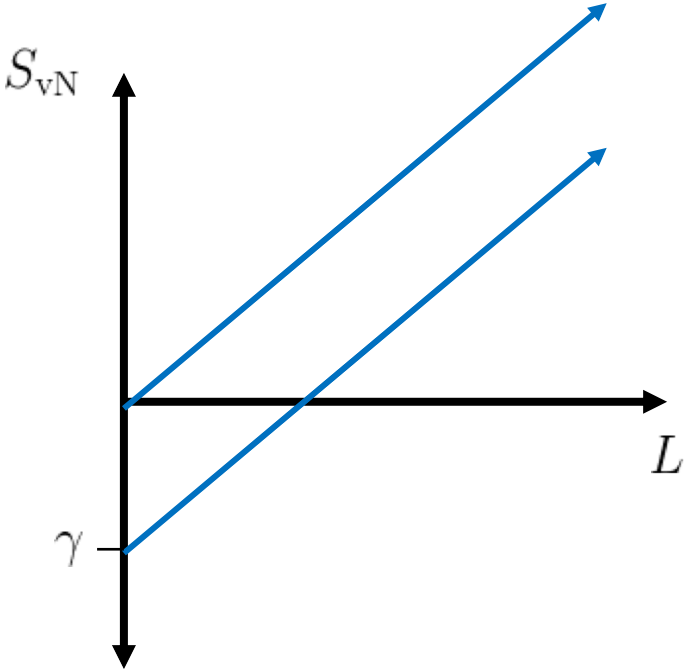
Topological Entanglement Entropy

$$S_{\mathrm{vN}} = \mathrm{Tr}\left(\rho_A \log_2 \rho_A\right)$$



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

$$S_{\mathrm{vN}} = \alpha L - \gamma + \mathcal{O}(1/L)$$



$$S_{\mathrm{topo}} = -\gamma = -\ln \mathcal{D}$$

$$\mathcal{D} \equiv \sqrt{\sum_i d_i^2}$$

Gapped Non abelian KSL

Vacuum $1 \sim d_1 = 1$

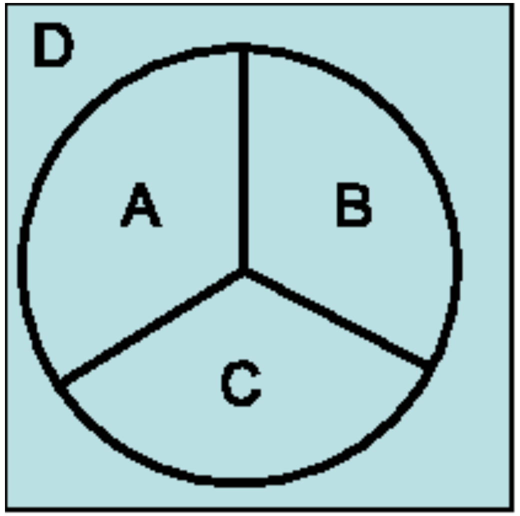
Fermion $\epsilon \sim d_\epsilon = 1$

} abelian

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

$$\to D = \sqrt{d_1^2 + d_\epsilon^2 + d_v^2}$$
$$= \sqrt{1+1+2}$$
$$= 2$$

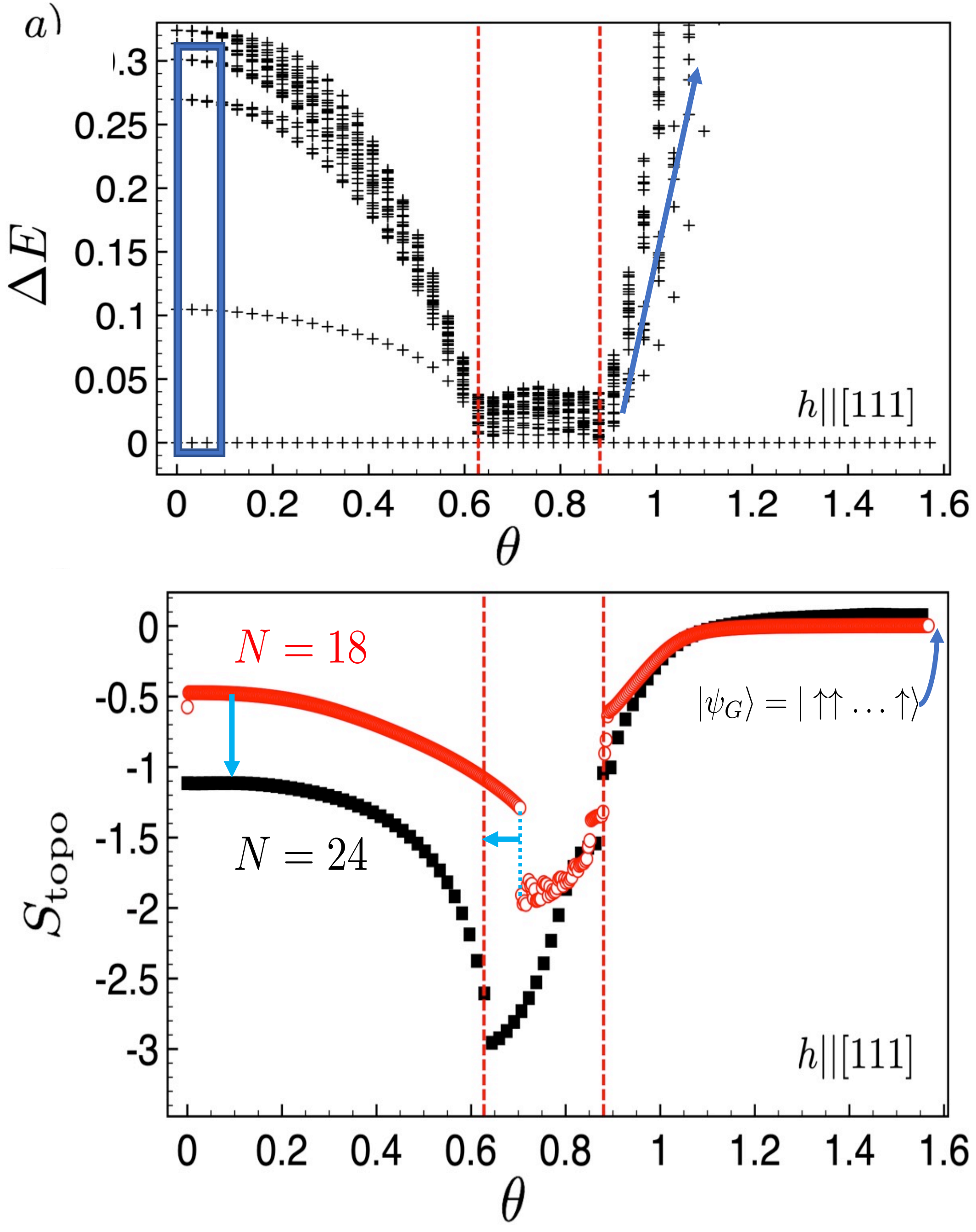
$$\to \gamma = \log D = \log 2$$



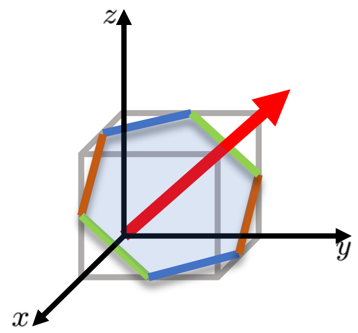
Kitaev-Preskill Construction

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

Energy Spectra



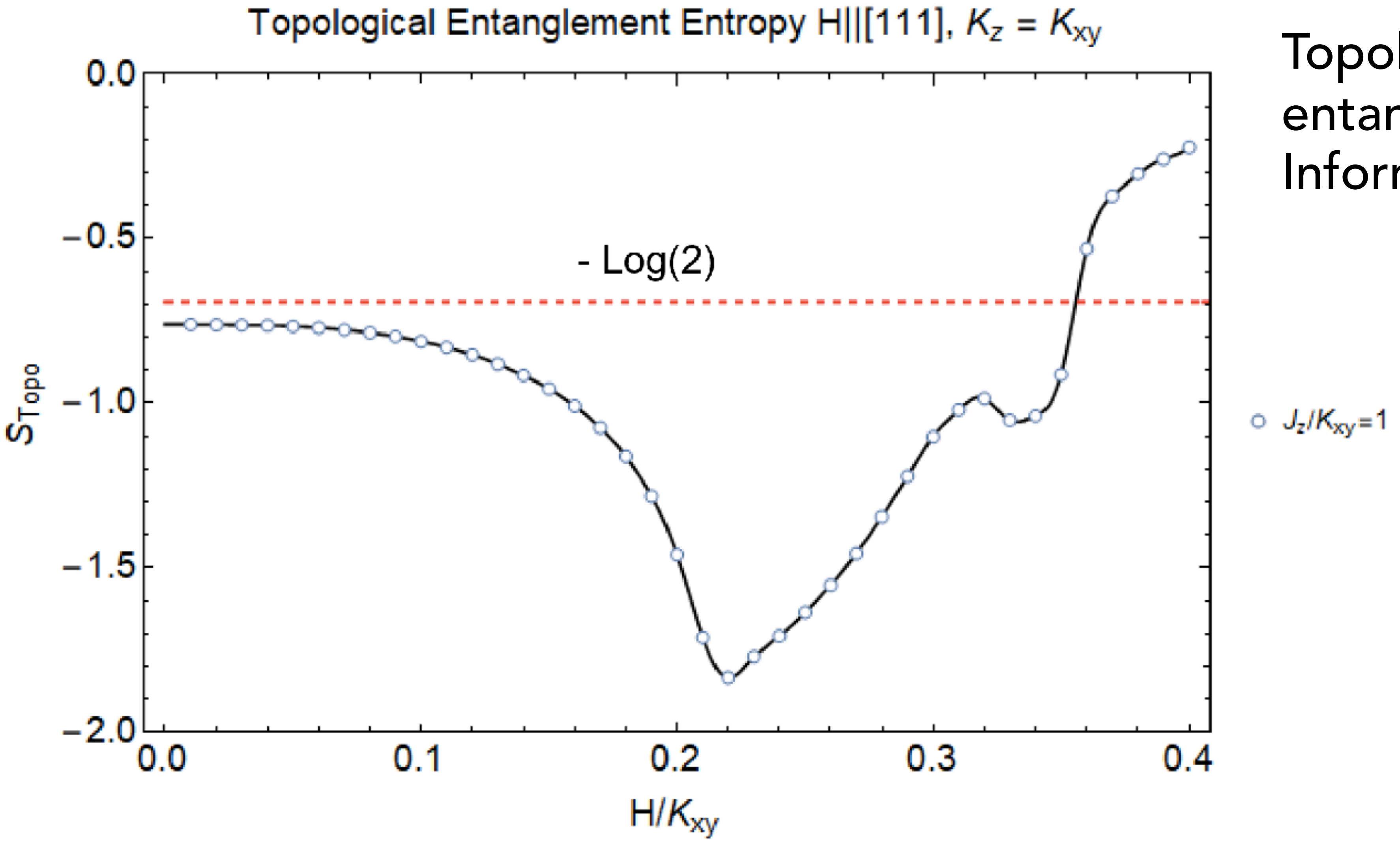
TEE



[111]

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

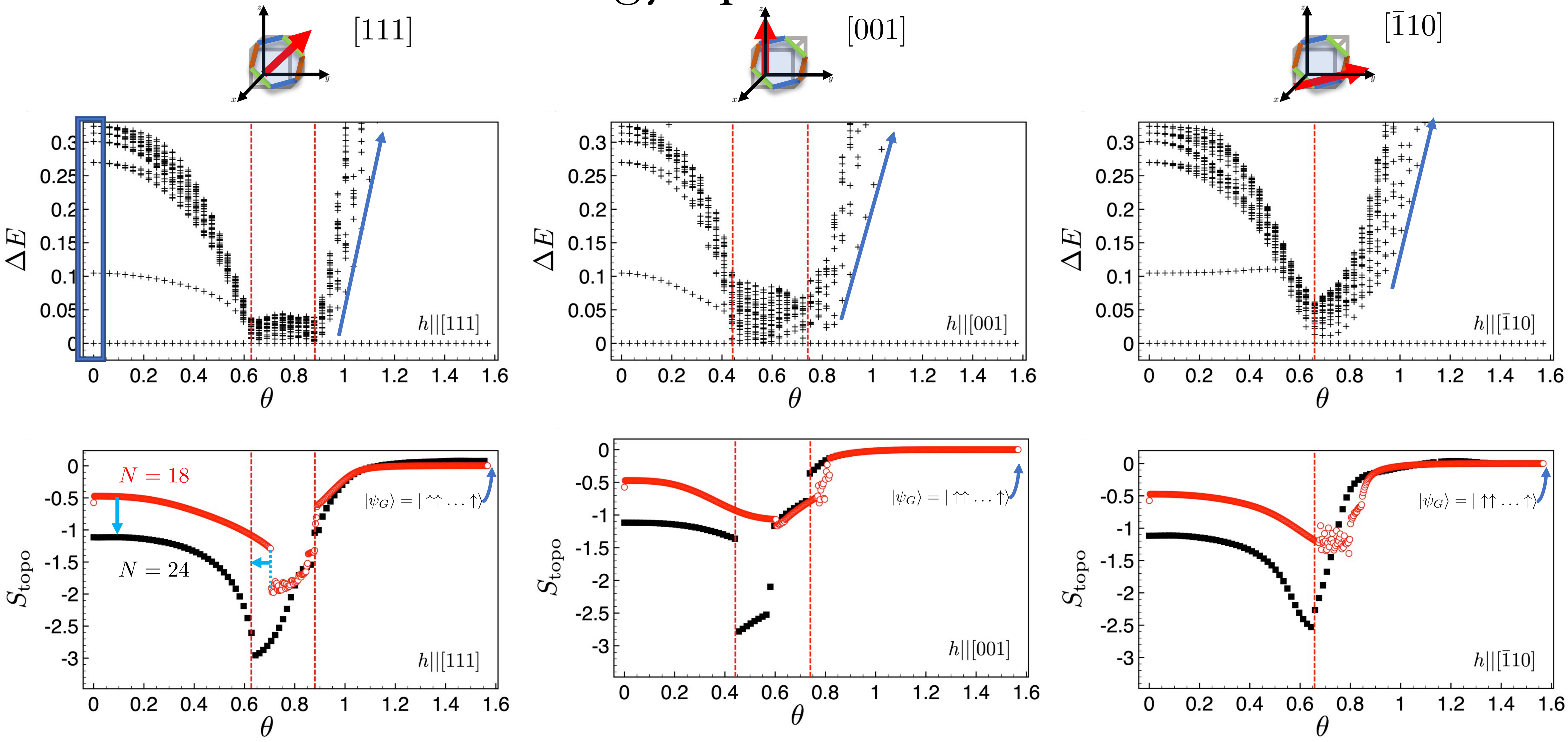
Ronquillo, Vengal, Trivedi,
PRB 99, 140413(R) (2019)



Topological entanglement entropy: Information resource

Ian Osbourne

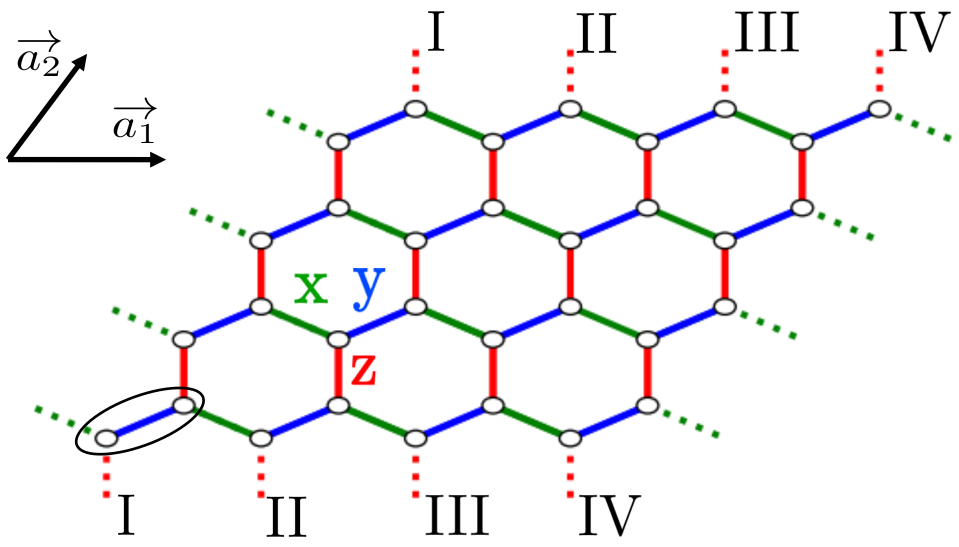
Energy Spectra & TEE



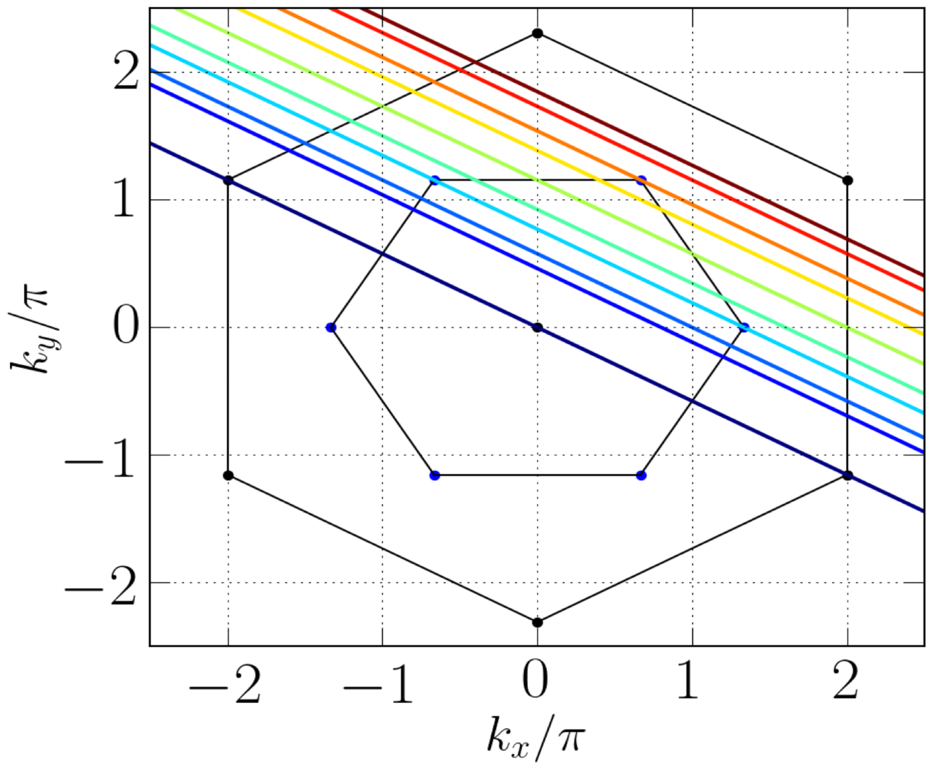
$\theta \sim |\vec{h}|/K$

Evidence for spinon Fermi surface

Kitaev Model: spin structure factor



Brillouin Zone: Momenta cuts

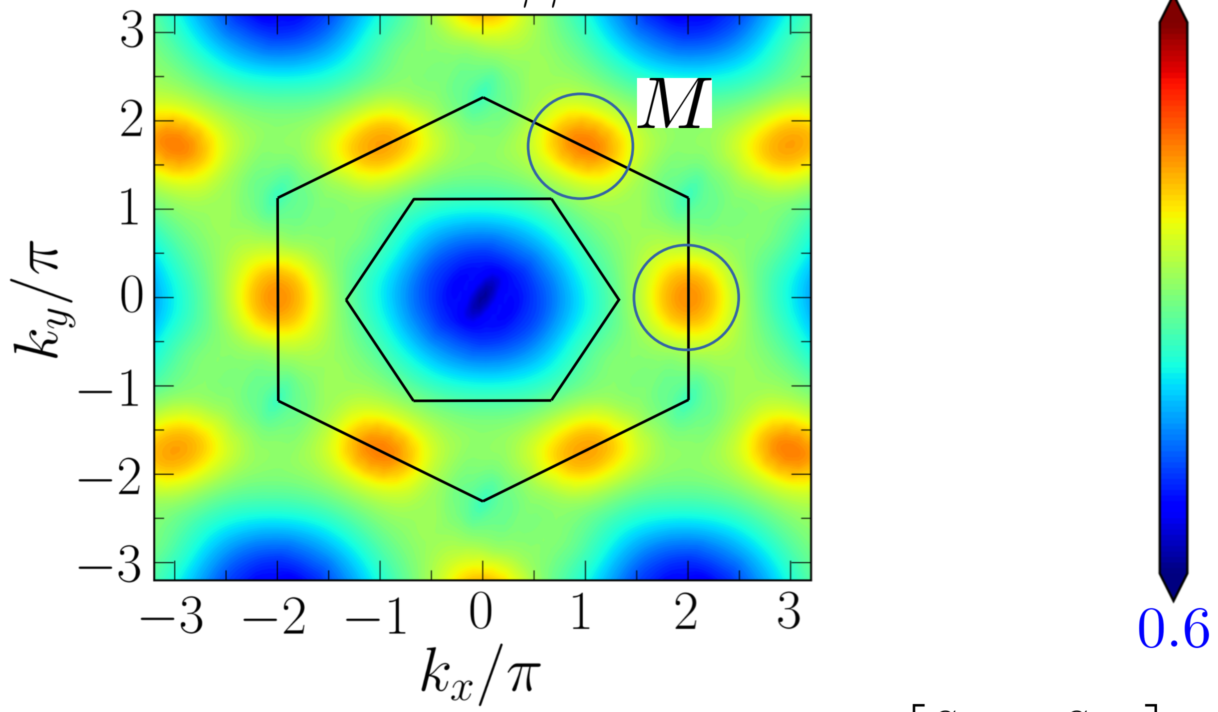


$$H_K = K \sum_{\langle ij \rangle} S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z$$

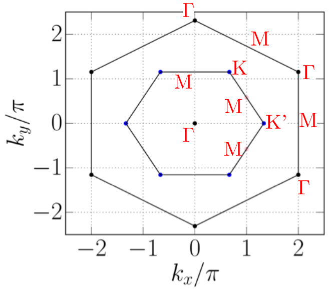
DMRG++ Open Source:
https://web.ornl.gov/~gz1/dmrgPlusPlus/

Structure Factor S(k) – Intermediate phase

$$\mathrm{S}_{tot} = \sum_{\gamma\gamma'} S_{\gamma\gamma'}$$



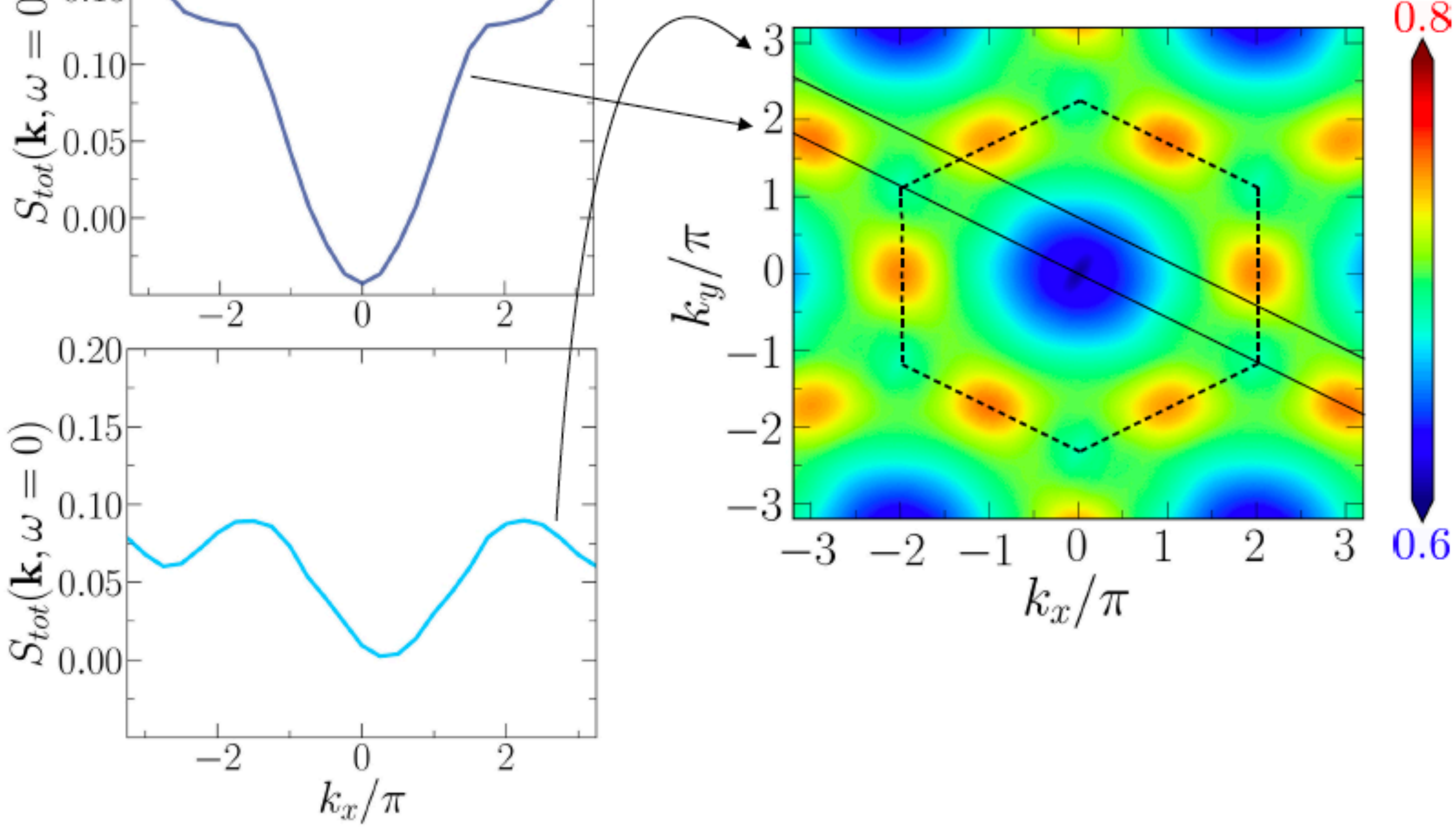
$$\mathrm{S(k)} = \begin{bmatrix} S_{AA} & S_{AB} \\ S_{BA} & S_{BB} \end{bmatrix}$$



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

Assumption: $\mathrm{S}_{tot}(\mathbf{k}) \simeq S_{tot}(\mathbf{k}, \omega = 0)$ ✓

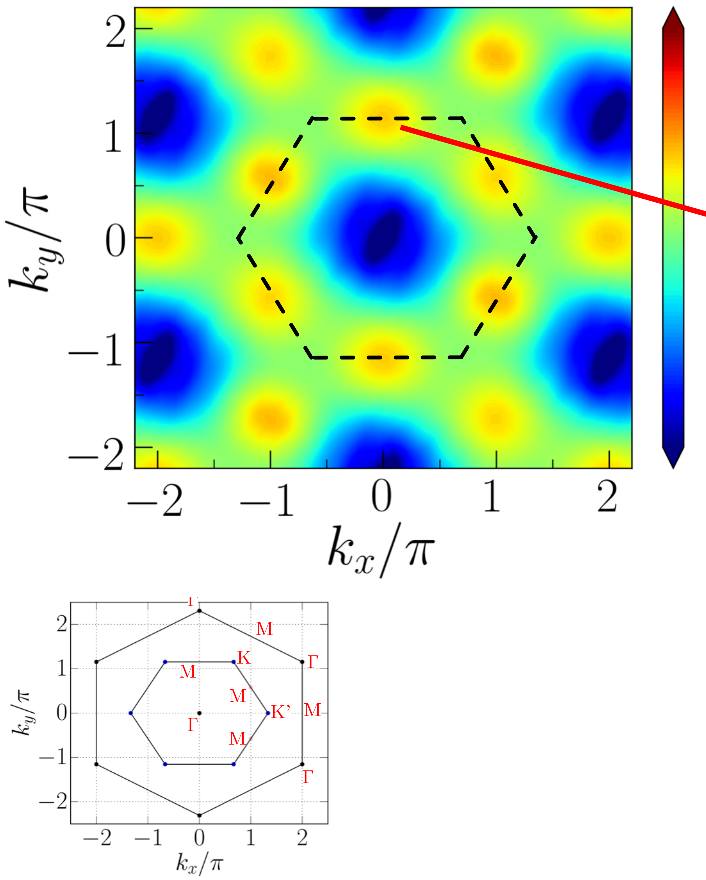
$\mathrm{S}_{tot}(\mathbf{k}) \propto \int_0^\infty S_{tot}(\mathbf{k}, \omega) d\omega$

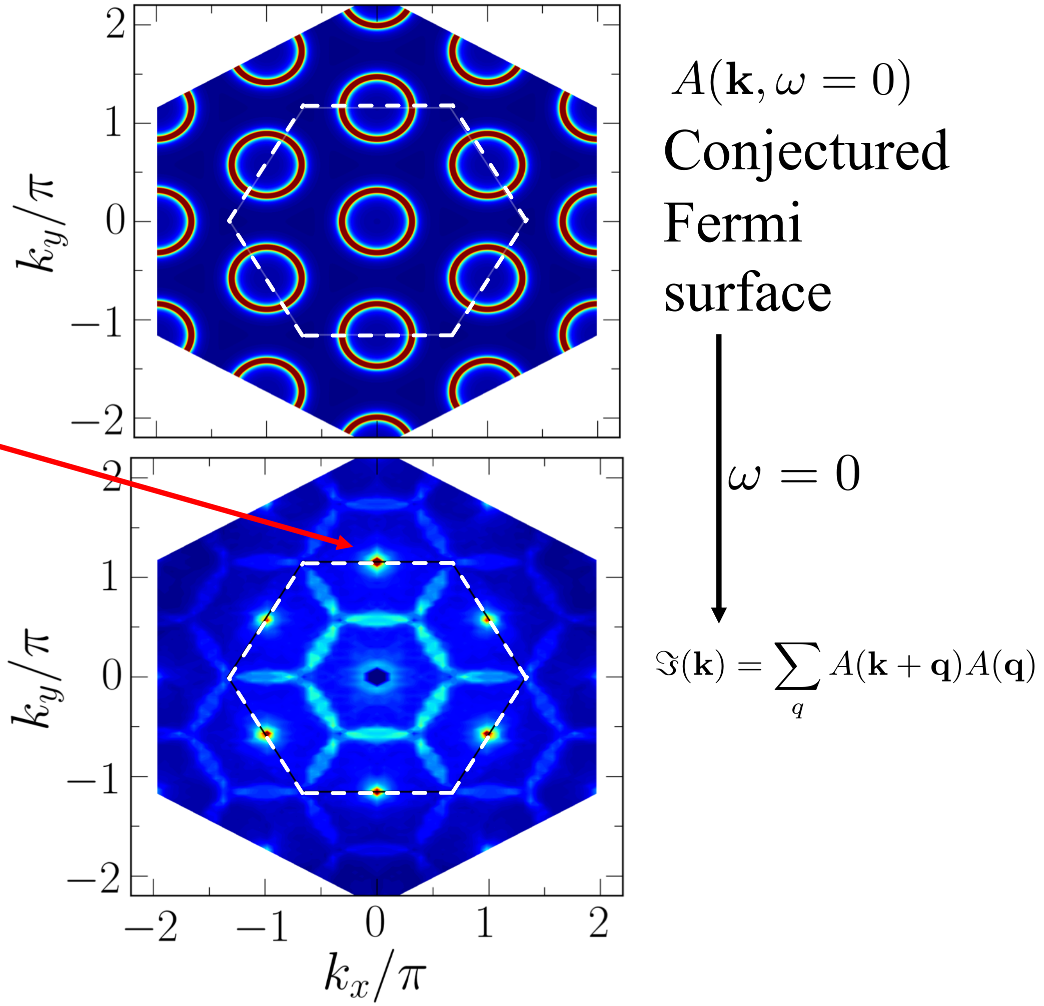


S(k) → spinon Fermi surface

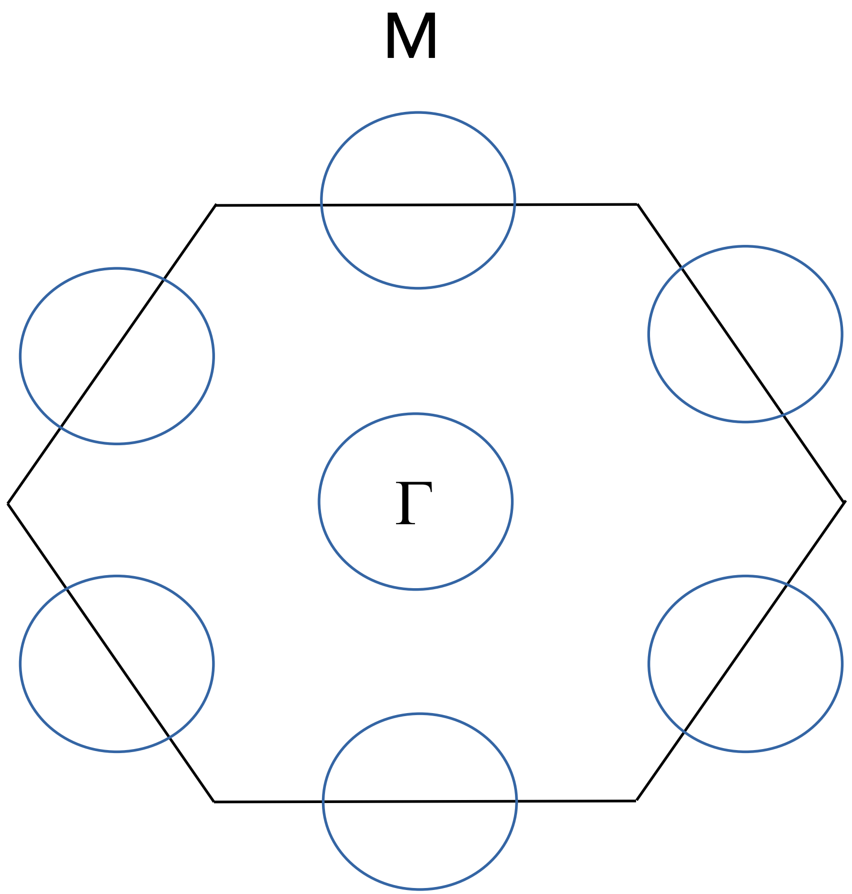
DMRG Results

$S_{tr} = \sum_\gamma S_{\gamma\gamma}$





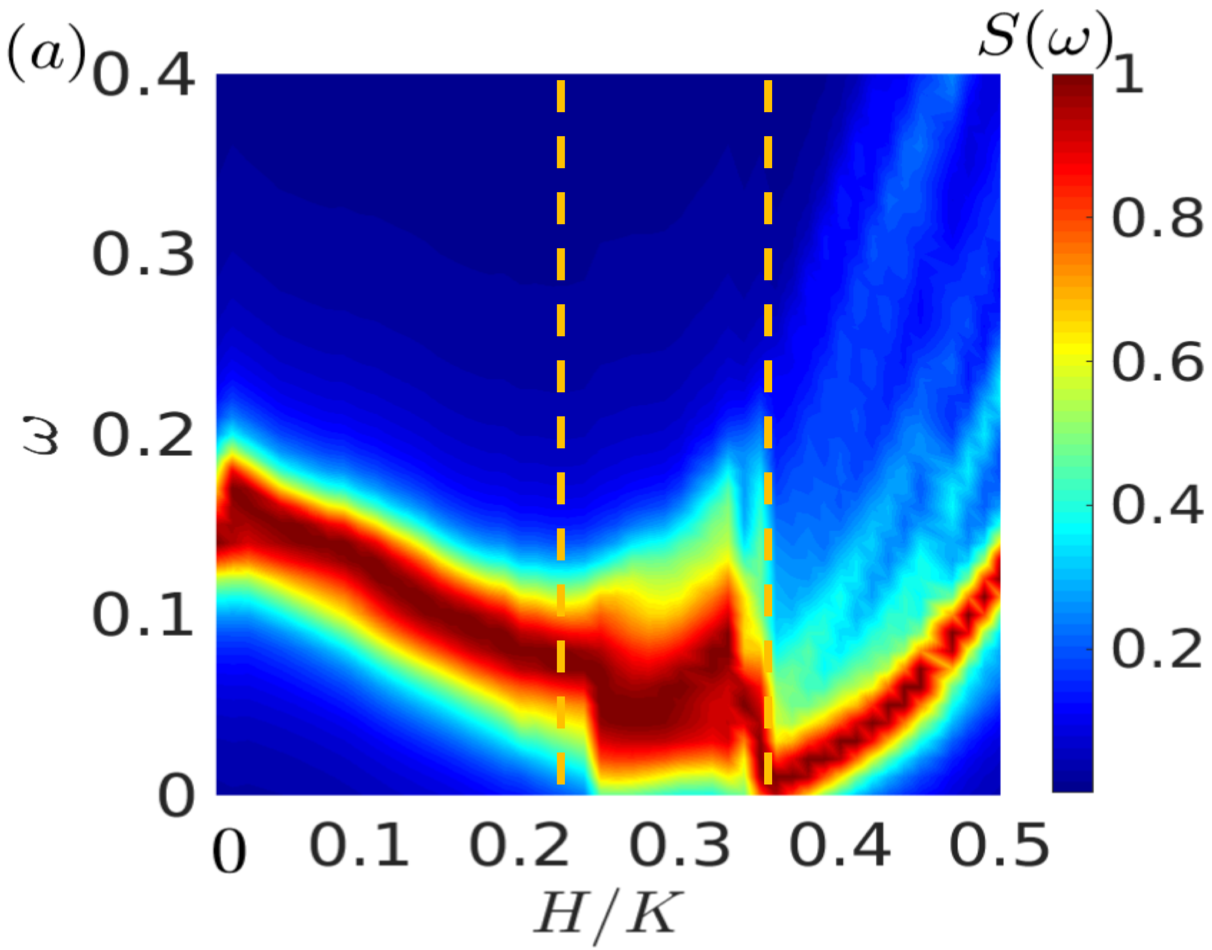
"Fermi Surface" of spinons in a Mott insulator!

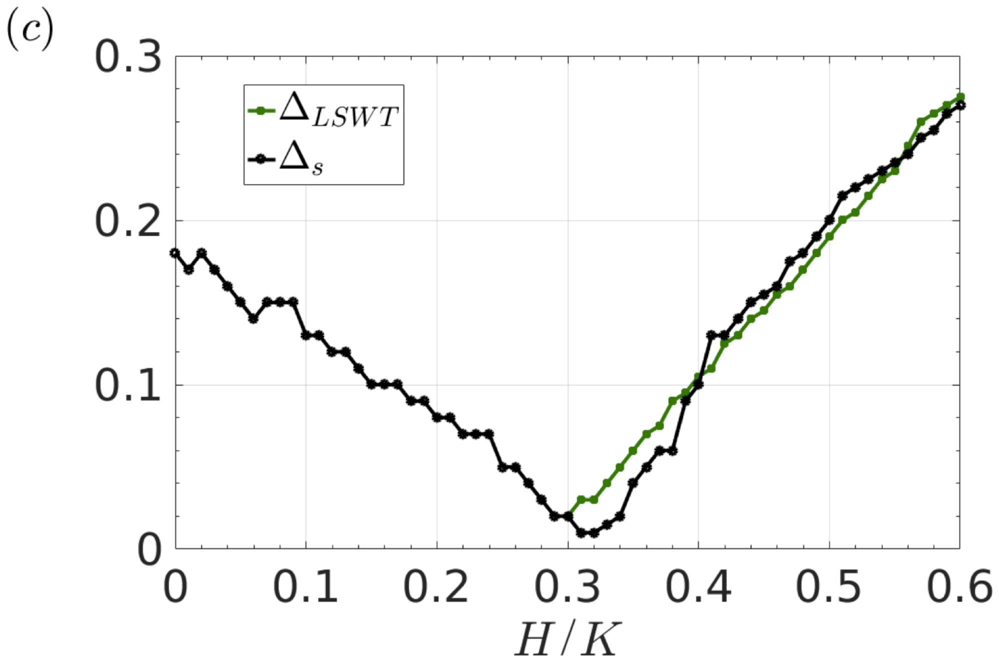


Singularities at all the M points related by C3 Rotations and Translations

Test using VMC on projected wave function

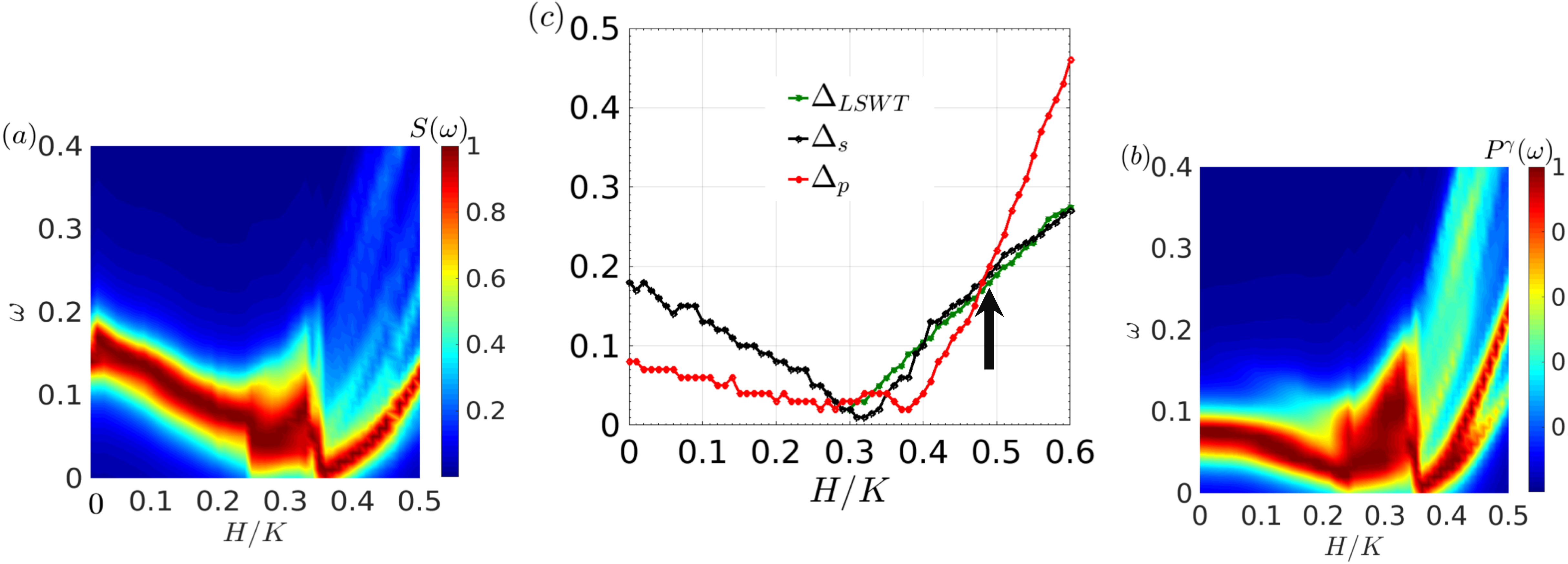
1-spin flip spectral functions





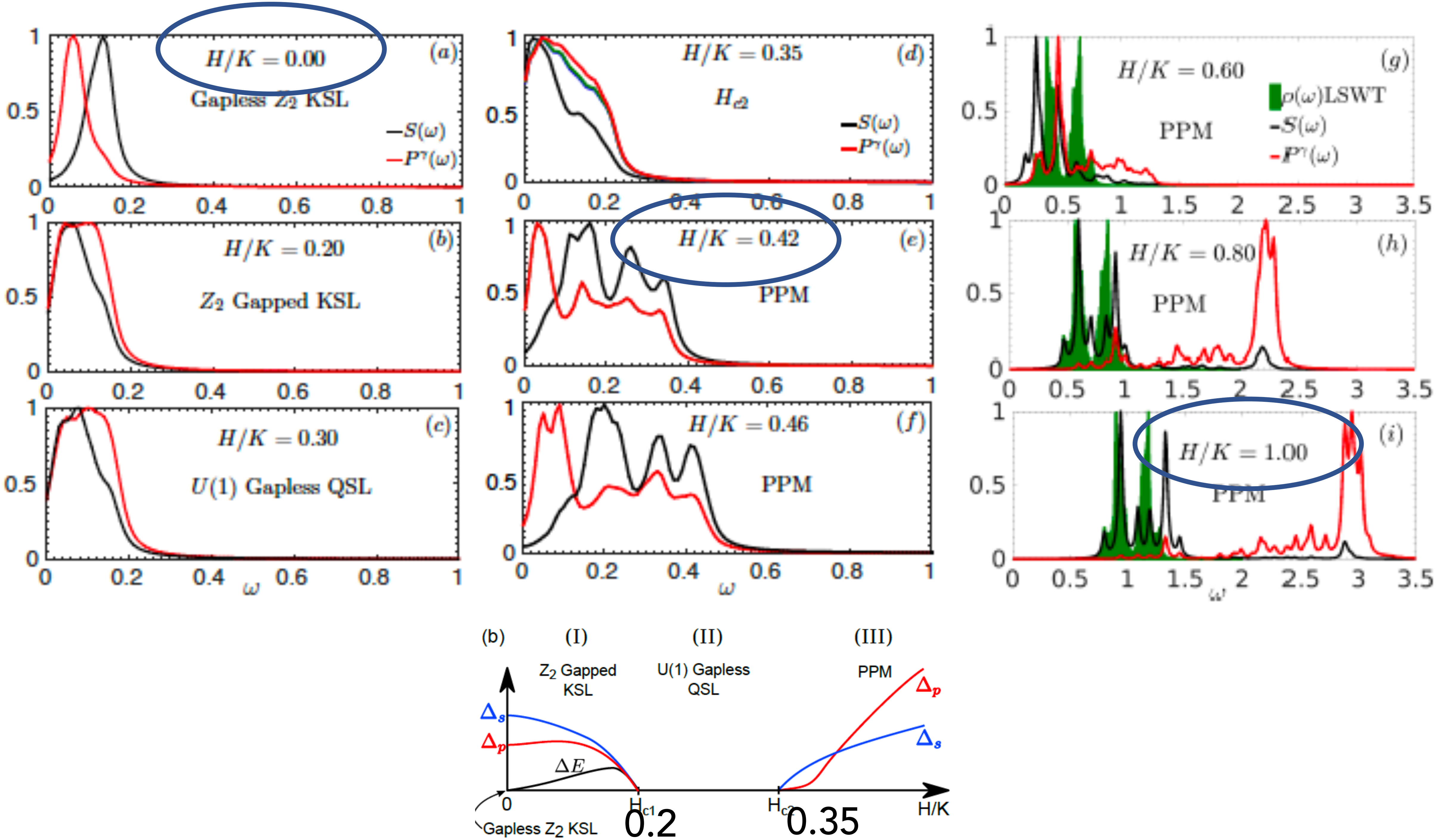
$$S(\omega) = \frac{-1}{N\pi} \mathrm{Im}\left[\sum_{\substack{m\neq 0, i \\ \alpha=+,-,z}} \frac{|\langle 0|S_i^\alpha|m\rangle|^2}{\omega + E_0 - E_m + i\eta} \right]$$

1-spin flip and 2 spin-flip spectral functions



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

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

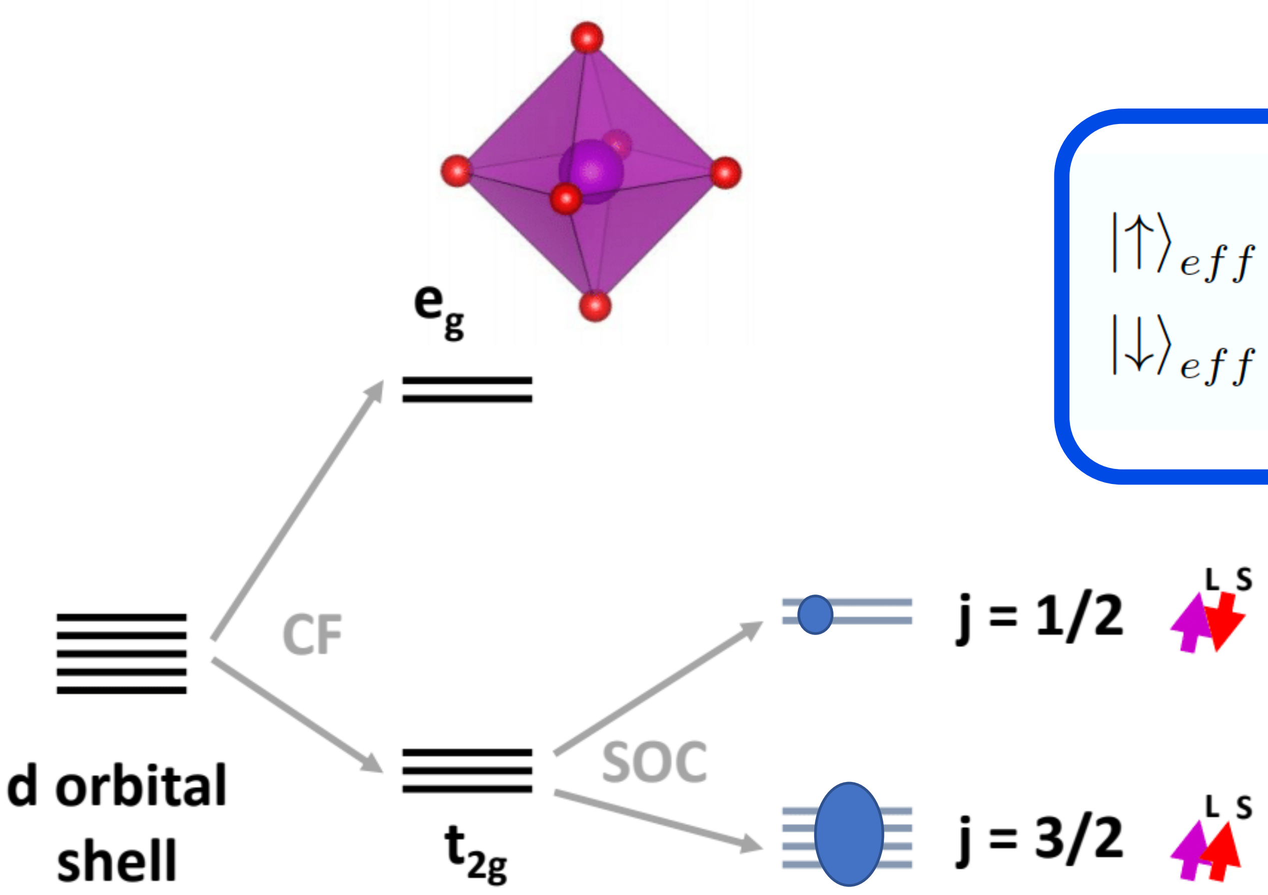


H/K = 0.00
Gapless Z2 KSL
(a)
S(ω)
P^γ(ω)
H/K = 0.20
Z2 Gapped KSL
(b)
H/K = 0.30
U(1) Gapless QSL
(c)
ω
H/K = 0.35
Hc2
(d)
S(ω)
P^γ(ω)
H/K = 0.42
PPM
(e)
H/K = 0.46
PPM
(f)
ω
H/K = 0.60
PPM
(g)
ρ(ω)LSWT
S(ω)
P^γ(ω)
H/K = 0.80
PPM
(h)
H/K = 1.00
PPM
(i)
ω
(b)
(I)
Z2 Gapped KSL
(II)
U(1) Gapless QSL
(III)
PPM
Δs
Δp
ΔE
0
Hc1
Hc2
H/K
Gapless Z2 KSL
0.2
0.35

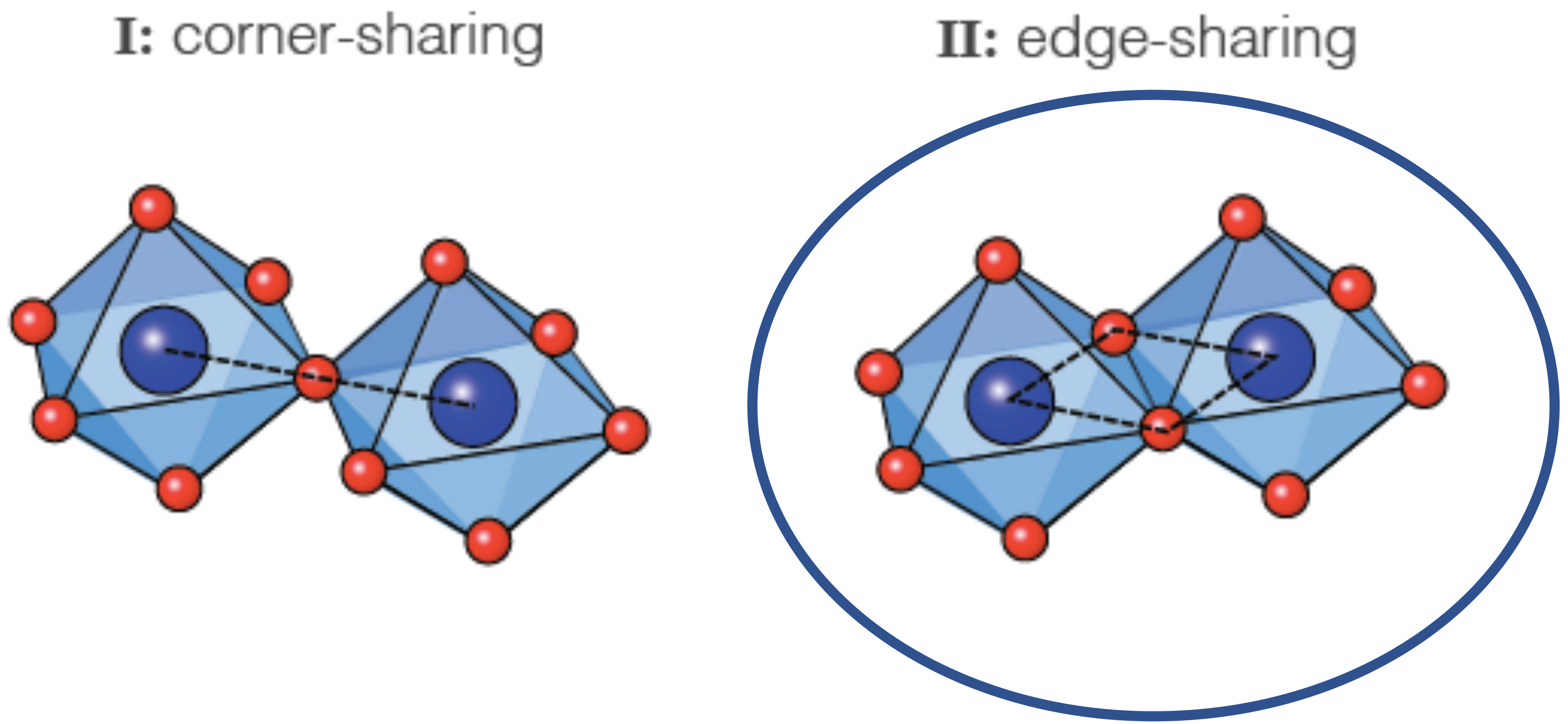
Main ingredients for Kitaev materials

Spin-Orbit coupled Mott Insulators

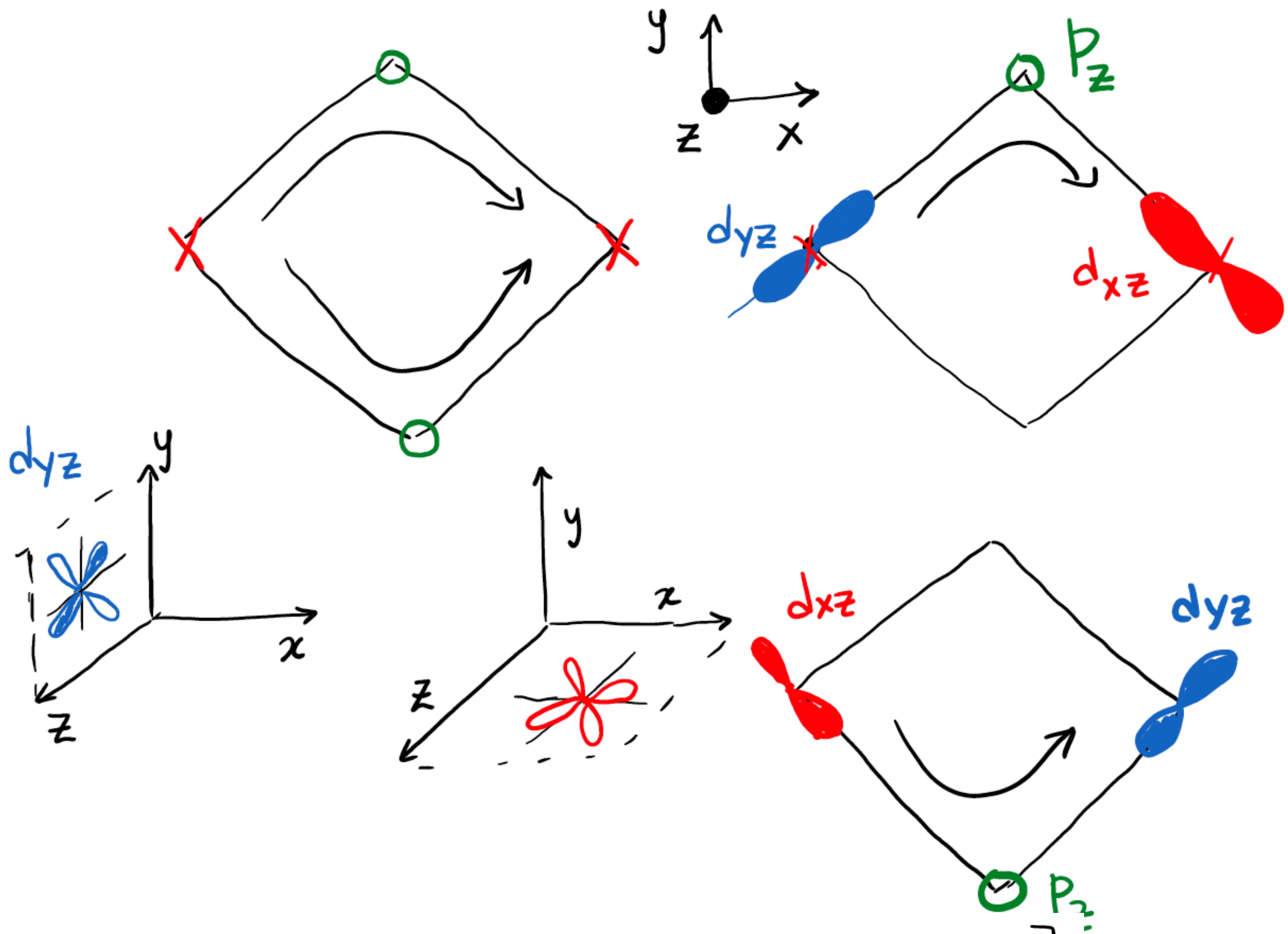
Mo	Tc	**Ru**	Rh
W	**Re**	**Os**	**Ir**



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



Destructive interference between the two pathways generates bond-dependent interactions

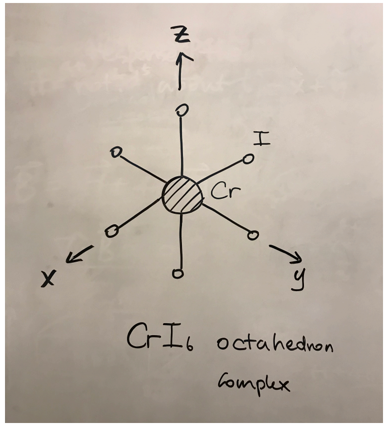


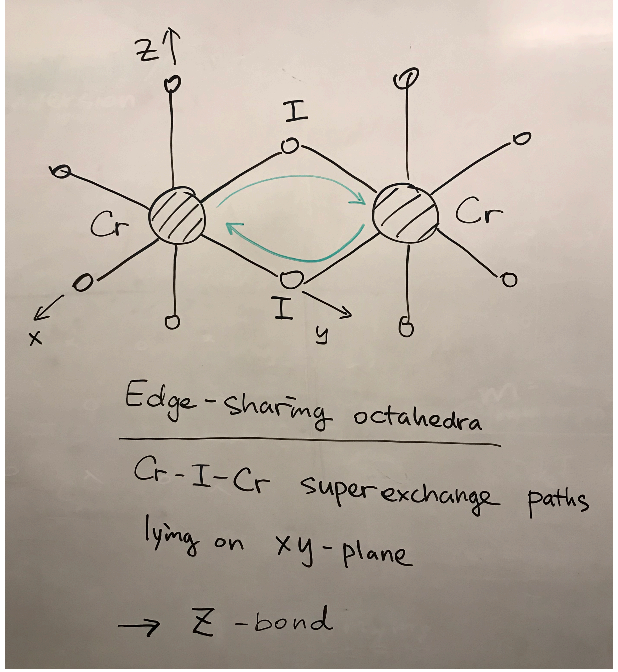
hopping via p_z orbital on ligand changes $d_{yz} \to d_{xz}$

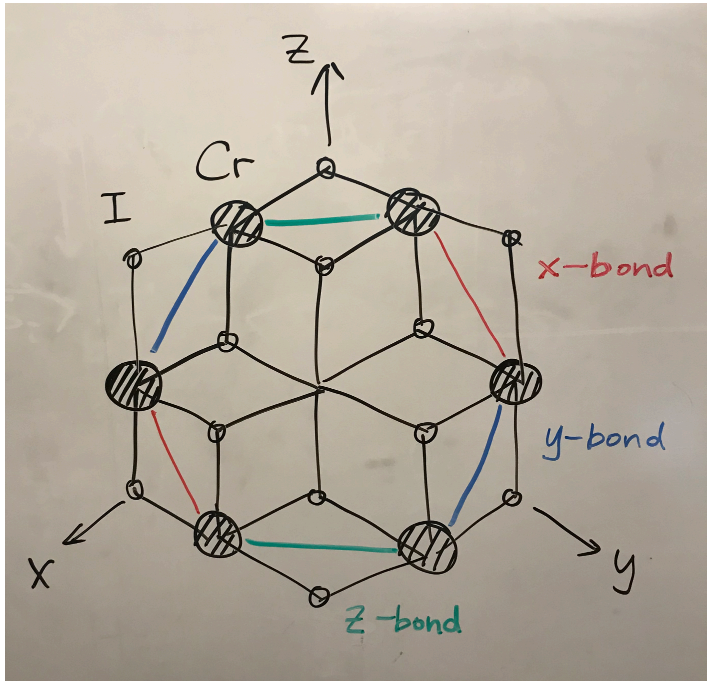
$d_{xz} \longrightarrow d_{yz}$

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

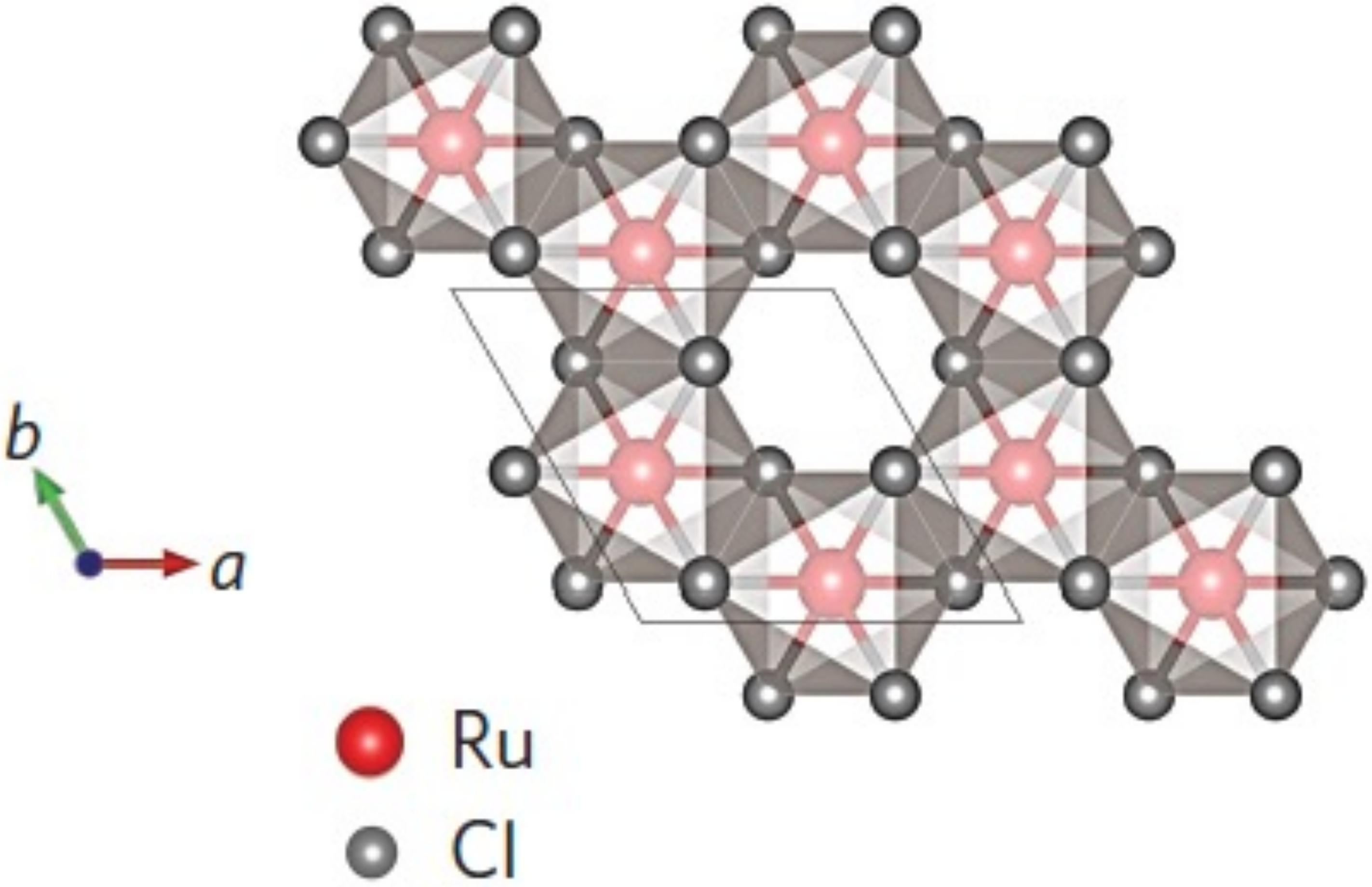
Crystal structure of α-$RuCl_3$
→ candidate Kitaev material

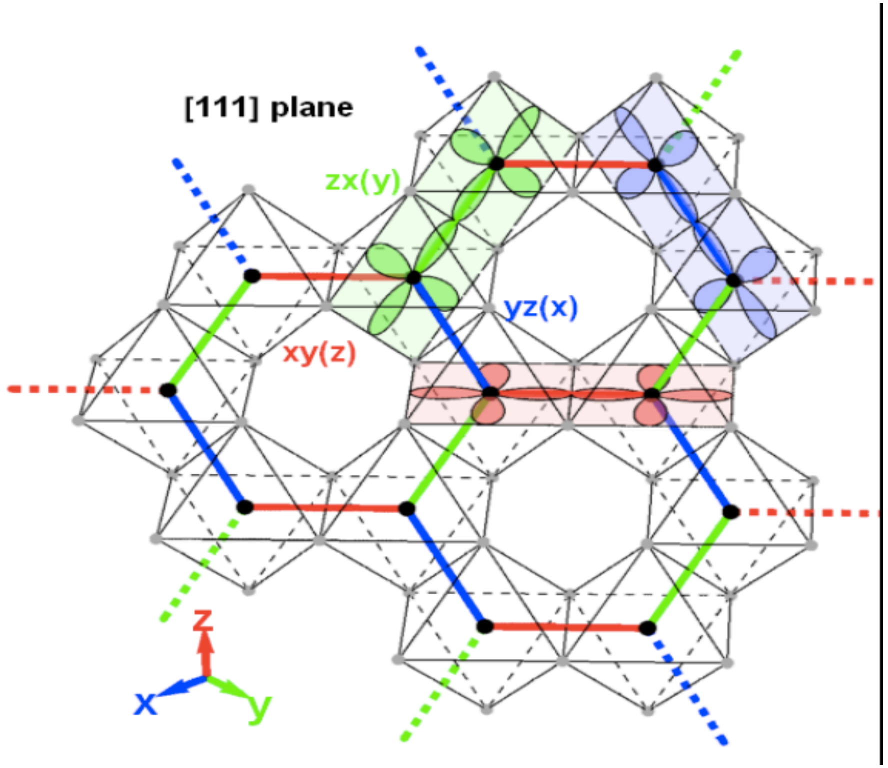






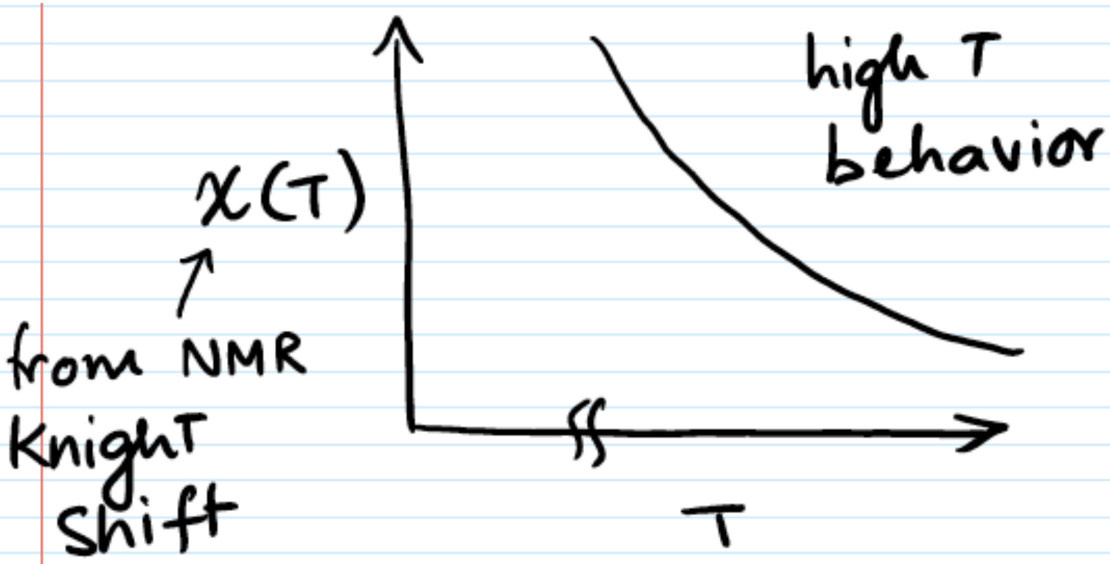
α-$RuCl_3$

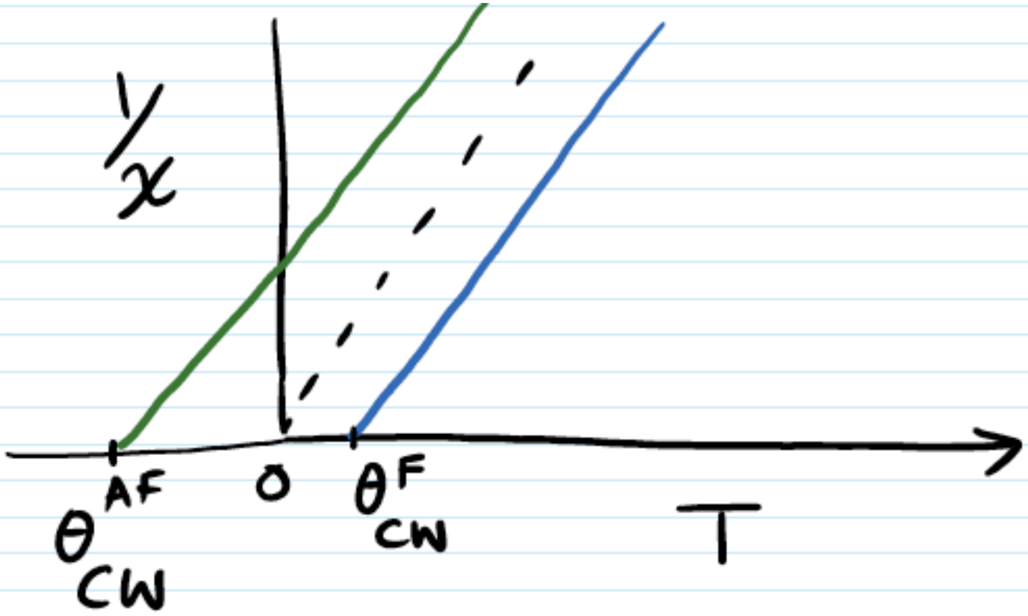




How do you detect a QSL?

Signatures of a QSL: large frustration parameter

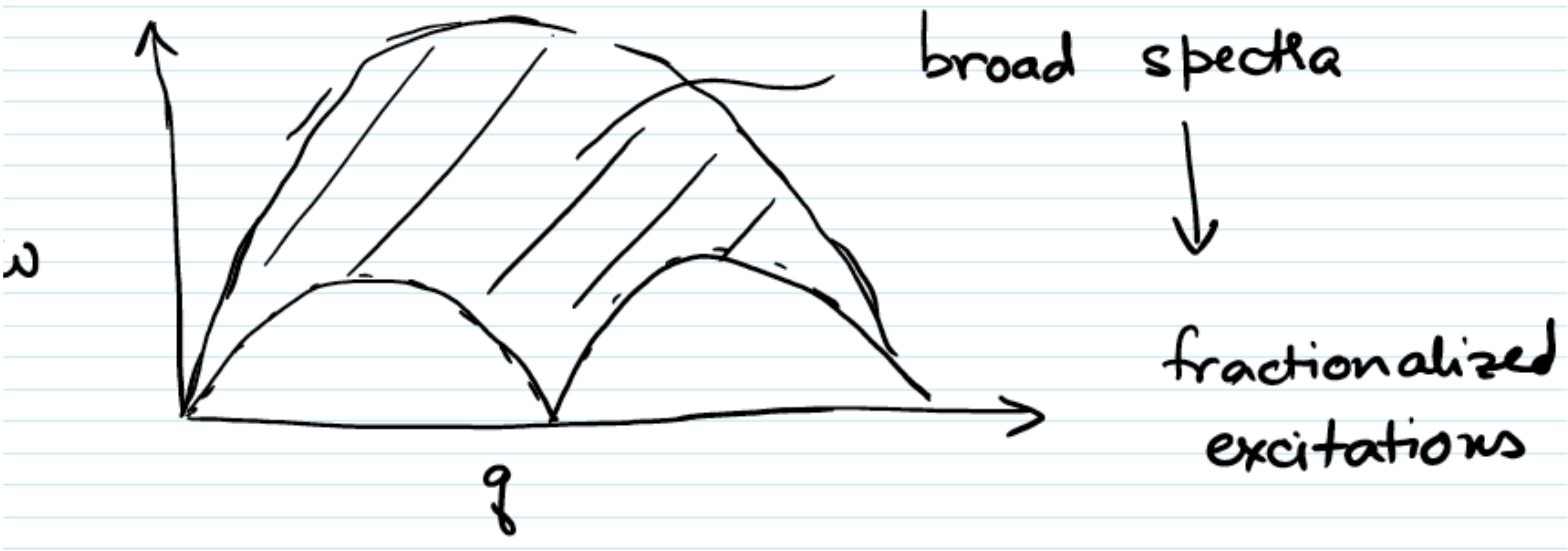




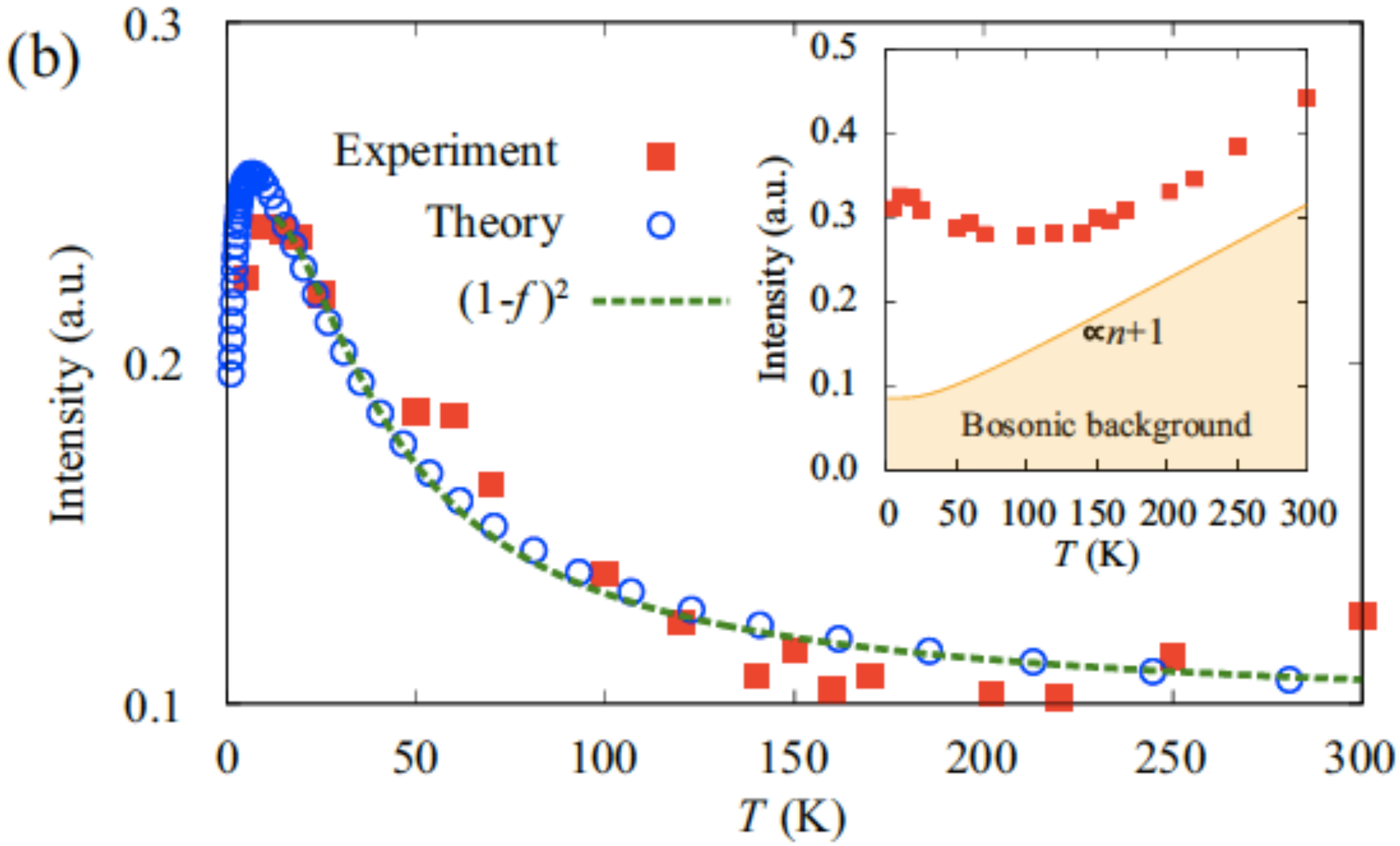
$$\chi(T) = \frac{C}{T - \theta_{cw}}$$

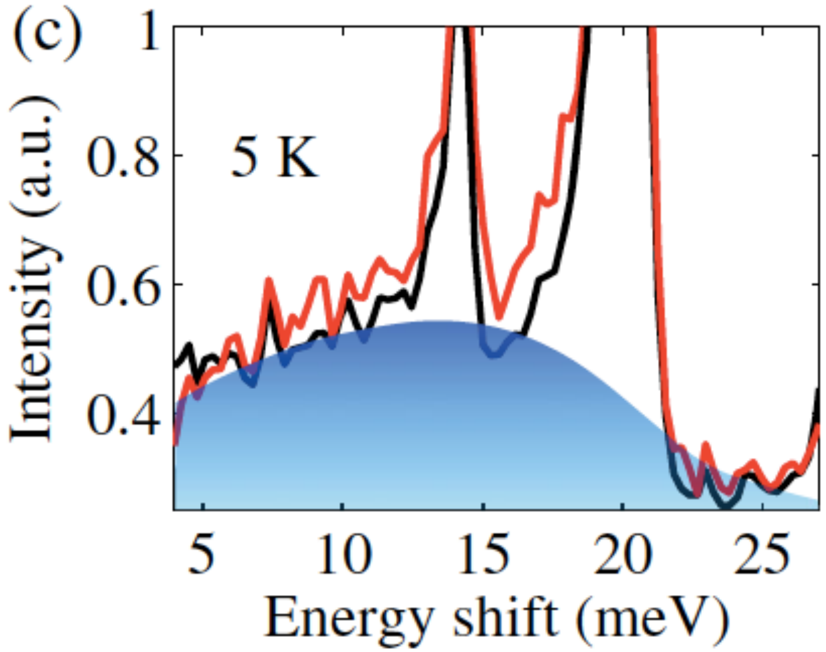
$$f = \frac{|\theta_{cw}|}{T_c}$$

Signatures of a QSL: broad spectrum of spin excitations



Signatures of a QSL: fermionic nature of spin excitations in Raman



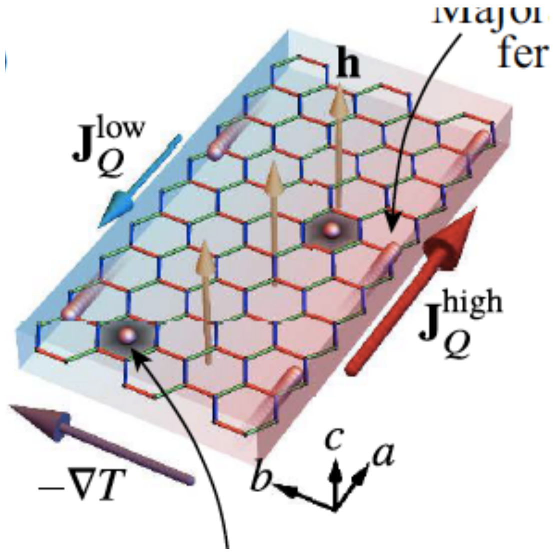


$$\mathcal{R} = \sum_{\langle ij \rangle_\mu} (\boldsymbol{\epsilon}_{\text{in}} \cdot \mathbf{d}^\mu)(\boldsymbol{\epsilon}_{\text{out}} \cdot \mathbf{d}^\mu) J_\mu S_i^\mu S_j^\mu$$

$$I(\omega) = \frac{1}{N} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \mathcal{R}(t) \mathcal{R} \rangle$$

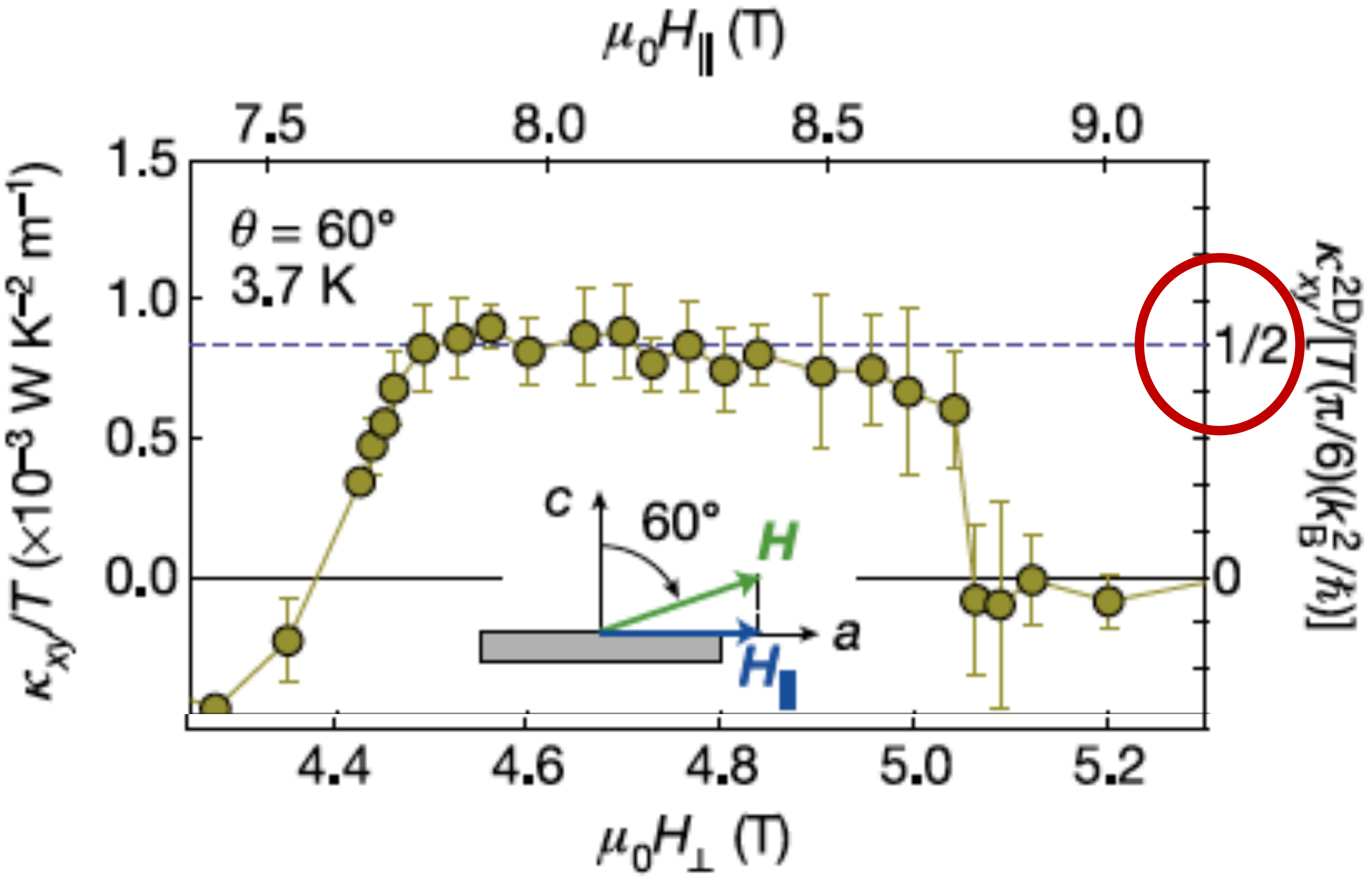
Luke J. Sandilands, Yao Tian, Kemp W. Plumb, and Young-June Kim, Kenneth S. Burch, PRL 114, 147201 (2015)

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



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

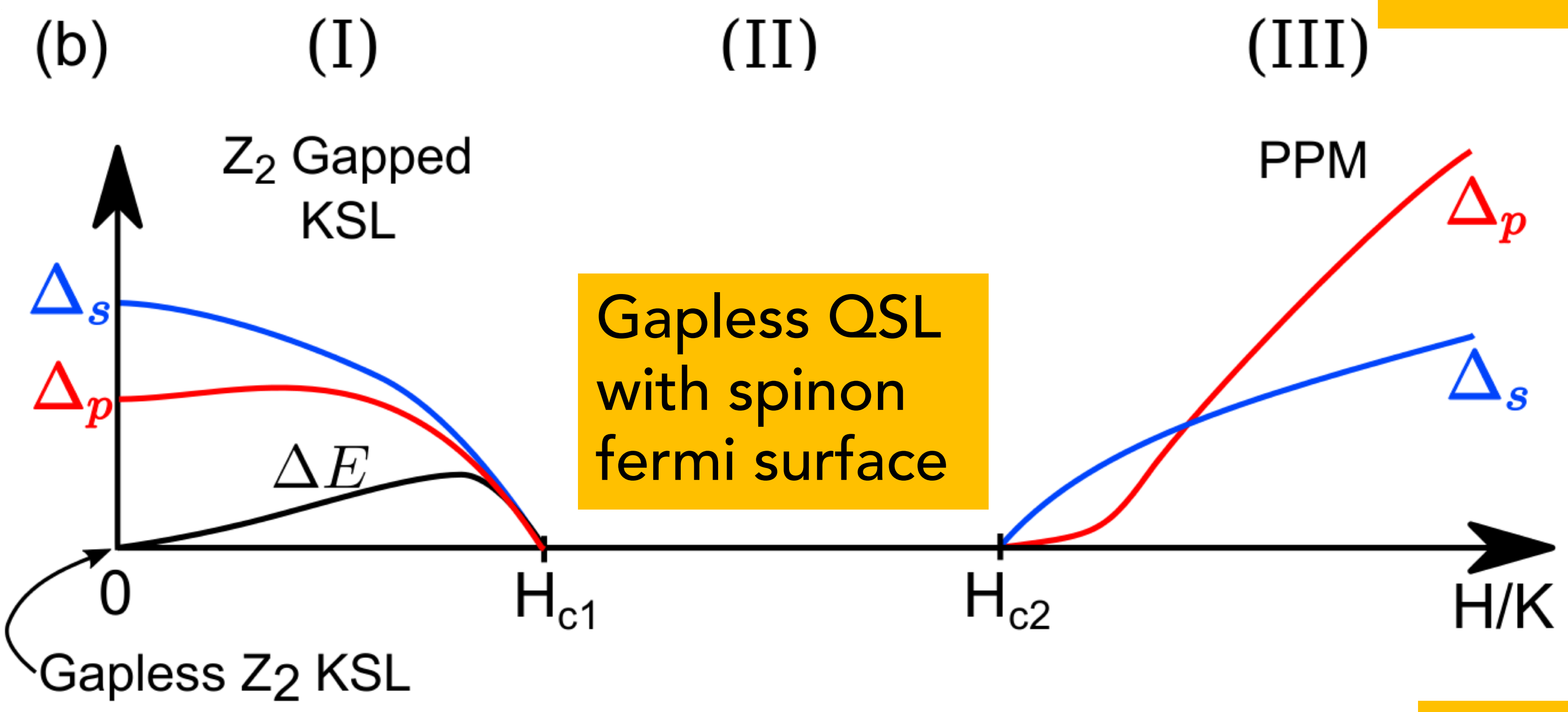
$$\kappa_{xy}^{2D} = \kappa_{xy} d$$



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).

Our Main Results: Kitaev Model in a Magnetic Field

K: AF exchange



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

PNAS 201821406 (2019)
Phys. Rev. B 99, 140413(R) (2019)
arXiv:1908.10877

K: F exchange
No gapless QSL

Theory — Spinon fermi surface

Materials — F and AF Kitaev materials

Phenomena — Spin fractionalization in pump-probe dynamics