Title: New topological phases in the Kitaev model as a function of magnetic field

Speakers: Nandini Trivedi

Collection: Quantum Criticality: Gauge Fields and Matter

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Abstract: The Kitaev model with anisotropic interactions on the bonds of a honeycomb lattice is a paradigmatic model for quantum spin liquids. Despite the simplicity of the model, a rich phase diagram with gapless and gapped quantum spin liquid phases, with abelian and non-abelian excitations, are revealed as a function of a magnetic field and bond couplings. Our results of the entanglement entropy, topological entanglement entropy, and the dynamical spin excitation spectrum, are obtained using exact diagonalization and density matrix renormalization group (DMRG) methods. We provide insights into the phases from the underlying effective field theories.

In collaboration with Shi Feng, Cullen Gantenberg, Adhip Agarwala, Subhro Bhattacharjee

[1] Signatures of magnetic-field-driven quantum phase transitions in the entanglement entropy and spin dynamics of the Kitaev honeycomb model, David C. Ronquillo, Adu Vengal, Nandini Trivedi, Phys. Rev. B 99, 140413 (2019)

[2] Magnetic field induced intermediate quantum spin-liquid with a spinon Fermi surface, Niravkumar D. Patel and Nandini Trivedi, Proceedings of the National Academy of Sciences 116, 12199 (2019).

[3] Two-Magnon Bound States in the Kitaev Model in a [111]-Field, Subhasree Pradhan, Niravkumar D. Patel, Nandini Trivedi, Phys. Rev. B 101, 180401 (2020)

[4] Symmetry Analysis of Tensors in the Honeycomb Lattice of Edge-Sharing Octahedra, Franz G. Utermohlen, Nandini Trivedi, Phys. Rev. B 103, 155124 (2021)

New topological phases in the Kitaev model as a function of magnetic field

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PERIMETER INSTITUTE Quantum Criticality: Gauge Fields and Matter

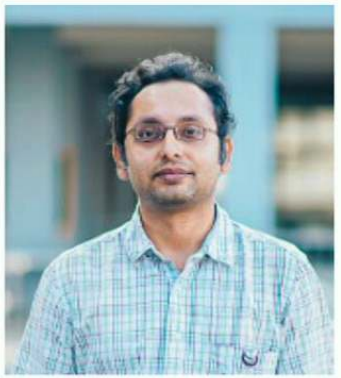
16-20 May 2022
America/Toronto timezone

Center of Emergent Materials
NSF MRSEC – DMR

Shi Feng, OSU

Adhip Agarwala, IIT Kanpur

Cullen Gantenberg, OSU



Subhro Bhattacharya, ICTS Bangalore

David Ronquillo

Adu Vengal

Ian Osborne.

Nirav Patel

Subhasree Pradhan

Franz Utermohlen

Gonzalo Alvarez

Field-orientation-dependent spin dynamics of the Kitaev honeycomb model PRB 99, 140413(R) (2019)

Magnetic field induced intermediate gapless spin-liquid phase with a spinon Fermi surface
PNAS 116, 12199 (2019)

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

Symmetry Analysis of Tensors in the Honeycomb Lattice of Edge-Sharing Octahedra,
PRB 103, 155124 (2021).

Gapless to gapless phase transitions in quantum spin chains, PRB 105, 014435 (2022)

Orbital Frustration and Topological Flatbands,
PRB 104, 235202 (2021)

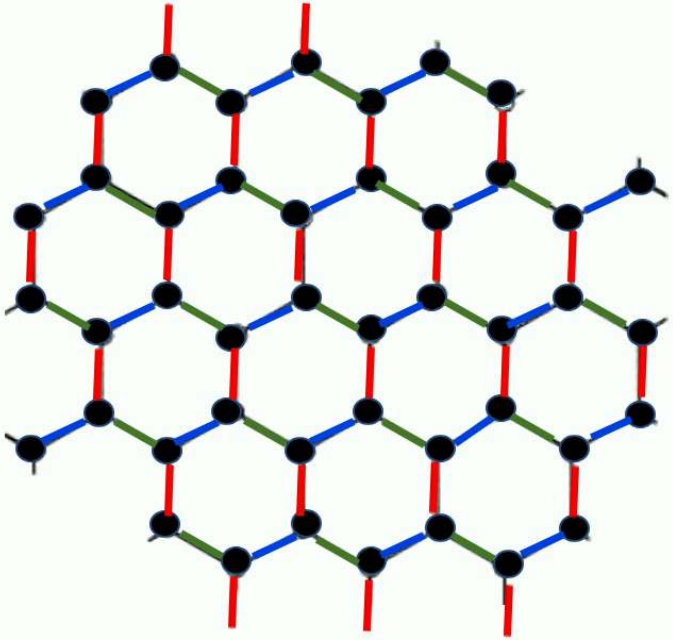
Wenjuan Zhang Zachary Addison

Related work:
Z. Zhu, Kimchi, D.N. Sheng, L. Fu,
PRB 97, 241110 (2018)
Gohlke, Moessner, Pollmann,
PRB 98, 014418 (2018)
C. Hickey and S. Trebst,
Nat. Comm. 10, 530 (2019)
H.C. Jiang, C.Y. Yang, B. Huang, Y.M. Lu,
arXiv 1809.08247
Y. Motome and J. Nasu,
J. Phys. Soc. Jpn. 89, 012002 (2020)

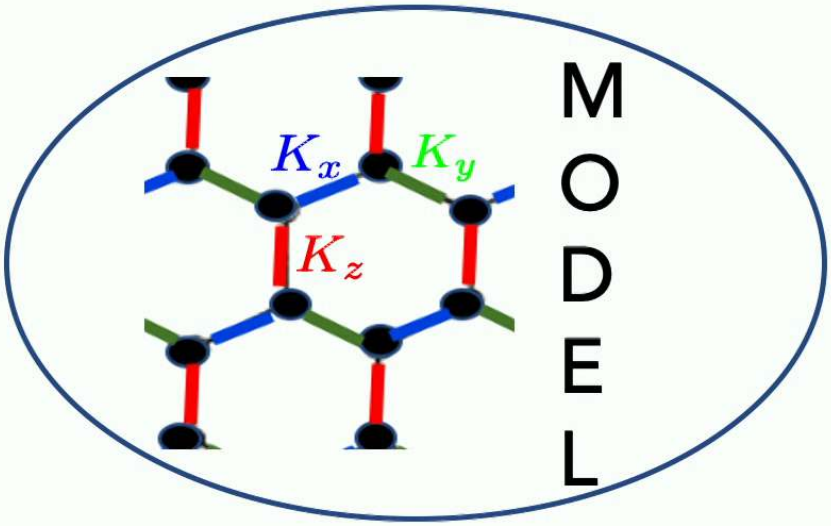
Kitaev Model: bond-dependent interactions

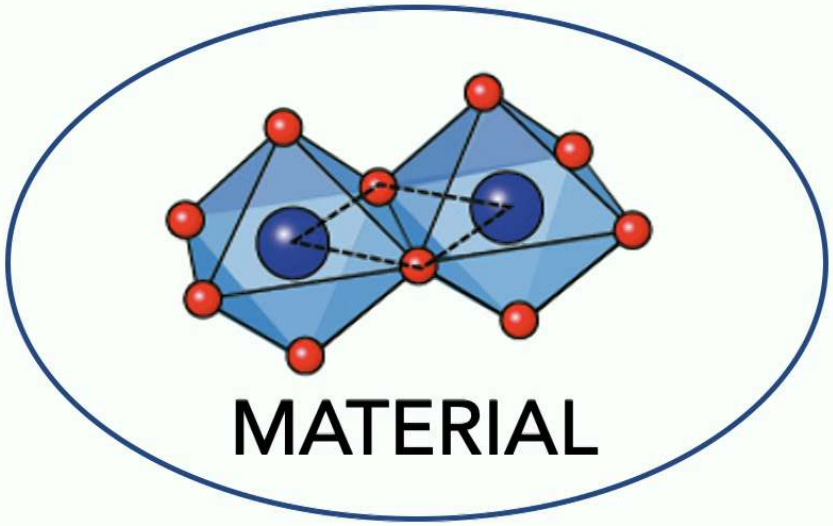
A. Kitaev, Annals of Physics 321, 2-111 (2006)

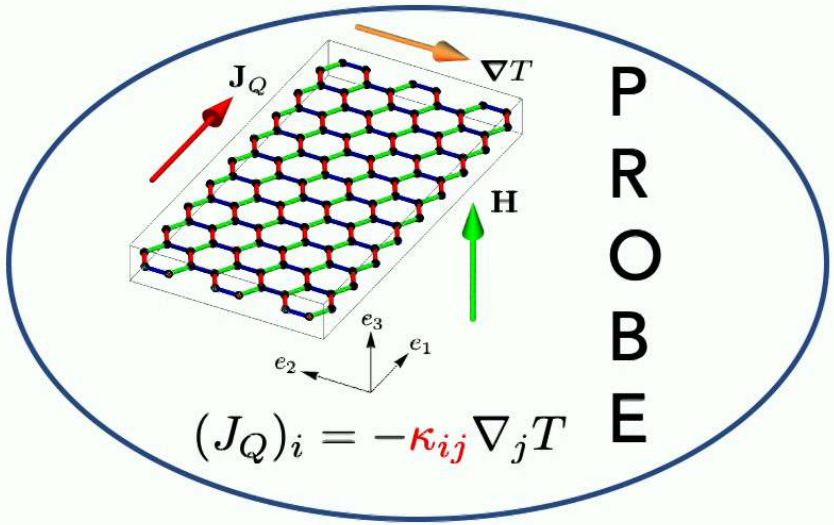
$$\mathcal{H} = K\left[\sum_{\langle ij\rangle \in x} \sigma_i^x \sigma_j^x + \sum_{\langle ij\rangle \in y} \sigma_i^y \sigma_j^y + \sum_{\langle ij\rangle \in z} \sigma_i^z \sigma_j^z\right]$$



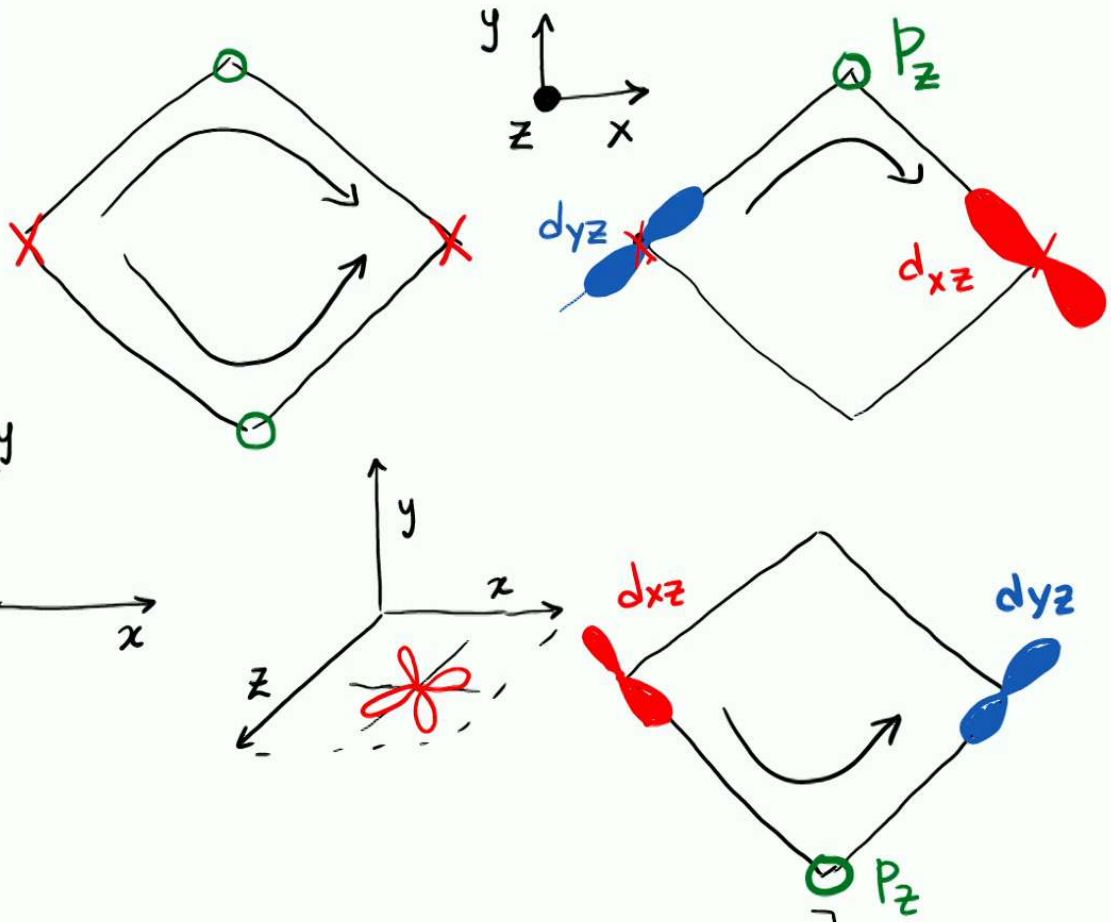
(2+1)D Quantum spin model:
Exact solution
No magnetic long range order
Topological order
→ Quantun spin liquid with
long range entanglement


K_x
K_y
K_z
MODEL


MATERIAL


$\mathbf{J}_Q$
∇T
$\mathbf{H}$
e_3
e_1
e_2
$(J_Q)_i = -\kappa_{ij}\nabla_j T$
PROBE

Jackeli and Khaliullin,
PRL 102, 017205 (2009)

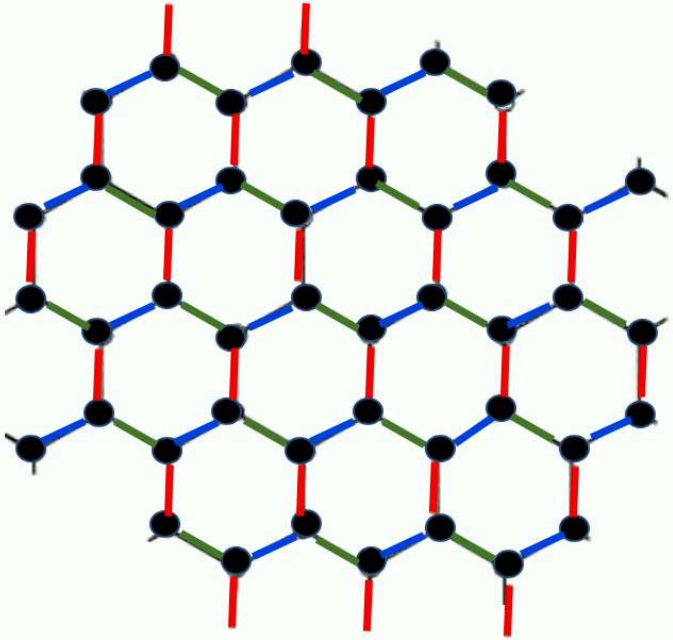


$$|J_z = +\tfrac{1}{2}\rangle = \frac{1}{\sqrt{3}}\left[|d_{xy}\uparrow\rangle + |d_{yz}\downarrow\rangle + i\,|d_{xz}\downarrow\rangle\right]$$

Kitaev Model: bond-dependent interactions

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

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

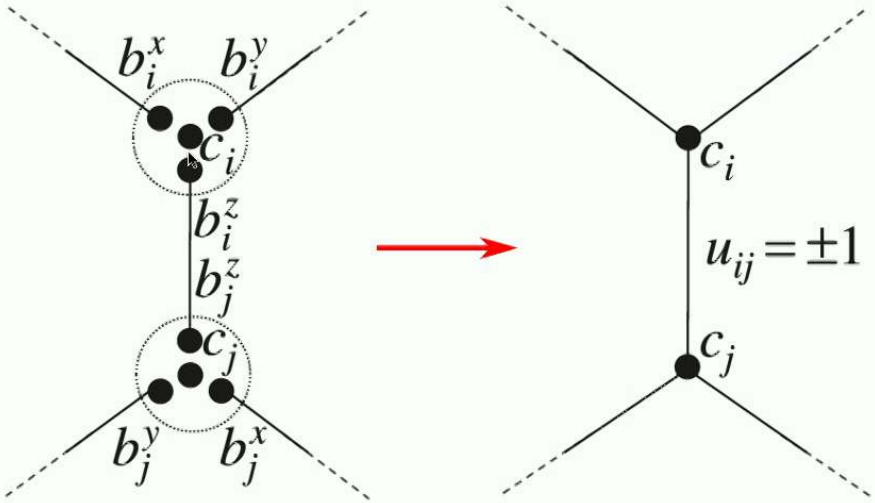


Parton construction:

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

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

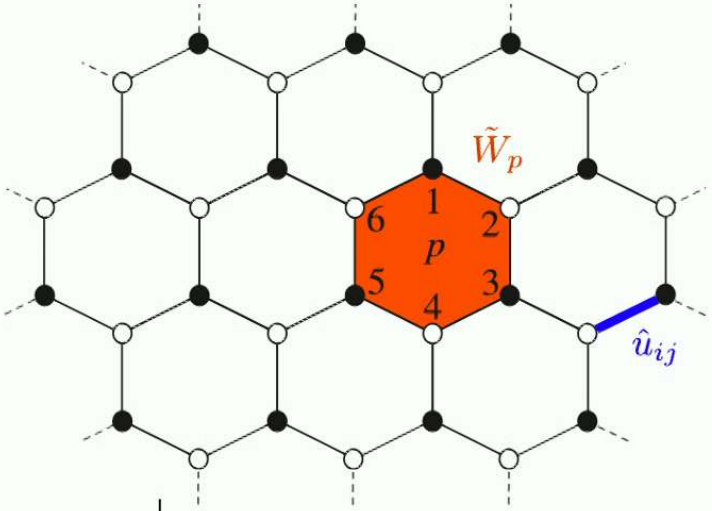
Link Operators (vector potential) and **Plaquette operators** (flux)

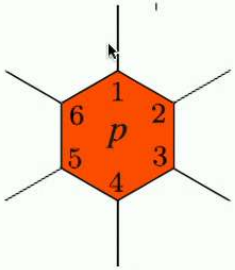


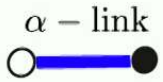
link operator: $\hat{u}_{ij} = i b_i^\alpha b_j^\alpha$

- $\hat{u}_{ij}$ is conserved: $[\hat{u}_{jk},\ H] = 0$.
- $\hat{u}_{jk}^2 = 1$, hence its eigen values are ± 1.

Link Operators (vector potential) and **Plaquette operators** (flux)







$$\tilde{W}_p = \tilde{\sigma}_1^x \tilde{\sigma}_2^y \tilde{\sigma}_3^z \tilde{\sigma}_4^x \tilde{\sigma}_5^y \tilde{\sigma}_6^z \qquad \hat{u}_{ij} = i b_i^\alpha b_j^\alpha$$

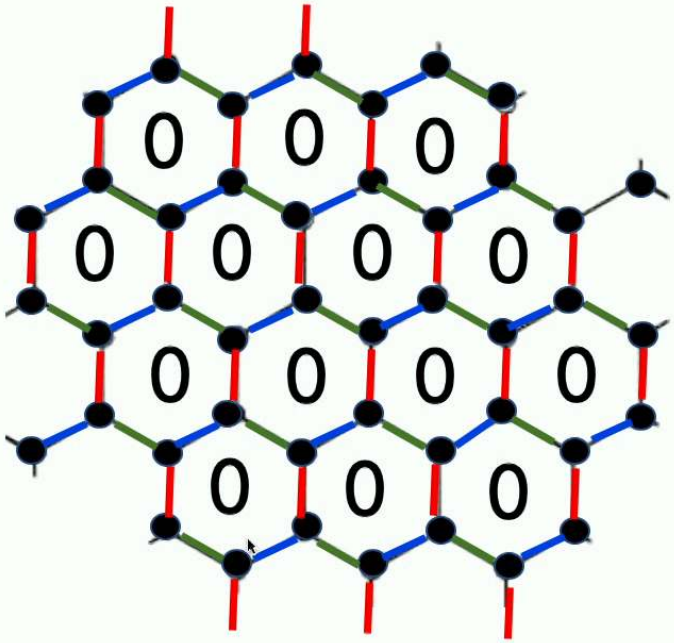
$$[\hat{u}_{ij}, H] = 0$$

$$[\tilde{W}_p, H] = 0$$

$$\downarrow$$

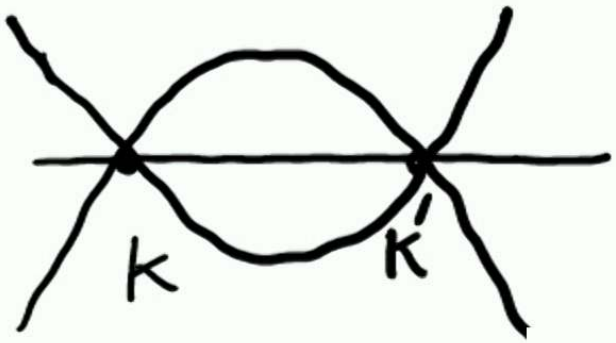
Extensive # of conserved quantites $\{W_p\}$ and $\{u_{ij}\}$

Ground State:

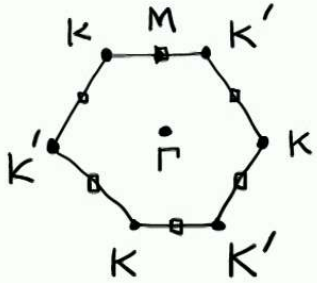


All plaquettes have zero flux

c- Majoranas

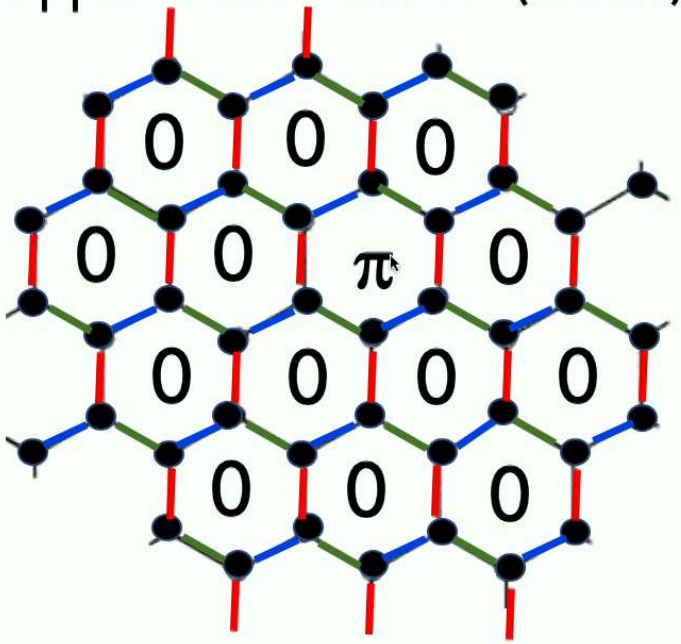


c-majorana fermions
have a Dirac dispersion

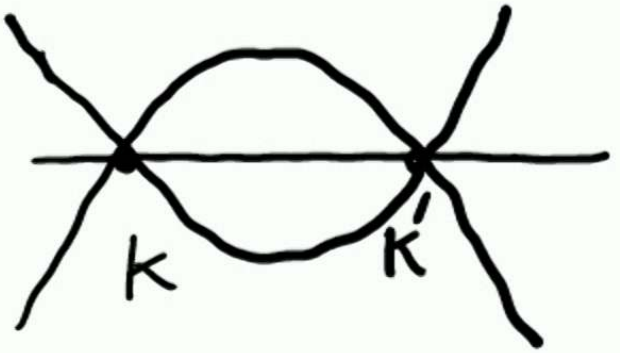


Excitations:

(1)Gapped flux excitation (visons)

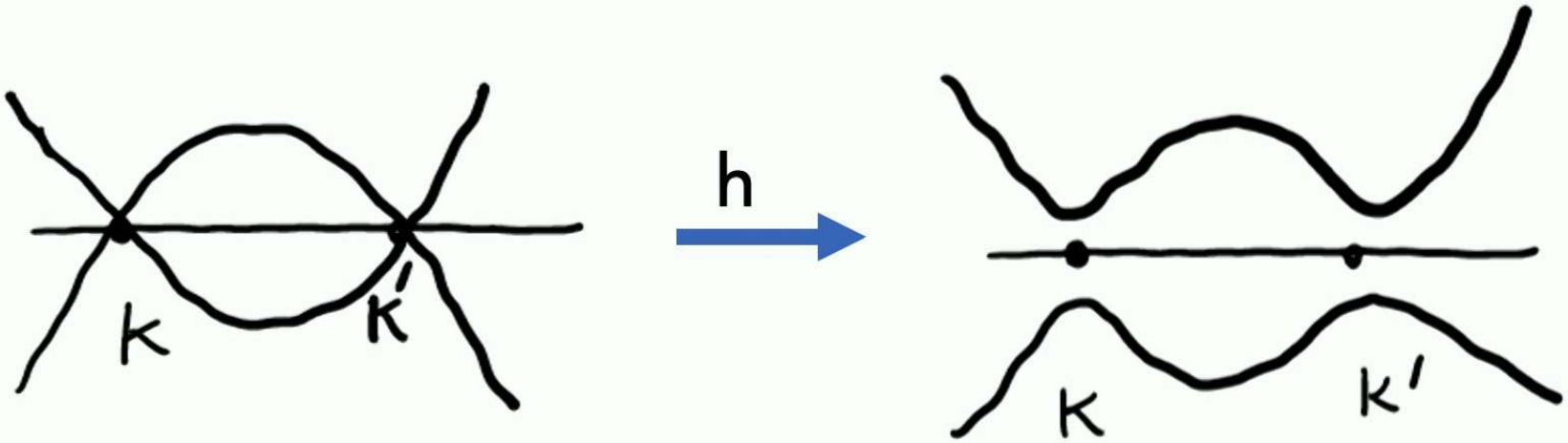


(2) Gapless majorana fermions



Gapless Z_2 Quantum Spin Liquid

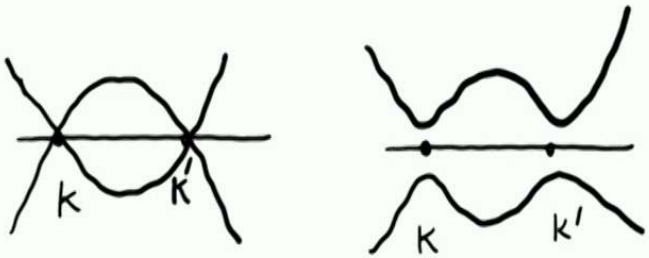
Non-abelian Z_2 gapped chiral spin liquid:



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

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

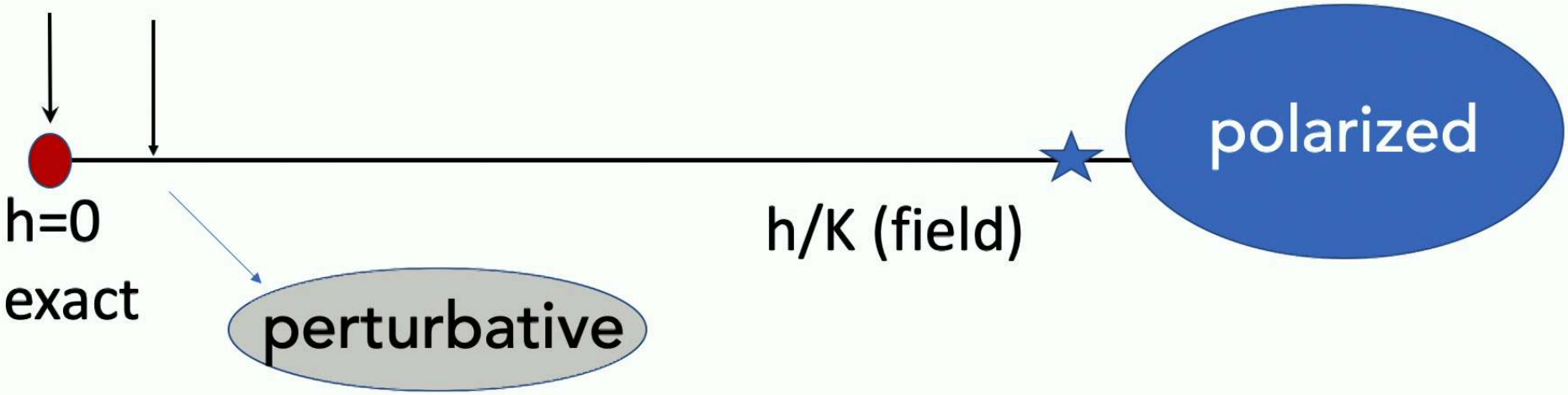
Known results (Kitaev):



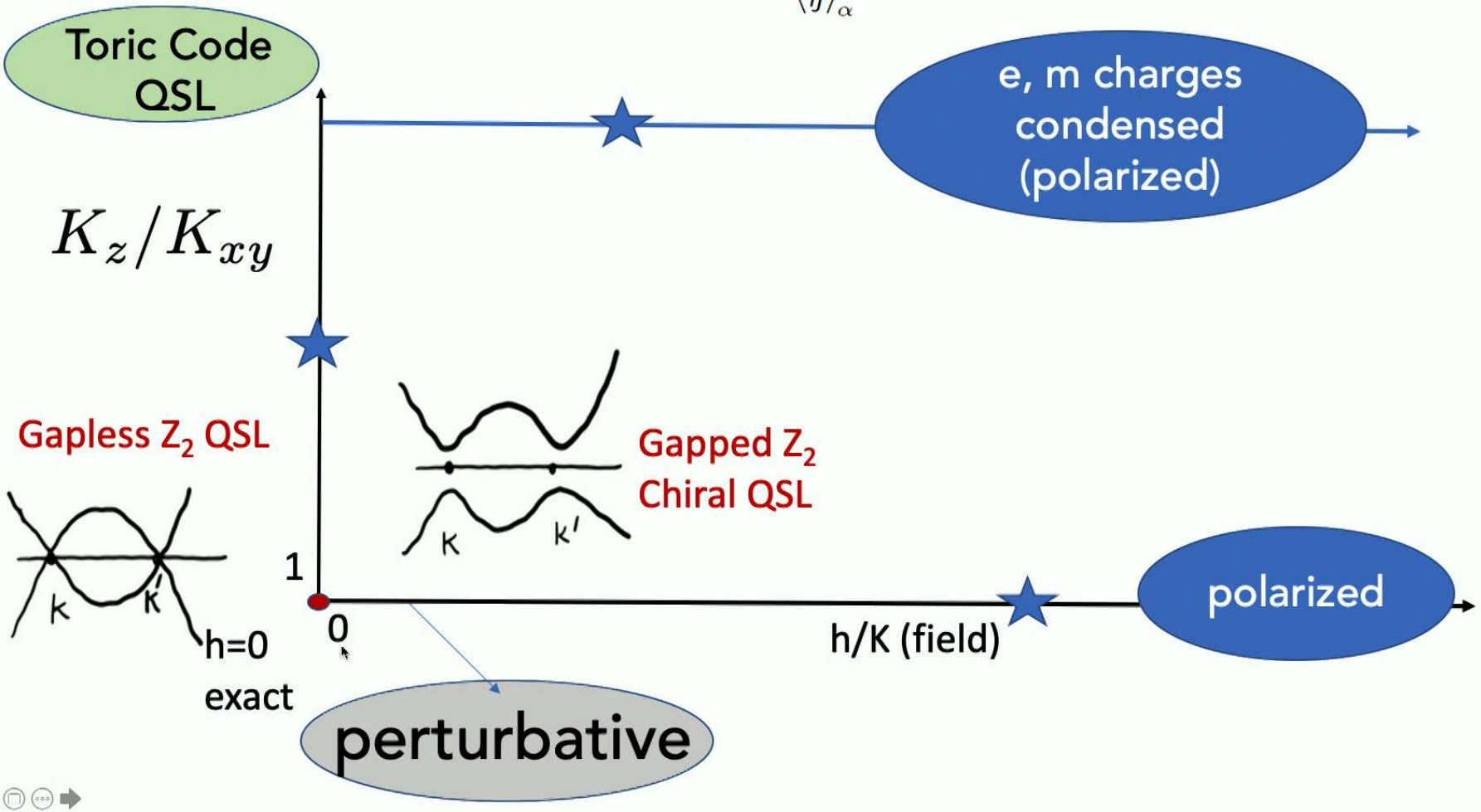
Gapless Z_2 QSL

Gapped Z_2 Chiral QSL

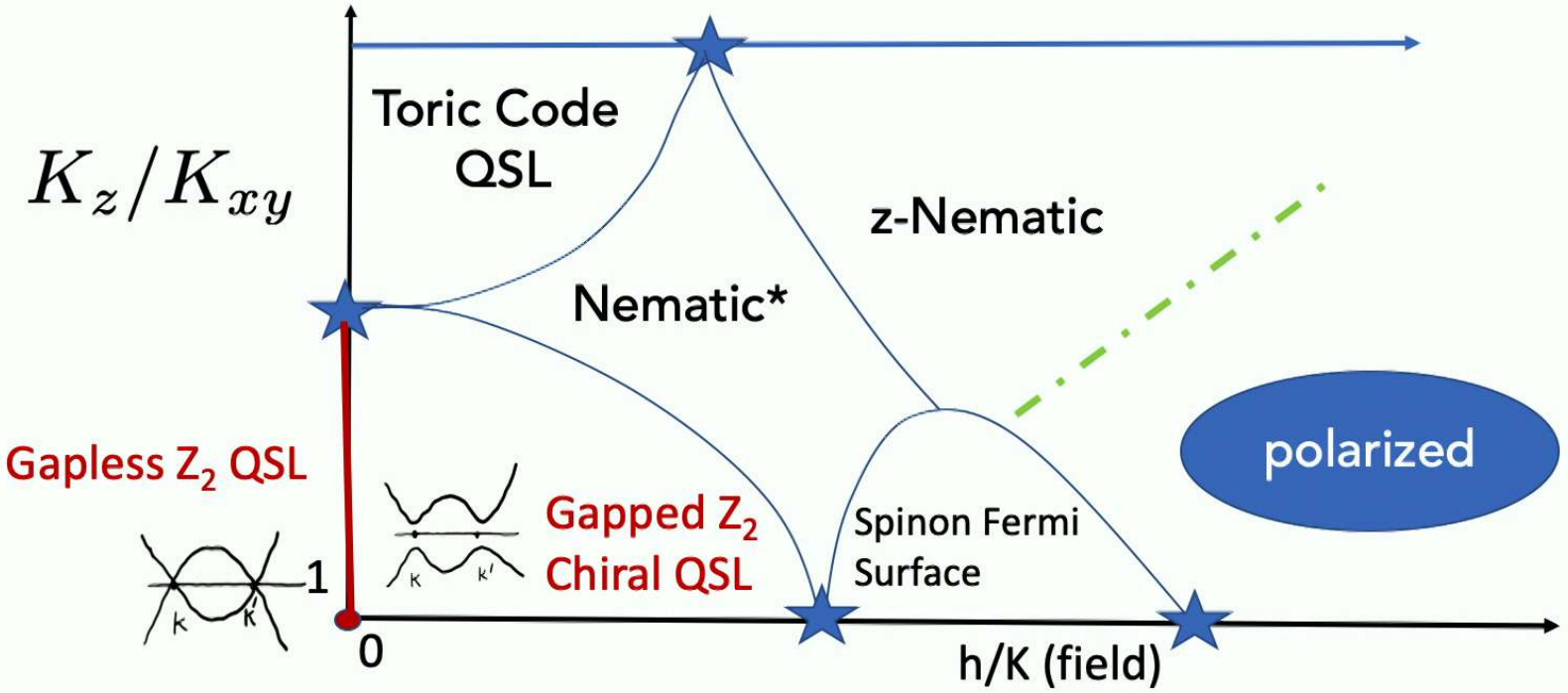
$$H = H_K + h \sum_{i\alpha} S_i^{\alpha}$$



Known results (Kitaev): $H = \sum_{\langle ij \rangle_\alpha} K_\alpha \sigma_i^\alpha \sigma_j^\alpha$



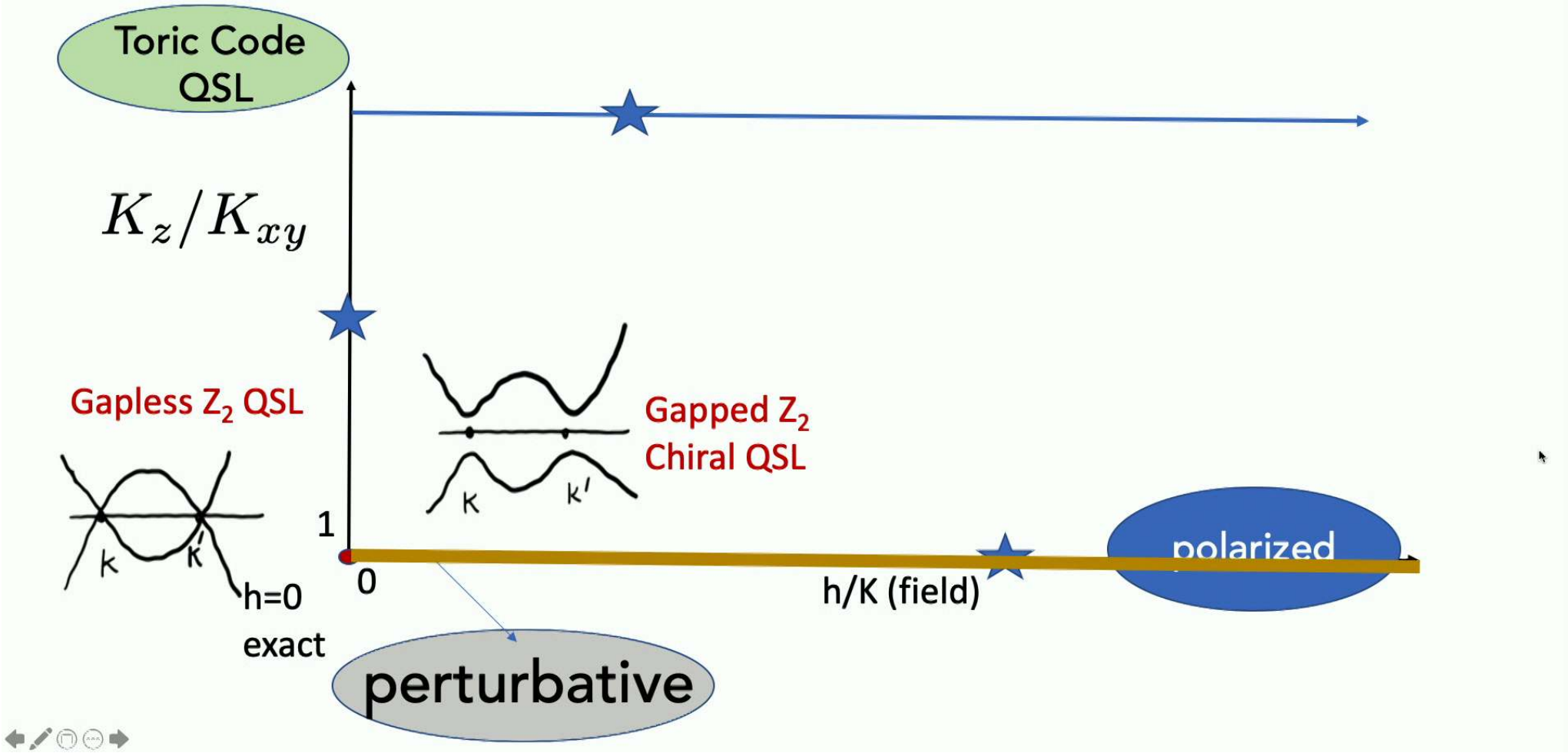
Our Main Results:



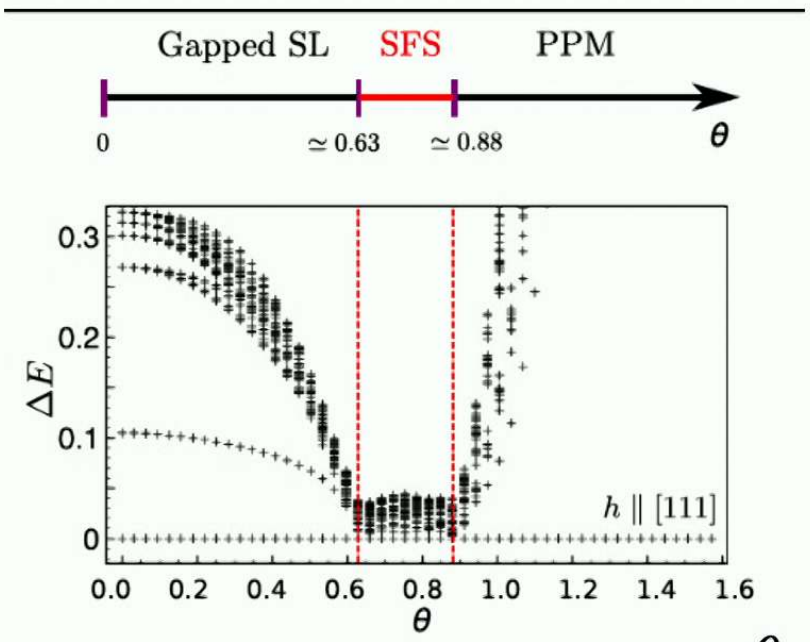
24 sites exact diagonalization
160 sites density matrix renormalization group

Perturbation theory
Mean field theory
Variational approach

Phases at the Isotropic point as a function of field



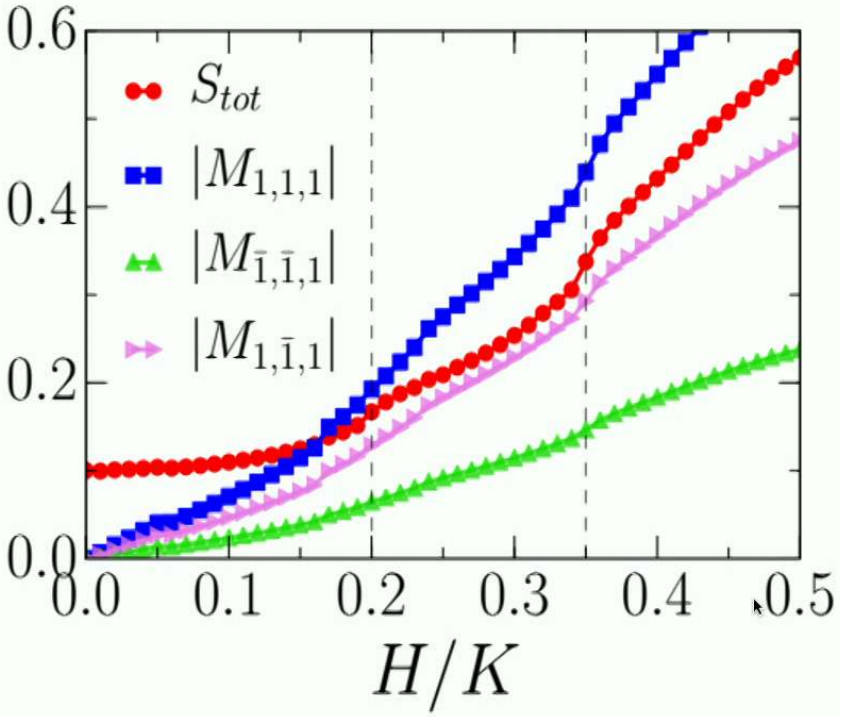
$h||[111]$



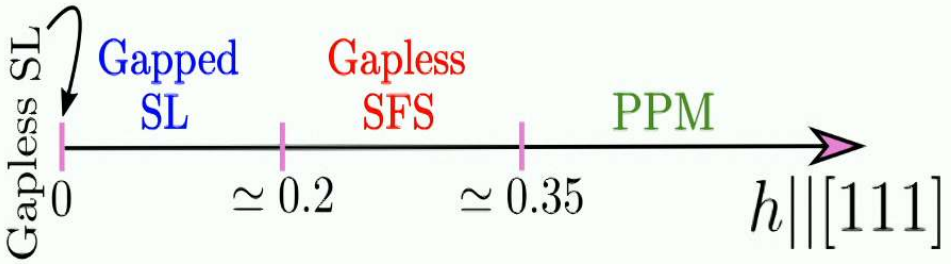
$\theta \approx h/K$

Exact diagonalization
24 sites

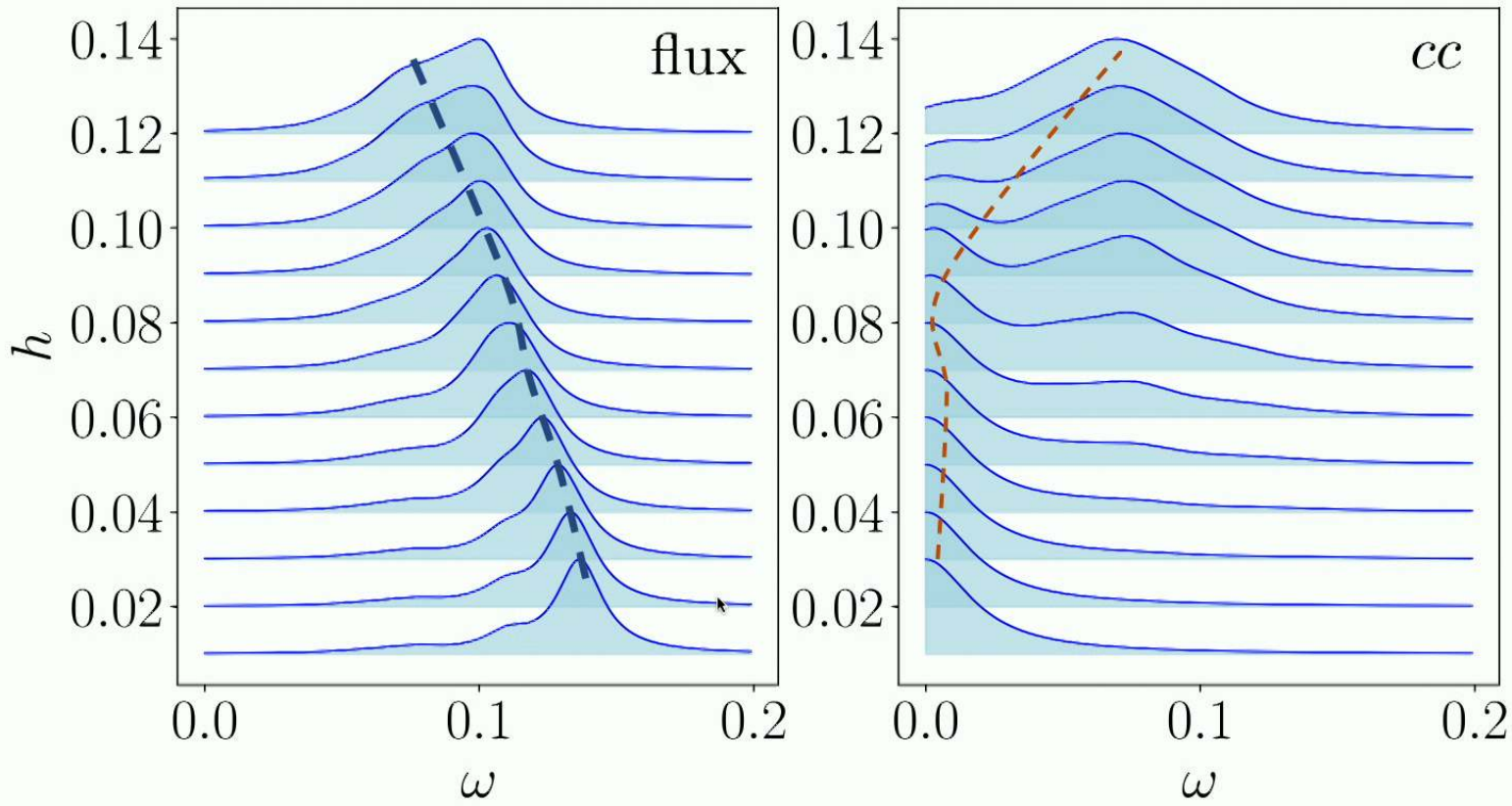
Kitaev Model + Magnetic field: magnetization $h||[111]$



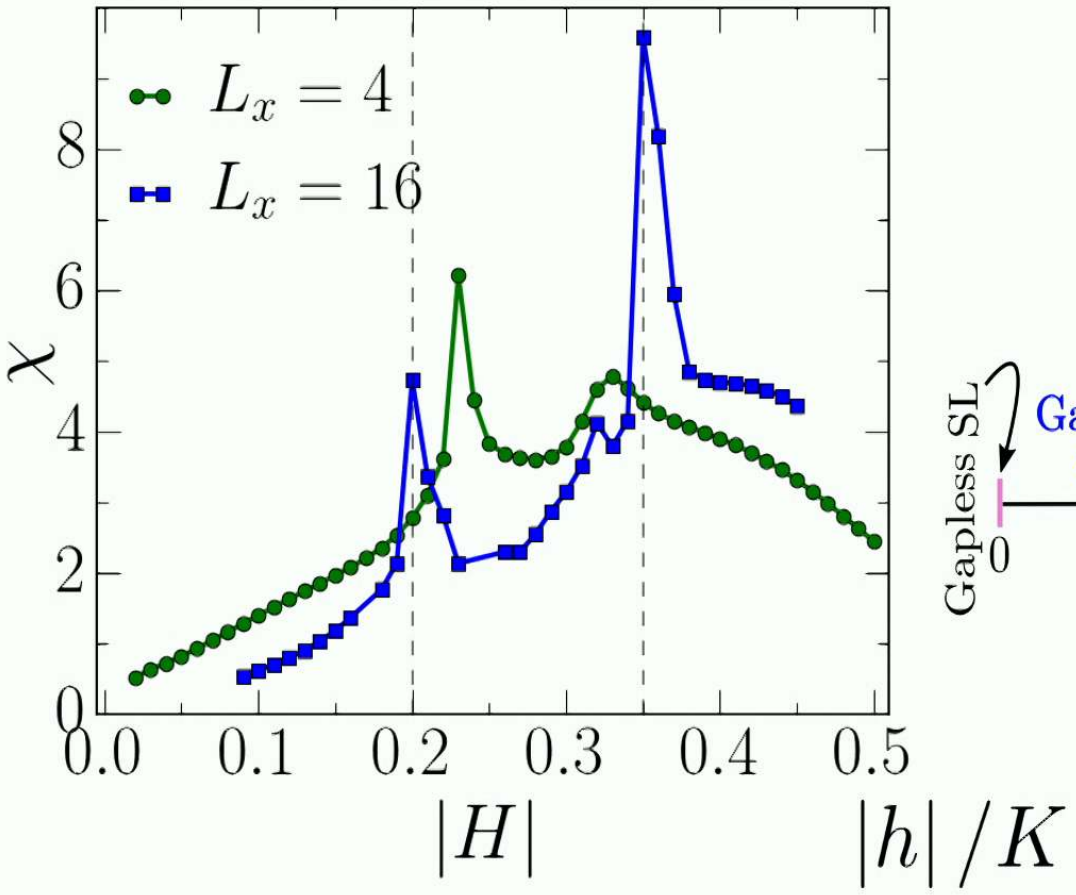
$$H = H_K + h \sum_{i\alpha} S_i^{\alpha}$$



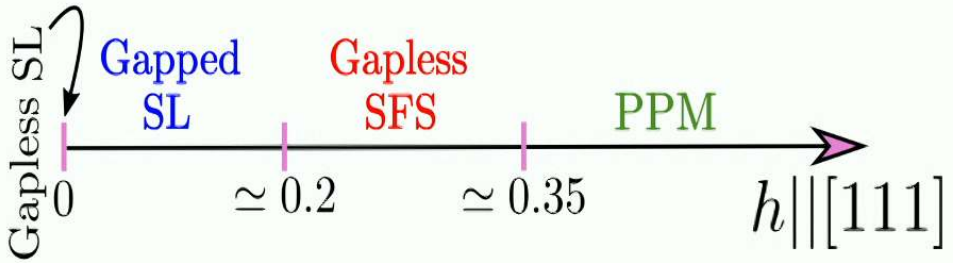
Density Matrix Renormalization Group calculations with 160 spins


flux
cc
h
ω
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.0
0.1
0.2

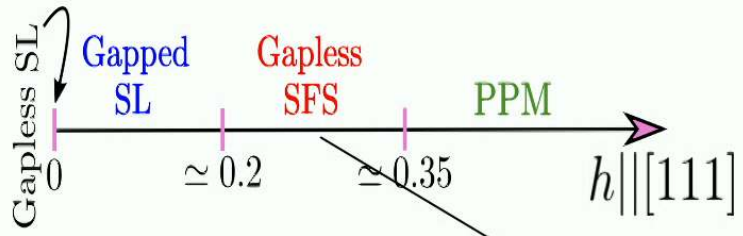
Kitaev Model + Magnetic field $h||[111]$
Evidence for Two Tranitions

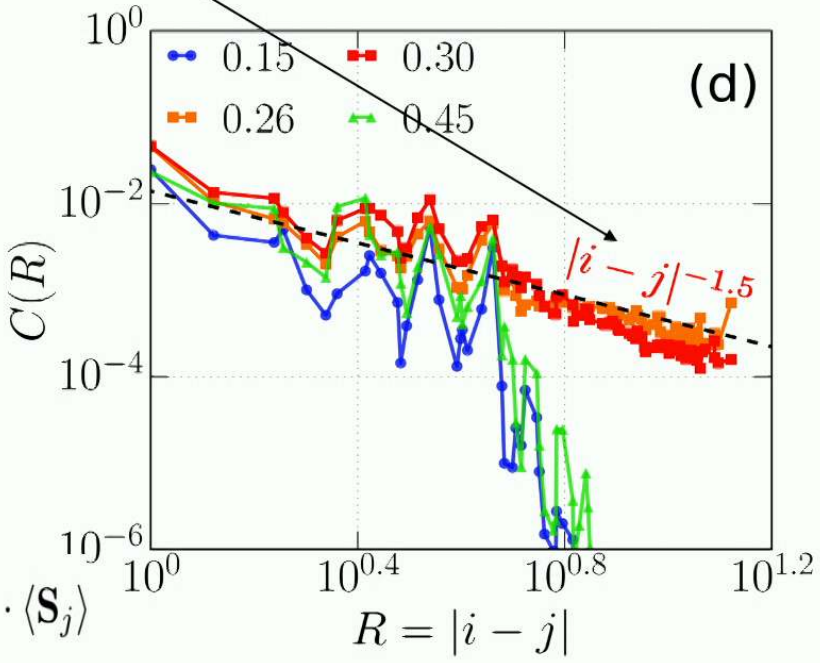


$$H = H_K + h \sum_{i\alpha} S_i^{\alpha}$$



Spin-Spin Correlations in Intermediate phase





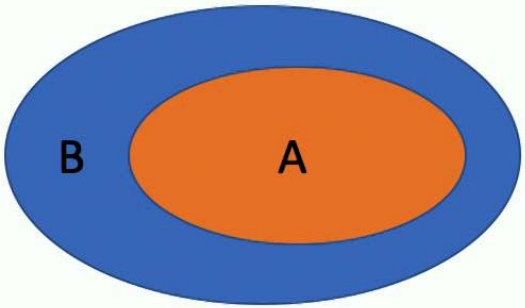
Distinct power law decay of real-space spin-spin correlations!

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

Topological Entanglement Entropy

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

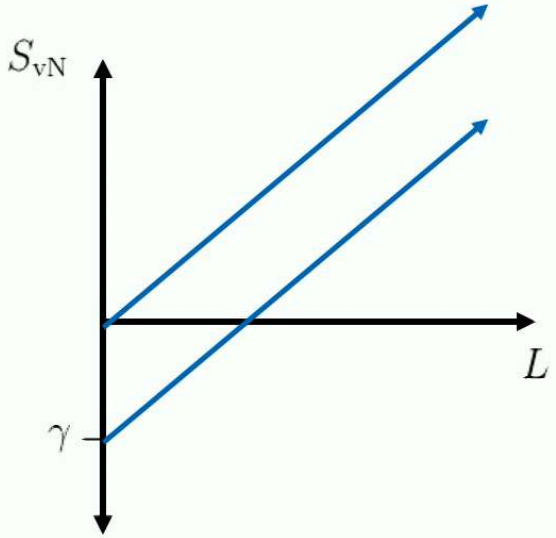
$$\rho_A \equiv \mathrm{Tr}_B(\rho)$$



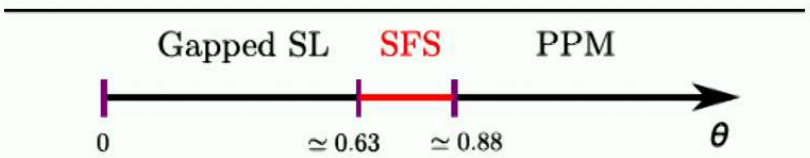
$$S_{\mathrm{vN}} = \alpha L - \gamma + \mathcal{O}(1/L)$$

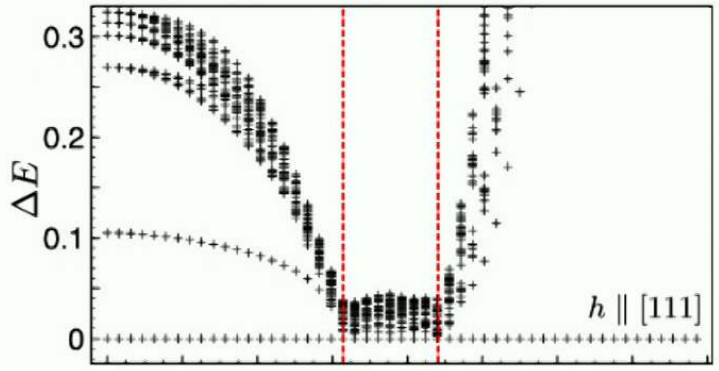
$$S_{\mathrm{topo}} = -\gamma = -\ln \mathcal{D}$$

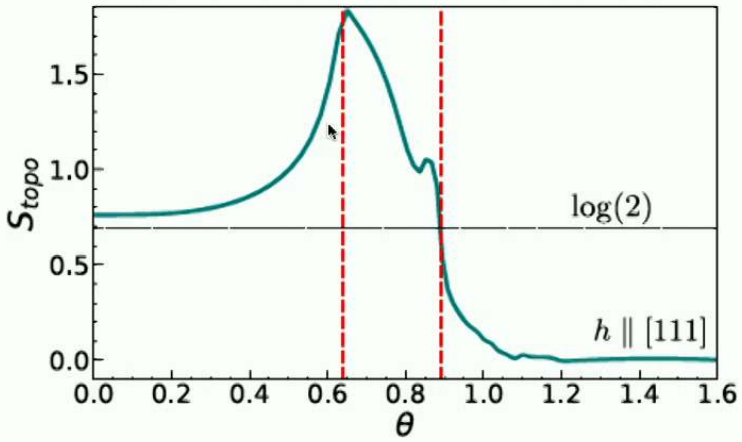
$$\mathcal{D} \equiv \sqrt{\sum_i d_i^2}$$



$h||[111]$



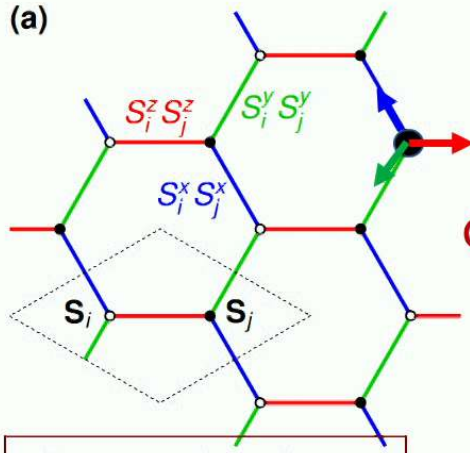




Exact diagonalization
24 sites

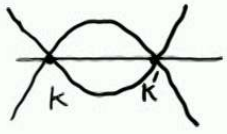
$\theta \approx h/K$

Predictions for Kitaev magnets in a field

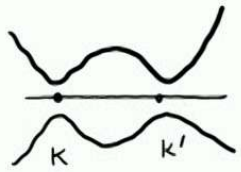


Frustration from bond-dependent interactions

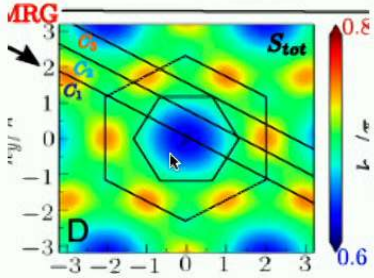
Kitaev (2006)
Jackeli, Khaliullin (2009)



Gapless Z_2 QSL



Gapped Z_2 QSL



Gapless U(1) QSL

Magnon bound states

pola rized

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!

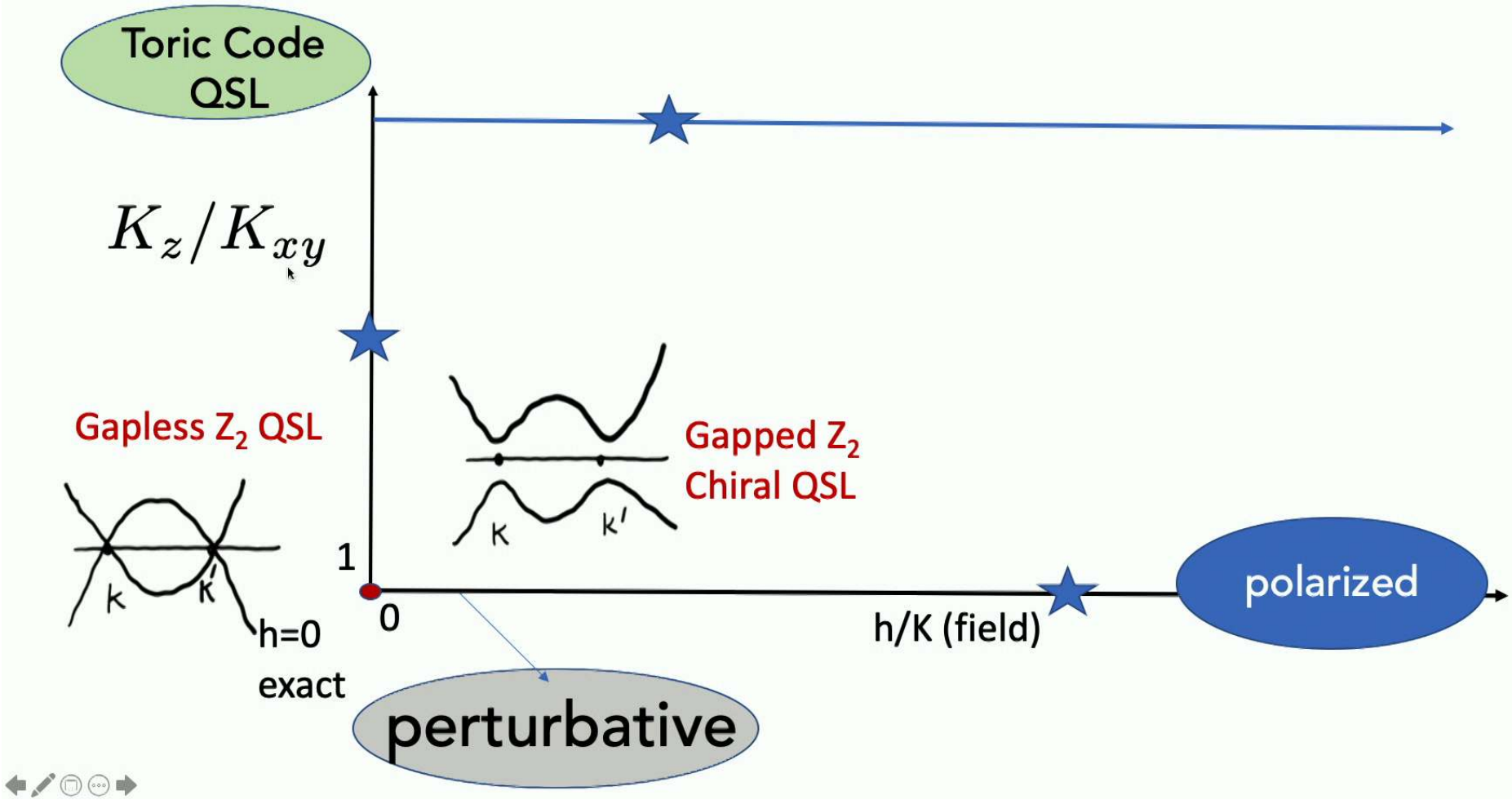
$\kappa_{xx} \sim T$

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)

33

Phases at as a function of bond anisotropy

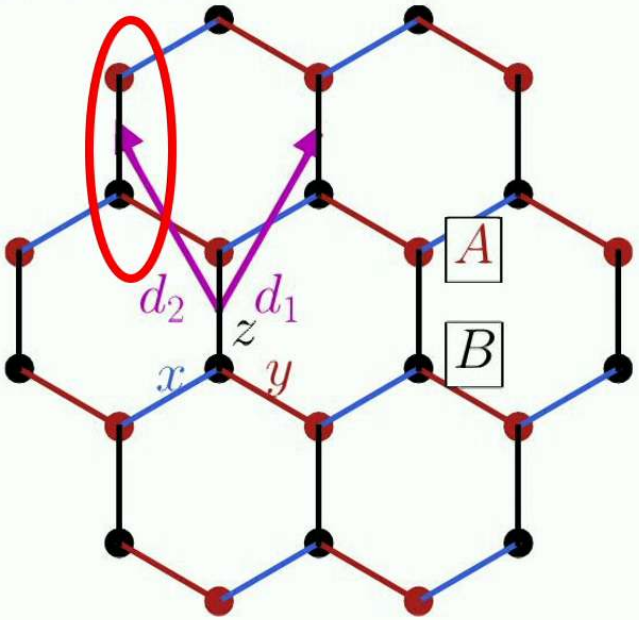


Large Anisotropy→ Toric Code

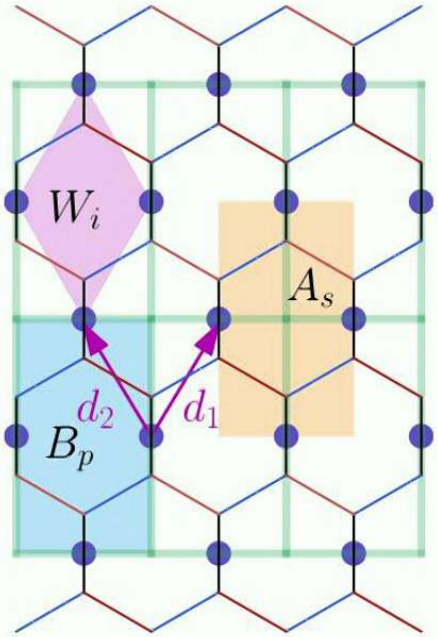
$|\uparrow\downarrow\rangle, \quad |\downarrow\uparrow\rangle$

Low energy manifold
(AF exchange)

Define a new spin
on every z-bond: $\tau^z = (\sigma_A^z - \sigma_B^z)/2$



(a)



(b)

Effective Hamiltonian
(after a unitary transformation):

$$H_{eff} = -J_{TC}\left[\sum_s A_s + \sum_p B_p\right]$$

$$J_{TC} = \frac{K^4}{16|K_z|^3}$$

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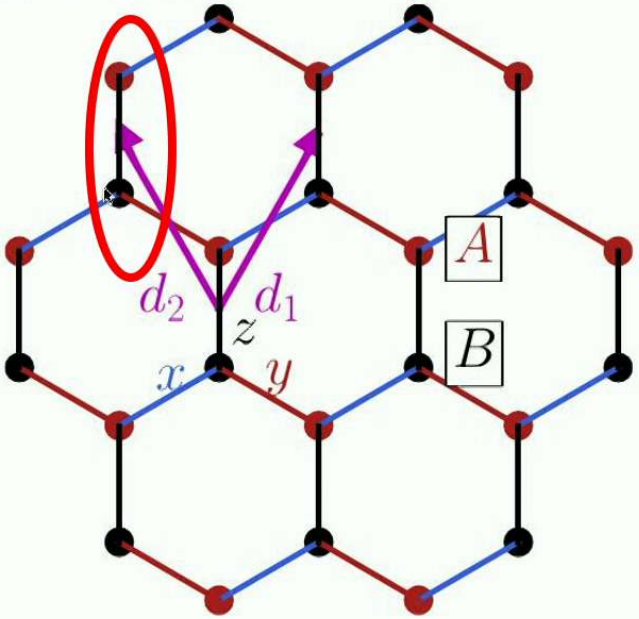
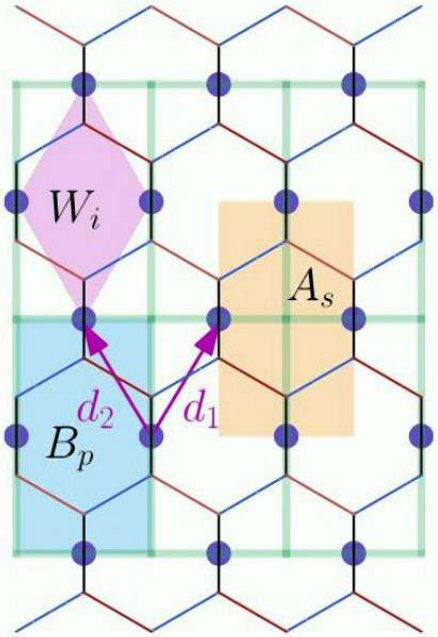


(a)



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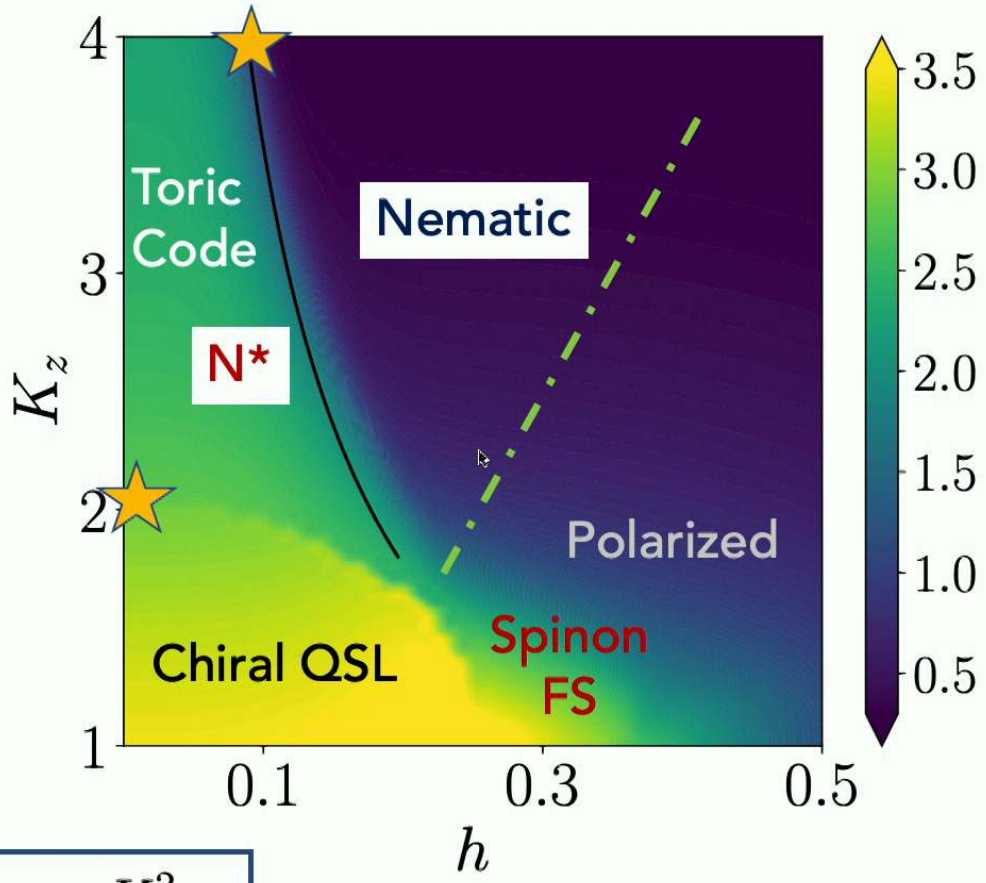
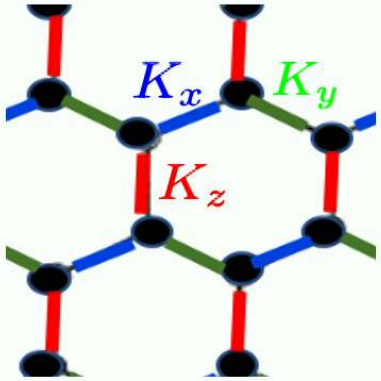


Bipartite Entanglement Entropy

$$\rho_A = \mathrm{Tr}_B |\Psi_0\rangle\langle\Psi_0|$$

$$S_{vN} = \mathrm{Tr}[\rho_A \log \rho_A]$$



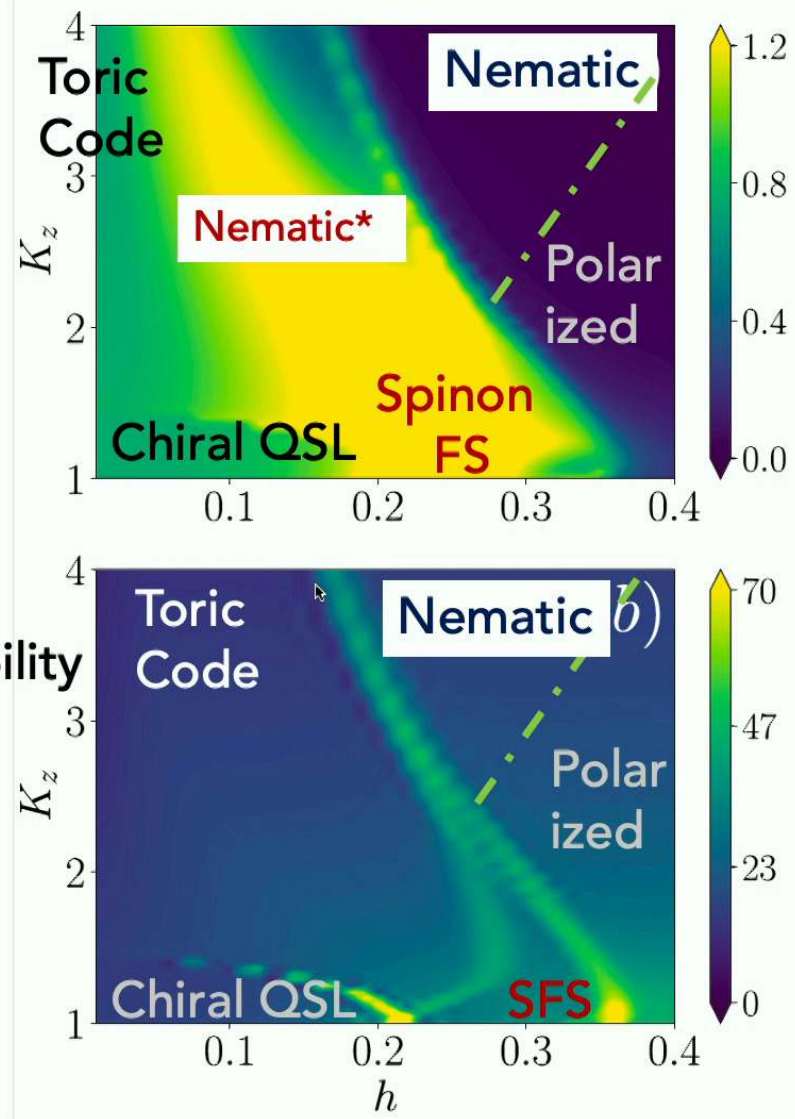
$$K_x = K_y = K$$

K: AF
h perpendicular to honeycomb plane

$$h_c = \frac{K^2}{4\sqrt{2}K_z}$$

Analytic result:

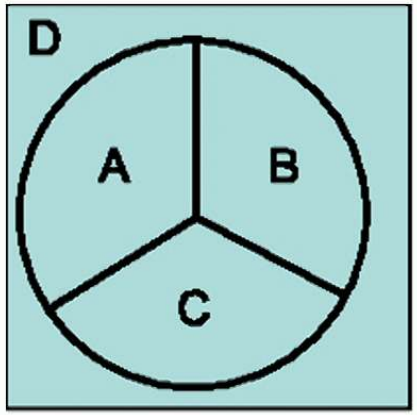
Magnetic Susceptibility



γ

Topological Entanglement Entropy

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



Kitaev-Preskill construction

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

Gapped non abelian Chiral QSL

Vacuum $1 \sim d_1 = 1$

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

} abelian

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

} Non abelian

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

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

$$= 2$$

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

Toric Code (abelian)

$$1, e, m, \epsilon$$

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

$$= 2$$

$$\gamma = \log 2$$

Matter and Gauge Sectors

In the majorana basis $\sigma_i^\alpha = i b_i^\alpha c_i$:

$$H = \sum_{\langle ij \rangle_\alpha} K_\alpha \sigma_i^\alpha \sigma_j^\alpha = i \sum_{\langle ij \rangle_\alpha} K_\alpha \hat{u}_{\langle ij \rangle_\alpha} c_i c_j$$

$$[\hat{u}_{ij}, H] = 0, \ [\hat{W}_p, H] = 0$$

Free majorana coupled to $\mathbb{Z}_2$ gauge field

$$|\Psi\rangle = |M_\mathcal{G}\rangle \otimes |\mathcal{G}\rangle$$

It gives additive von-Neumann entropies:

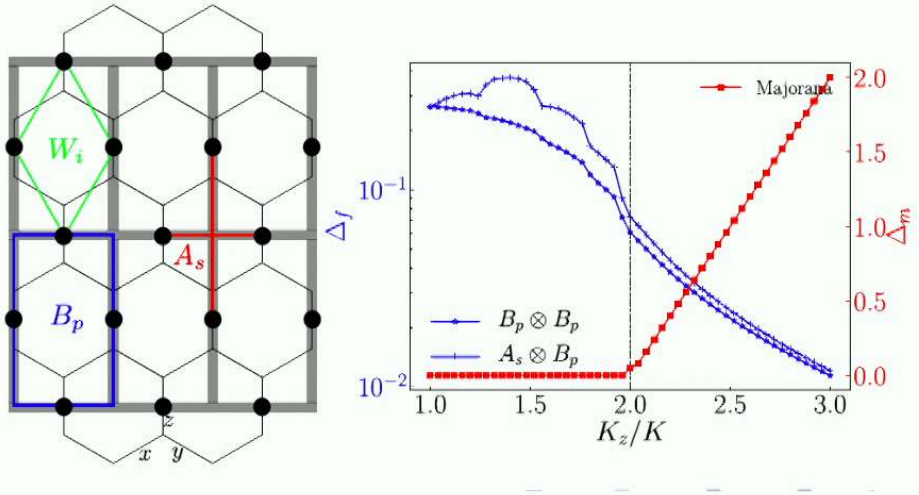
$$S = S_\mathcal{G} + S_M$$

$$S_M \sim \alpha L, \ S_\mathcal{G} \sim L \log 2 - \log 2$$

Excitations:

$|M_\mathcal{G}\rangle$: Free majorana particles

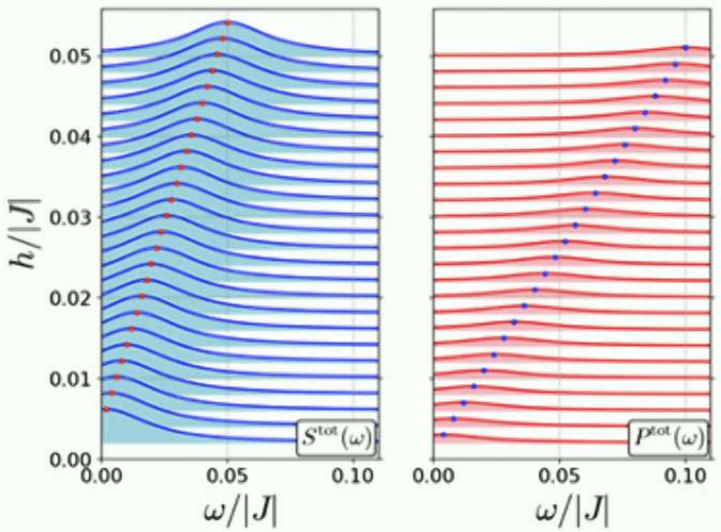
$|\mathcal{G}\rangle$: massive fluxes

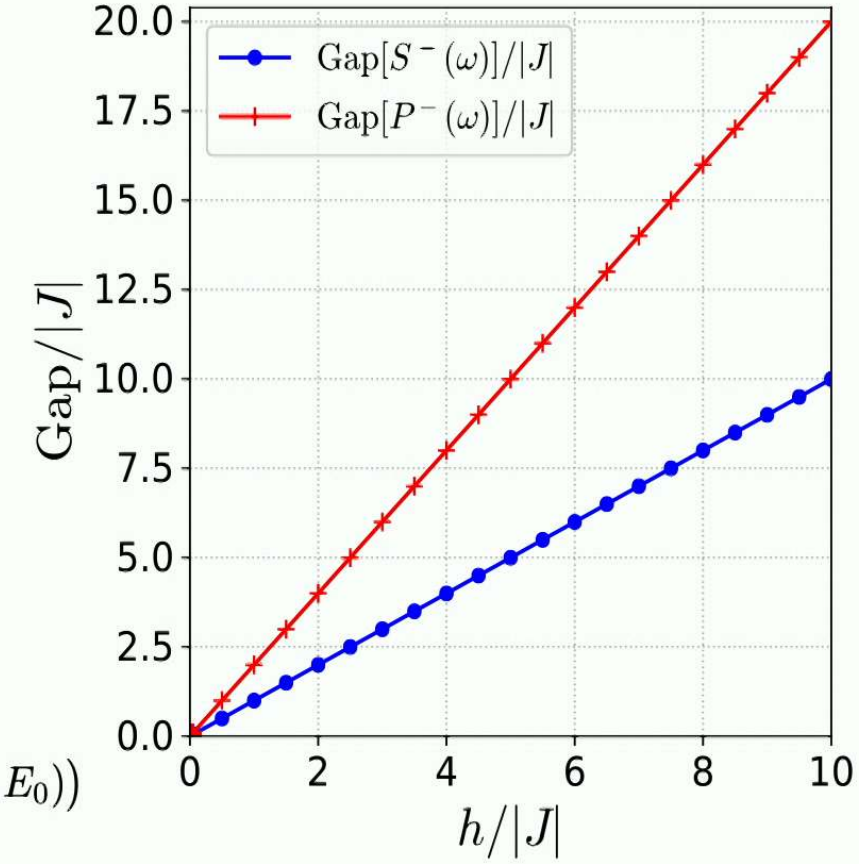


One- and Two-Magnon DOS Gaps

Heisenberg

Ferromagnet





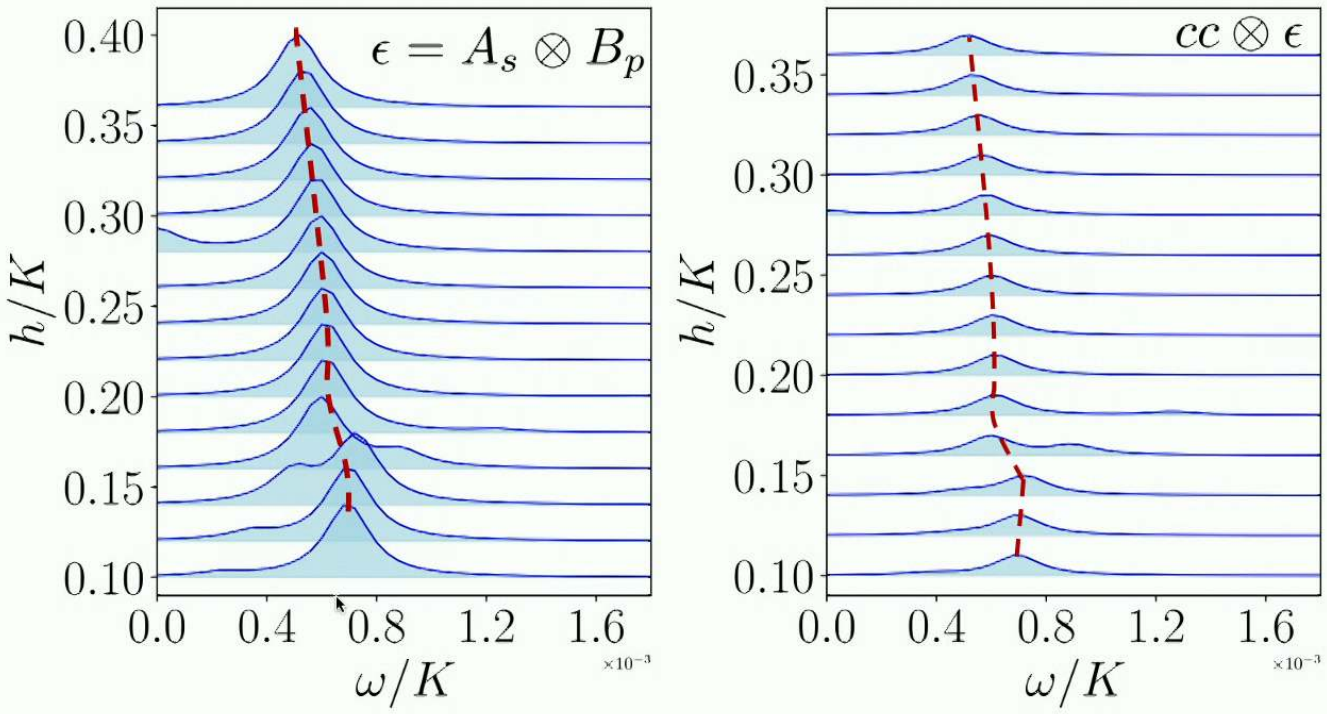
One magnon: $$S^{\alpha}(\omega) \equiv 2\pi \sum_{m\neq 0} \sum_{j} \left|\langle m|\hat{S}^{\alpha}_{j}|0\rangle\right|^2 \delta\left(\omega - (E_m - E_0)\right)$$

Two magnons: $$P^{\alpha}(\omega) \equiv 2\pi \sum_{m\neq 0} \sum_{\langle jj'\rangle} \left|\langle m|\hat{S}^{\alpha}_{j}\hat{S}^{\alpha}_{j'}|0\rangle\right|^2 \delta\left(\omega - (E_m - E_0)\right)$$

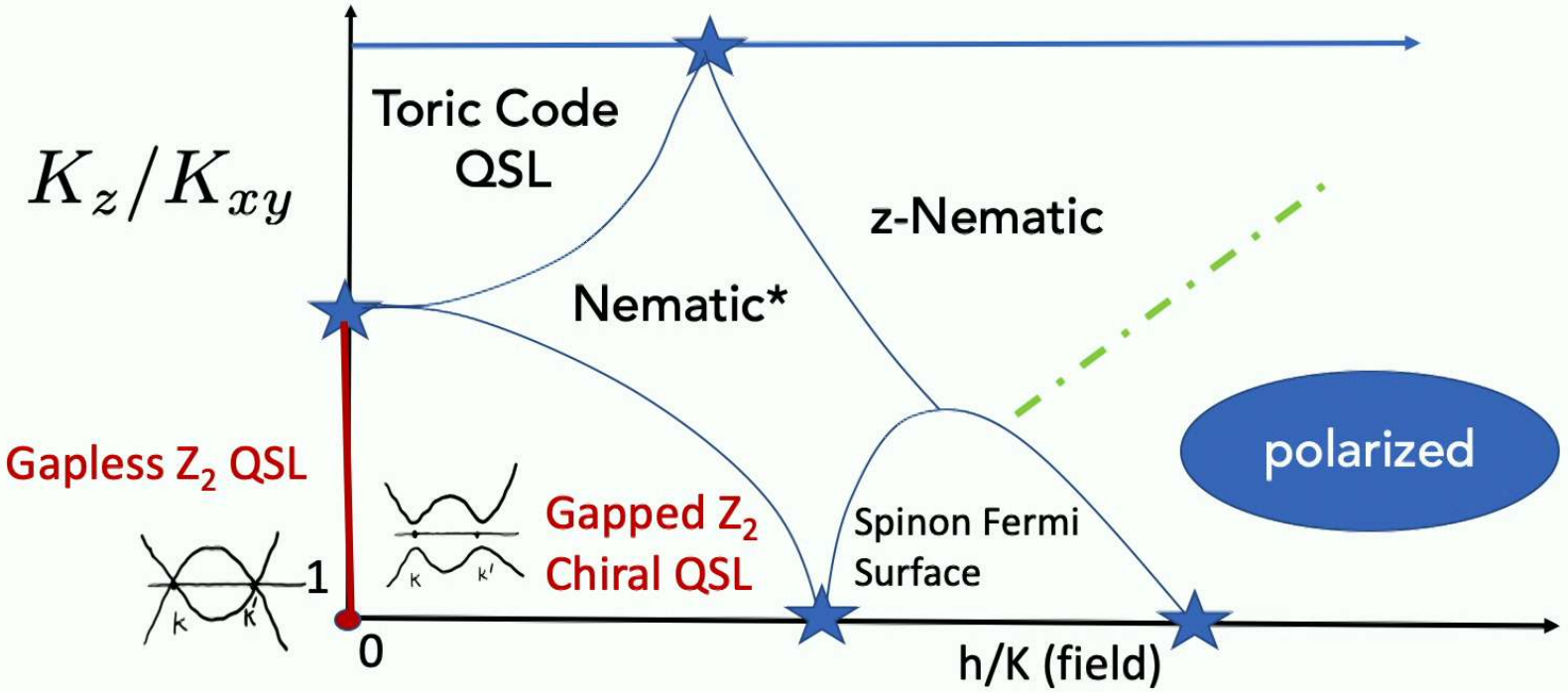
$$E_{2\text{ magnons}} = 2E_{1\text{ magnon}}$$

Gauge + Matter coupling→ bound state

$K_z = 3K$



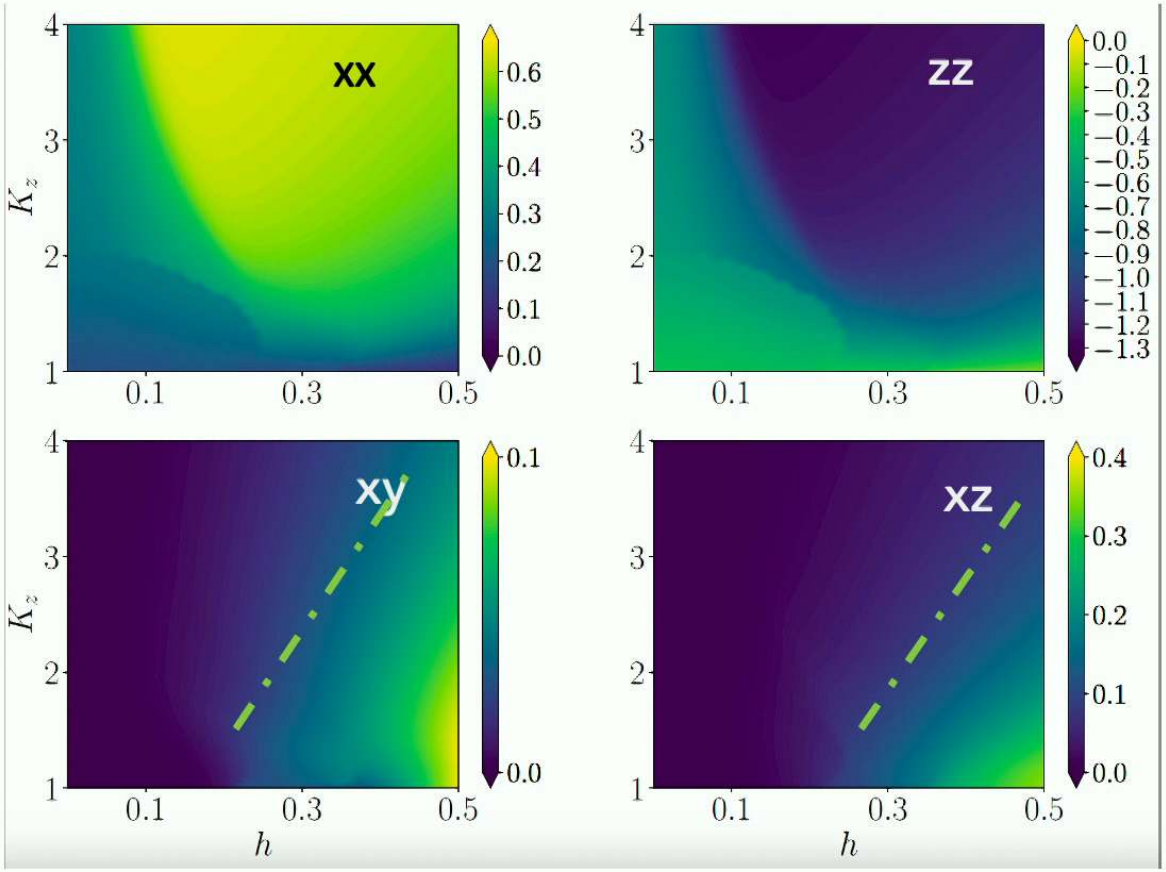
Our Main Results:



24 sites exact diagonalization
160 sites density matrix renormalization group

Perturbation theory
Mean field theory
Variational approach

Nematic Order Parameter



$$\hat{Q}^{\alpha\beta}_{pp'} = \left(\frac{\sigma^{\alpha}_{p}\sigma^{\beta}_{p'} + \sigma^{\beta}_{p}\sigma^{\alpha}_{p'}}{2} - \frac{\delta_{\alpha\beta}}{3}\boldsymbol{\sigma}_{p}.\boldsymbol{\sigma}_{p'} \right)$$

Z-nematic

$$\langle\psi|\,\hat{Q}^{\alpha\beta}_{pp'}\,|\psi\rangle = \begin{bmatrix} \frac{2}{3} & 0 & 0 \\ 0 & \frac{2}{3} & 0 \\ 0 & 0 & -\frac{4}{3} \end{bmatrix}$$

Fully polarized

$$\langle\psi|\,\hat{Q}^{\alpha\beta}_{pp'}\,|\psi\rangle = \begin{bmatrix} 0 & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & 0 \end{bmatrix}$$