

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

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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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America/Toronto timezone



Center of Emergent Materials  
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Cullen Gantenberg,  
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Subhro Bhattacharya,  
ICTS Bangalore



David  
Ronquillo



Adu Vengal



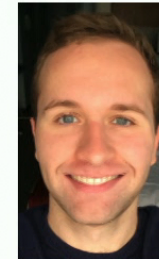
Ian Osborne.



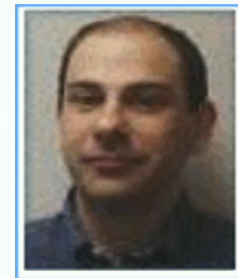
Nirav Patel



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

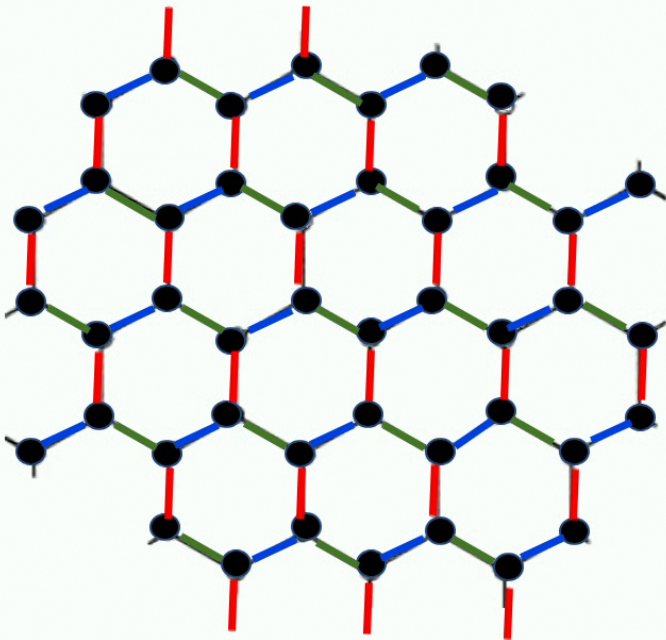
Y. Motome and J. Nasu,  
J. Phys. Soc. Jpn. 89, 012002 (2020)

# Kitaev Model: bond-dependent interactions



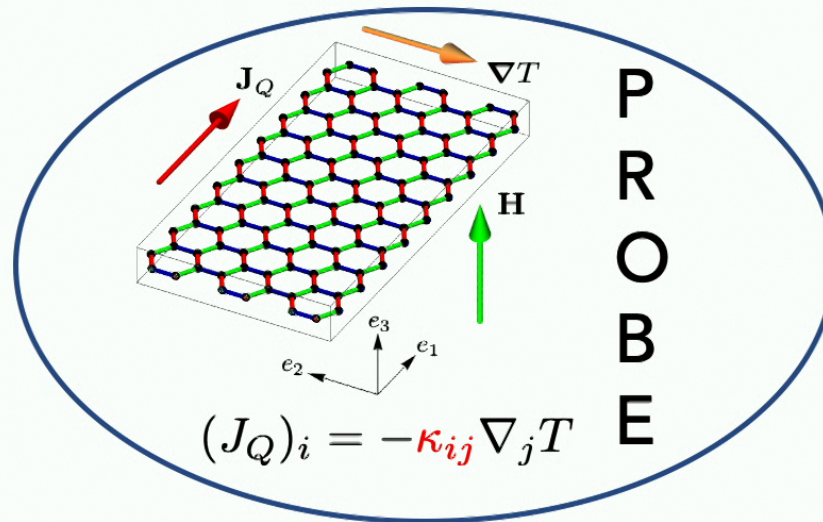
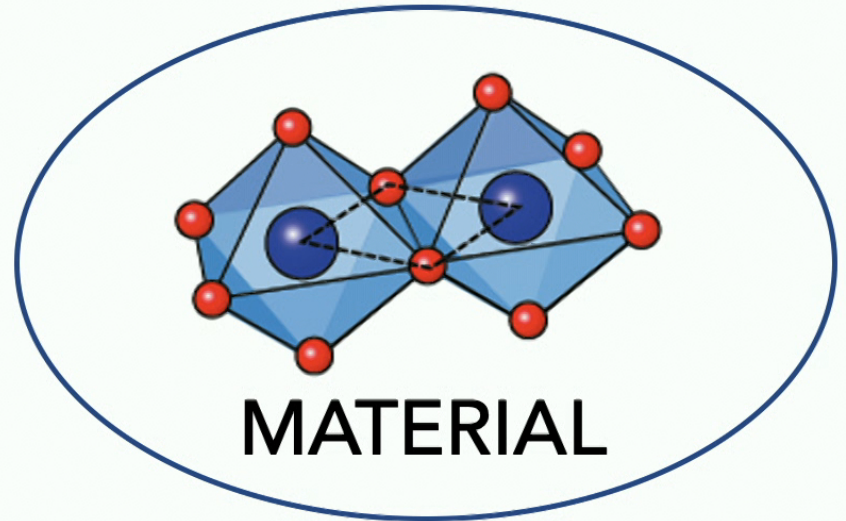
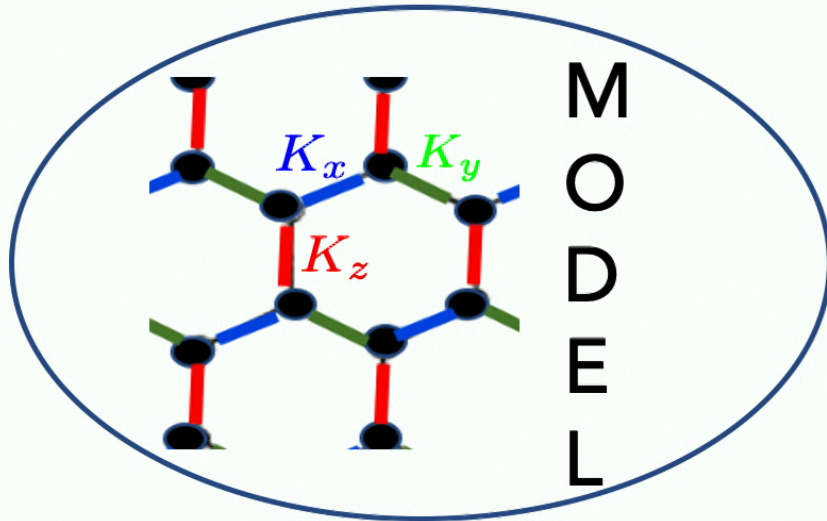
A. Kitaev, Annals of  
Physics 321, 2-111  
(2006)

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



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



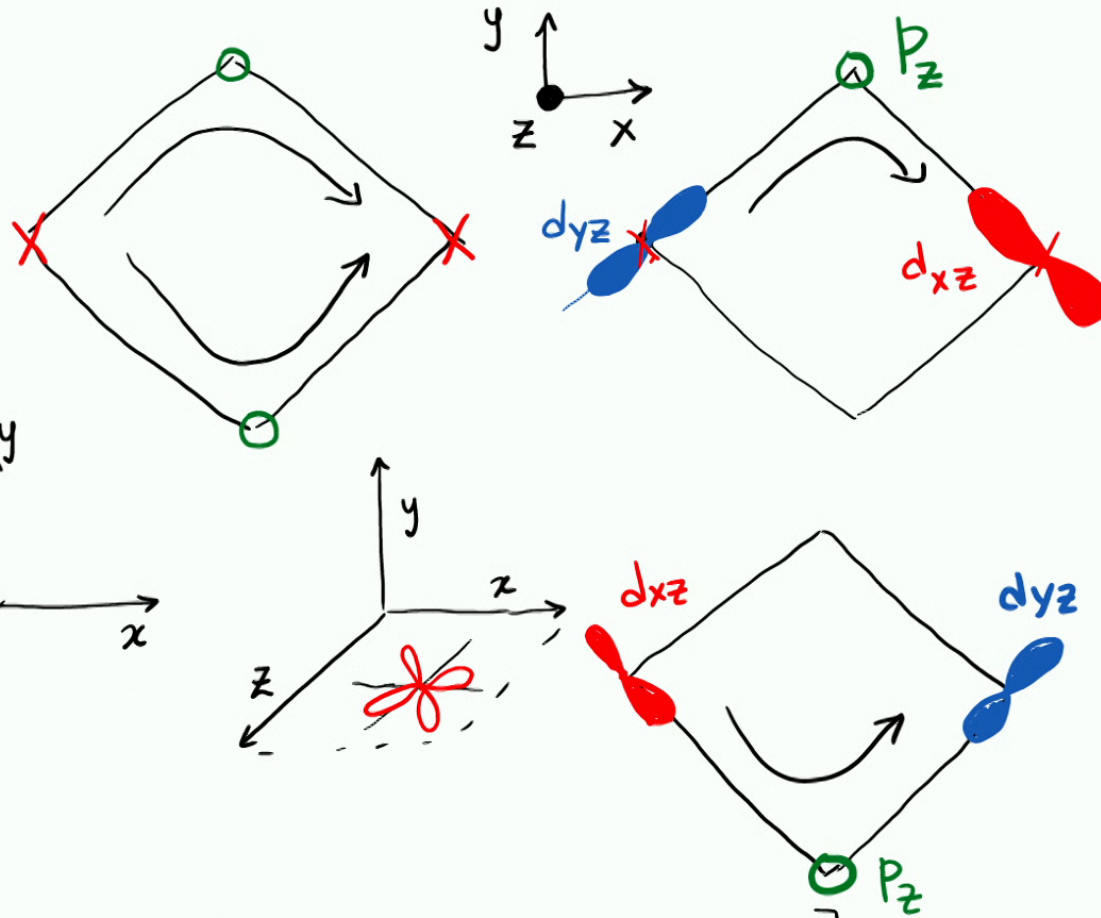


$$(J_Q)_i = -\kappa_{ij} \nabla_j T$$





Jackeli and Khaliullin,  
PRL 102, 017205 (2009)



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

$d_{xz} \rightarrow d_{yz}$

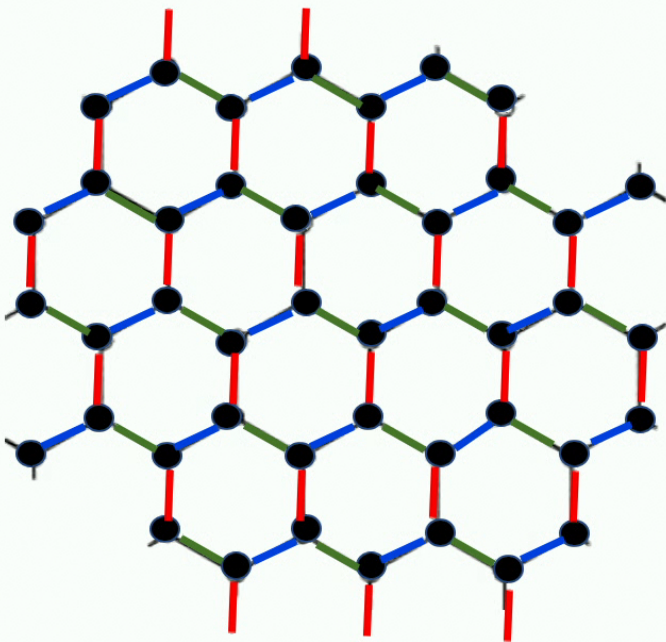
$$|j_z = +\frac{1}{2}\rangle = \frac{1}{\sqrt{3}} \left[ |d_{xy}\uparrow\rangle + |d_{yz}\downarrow\rangle + i |d_{xz}\downarrow\rangle \right]$$

# Kitaev Model: bond-dependent interactions



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

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



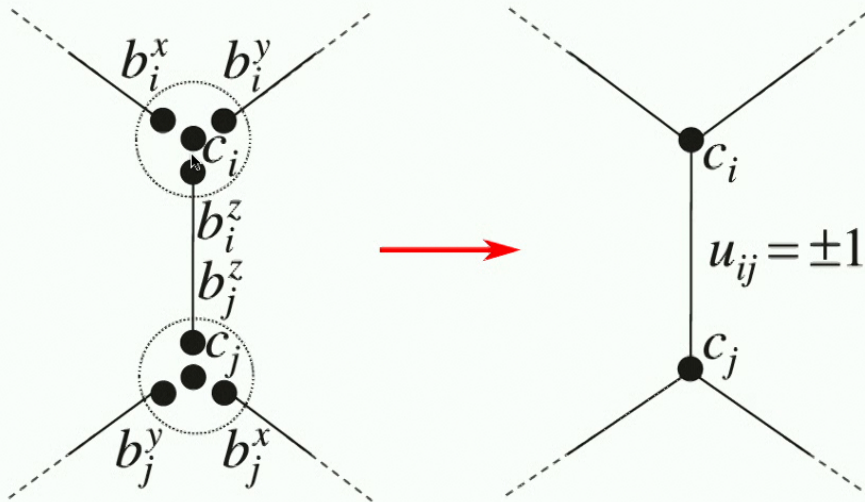
Parton construction:

$$\sigma^d = i b^d c$$

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



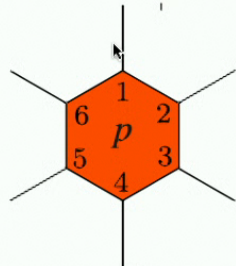
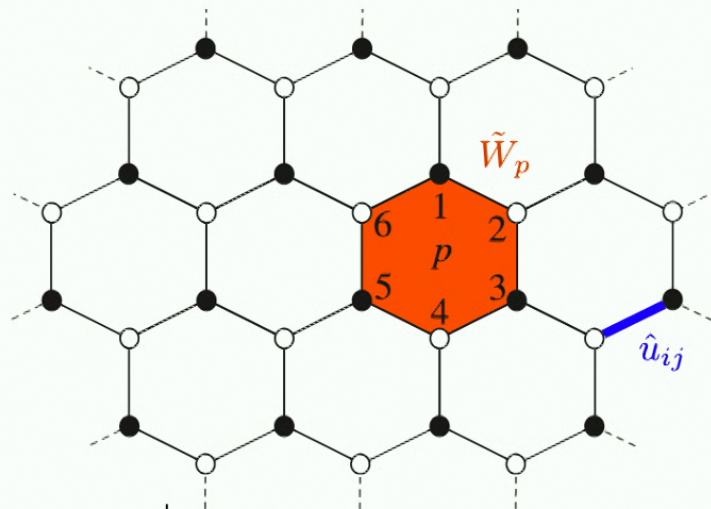
## Link Operators (vector potential) and Plaquette operators (flux)



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

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

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



$\alpha$  - link

$$\tilde{W}_p = \tilde{\sigma}_1^x \tilde{\sigma}_2^y \tilde{\sigma}_3^z \tilde{\sigma}_4^x \tilde{\sigma}_5^y \tilde{\sigma}_6^z$$

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

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

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

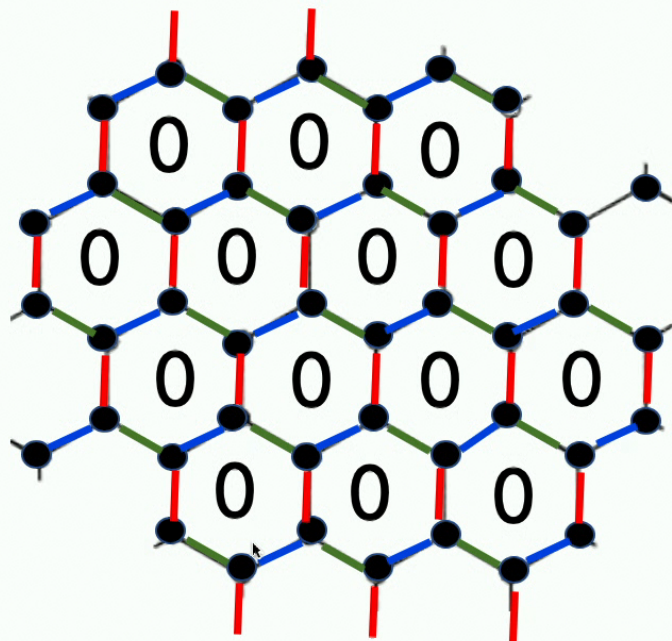


Extensive # of conserved quantities  
 $\{W_p\}$  and  $\{u_{ij}\}$



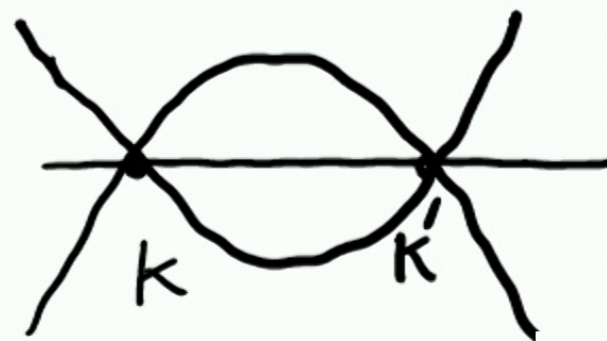


# Ground State:

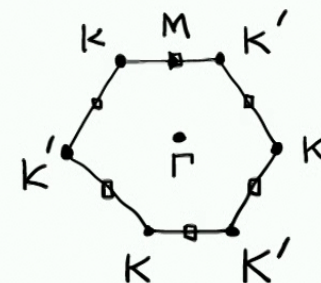


All plaquettes have zero flux

c-Majoranas

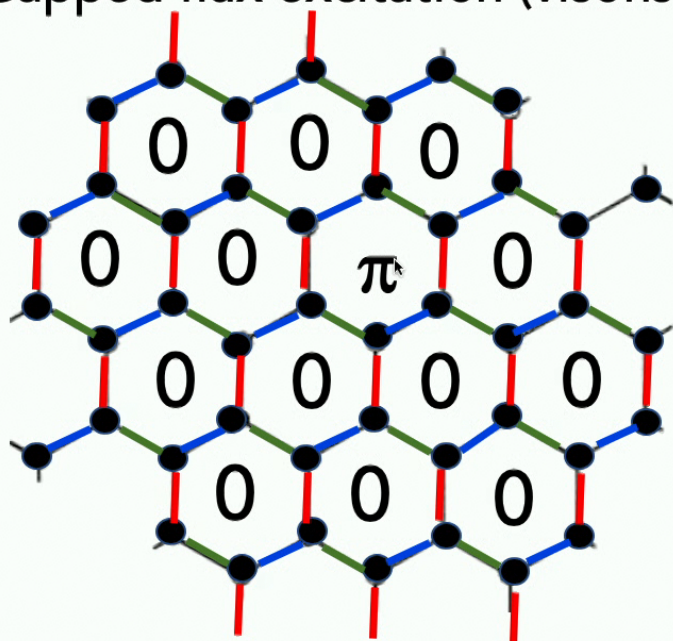


c-majorana fermions  
have a Dirac dispersion

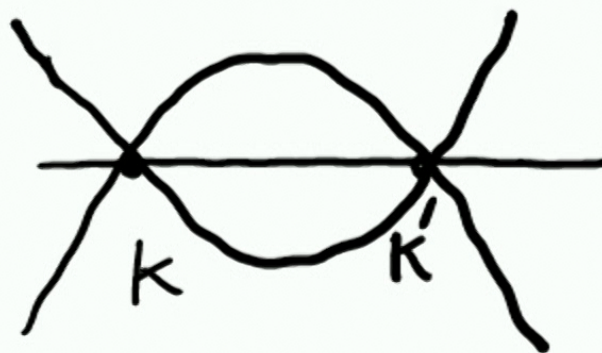


# Excitations:

(1) Gapped flux excitation (visons)



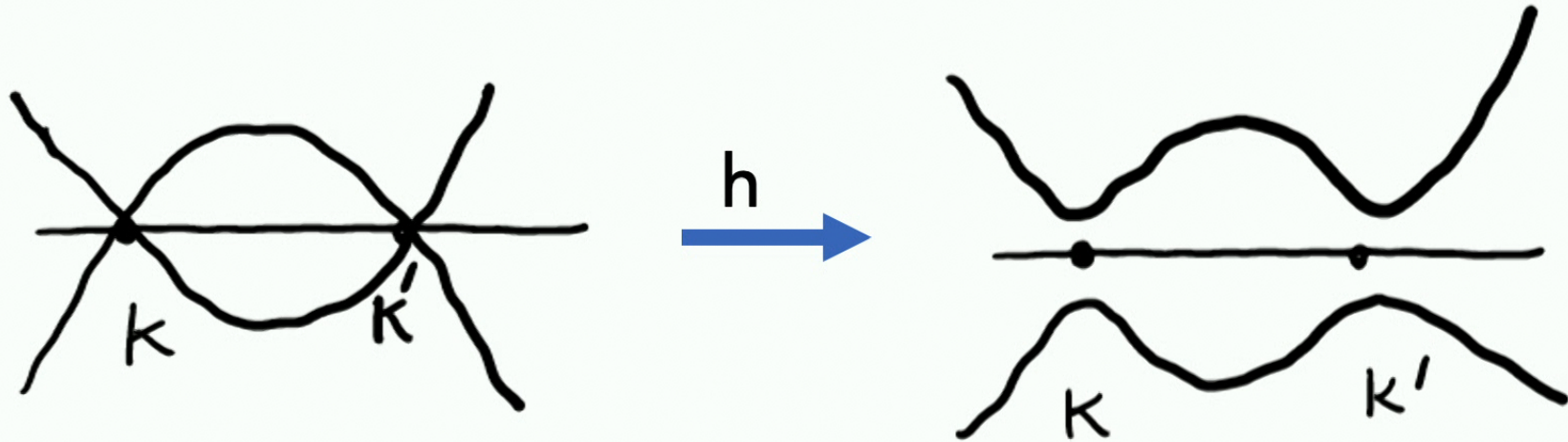
(2) Gapless majorana fermions



## Gapless $Z_2$ Quantum Spin Liquid

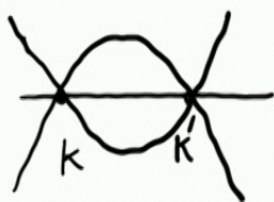


# Non-abelian $Z_2$ gapped chiral spin liquid:

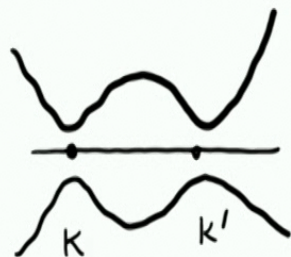


- Majorana fermions get gapped
- Chern insulator
- Chiral edge mode with thermal Hall conductance  $\kappa_{xy}/T = (1/2) (\pi/6) (k_B^2/\hbar)$

# Known results (Kitaev):

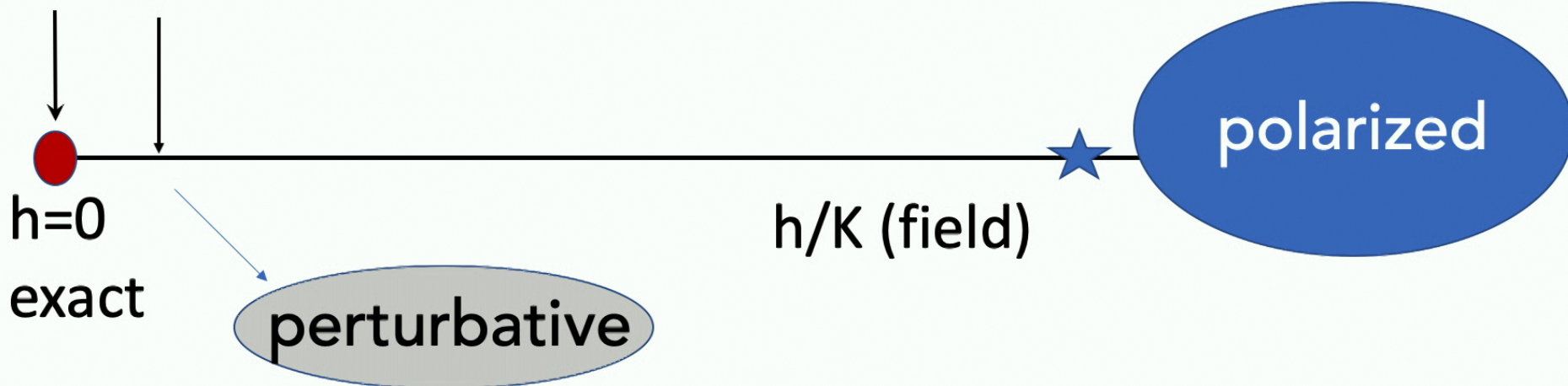


Gapless  $Z_2$  QSL



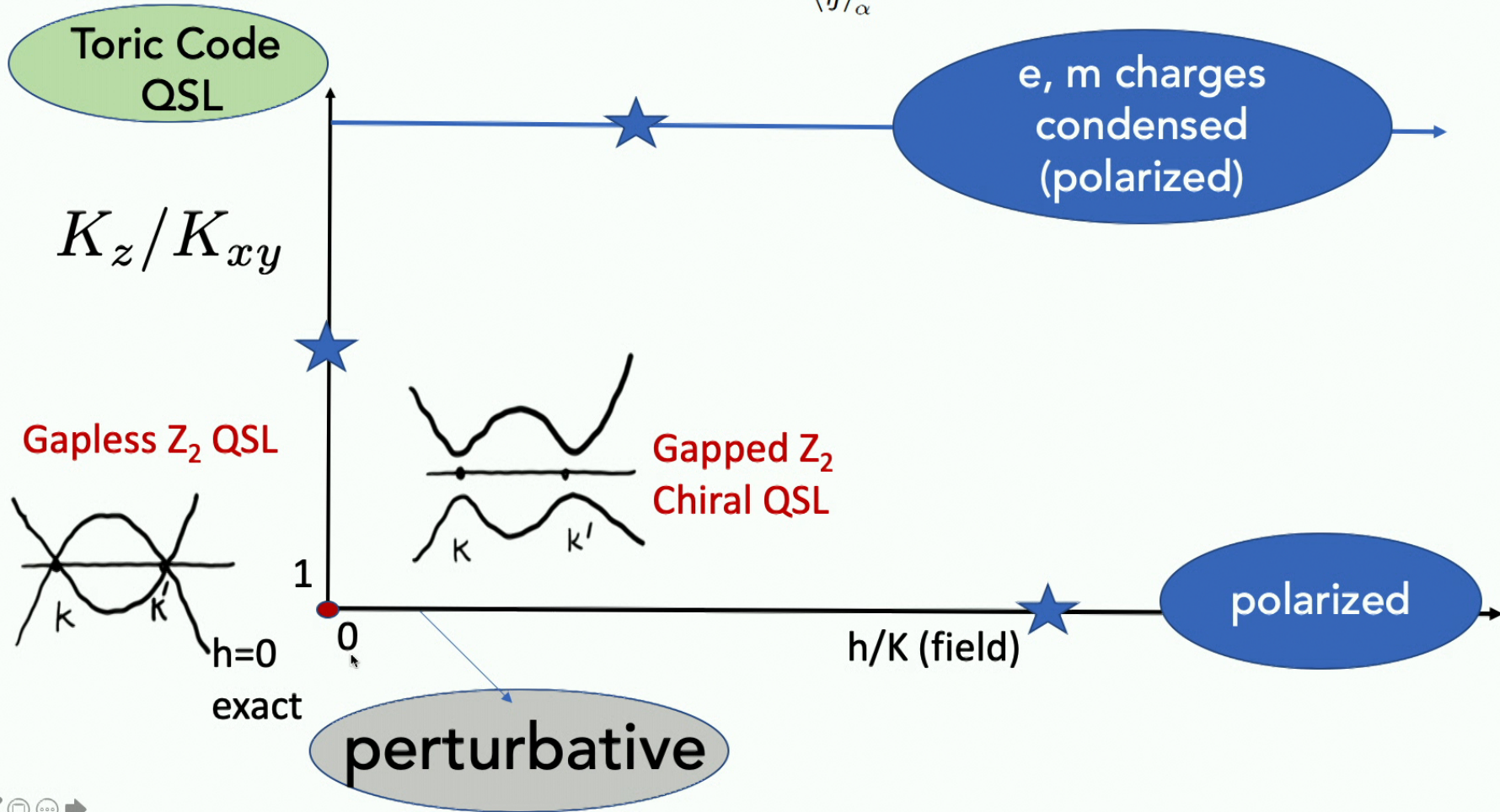
Gapped  $Z_2$  Chiral QSL

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

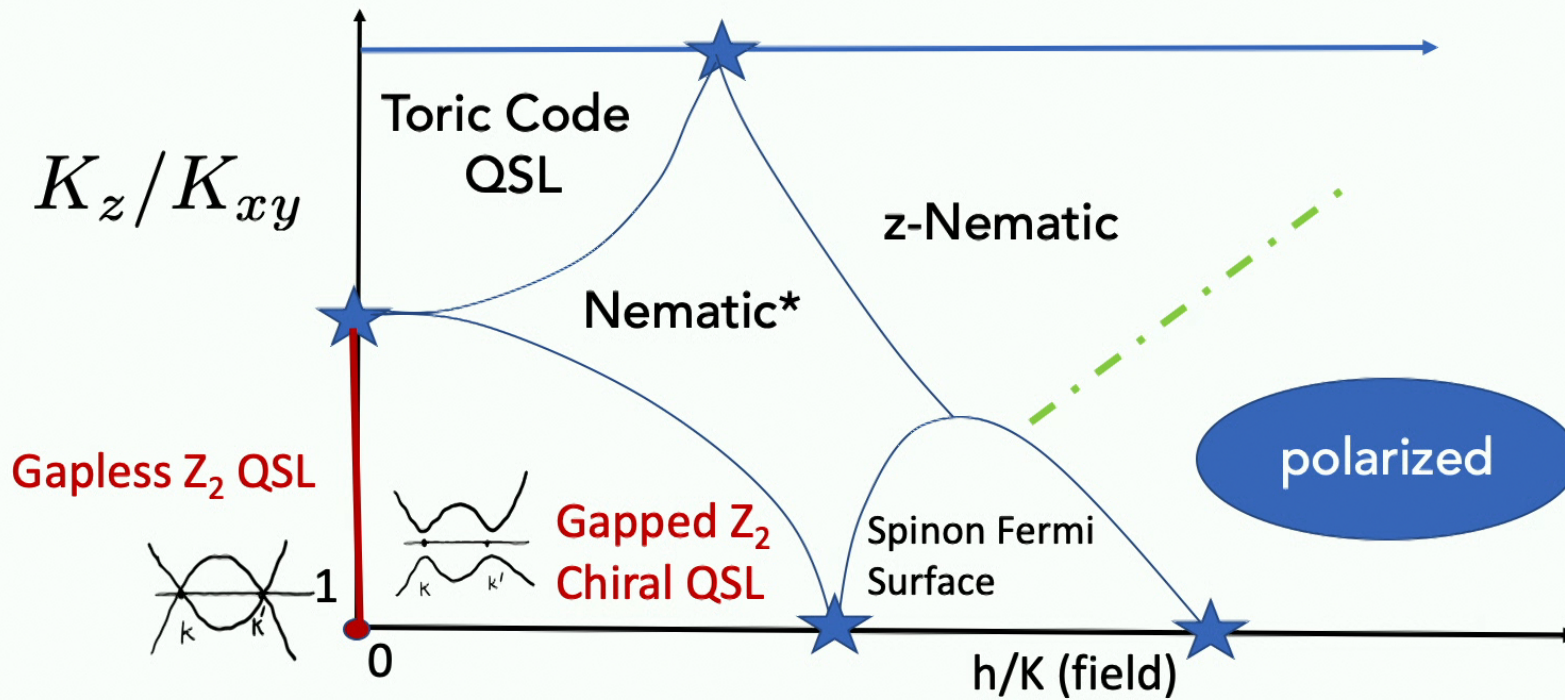




# Known results (Kitaev): $H = \sum_{\langle ij \rangle_\alpha} K_\alpha \sigma_i^\alpha \sigma_j^\alpha$



# Our Main Results:

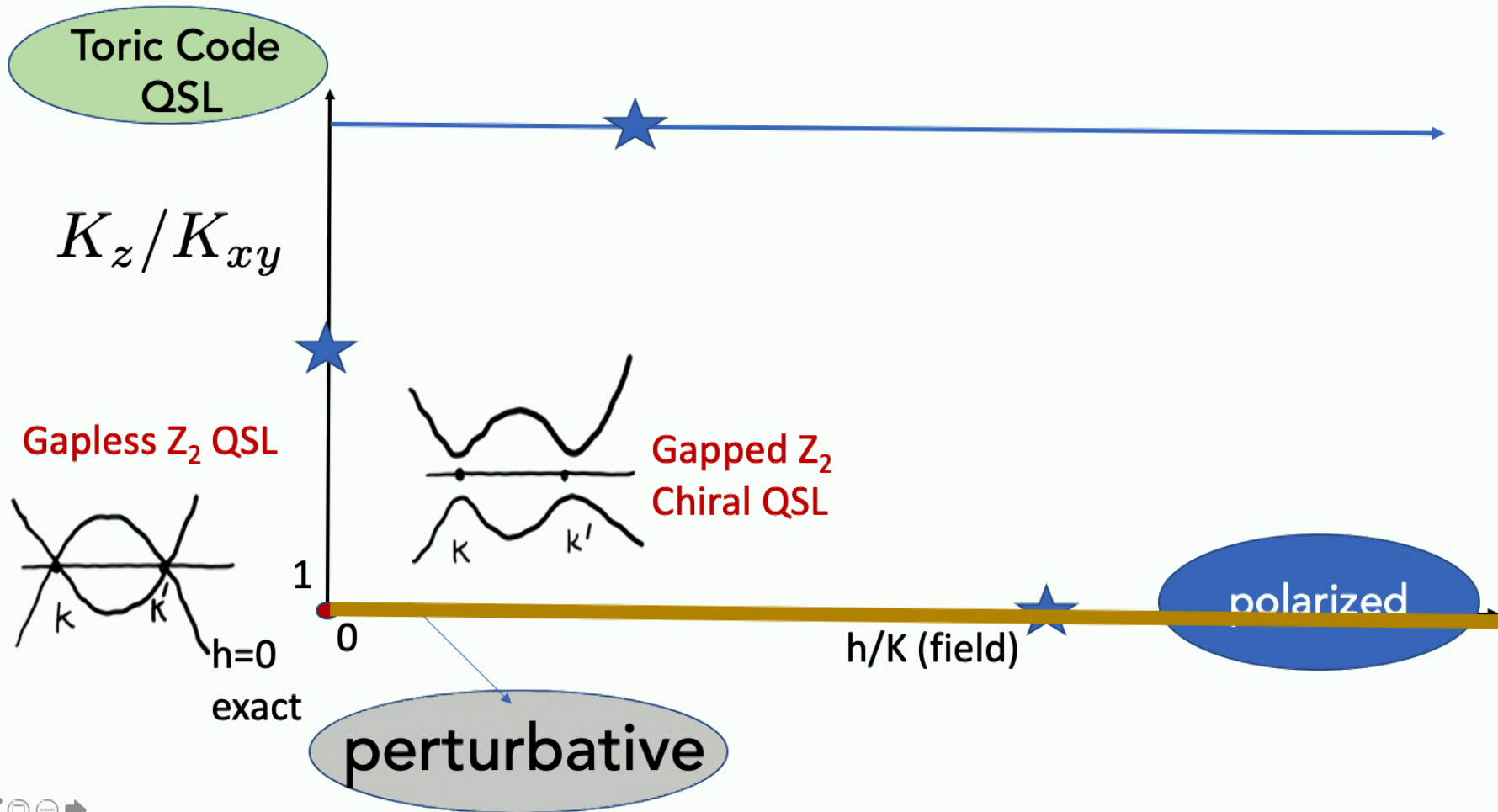


24 sites exact diagonalization  
 160 sites density matrix renormalization group

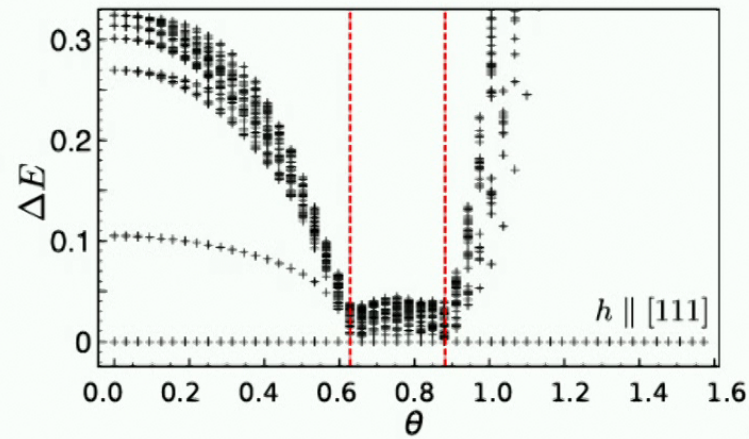
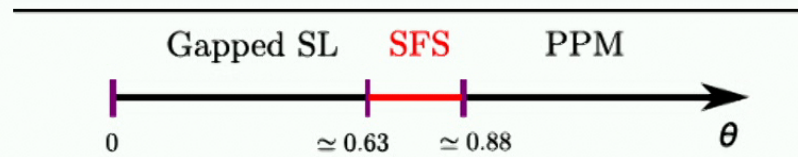
Perturbation theory  
 Mean field theory  
 Variational approach



# Phases at the Isotropic point as a function of field



$$h \parallel [111]$$

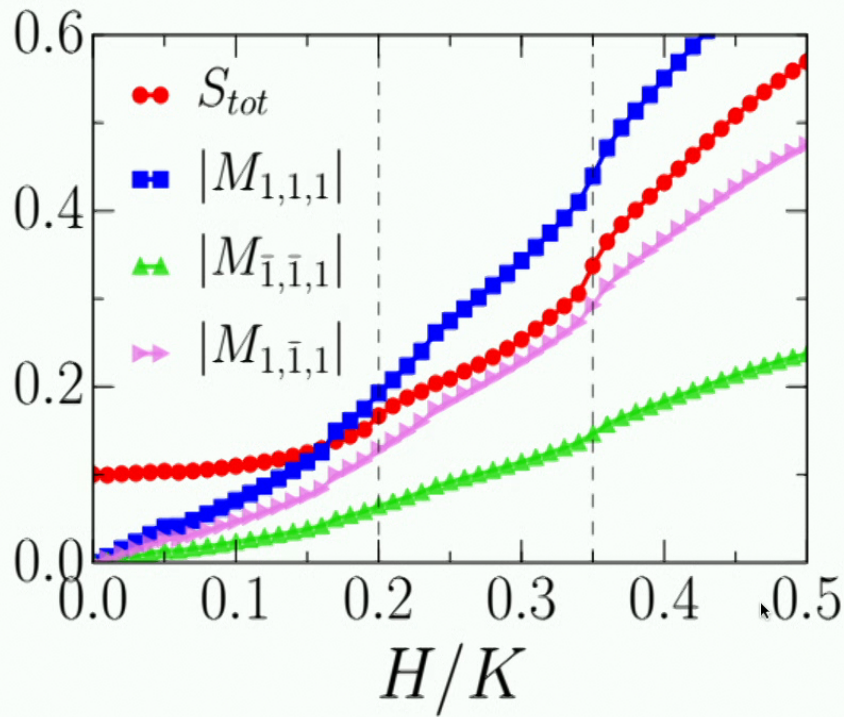


$$\theta \approx h/K$$

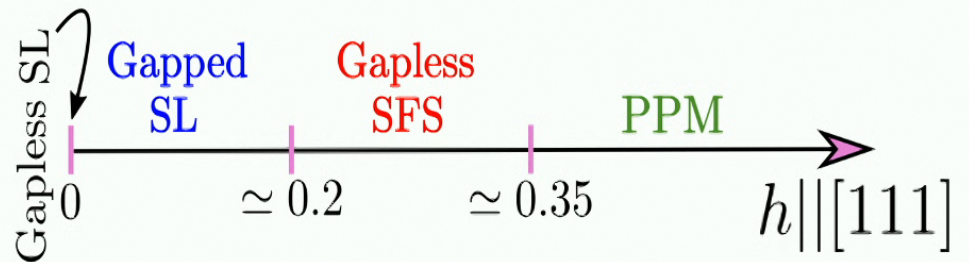
Exact diagonalization  
24 sites



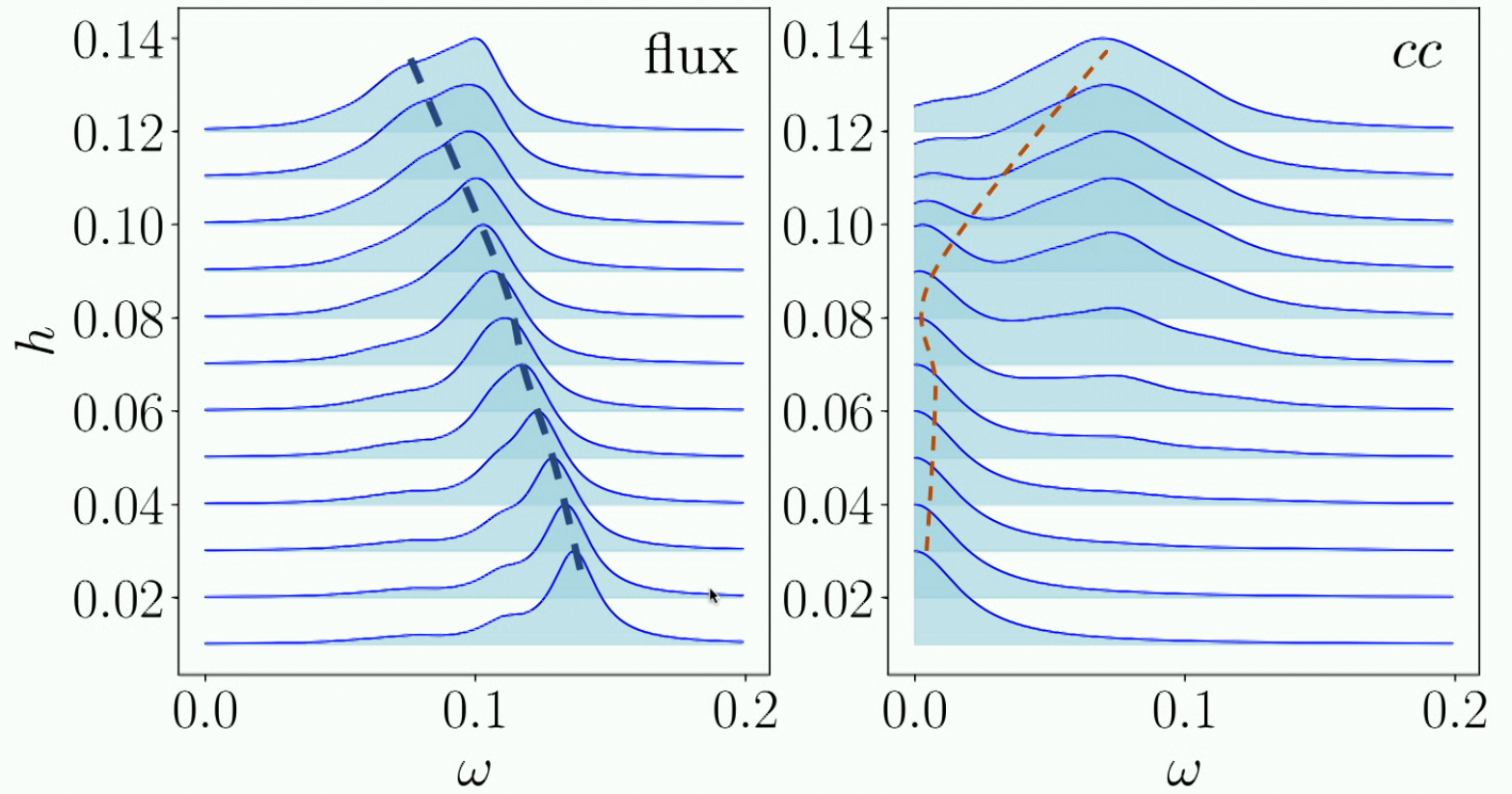
# Kitaev Model + Magnetic field: $h||[111]$ magnetization



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



Density Matrix Renormalization Group calculations with 160 spins

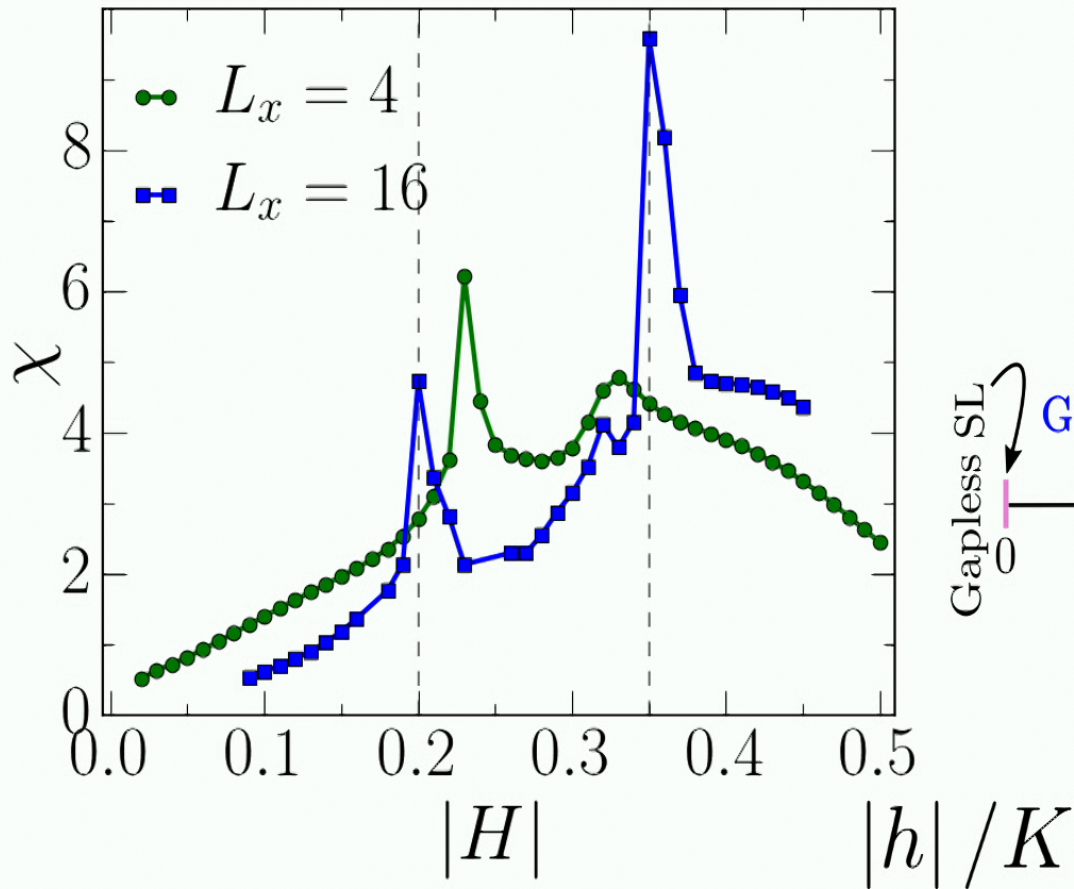




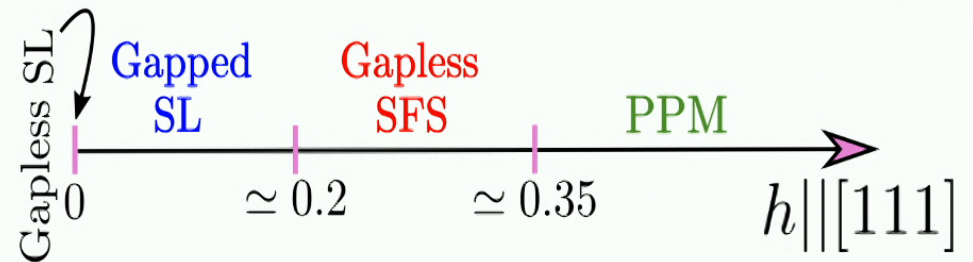
# Kitaev Model + Magnetic field

## Evidence for Two Transitions

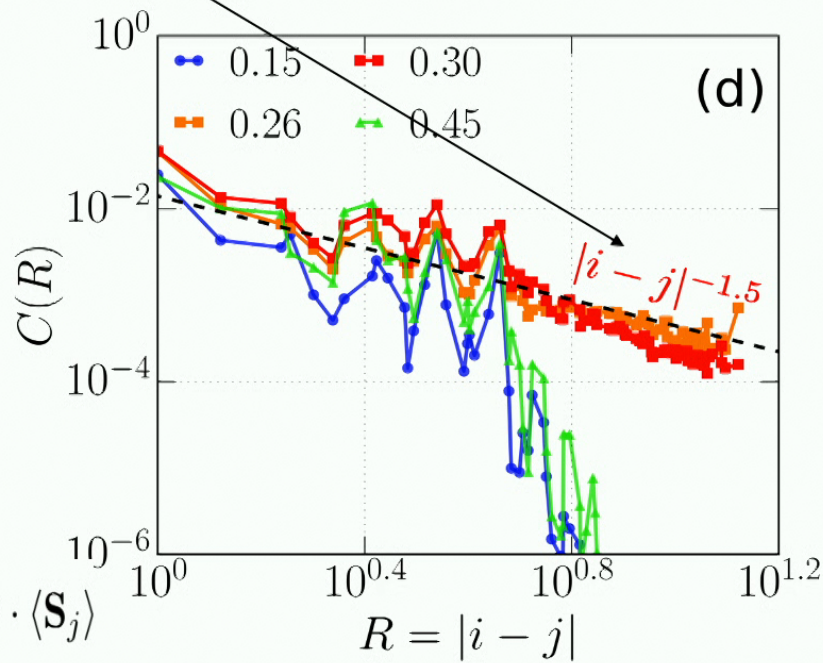
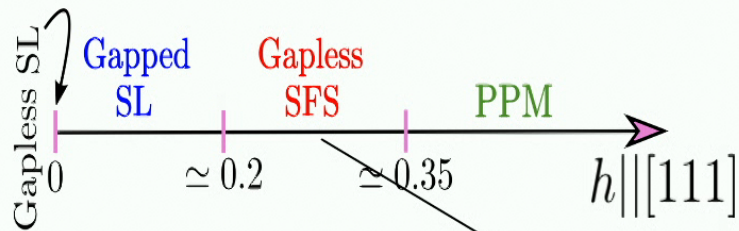
$h \parallel [111]$



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



# 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

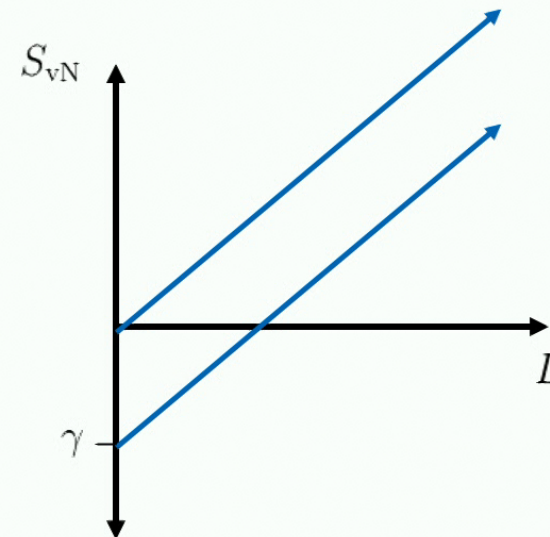
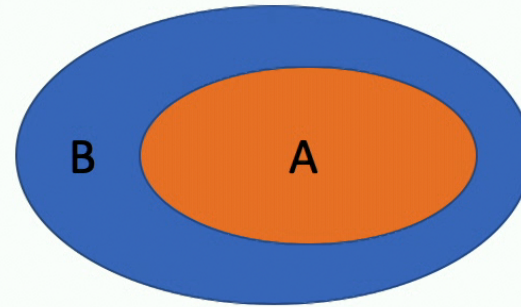
$$S_{\text{vN}} = \text{Tr}(\rho_A \log_2 \rho_A)$$

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

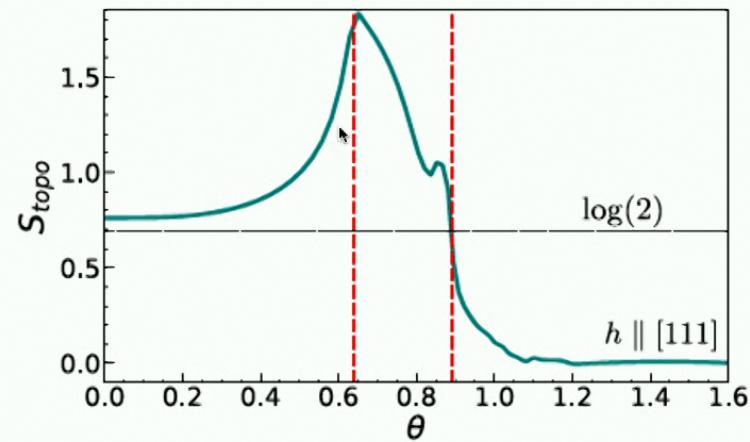
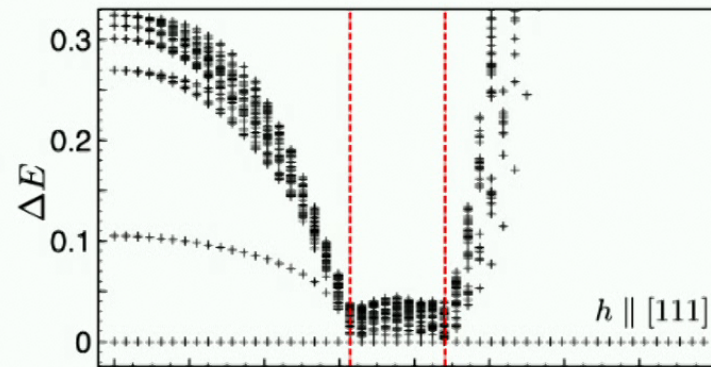
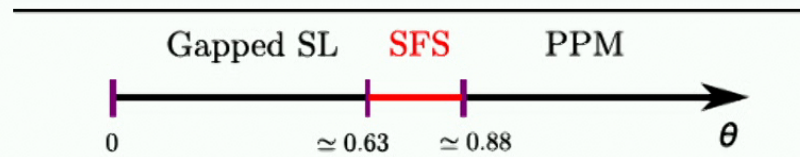
$$S_{\text{vN}} = \alpha L \underbrace{-\gamma}_{\text{topo}} + \mathcal{O}(1/L)$$

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

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



$$h \parallel [111]$$



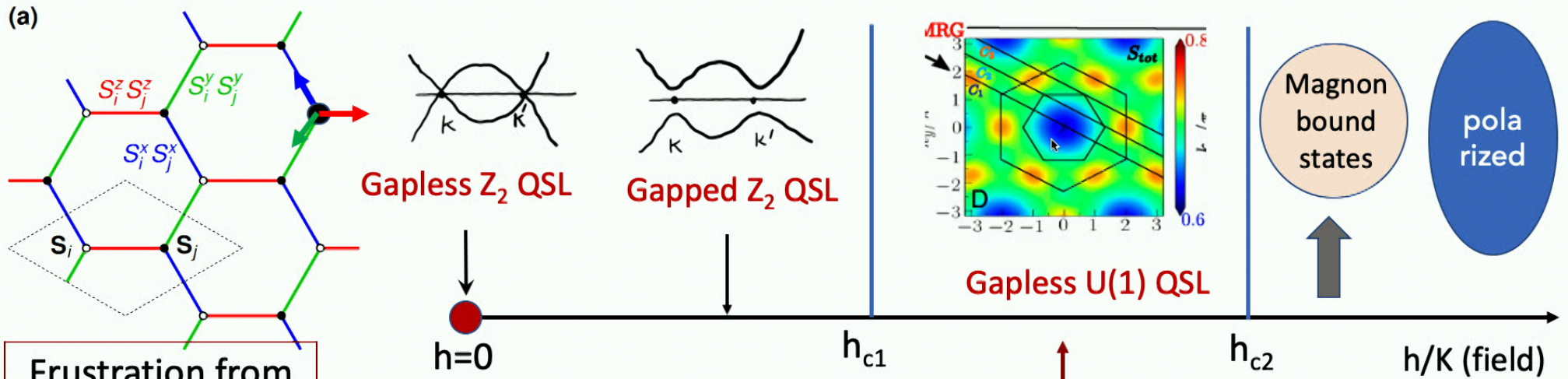
Exact diagonalization  
24 sites

$$\theta \approx h/K$$





# Predictions for Kitaev magnets in a field



Frustration from bond-dependent interactions

Kitaev (2006)

Jackeli, Khaliullin (2009)

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

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

Fermi surface of neutral, gapless spinons in an insulator!

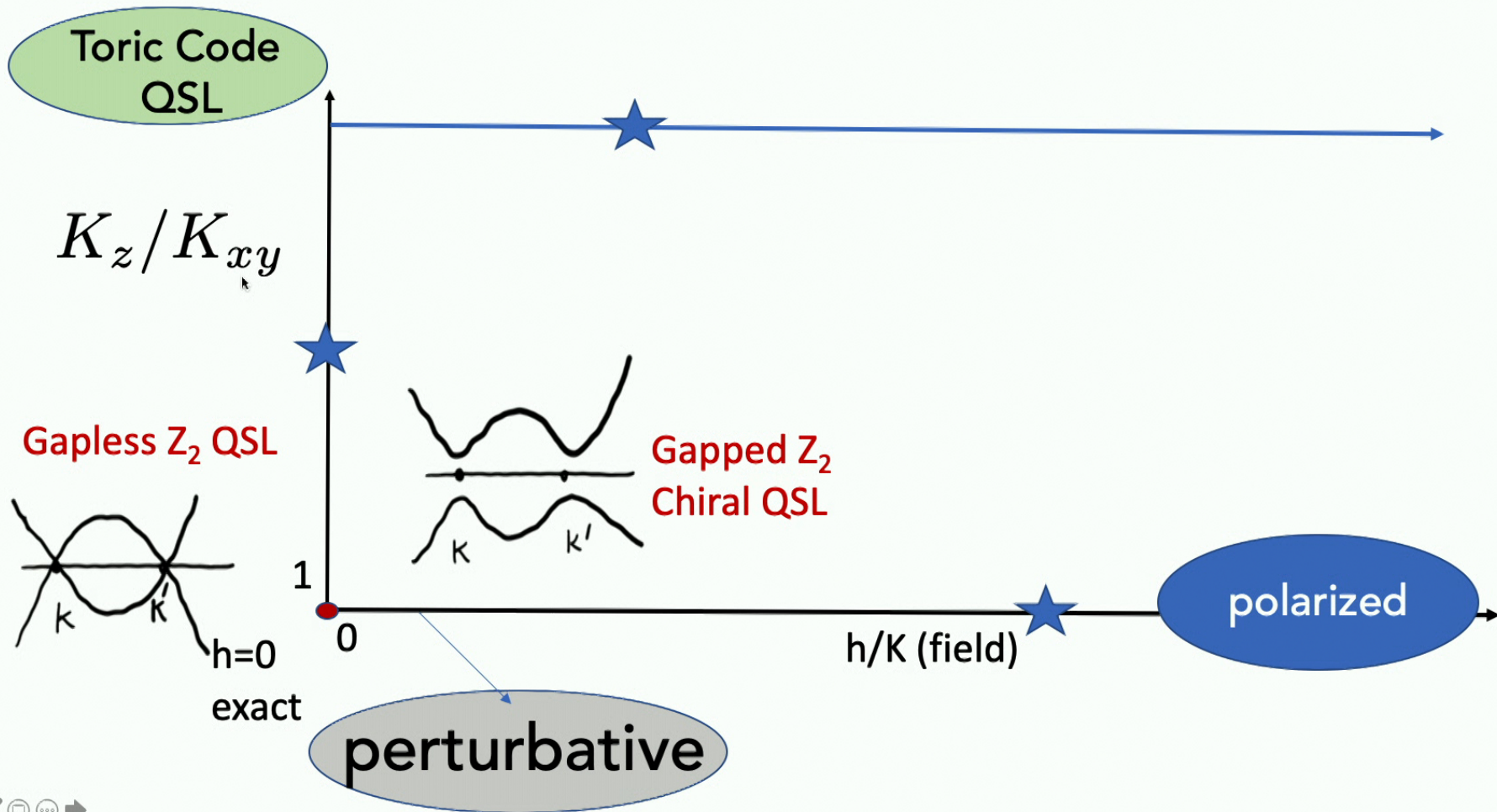
$$\kappa_{xx} \sim T$$

Chiral spinon edge mode  $\rightarrow$  Quantized thermal Hall conductance

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



# Phases at as a function of bond anisotropy





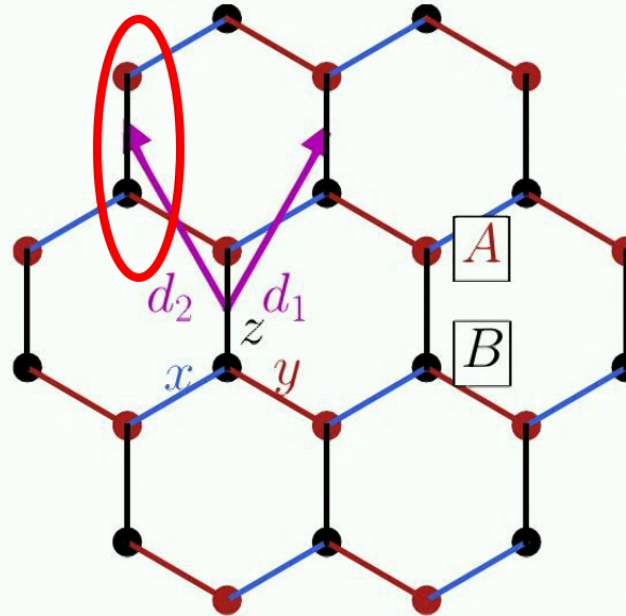
# Large Anisotropy $\rightarrow$ Toric Code

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

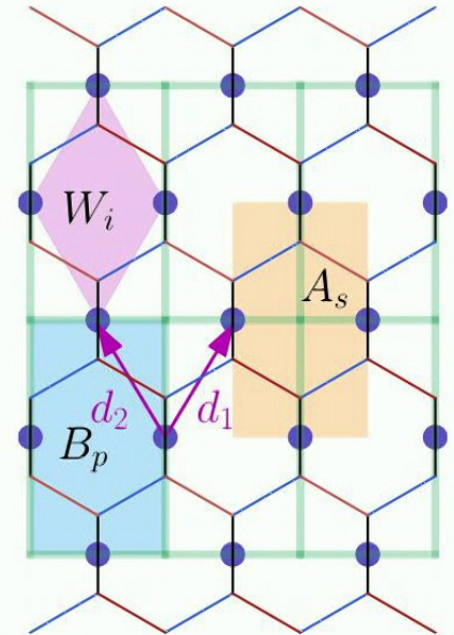
Low energy manifold  
(AF exchange)

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):

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

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

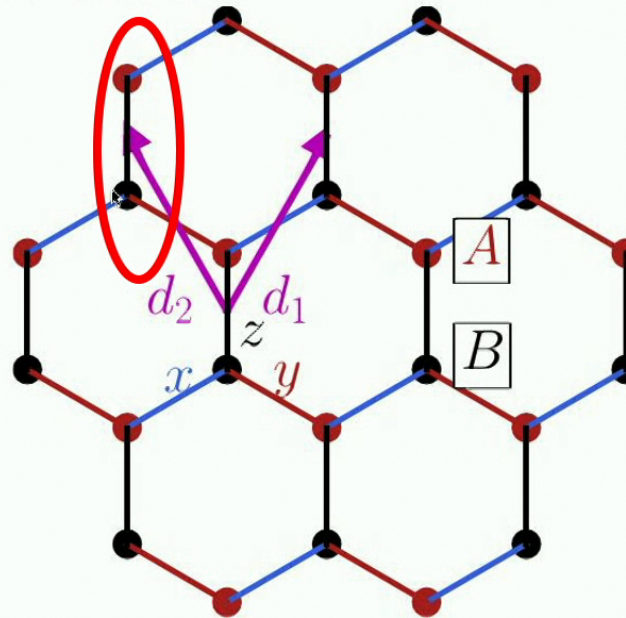
# Large Anisotropy $\rightarrow$ Toric Code

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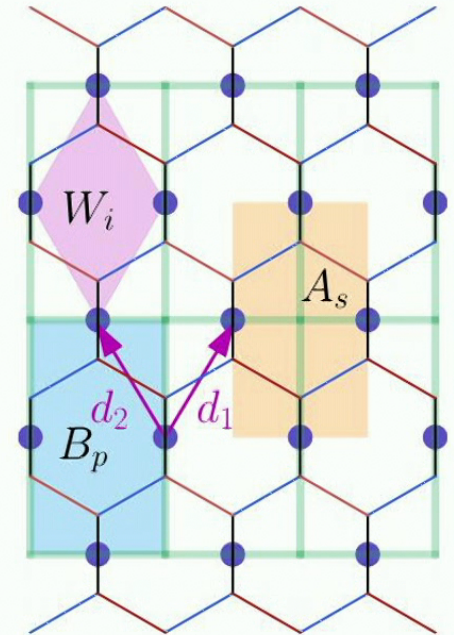
Low energy manifold  
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(b)

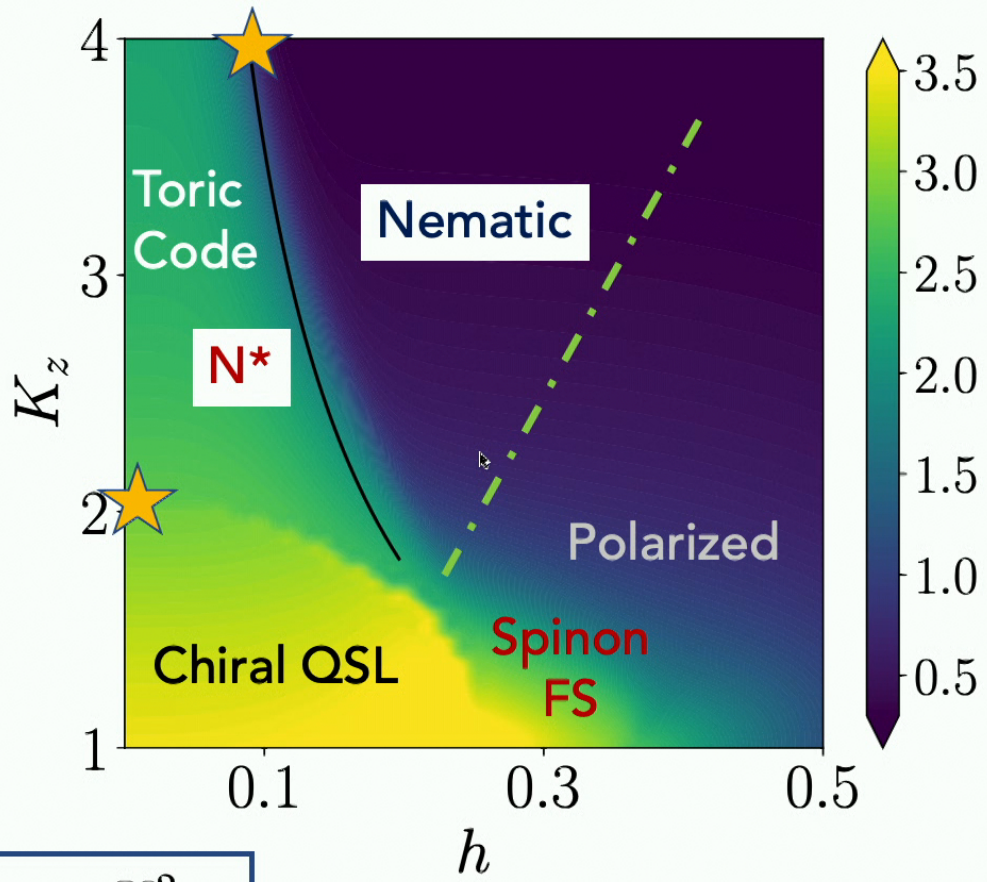
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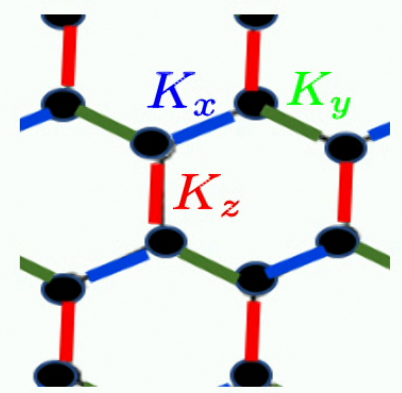




**Bipartite Entanglement Entropy**

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

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

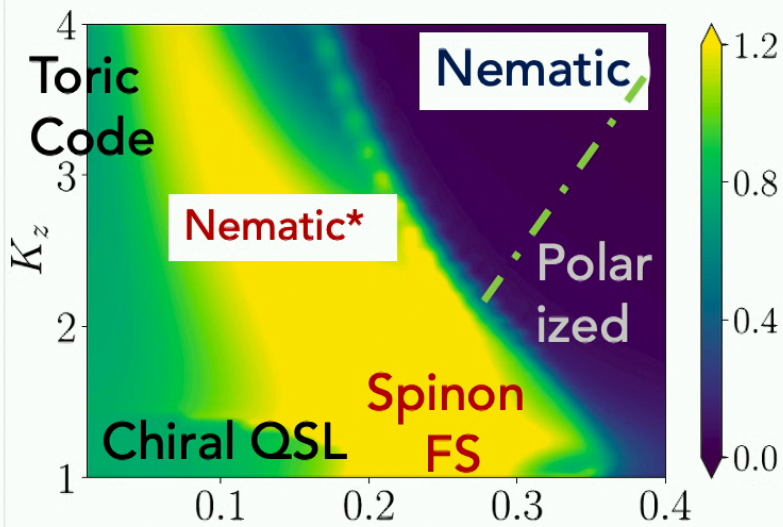


$$K_x = K_y = K$$

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

Analytic result:

K: AF  
h perpendicular to honeycomb plane

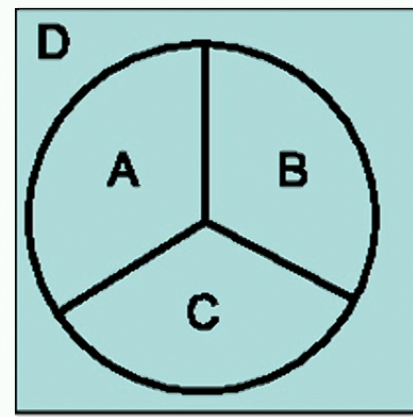
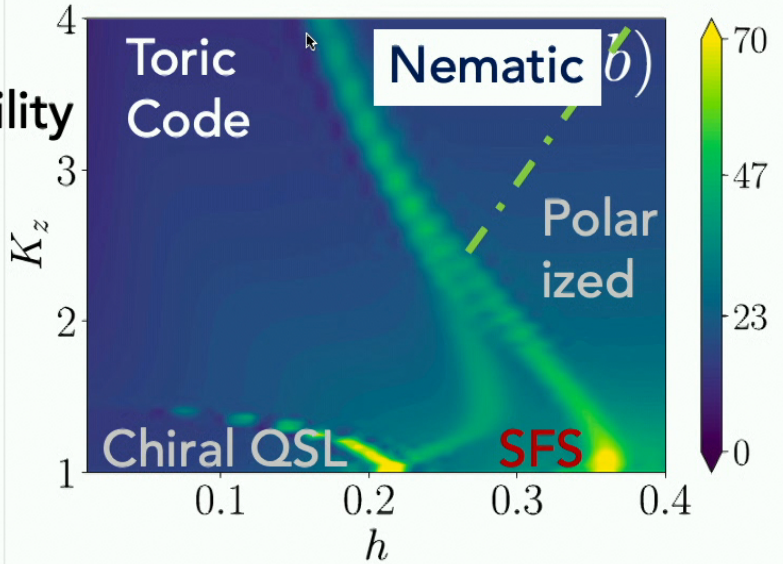


$\gamma$

Topological Entanglement Entropy

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

Magnetic Susceptibility



Kitaev-Preskill construction

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



## Gapped non abelian Chiral QSL

Vacuum  $1 \sim d_1 \stackrel{!}{=} 1$

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

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

} abelian

} 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  $\sigma_i^\alpha = ib_i^\alpha c_i$ :

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

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

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

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

It gives additive von-Neumann entropies:

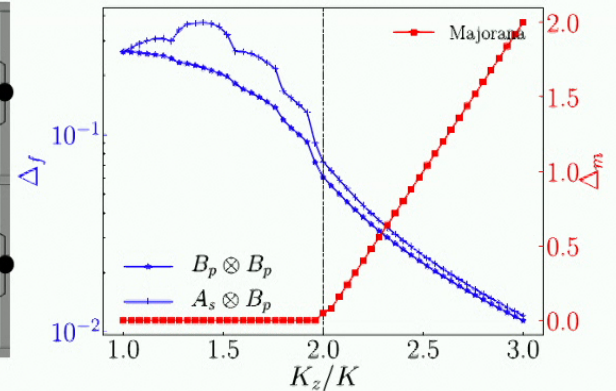
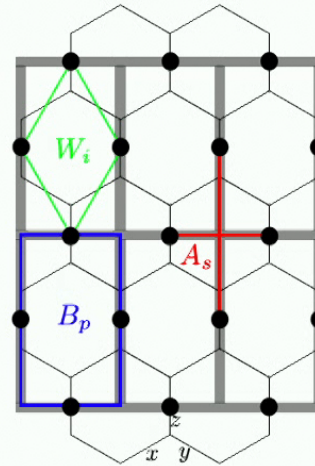
$$S = S_G + S_M$$

$$S_M \sim \alpha L, S_G \sim L \log 2 - \log 2$$

Excitations:

$|M_G\rangle$  : Free majorana particles

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

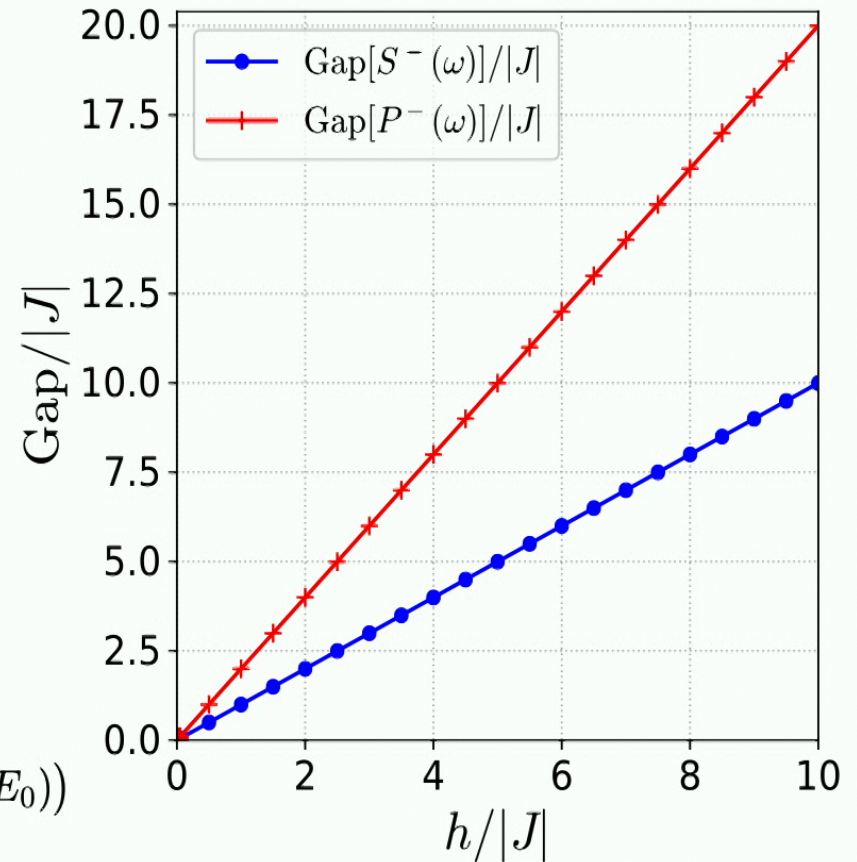
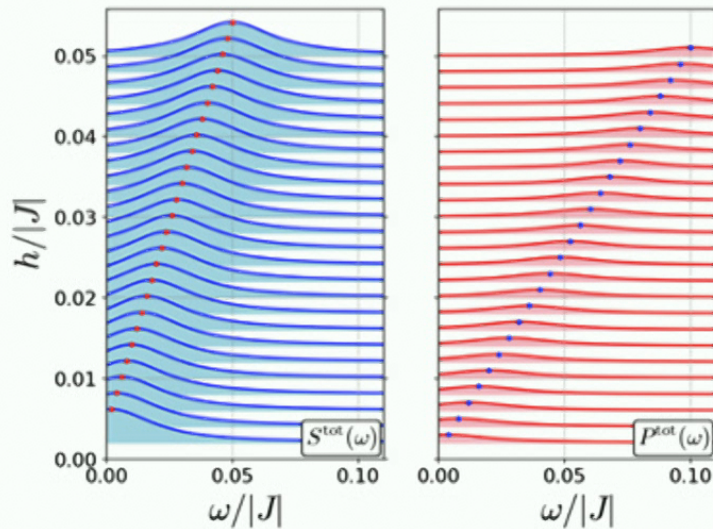




# One- and Two-Magnon DOS Gaps

Heisenberg

Ferromagnet

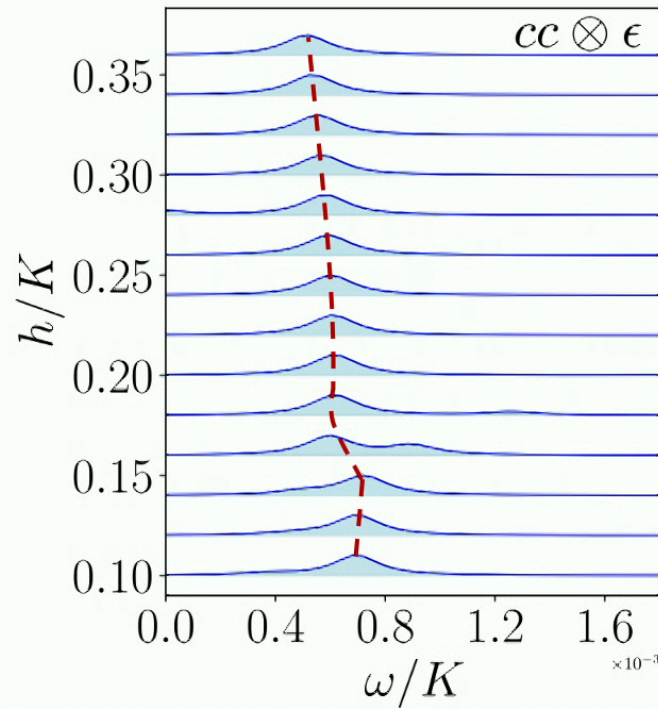
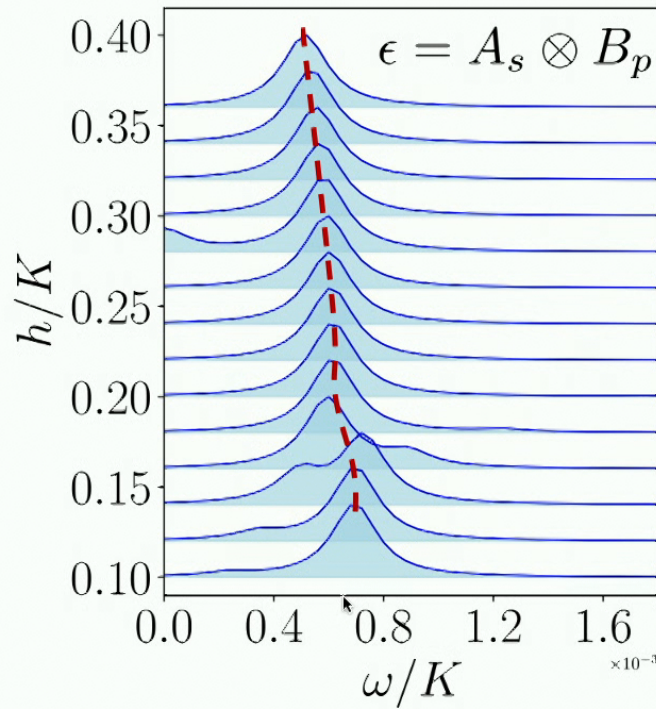


One magnon: 
$$S^\alpha(\omega) \equiv 2\pi \sum_{m \neq 0} \sum_j |\langle m | \hat{S}_j^\alpha | 0 \rangle|^2 \delta(\omega - (E_m - E_0))$$

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

$E_2$  magnons =  $2E_1$  magnon

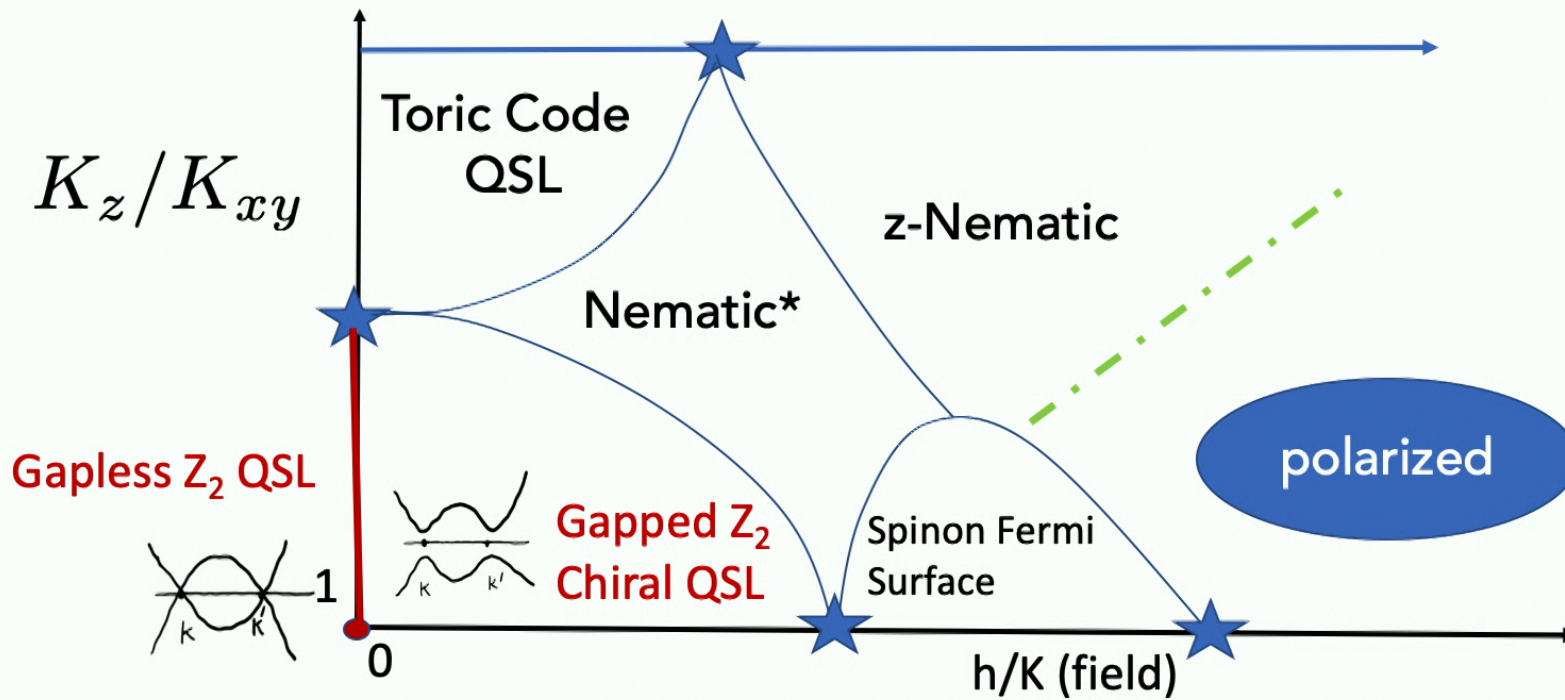
# Gauge + Matter coupling $\rightarrow$ bound state



$$K_z = 3K$$



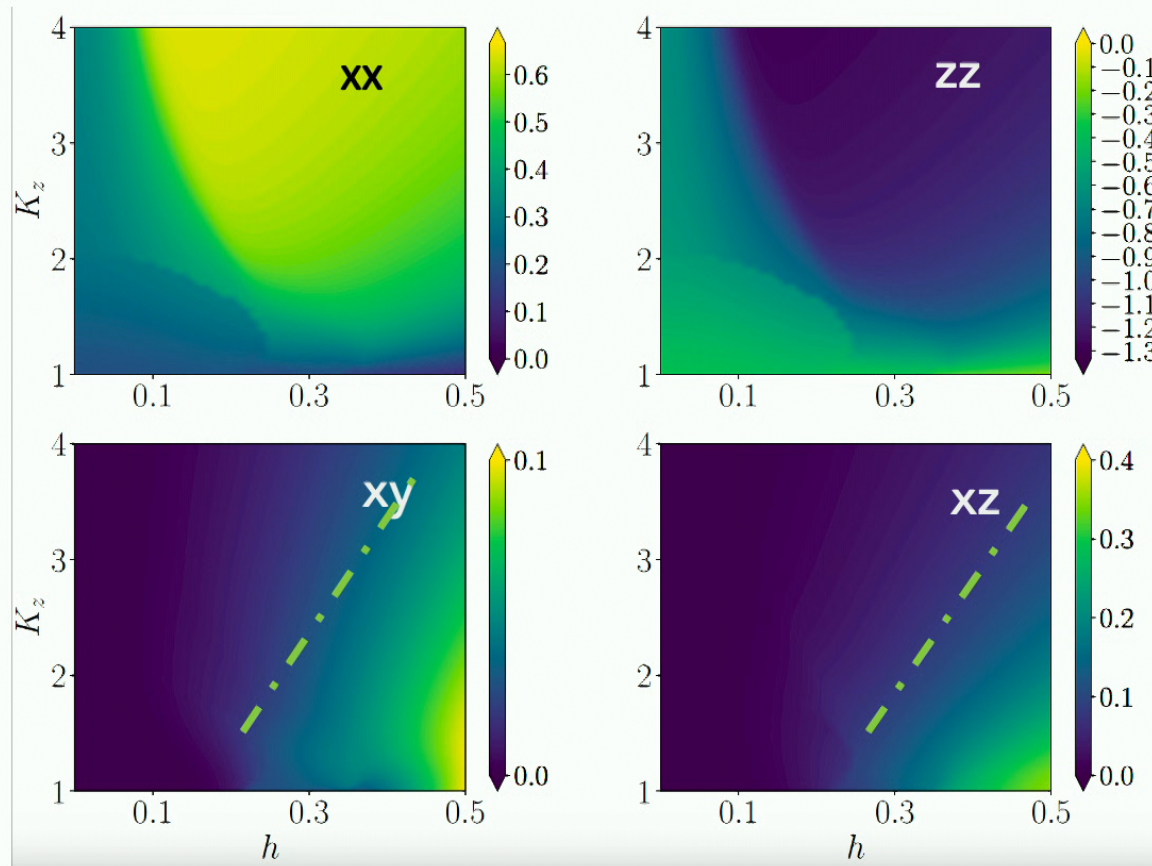
# Our Main Results:



24 sites exact diagonalization  
 160 sites density matrix renormalization group

Perturbation theory  
 Mean field theory  
 Variational approach

# Nematic Order Parameter



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

**Z-nematic**

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

**Fully polarized**

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