Title: Machine learning feature discovery of spinon Fermi surface

Speakers:

Series: Machine Learning Initiative

Date: September 22, 2023 - 2:30 PM

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Abstract: With rapid progress in simulation of strongly interacting quantum Hamiltonians, the challenge in characterizing unknown phases becomes a bottleneck for scientific progress. We demonstrate that a Quantum-Classical hybrid approach (QuCl) of mining the projective snapshots with interpretable classical machine learning, can unveil new signatures of seemingly featureless quantum states. The Kitaev-Heisenberg model on a honeycomb lattice with bond-dependent frustrated interactions presents an ideal system to test QuCl. The model hosts a wealth of quantum spin liquid states: gapped and gapless Z2 spin liquids, and a chiral spin liquid (CSL) phase in a small external magnetic field. Recently, various simulations have found a new intermediate gapless phase (IGP), sandwiched between the CSL and a partially polarized phase, launching a debate over its elusive nature. We reveal signatures of phases in the model by contrasting two phases pairwise using an interpretable neural network, the correlator convolutional neural network (CCNN). We train the CCNN with a labeled collection of sampled projective measurements and reveal signatures of each phase through regularization path analysis. We show that QuCl reproduces known features of established spin liquid phases and ordered phases. Most significantly, we identify a signature motif of the field-induced IGP in the spin channel perpendicular to the field direction, which we interpret as a signature of Friedel oscillations of gapless spinons forming a Fermi surface. Our predictions can guide future experimental searches for U(1) spin liquids.

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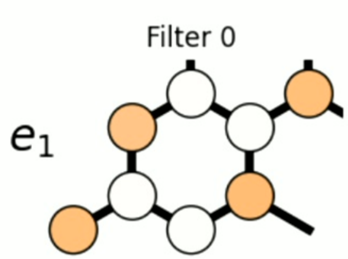
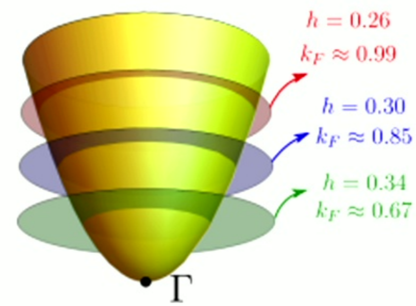
Zoom link: https://pitp.zoom.us/j/94233944575?pwd=OVljLzMrZzlKeUErNHZQRkEzMFRKUT09

Machine learning feature discovery of spinon Fermi surface

Kevin Zhang @ PI
Cornell University





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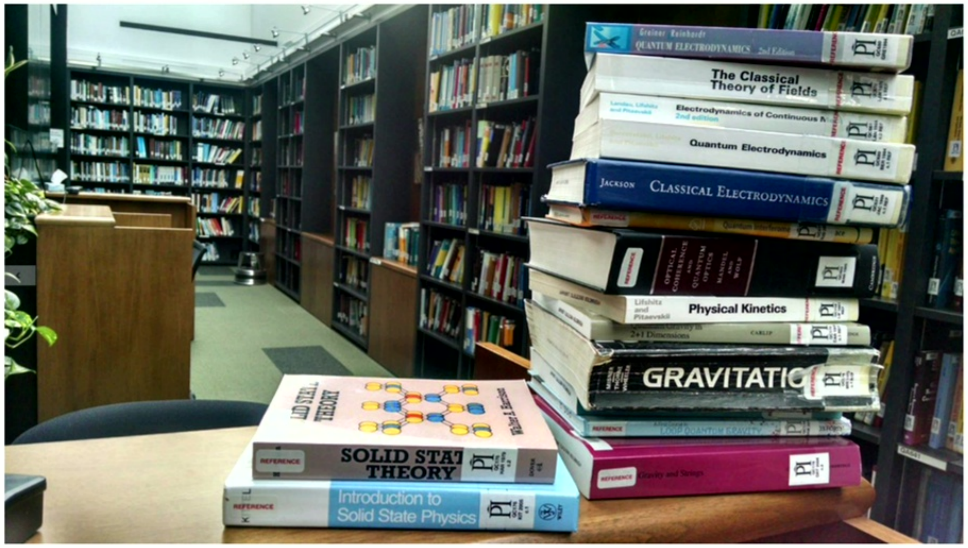
Characterizing quantum many-body states

32 spins: 2^{32} complex numbers = 60GB

How much information in PI library?

What can we do with wf data?

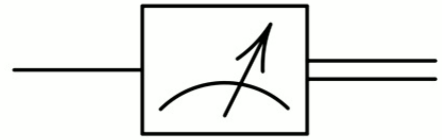


measure observables $\langle\Psi|O|\Psi\rangle$

or

snapshots $P_i \sim |c_i|^2$

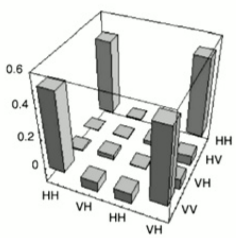
Projective measurements



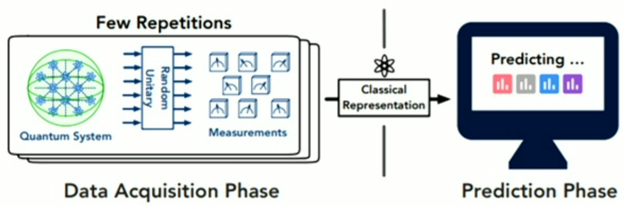
States on a quantum simulator are accessed through **projective measurements** e.g. bitstrings 001001110, 111010111, …

Things we can do with bitstrings

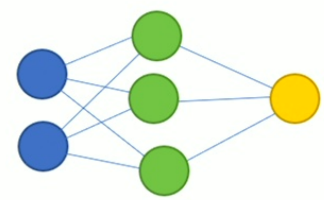
Fewer samples needed



Full tomography
James et al. (PRA 2001)



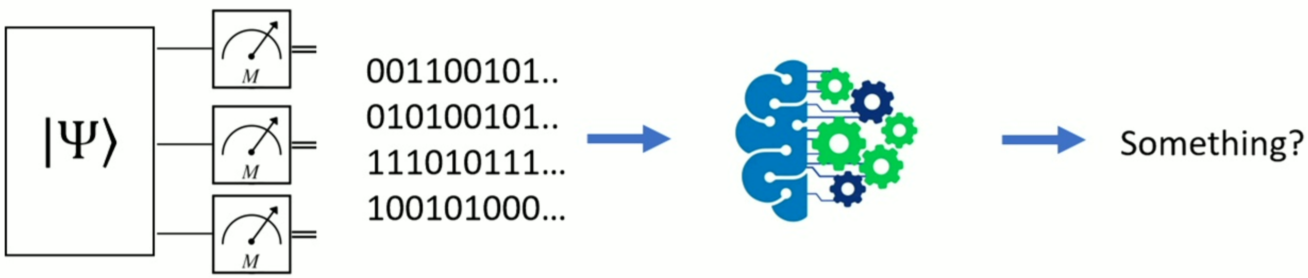
“Classical shadows”
Huang et al. (Nat. Phys. 2020)



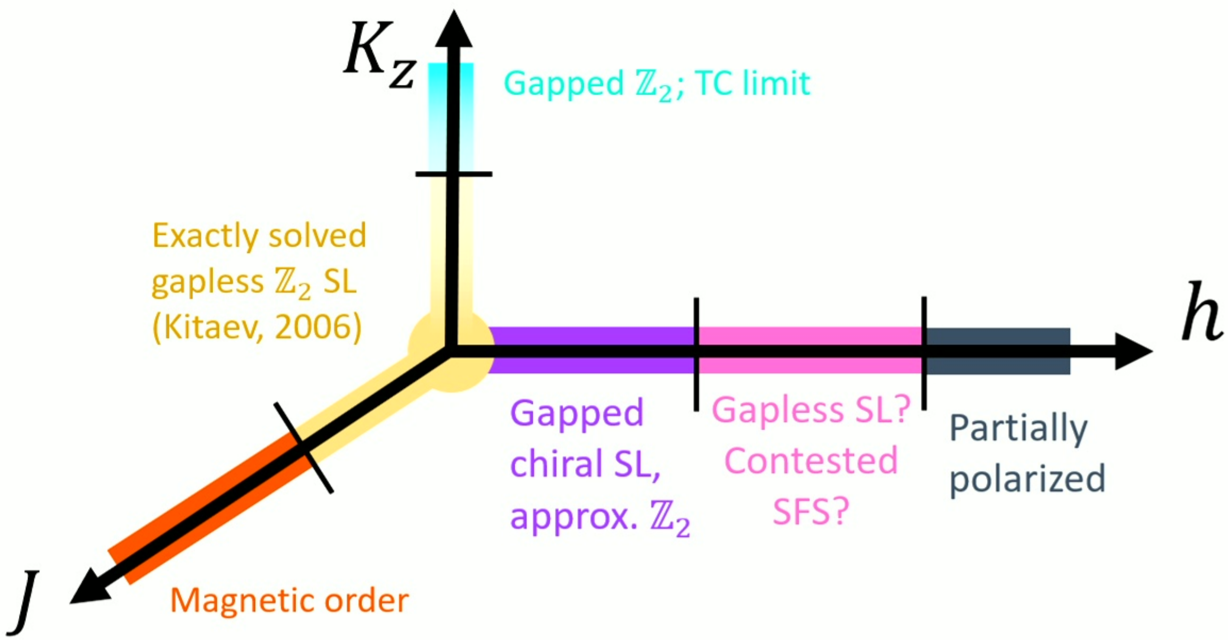
Machine learning?

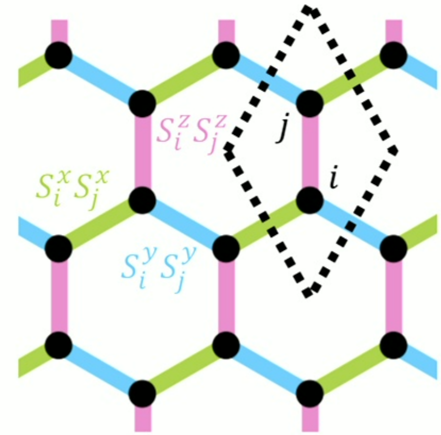
Machine learning with snapshots

- Snapshots are suitable for machine learning:
  - Large volume of data points drawn from distribution
  - Snapshots have consistent structure (lattice sites, symmetries, …)
  - Ensemble of snapshots reconstructs all* of original state

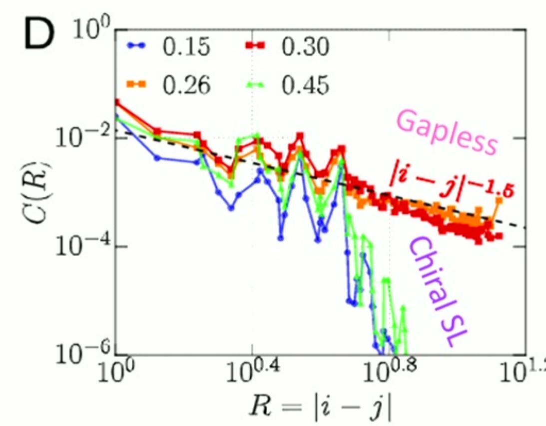


New developments in Kitaev model



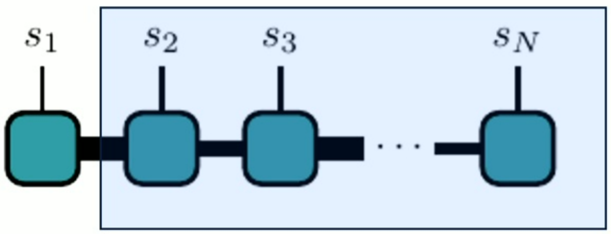


Patel, Trivedi (PNAS, 2019)

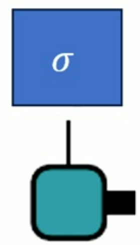


$$H = \sum_{\langle ij \rangle_\gamma} K_\gamma S_i^\gamma S_j^\gamma - J\boldsymbol{S_i} \cdot \boldsymbol{S_j} - \sum_{\boldsymbol{i}} h \cdot S_i$$

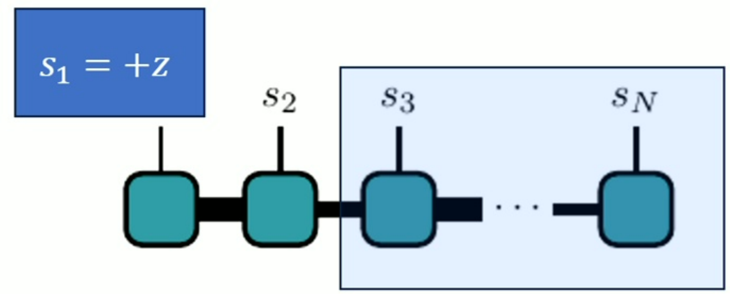
Snapshots from DMRG



trace out rest of system



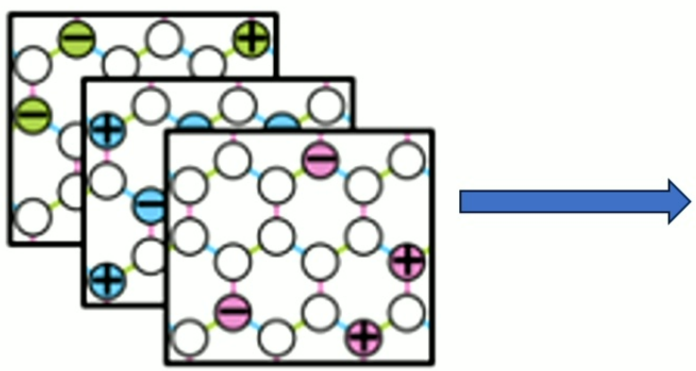
rotate into some spin basis
and sample spin +1 or -1
from RDM



project and move on

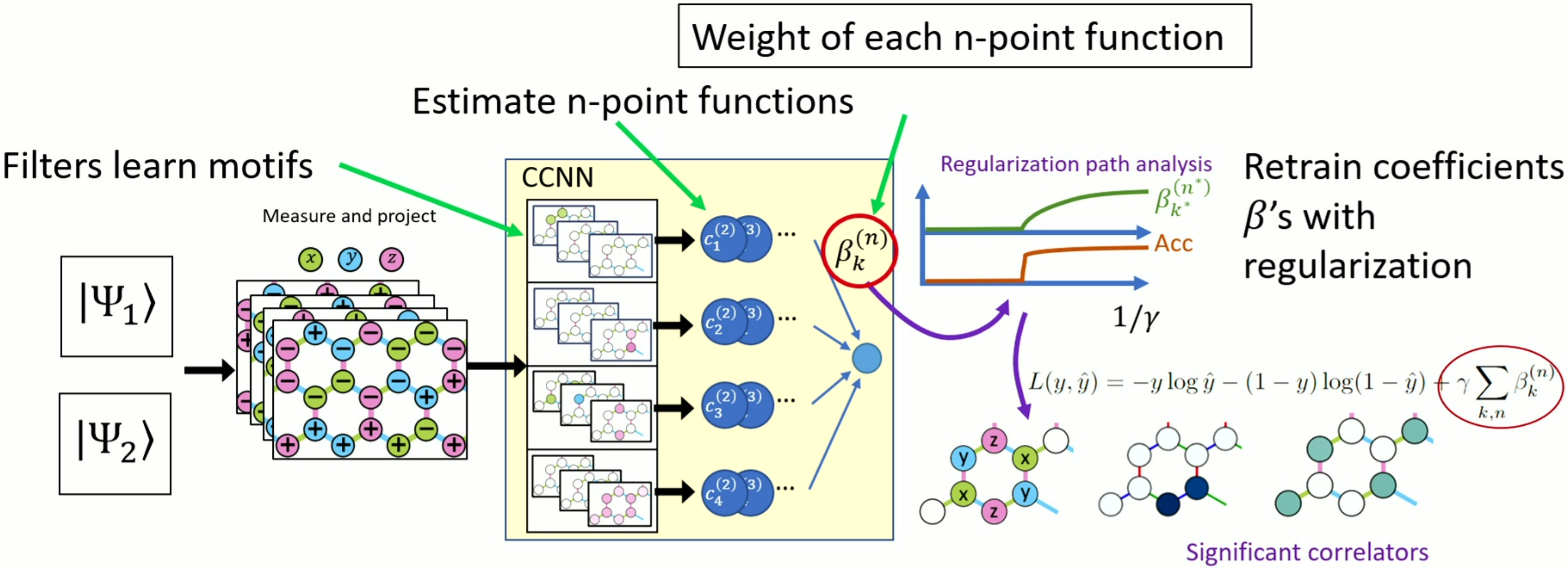
DMRG snapshots and ML

- Which axis to measure in? Depends on the specific training
- Basis direction encoded in snapshot channel "RGB"
- Honeycomb lattice maps to array



3 x 2W x L tensor of {-1,0,1}

Architecture



Architecture

- How to think about learning different n-point functions?
- Consider an expansion of some activation function (nonlinearity)

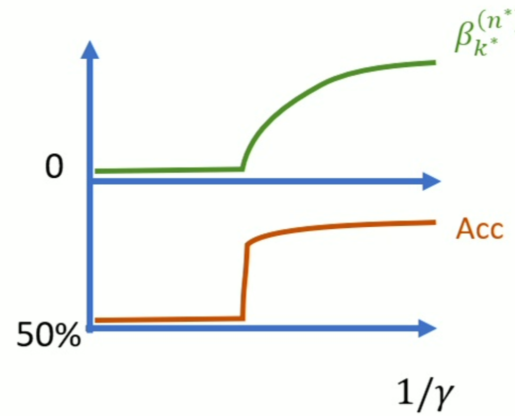
$$f(z) \sim \beta_0 + z\beta_1 + \frac{z^2}{2} a_2 \ldots$$

- Now $z = \sum x_i w_i$, the convolution output of input data x with filter weights w

$$f(z) \sim \beta_0 + \beta_1 \underbrace{\sum B_i w_i}_{\text{1pt fns}} + \beta_2 \underbrace{\sum B_i B_j w_i w_j}_{\text{2pt fns}} \ldots$$

-> learning an activation function is equivalent to learning weights for different orders of correlations

Interpreting filters



- Suppose β_k^n is first to increase in RPA
- Look for filter #k

$$f(z) \sim \beta_0 + \beta_1 \sum B_i w_i + \beta_2 \sum B_i B_j w_i w_j \ldots$$

- Correlation function is the term that is multiplied by β_k^n, for example

$$c_k^n(a) = \sum_{xy} w(x) w(y) B(a+x) B(a+y)$$

- Weighted sum of k-pt fns

#1

#2

#3

#4

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Output prediction

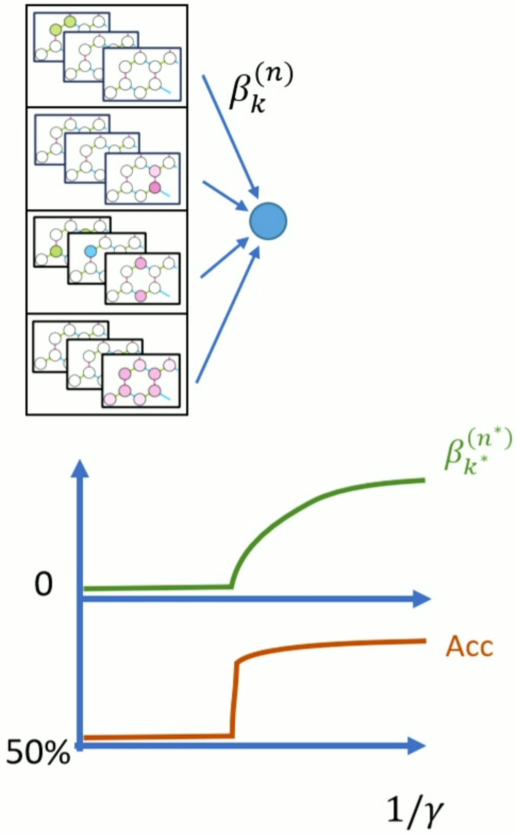
- Full NN representation:

$$y = \frac{1}{1 + \exp(\sum_{nk} \beta_k^n (\sum_x w_k(x) B(x+d))^n)}$$

Coefficients select particular correlations to be used

Learnable weights govern spatial layout of correlators

Regularization path analysis



$$L(y, \hat{y}) = -y \log \hat{y} - (1-y)\log(1-\hat{y}) + \gamma \sum_{k,n} \beta_k^{(n)}$$

- RPA: feature selection
- For RPA, retrain with filters w_k fixed but allow couplings β_k^n to vary as we change the L1 regularization γ
- Look for the moment where the first β_k^n becomes nonzero

Interpreting filters

- Suppose β_k^n is first to increase in RPA
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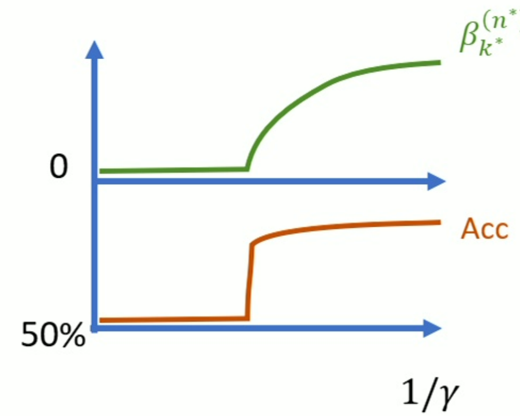

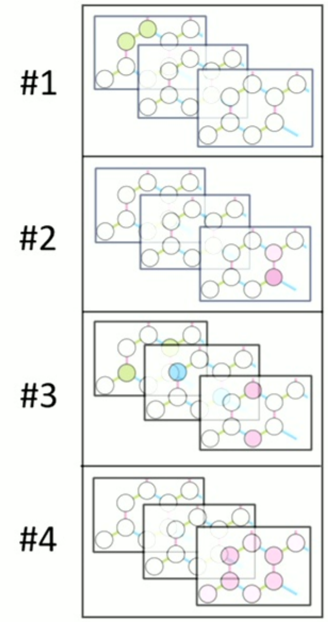

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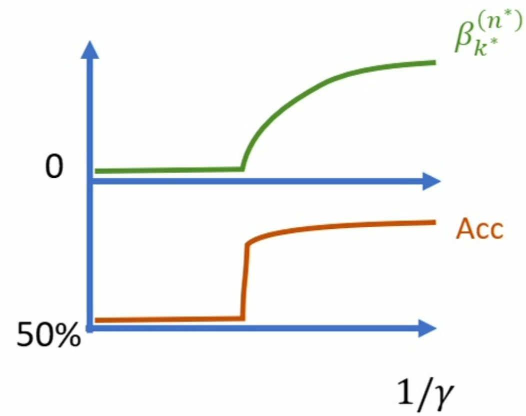

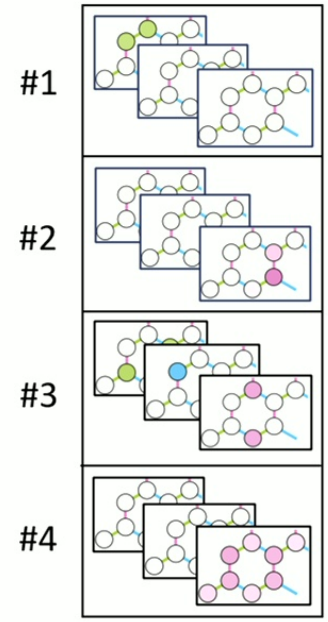

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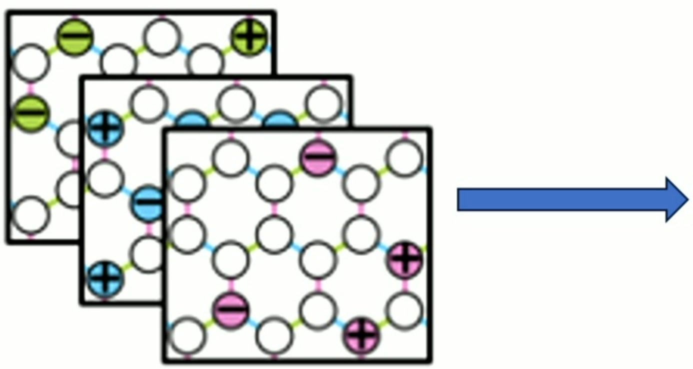

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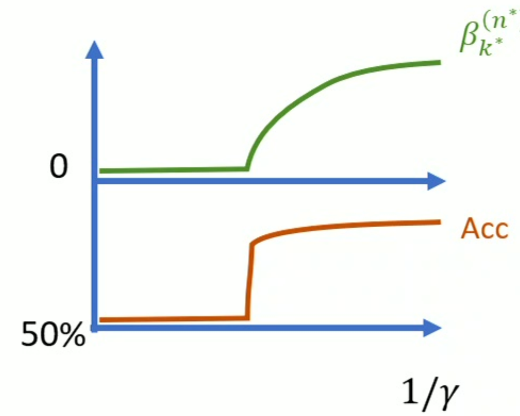
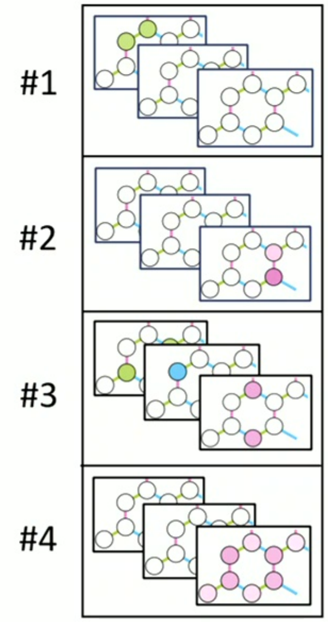
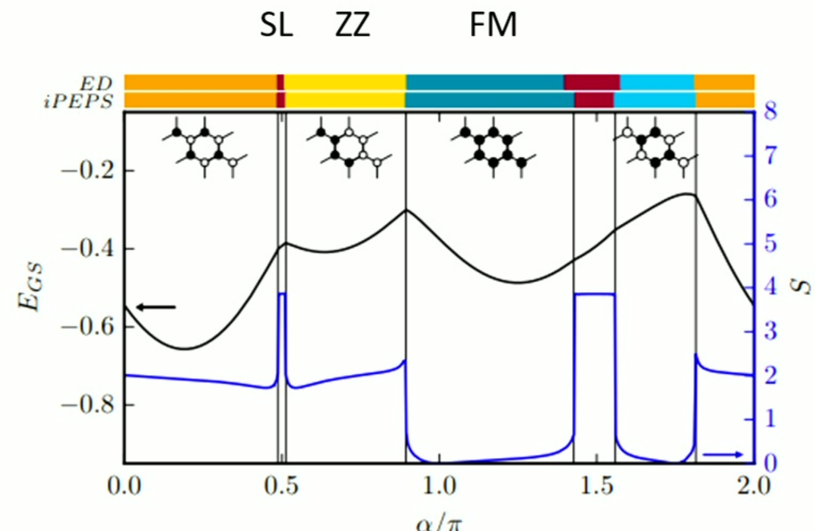


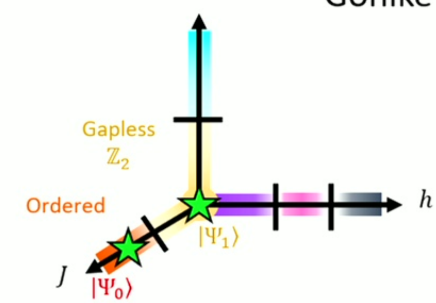


Benchmark: Kitaev vs FM

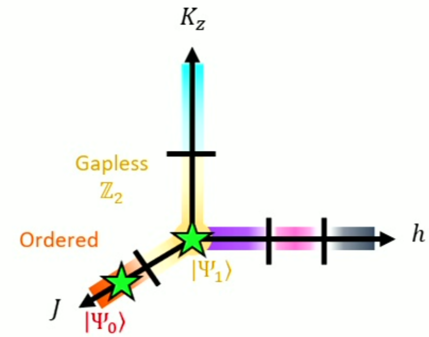
- Known transition from SL to order
- Sneakily skip past zigzag order to learn feature of FM
- Training procedure:
  9000 training, 1000 test
- Binary classification between $K_x = K_y = K_z$ SL and ordered FM states



Gohlke 2017



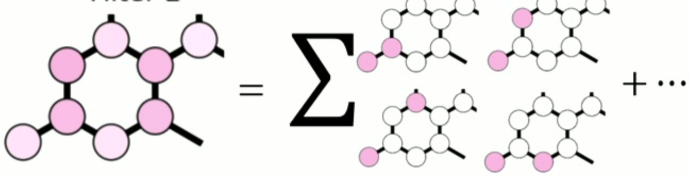
Benchmark: Kitaev vs FM



- RPA shows most important correlators are 2-point functions of

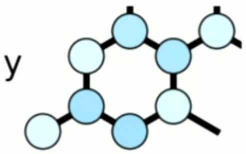
Filter 2

z



and y

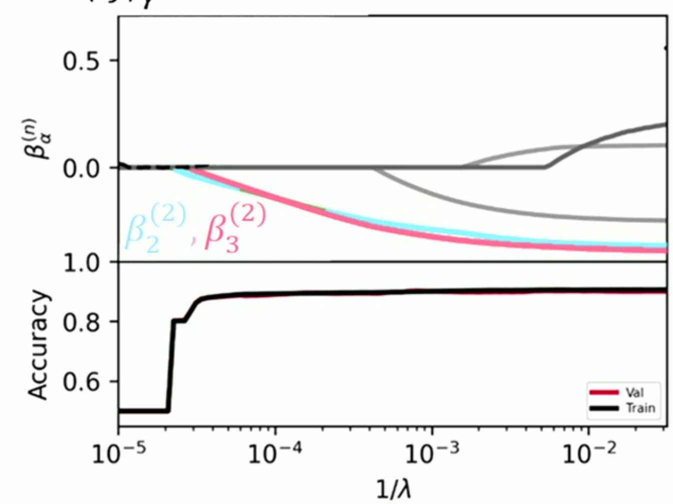
Filter 3



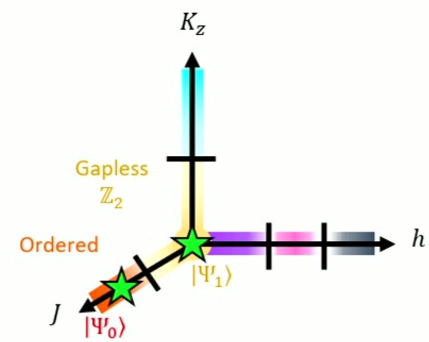
which represent

$$\langle |S^z(0)|^2\rangle, z \leftrightarrow y$$

$$H = \sum_{\langle ij\rangle_\gamma} K_\gamma S_i^\gamma S_j^\gamma - J\boldsymbol{S}_i \cdot \boldsymbol{S}_j$$



Benchmark: Kitaev vs FM



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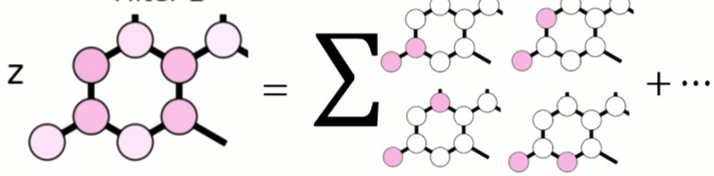
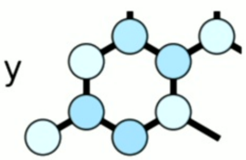
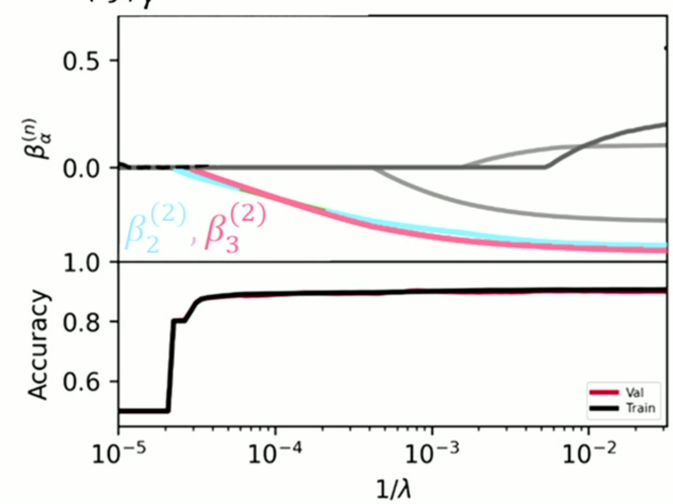


and y

Filter 3



$$H = \sum_{\langle ij \rangle_\gamma} K_\gamma S_i^\gamma S_j^\gamma - J \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$



which represent

$$\langle |S^z(0)|^2 \rangle, z \leftrightarrow y$$

- Signature of Heisenberg ferromagnet

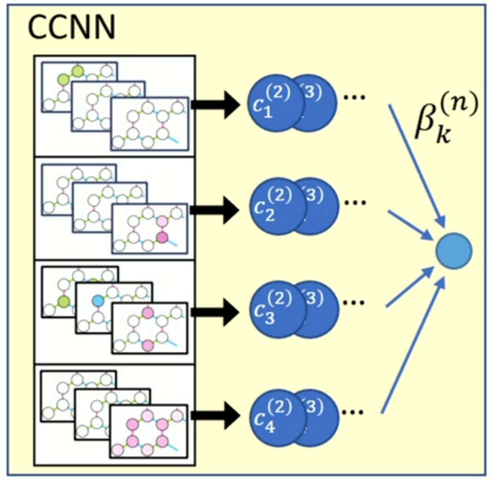
Output prediction

- Full NN representation:

$$y = \frac{1}{1 + \exp(\sum_{nk} \beta_k^n (\sum_x w_k(x) B(x+d))^n)}$$

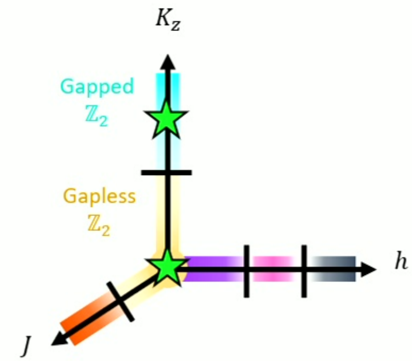
Coefficients select particular correlations to be used

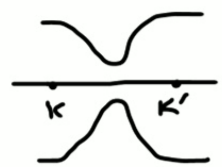
Learnable weights govern spatial layout of correlators

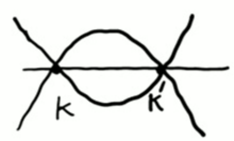


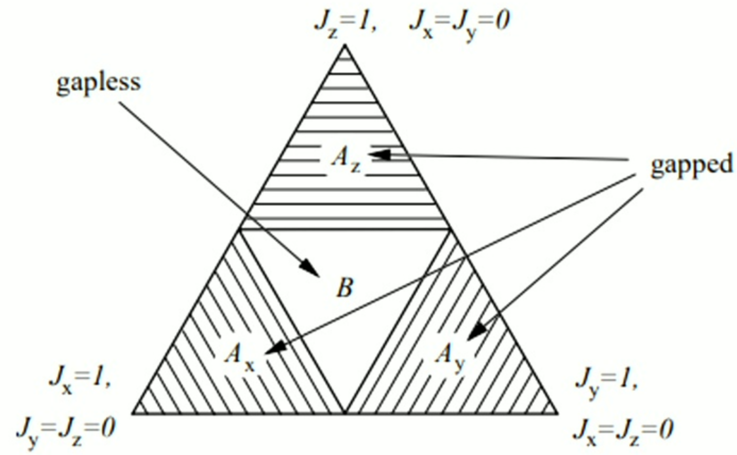
Benchmark: Z_2 SLs

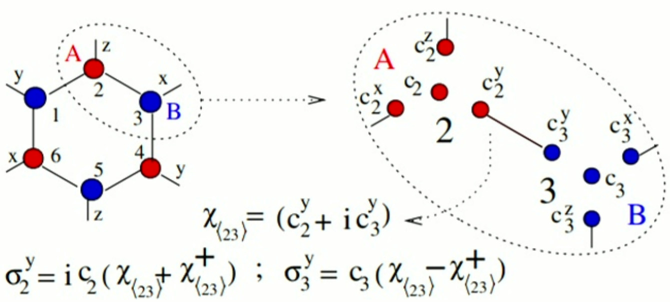
- Transition from gapless to gapped Z_2 upon tuning K_z
- Exact solution in terms of bond fermions and majoranas





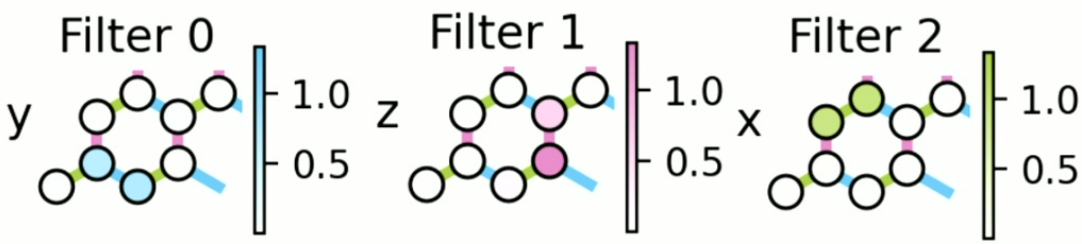






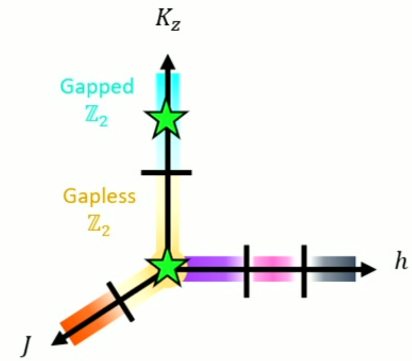
Benchmark: Z_2 SLs

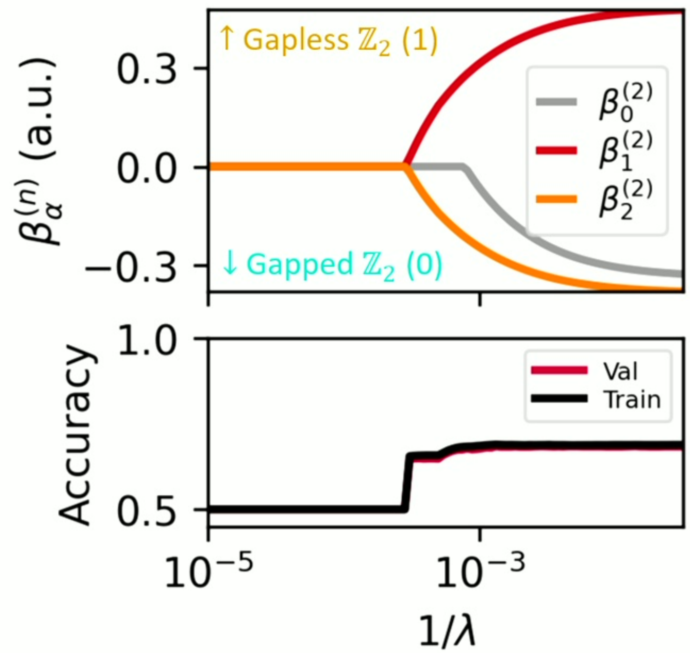
- Random x, y, z basis
- Filters:



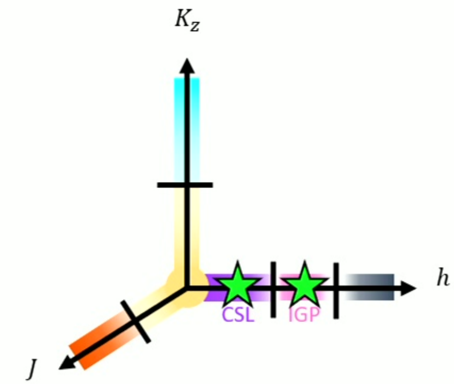
- Exact solution: spin-spin correlation

$$\langle \sigma_i^z \sigma_j^z \rangle \equiv S^{zz}_{\langle ij \rangle z}(0) = \frac{\sqrt{3}}{16\pi^2} \int_{BZ} \cos\theta(k_1, k_2) dk_1 dk_2,$$

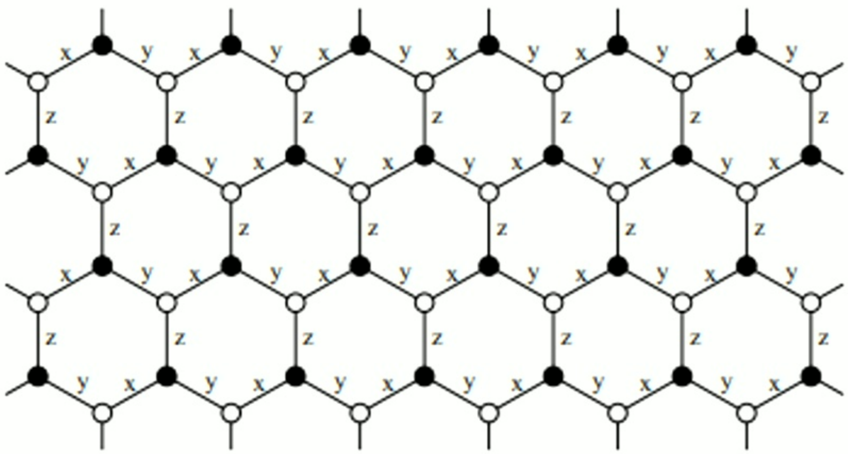


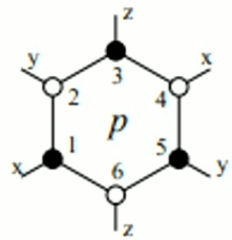


Structure of chiral phase



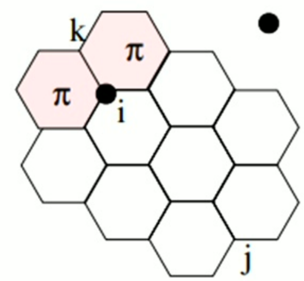
- CSL is has approximate Z_2 gauge theory



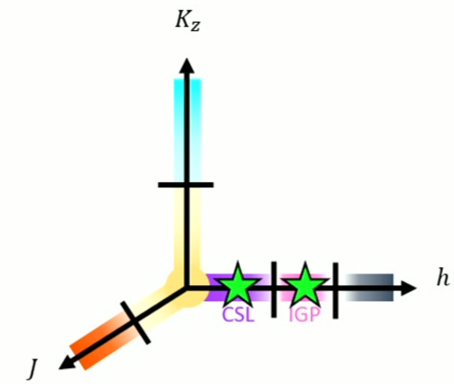


$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

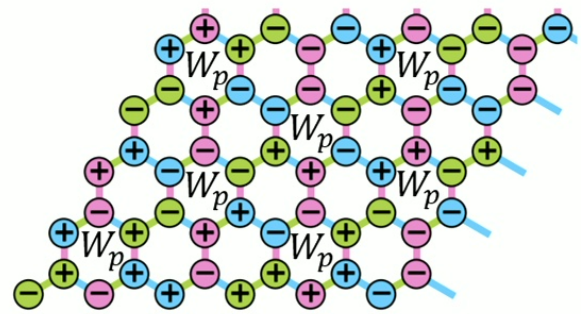
[W, H] = 0



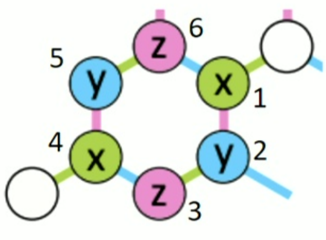
Topological feature in chiral phase

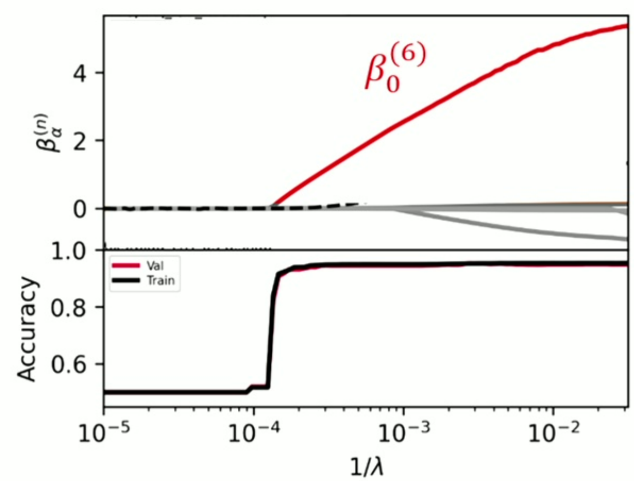


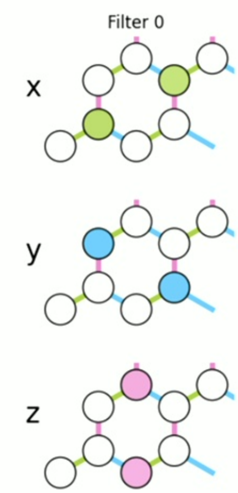
- Snapshot in plaquette basis: Wilson loop of gauge theory
- 6-point function learned by NN is the Wilson loop



$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

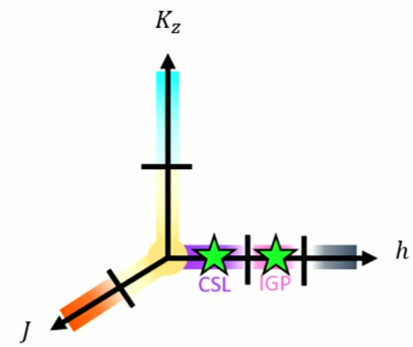


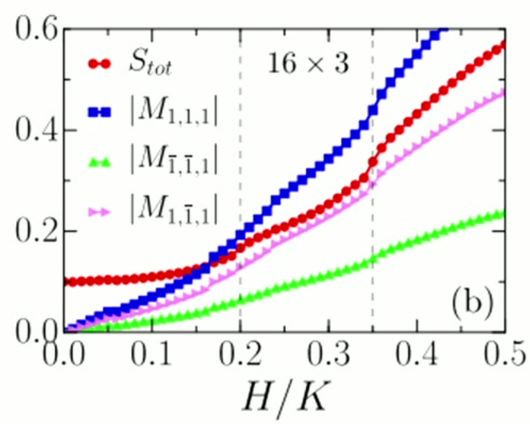


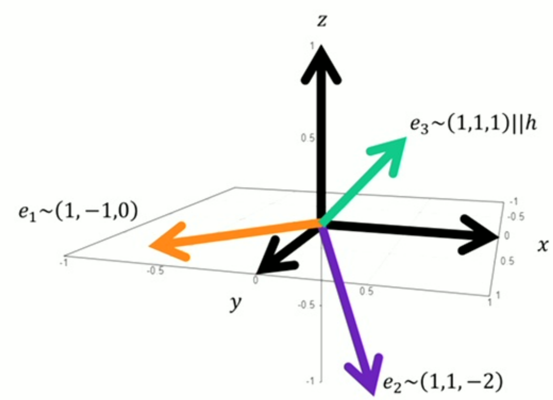


Discovering new feature of gapless phase

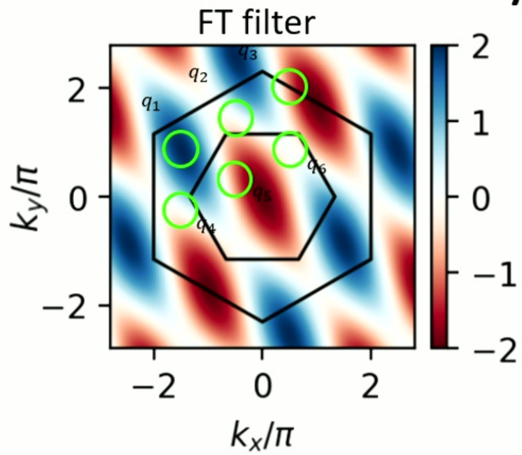
- Naively the NN would learn the total magnetization (since correlation functions are not connected)
- How to suppress effect of h?
- Switch to a basis $e_{1,2,3}$ where magnetization can be absorbed into e_3 direction, and take snapshots in random e_1, e_2 basis

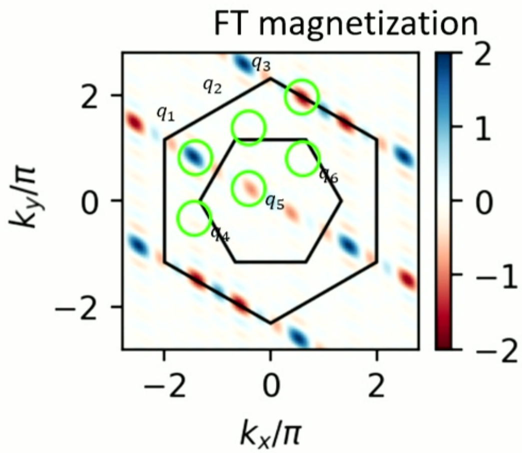




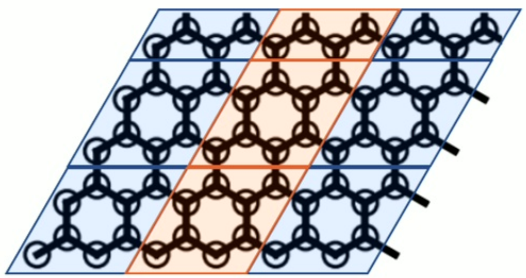


Fourier analysis and magnetization





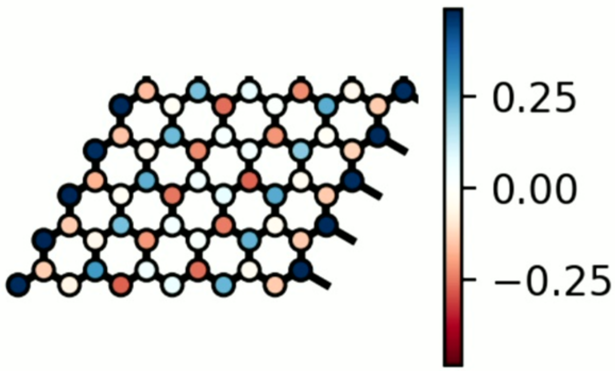
- Conjecture an AF tiling of the filter $\langle S_{e_1} \rangle = 0$

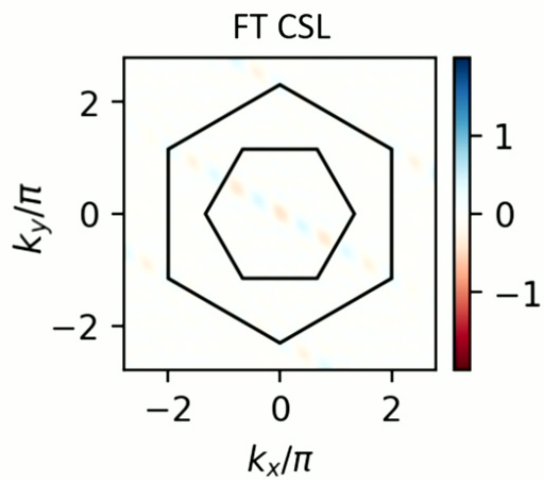


- Bragg peaks associated with AF tiling consistent with DMRG measurement

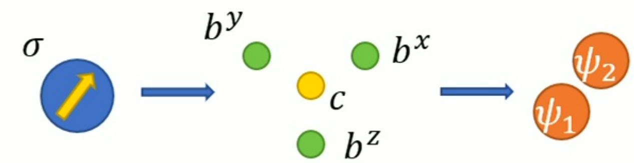
Real-space magnetization feature

- Real-space magnetization pattern consistent with filter
- Oscillation captured by 2-pt fn
- Feature is not present in CSL phase: what physics does it signify?





Spinon mapping



- Transformation of majoranas into spinons

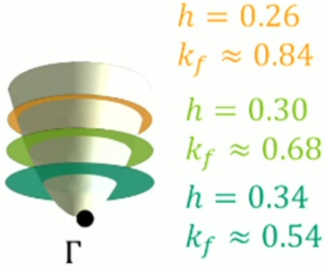
$$c_i = (\psi_{i,1} + \psi^\dagger_{i,1}),\ b_i^{e_1} = i(\psi^\dagger_{i,1} - \psi_{i,1}),\ b_i^{e_2} = \psi_{i,2} + \psi^\dagger_{i,2},\ b_i^{e_3} = i(\psi^\dagger_{i,2} - \psi_{i,2}),$$

- Mapping from spin to spinon density

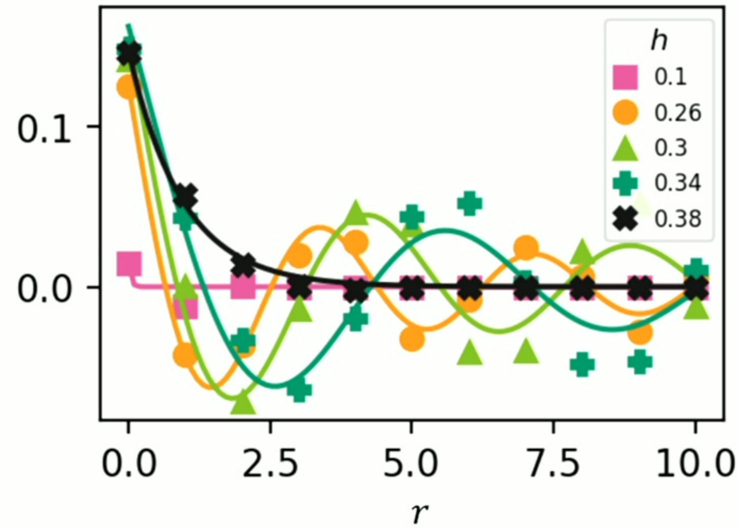
$$S_i^{e_1} = ic_i b_i^{e_1} = -(\psi_{i,1} + \psi^\dagger_{i,1})(\psi^\dagger_{i,1} - \psi_{i,1}) = 2\psi^\dagger_{i,1}\psi_{i,1} - 1$$
$$S_i^{e_2} = ic_i b_i^{e_2} = i(\psi_{i,1} + \psi^\dagger_{i,1})(\psi^\dagger_{i,2} + \psi_{i,2}) = i\psi_{i,1}\psi_{i,2} + i\psi_{i,1}\psi^\dagger_{i,2} + i\psi^\dagger_{i,1}\psi_{i,2} + i\psi^\dagger_{i,1}\psi^\dagger_{i,2}$$
$$S_i^{e_3} = ic_i b_i^{e_3} = -(\psi_{i,1} + \psi^\dagger_{i,1})(\psi_{i,2} - \psi^\dagger_{i,2}) = -\psi_{i,1}\psi_{i,2} + \psi_{i,1}\psi^\dagger_{i,2} - \psi^\dagger_{i,1}\psi_{i,2} + \psi^\dagger_{i,1}\psi^\dagger_{i,2}$$

Field dependence of Friedel oscillations

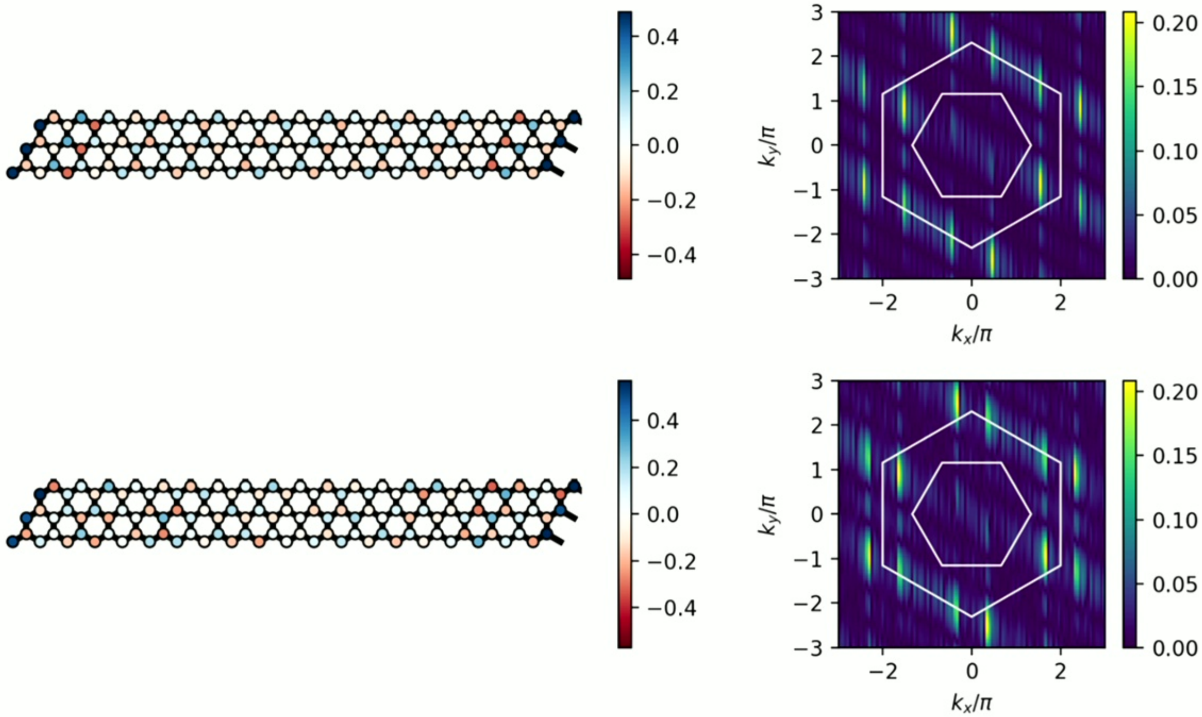
- Friedel oscillations reveal Fermi surface size
- Probe field dependence by fitting to functional form



$$\langle S^{e_1}(r)\rangle \sim \langle n_1(r)\rangle \sim \frac{k_F}{\pi}\left[1 - \frac{\sin(2k_F r)}{2k_F r}\right]$$

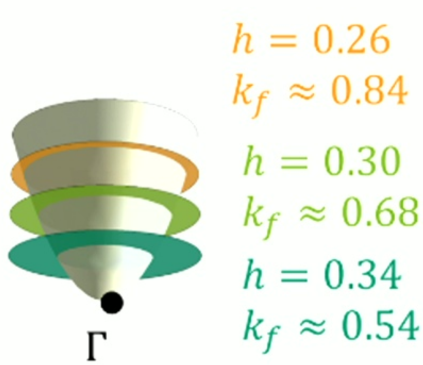


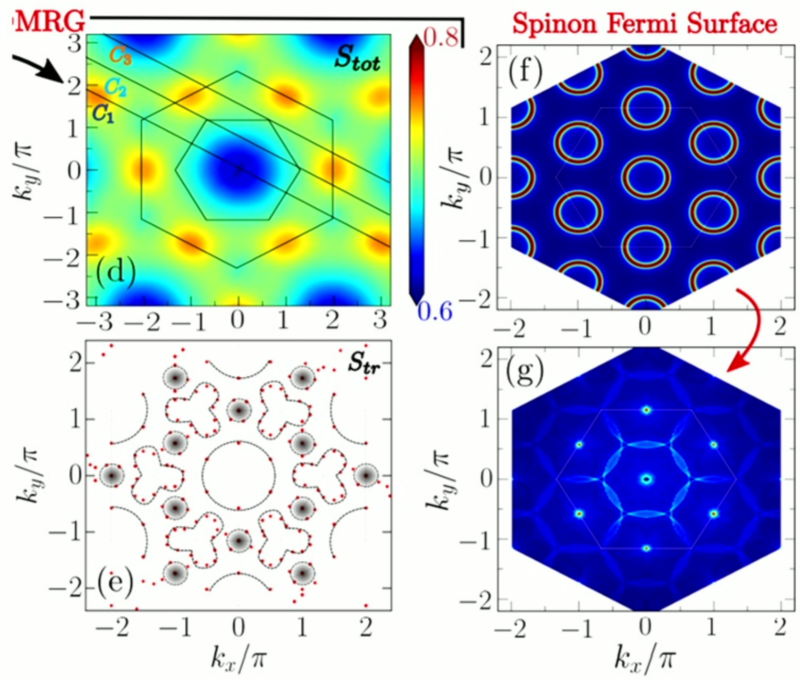
Longer systems



Sketch and comparison of conjecture

- Previous conjecture (Patel & Trivedi) of FS size consistent with our results





Significance and conclusions

- ML-led discovery of a characteristic feature (Friedel oscillations) in re-entrant gapless phase of Kitaev model
- Potential probe in experiments: measurement of correlations in specific axis rather than total $S \cdot S$

Collaborators

- Feng Shi, Nandini Trivedi (OSU)
- Yuri Lensky, Eun-Ah Kim (Cornell)




Architecture

- How to think about learning different n-point functions?
- Consider an expansion of some activation function (nonlinearity)

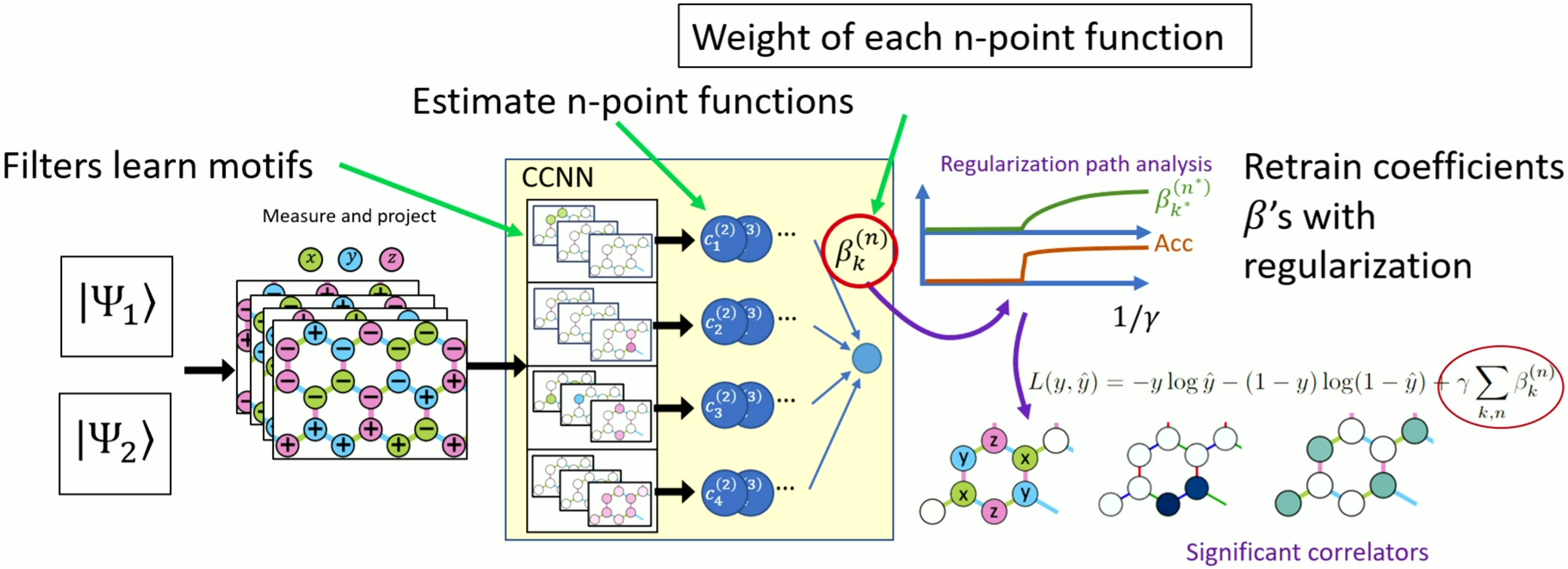
$$f(z) \sim \beta_0 + z\beta_1 + \frac{z^2}{2} a_2 \ldots$$

- Now $z = \sum x_i w_i$, the convolution output of input data x with filter weights w

$$f(z) \sim \beta_0 + \underbrace{\beta_1 \sum B_i w_i}_{\text{1pt fns}} + \underbrace{\beta_2 \sum B_i B_j w_i w_j}_{\text{2pt fns}} \ldots$$

-> learning an activation function is equivalent to learning weights for different orders of correlations

Architecture



- Dominant filter weight $\beta_{k^*}^{(n^*)}$ <-> spatial motifs

Miles et al. (Nat. Comm. 2021)