# Exploiting Machine Learning for Quantum Chaos and Quantum Information


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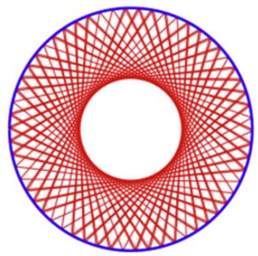
# Outline

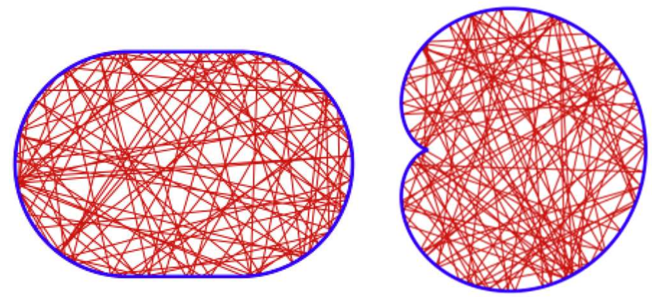
- Scars in billiard systems
- Problem statement
- Convolutional neural network
- Few shot classification algorithm
- Detect quantum scars in heart billiard

# Scars in chaotic billiard systems

- Billiard systems

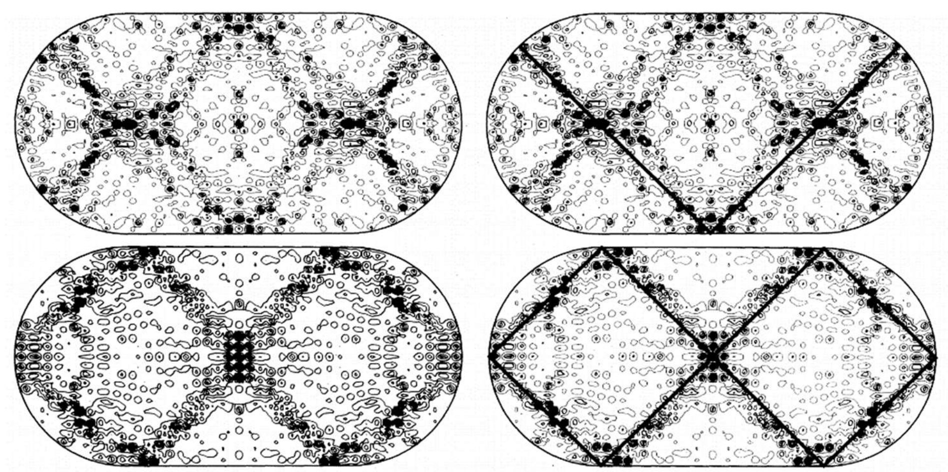


Classical integrable



Classical chaotic

- Quantum scars

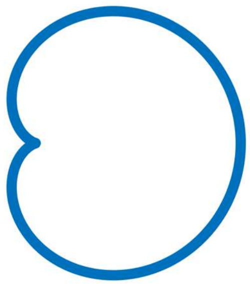


Heller, E. J. *Phys. Rev. Lett.*, ***53***, 1515. (1984).

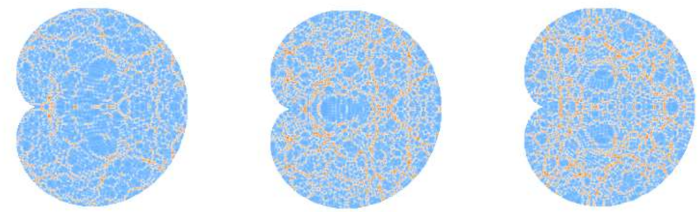
# Problem statement

Eigenstates

~15,000



Normal states



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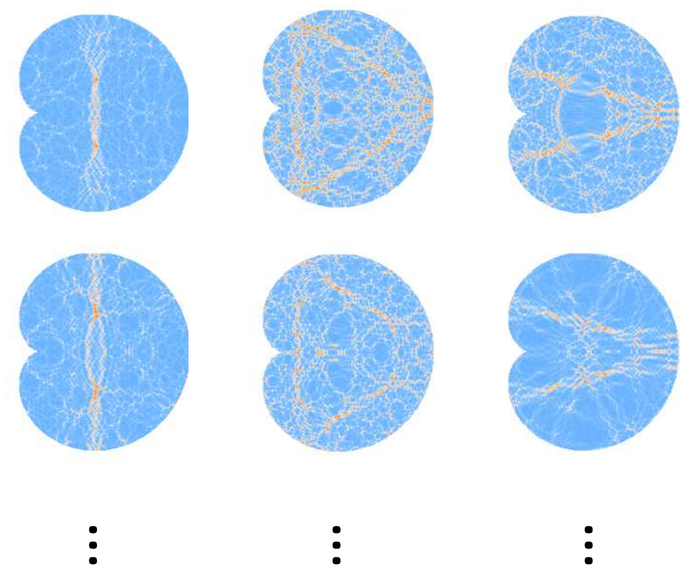
Quantum scars (5%-10%)

period 2 period 3 period 4



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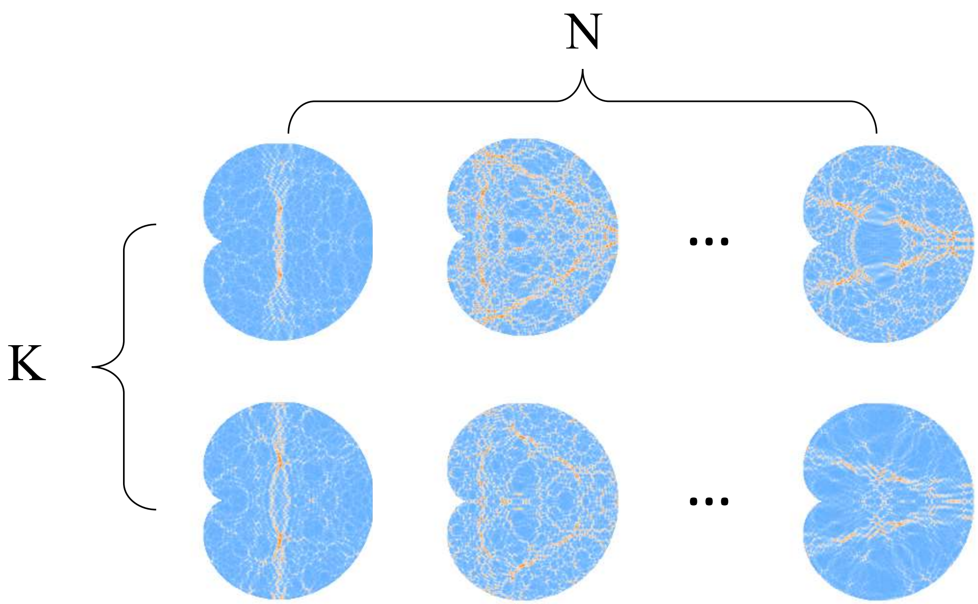
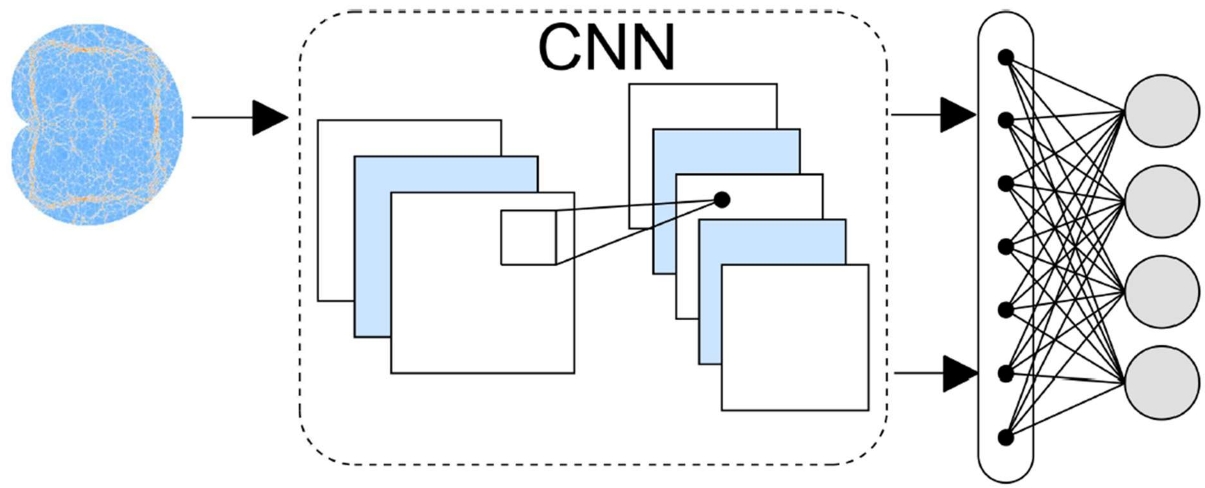
- ➢ Detecting quantum scars relying mostly on human visualization of eigenstates
- ➢ Efficiently detecting quantum scars has remained to be challenging
- ➢ Machine learning approach to detecting quantum scars

# Convolutional neural network (CNN)

- Training dataset



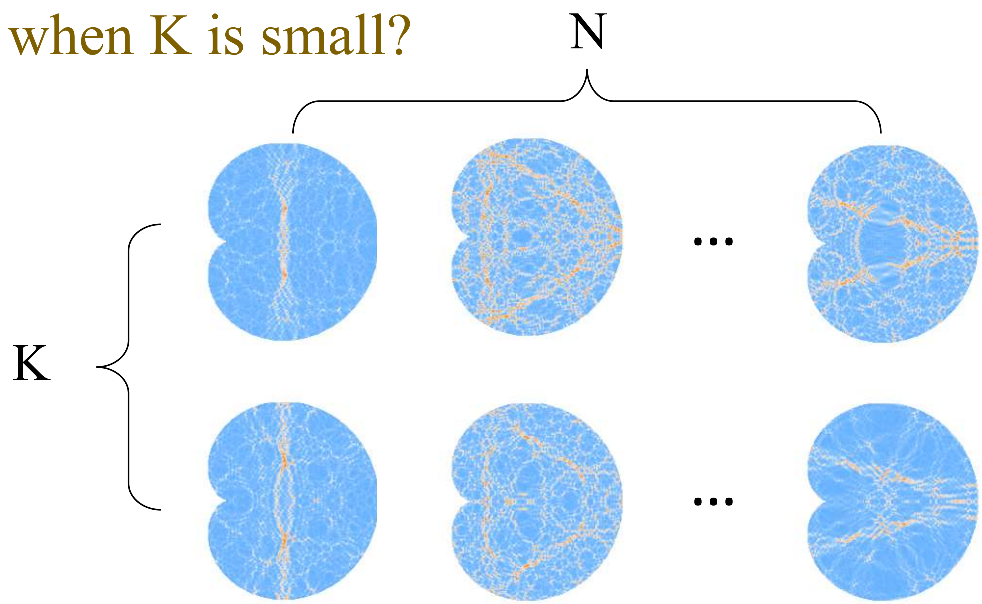

- Convolutional neural network




Krizhevsky, A., et al. Int. Conf. Neural Inf. Process. Syst.1097-1105. (2012)

# Meta learning: Few shot classification (idea)

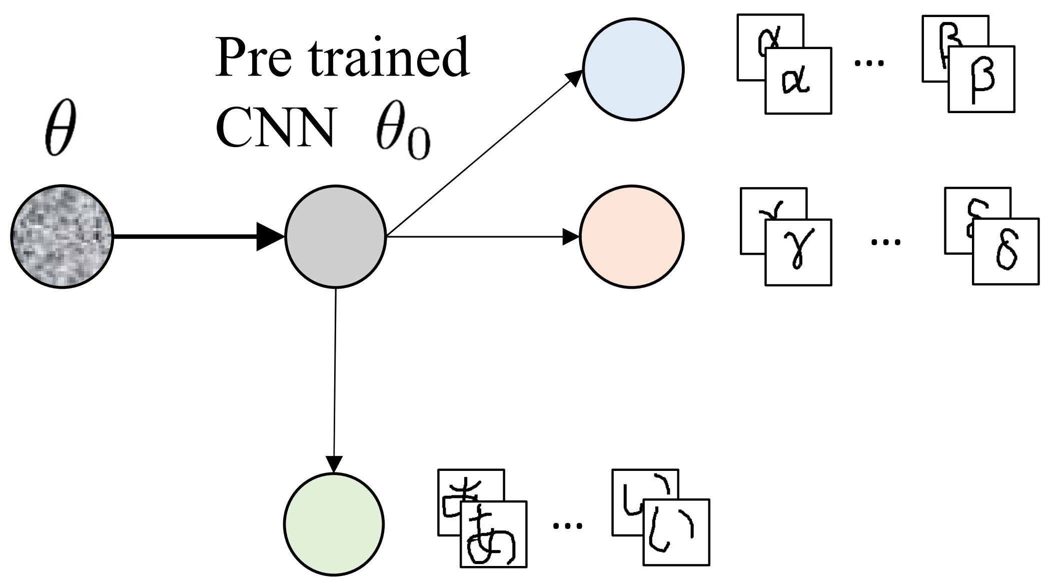
- What will happen when K is small?




- Meta learning: learn how to learn

Finn, C., et al. *PMLR*. 1126 (2017)
Nichol, A., et al. *arXiv* **1803**, 02999 (2018)

$\theta$ weights and biases in CNN




Omniglot dataset

B. M. Lake, et al. *Science* **350**, 1322 (2015)

# Meta learning: Few shot classification (algorithm) → CNN $\boldsymbol{\theta_0}$

- Example of hyperparameter optimization

Hyperparameters
(initial weights/biases, learning rate, …) $\longrightarrow$ Loss

| | Initial weight | Loss |
|---|---|---|
| Trial 1 | 0.01 | 1 |
| Trial 2 | 0.009 | 0.8 |
| Trial 3 | ? | |

- Meta learning (optimization based)

Finn, C., et al. *PMLR.* 1126 (2017)
Nichol, A., et al. *arXiv* **1803**, 02999 (2018)

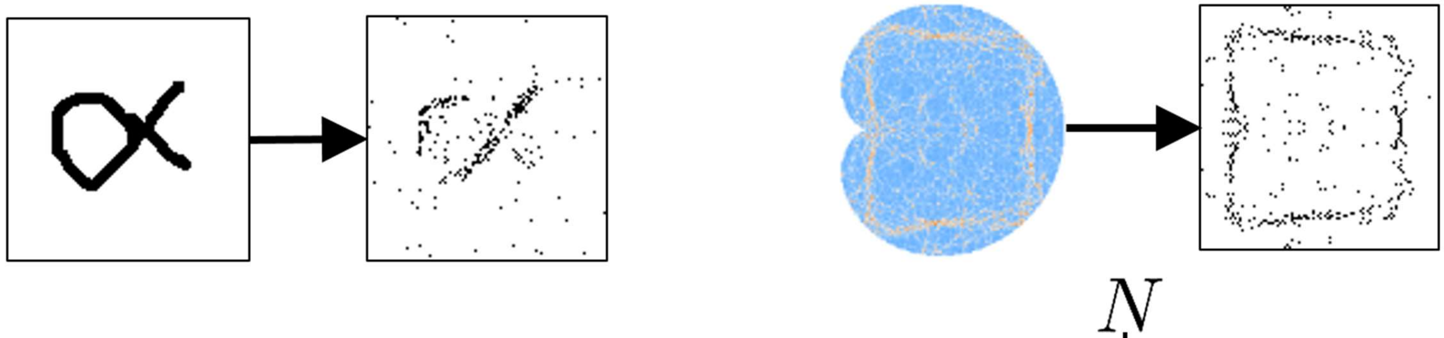
$\theta$ Weights and biases in CNN $\underset{\frac{\partial \mathcal{L}}{\partial \theta}}{\overset{\mathcal{L}(\theta)}{\rightleftarrows}}$ Loss

# Training steps

- Step 1:

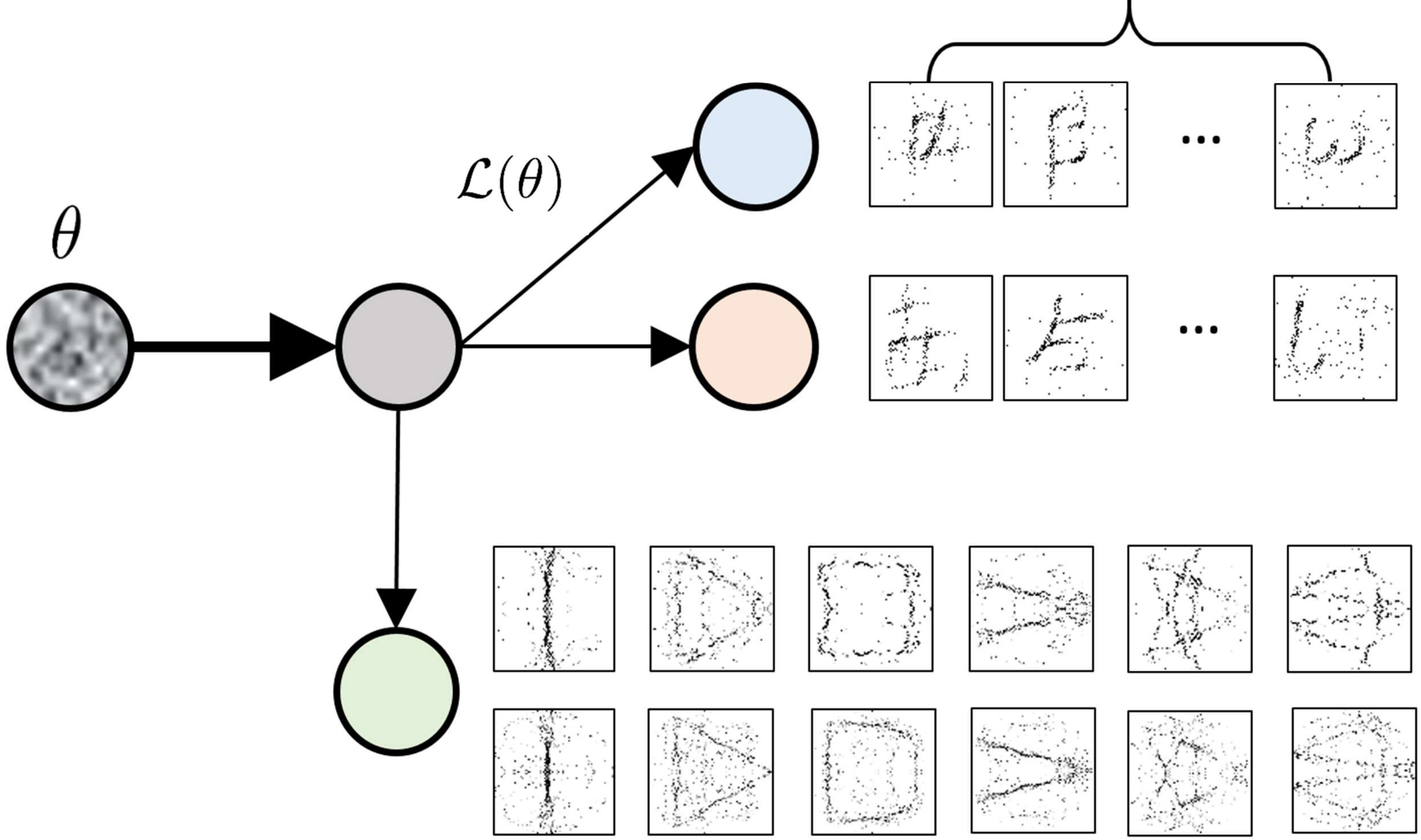
Omniglot dataset

B. M. Lake, et al. *Science* **350**, 1322 (2015)



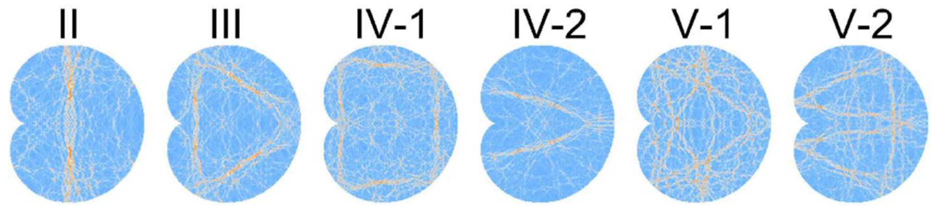

- Step 2:

Nichol, A., et al. *arXiv* **1803**, 02999 (2018)

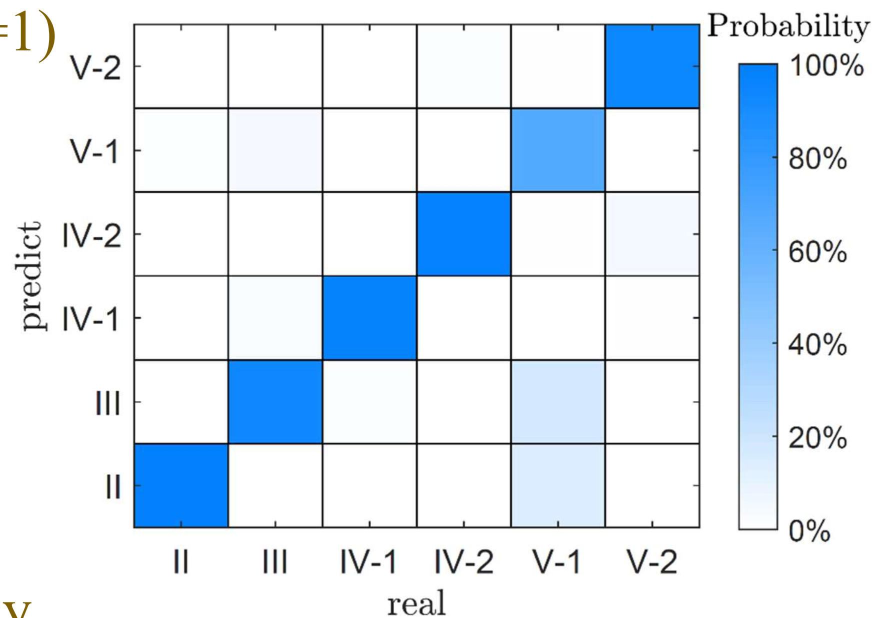



- Step 3:

# Few shot classification of scars in heart billiard




- Confusion matrix (K=1)




- Classification accuracy

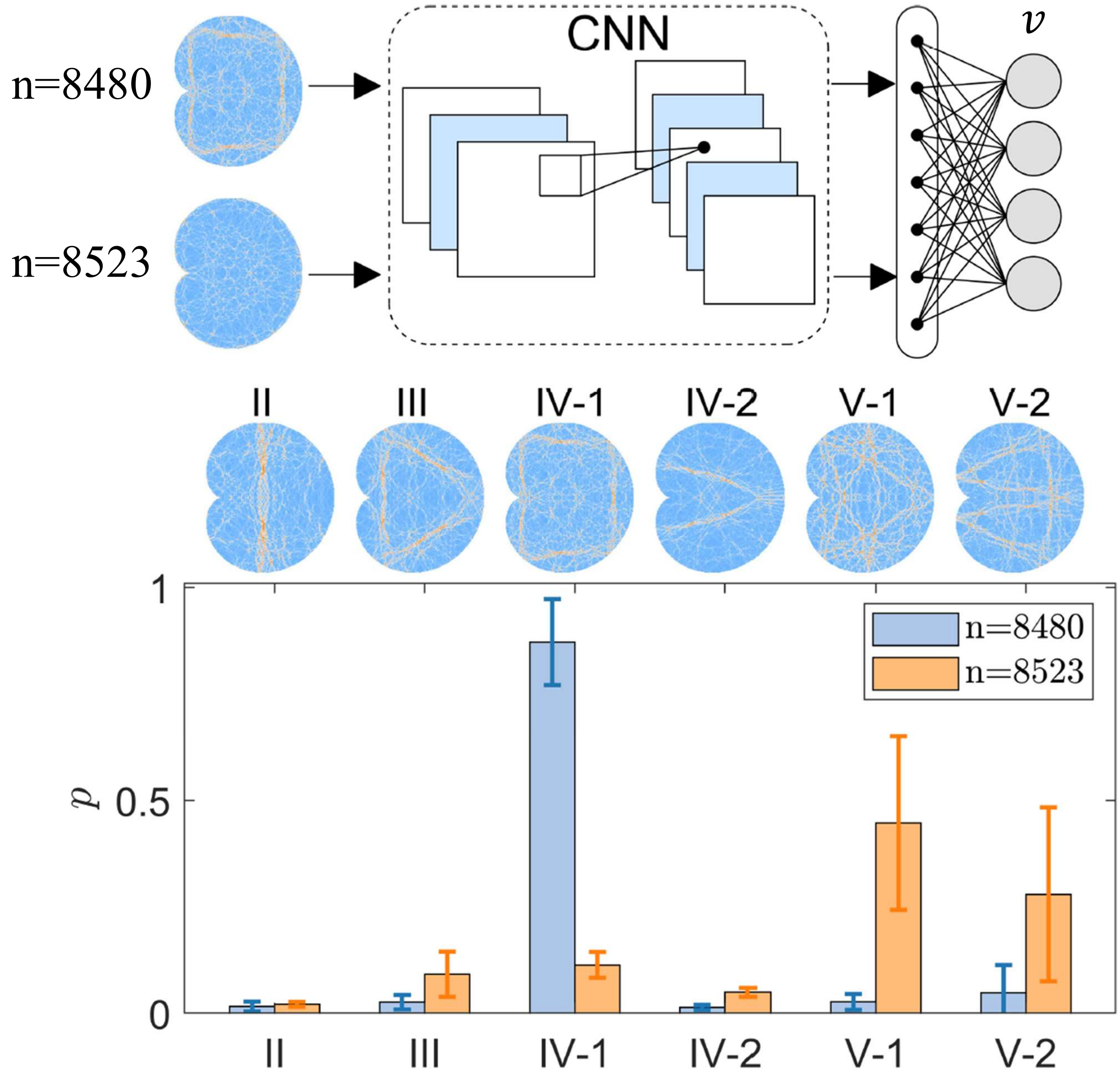
| shot | accuracy |
| --- | --- |
| $K = 1$ | $90.16\% \pm 1.41\%$ |
| $K = 2$ | $95.30\% \pm 0.68\%$ |
| $K = 5$ | $98.58\% \pm 0.32\%$ |

# Ensemble of neural networks

Mode index: n

$$p_i = \frac{\exp(v_i)}{\sum_i \exp(v_i)}$$

Ensemble of NNs under 1 shot



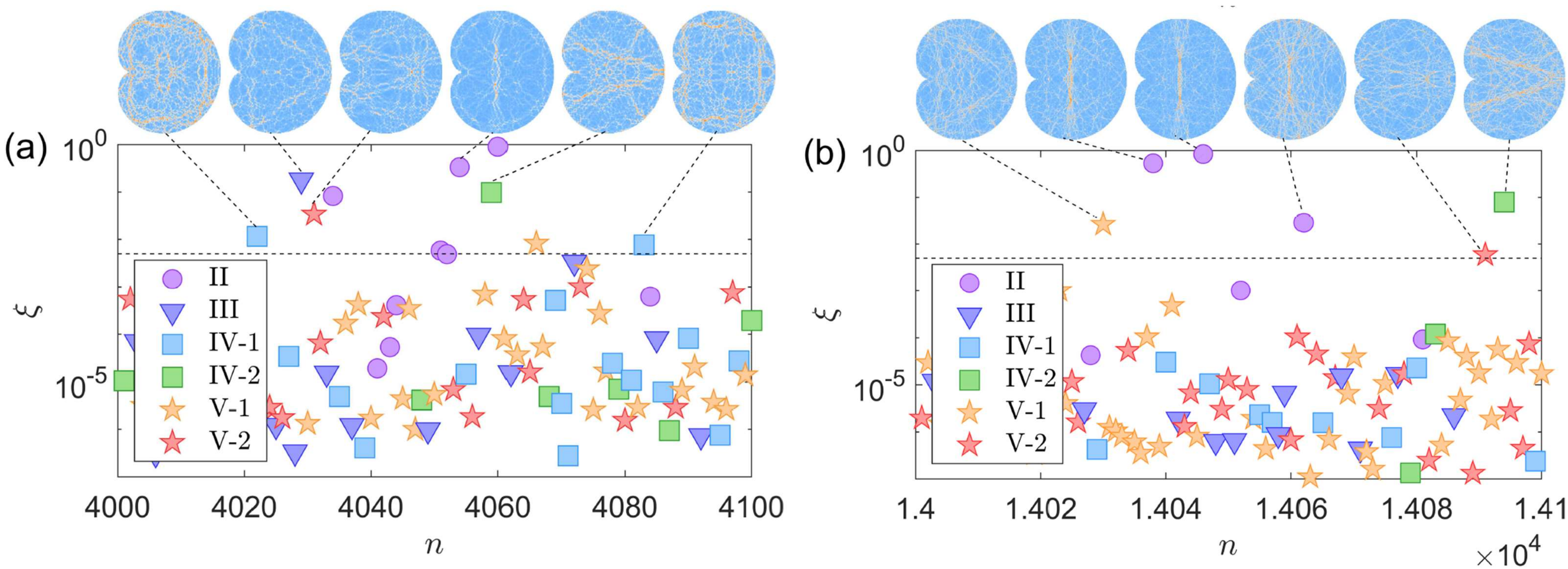
# Automated scar detector

Mode index: n

$$\xi(n) = \max\left(\prod_i p_j^{(i)}(n)\right)$$

Different neural networks

Different scars




Counting region: n ∈ [4000, 15000]

Criteria: $\xi(n) > 5 \times 10^{-3}$

# Comparison with semiclassical theory

$$\eta(n) = \frac{|k_n - k_0|}{\delta k} - \left[\frac{|k_n - k_0|}{\delta k}\right],$$

$\{0, 1\}$

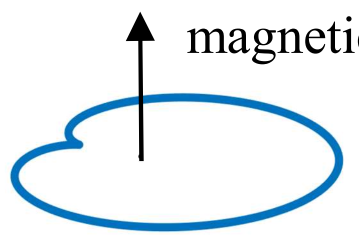
$\{0, 0.5, 1\}$

$k_n$ : wavevector for mode n

$k_0$: wavevector for reference state

$\delta k$ : scar dependent number

- Magnetic flux



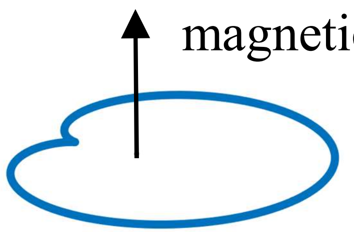
magnetic flux $\alpha$

$$\alpha = q\Phi/(hc)$$

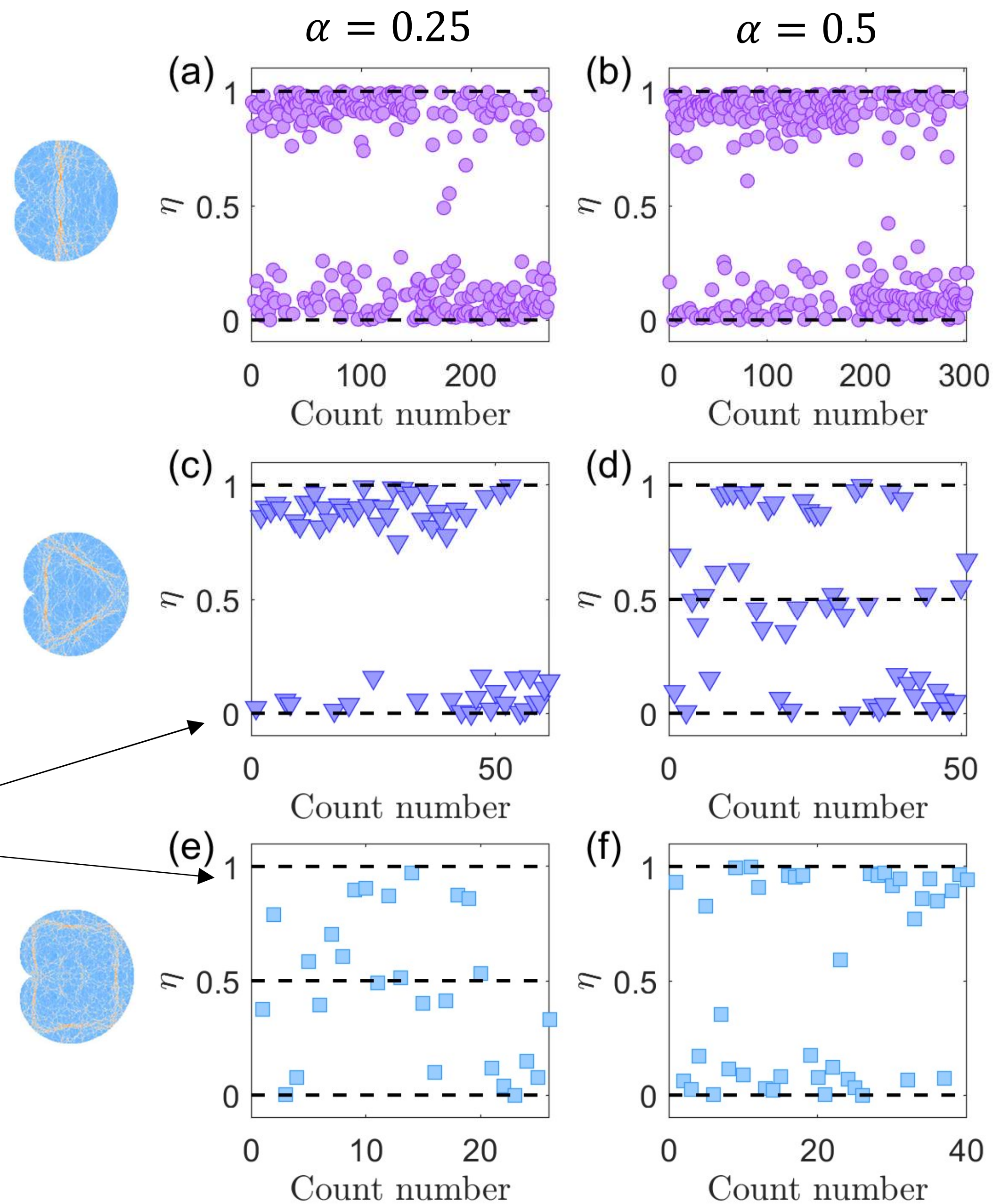
C.-Z. Wang, L. Huang, and K. Chang, Scars in Dirac fermion systems: The influence of an Aharonov-Bohm flux, *New J. Phys.* **19**, 013018 (2017).

# Comparison with semiclassical theory

- Semiclassical theory




Prediction from semiclassical theory




C.Z. Wang, et al. *New J. Phys.* **19**, 013018 (2017)

# Summary

*Previous results*

- Meta learning for Omniglot dataset/Imagenet dataset
- Computational method for quantum scars
- Semiclassical theory for relativistic quantum scars

*Our results*

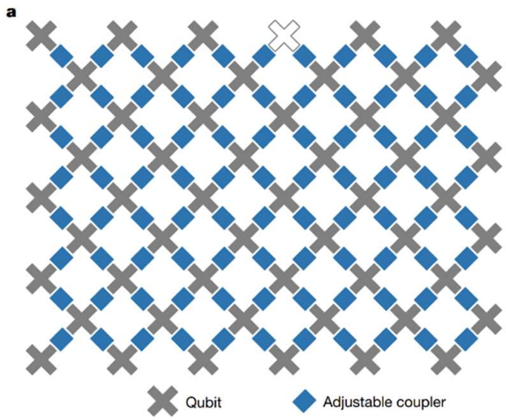
- Extended Meta learning to physics systems
- Constructed a few-shot classification algorithm for quantum scars
- Developed a machine learning approach to detecting quantum scars

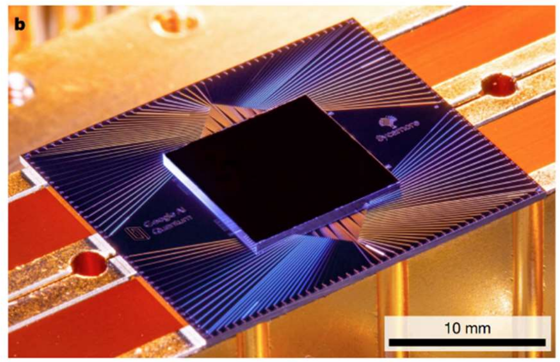
- **Chen-Di Han**, Cheng-Zhen Wang, and Ying-Cheng Lai. "Classifying and detecting quantum scars by machine learning." *To be submitted.*

# Outline

- Quantum computing and qubit systems
- Network tomography
- Heisenberg neural network
- Results for Hamiltonian based on two-body interactions
- Results for Hamiltonian based on long-range interactions

- Quantum computing




Arute, F., et al. *Nature*. **574**, 505 (2019)

- Toffoli gate (CCNOT gate)

| INPUT | | | OUTPUT | | |
|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 0 | 0 | 1 |
| 0 | 1 | 0 | 0 | 1 | 0 |
| 0 | 1 | 1 | 0 | 1 | 1 |
| 1 | 0 | 0 | 1 | 0 | 0 |
| 1 | 0 | 1 | 1 | 0 | 1 |
| 1 | 1 | 0 | 1 | 1 | 1 |
| 1 | 1 | 1 | 1 | 1 | 0 |

Table from Wikipedia

$$H_{\text{Toffoli}} = \frac{\pi}{8}(\mathbb{I}_2 - \sigma_3^1)(\mathbb{I}_2 - \sigma_3^2)(\mathbb{I}_2 - \sigma_1^3).$$

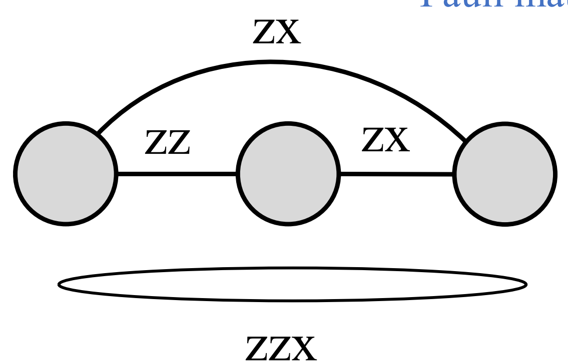
# Spin networks

- Hamiltonian for Toffoli gate

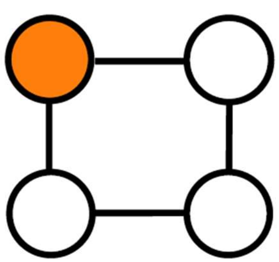
Different qubits

$$H_{\text{Toffoli}} = \frac{\pi}{8}(\mathbb{I}_2 - \sigma_3^1)(\mathbb{I}_2 - \sigma_3^2)(\mathbb{I}_2 - \sigma_1^3).$$

Pauli matrix




- Relationship to classical networks



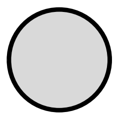
nodes $\leftrightarrow$ qubits

links $\leftrightarrow$ $\sigma^i \otimes \sigma^j$

Adjacency matrix $\leftrightarrow$ Hamiltonian

# Matrix representation of Hamiltonian

- Hamiltonian for single qubit

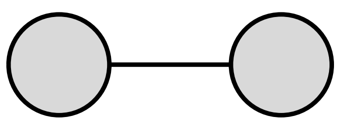


$|\uparrow\rangle, |\downarrow\rangle$

$$\begin{aligned} H &= c_0 I + c_1\sigma_x + c_2\sigma_y + c_3\sigma_z \\ &= c_0\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + c_1\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + c_2\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} + c_3\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\end{aligned}$$

- Hamiltonian for two qubits

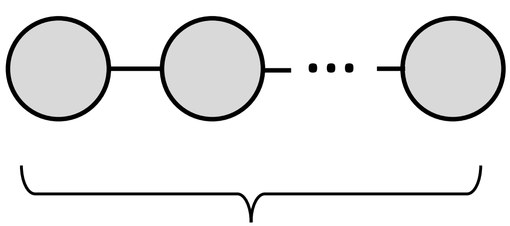
$$\mathbb{A}\otimes\mathbb{B} = \begin{pmatrix} a_{11}\mathbb{B} & \cdots & a_{1n}\mathbb{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathbb{B} & \cdots & a_{mm}\mathbb{B}\end{pmatrix}$$



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

$$H = c_{ij}\ \underbrace{\{\mathbb{I}^1, \sigma_x^1, \sigma_y^1, \sigma_z^1\} \otimes \{\mathbb{I}^2, \sigma_x^2, \sigma_y^2, \sigma_z^2\}}_{\text{16 terms}}$$

- Hamiltonian n qubits



n qubits

$2^n$ linearly independent states

$4^n$ Pauli terms for Hamiltonian

# Spin network tomography

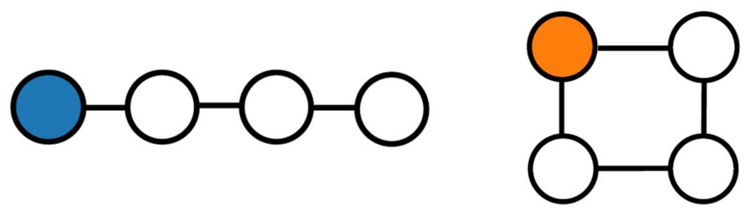
- Schrödinger equation

$$i\hbar\frac{d}{dt}\psi = H\psi \longrightarrow \psi(t) \longrightarrow \langle\psi(t)|A|\psi(t)\rangle$$

- Inverse problem n: number of qubits

Enough observations ($4^n$) × Enough initial states ($4^n$)

- Incomplete observations



- Time independent H:

Zhang, J., et al. *Phys. Rev. Lett.* **113**, 080401 (2014)

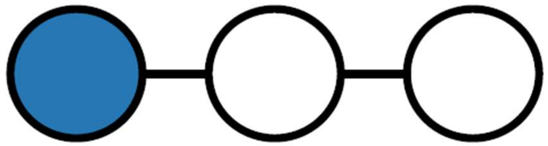
- Time dependent H:

?

# System description

- Step 1

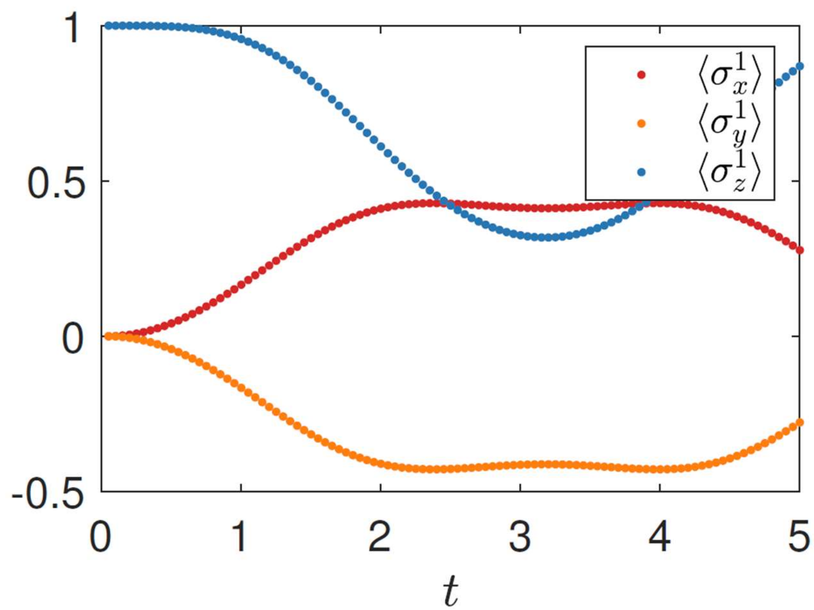
$$H(t) = \sin(t)\left(\sum_{i=1}^{3}\sum_{j=1}^{2}\sigma_j^i + \sum_{i=1}^{2}\sum_{l=1}^{3}\sum_{m=1}^{2}\sigma_l^i\sigma_m^{i+1}\right).$$



- Step 2

$$i\hbar\frac{d}{dt}\psi = H\psi$$

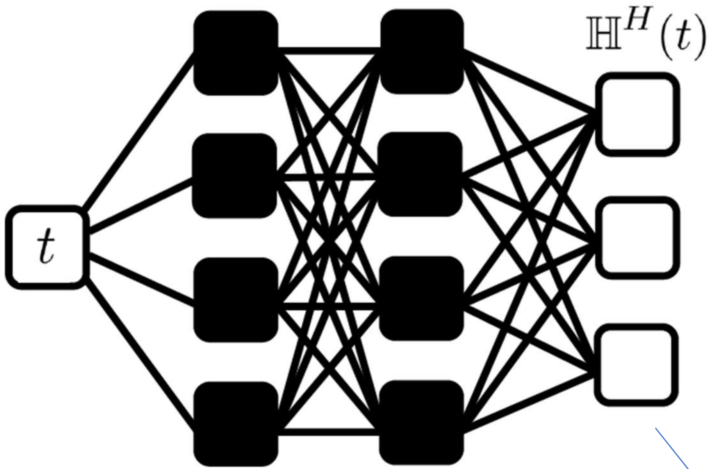
Randomly generate $\psi$




Example for $\frac{|1\rangle+i|0\rangle}{\sqrt{2}}|11\rangle$

# Training process

- Step 3




$$\frac{dA^H}{dt} = i[H^H(t), A^H(t)],$$

Heisenberg equation

$$\mathcal{L} = \sum_{\text{Observations}} \left| \langle \dot{A}(t) \rangle_{\text{real}} - \langle \dot{A}(t) \rangle_{\text{pred}} \right|^2$$

This neural network automatically satisfies Heisenberg equation

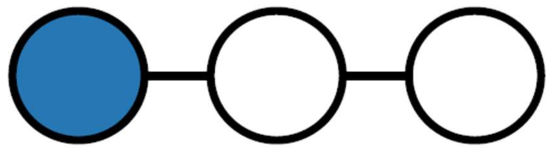
- Step 4

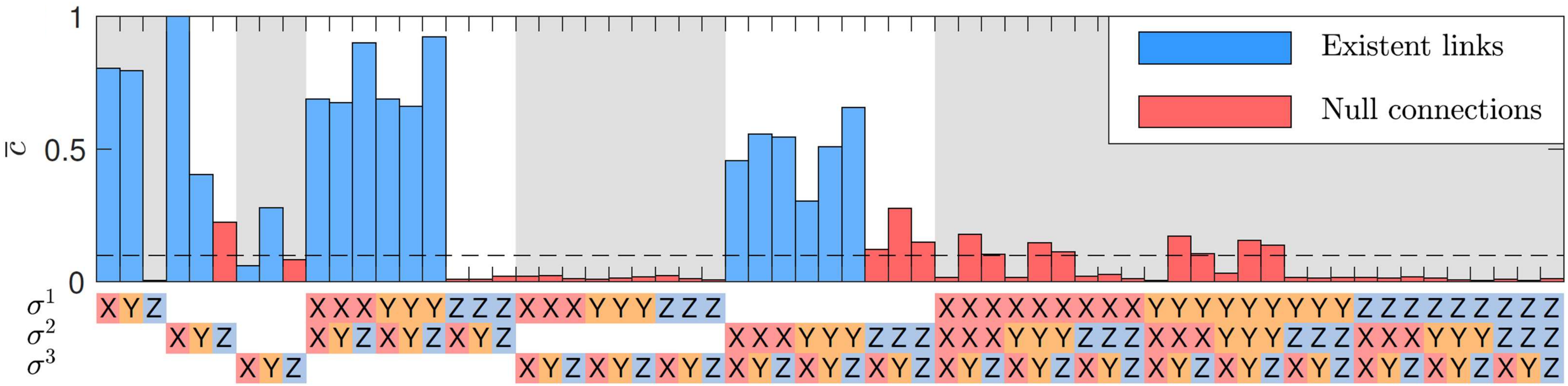
$$\begin{aligned}\mathbb{H}(t) = c_0(t)\mathbb{I} &+ \sum_{i,j} c_{i,j}(t)\sigma_j^i \\ &+ \sum_{i,j,m,n} c_{ijmn}(t)\sigma_j^i\sigma_n^m \\ &+ \sum_{i,j,m,n,k,l} c_{ijmnkl}(t)\sigma_j^i\sigma_n^m\sigma_l^k.\end{aligned}$$

$$\overline{c}_i = \int |c_i(t)| dt.$$

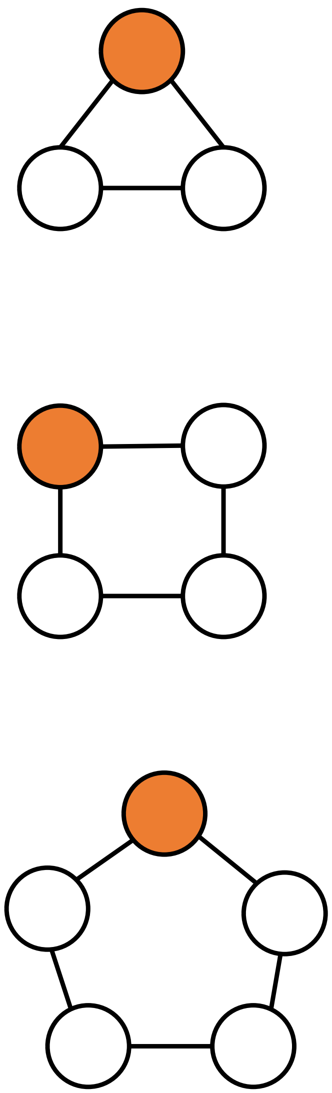
# Training process

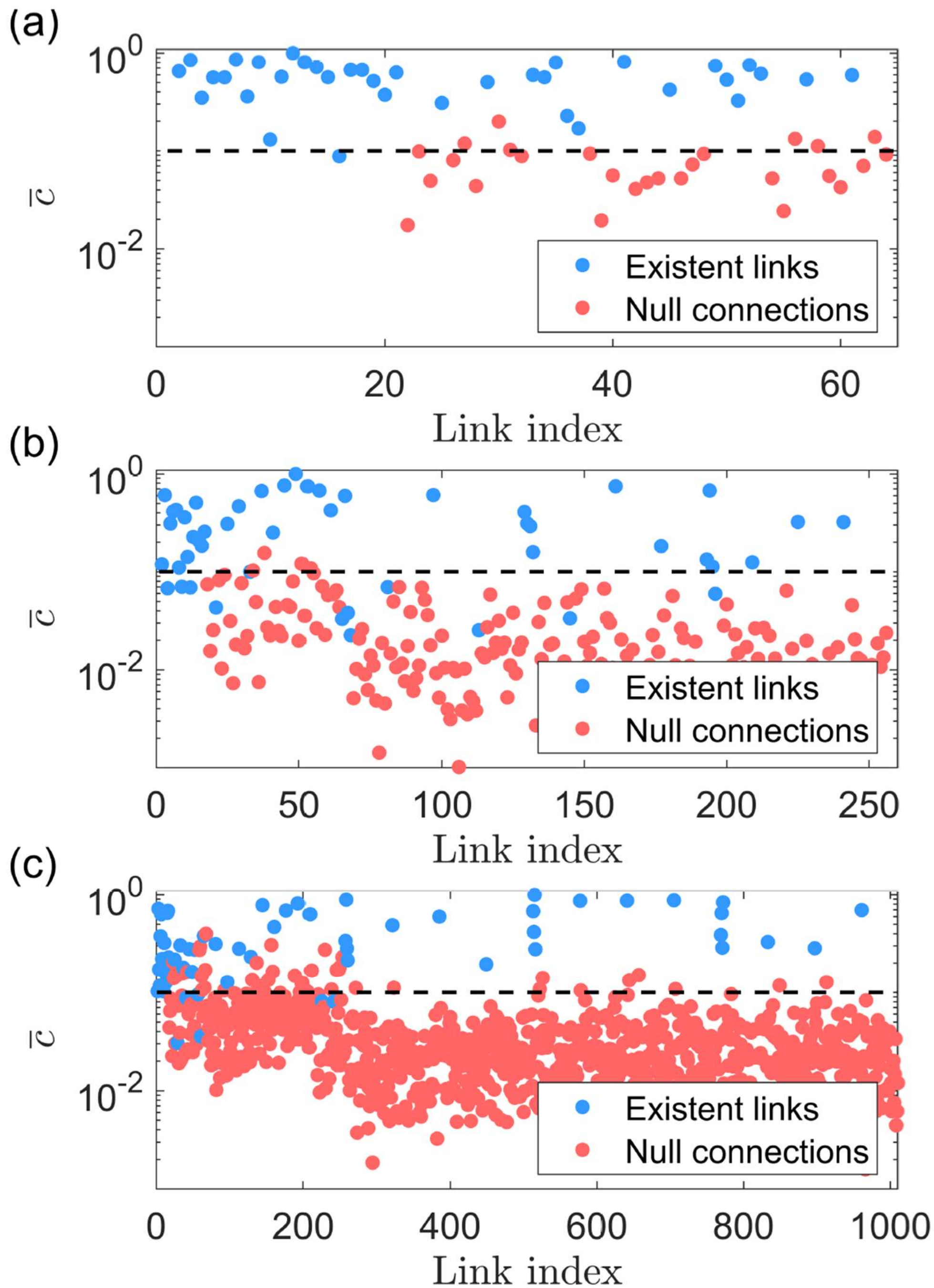
- Step 5:





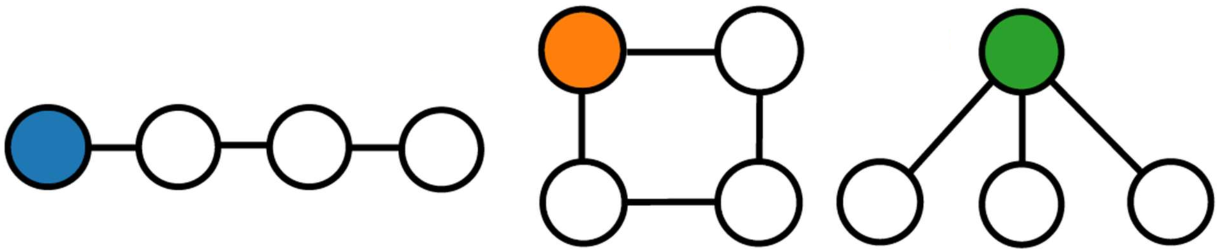
# Hamiltonian based on two-body interactions

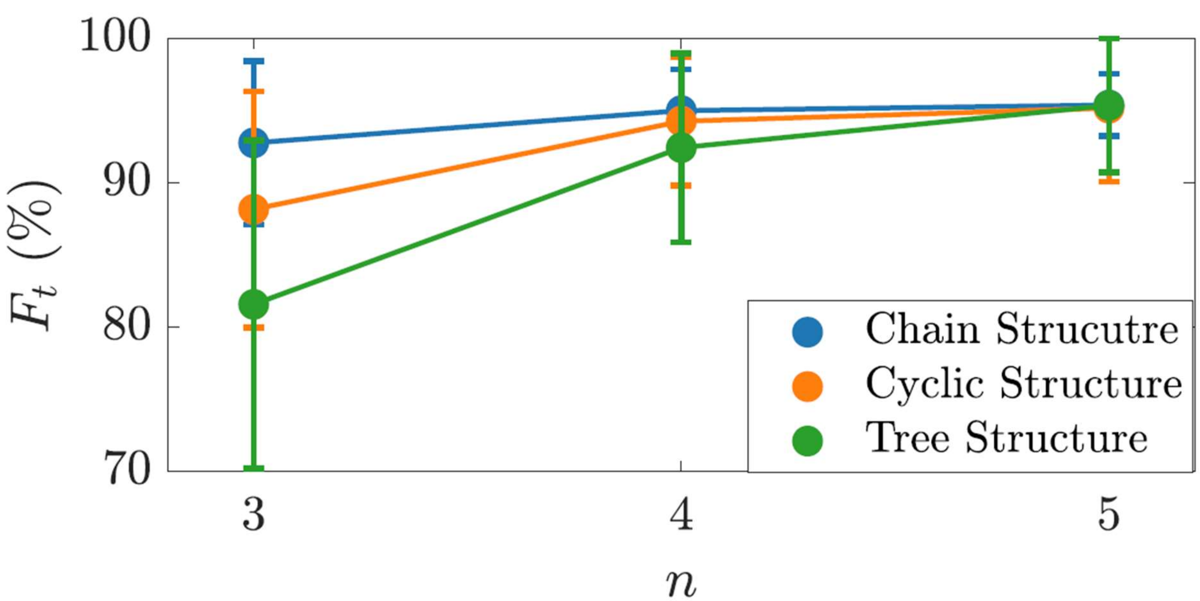




# Hamiltonian based on two-body interactions

$$F_t = \frac{4^n - 1 - (\#\text{ of missing links})}{4^n - 1},$$

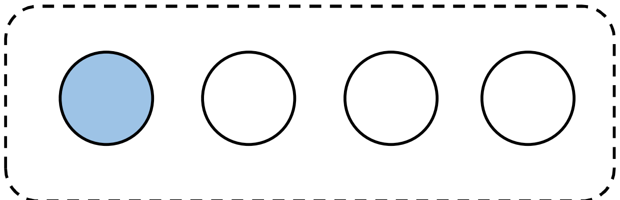


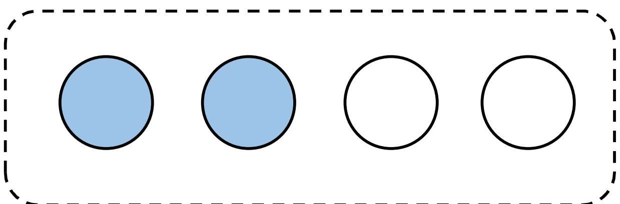


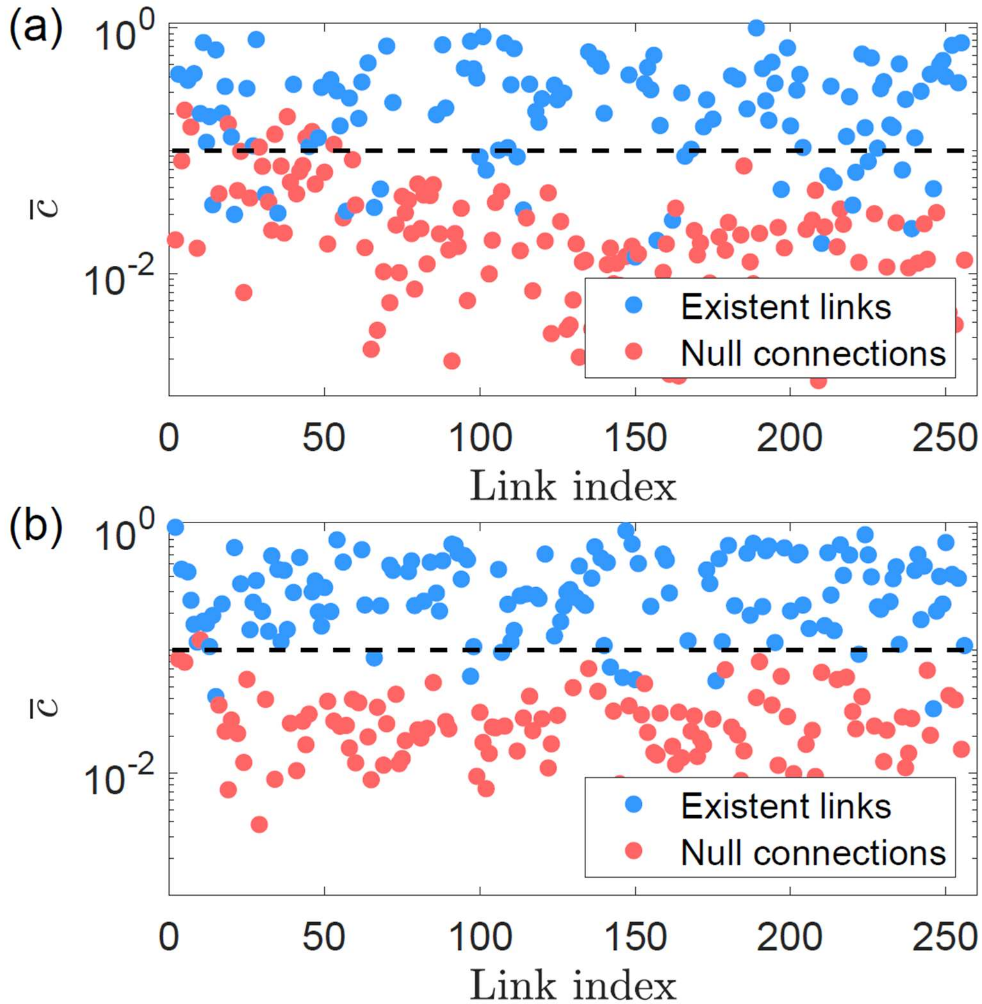
# Hamiltonian based on long-range interactions

$$H(t) = h^{(1)} + f(t)h^{(2)},$$

$$h^{(1,2)} = \sum_{i_1,i_2,\cdots,i_n=0}^{3} rc^{(1,2)}_{i_1 i_2 \cdots i_n} \sigma^1_{i_1} \sigma^2_{i_2} \cdots \sigma^n_{i_n},$$

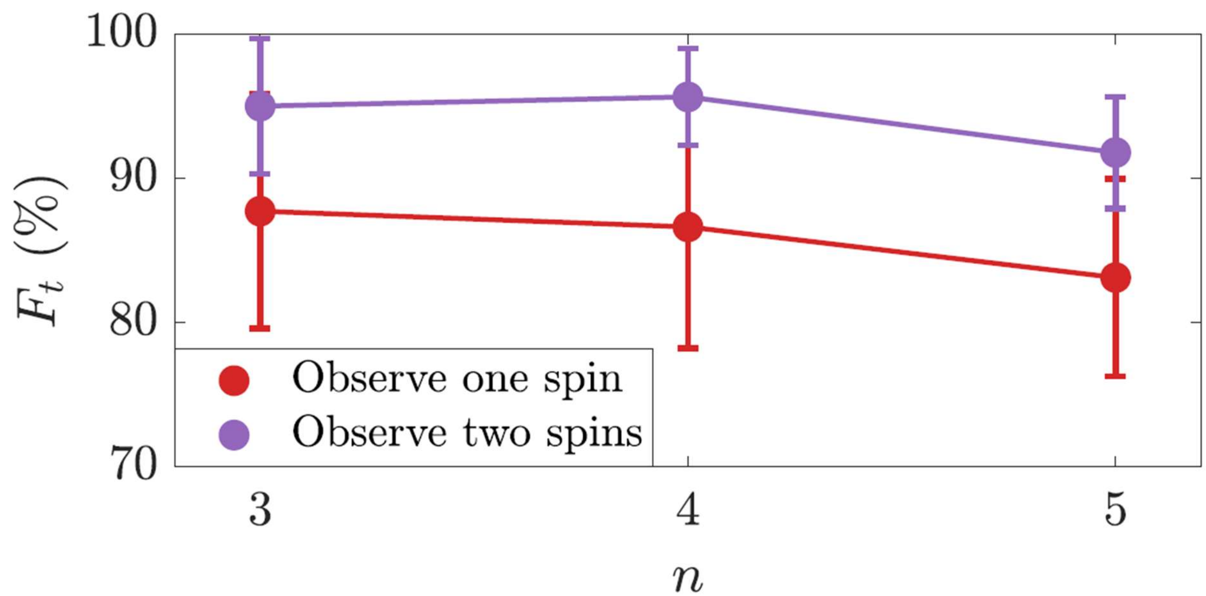






## Hamiltonian based on long-range interactions

$$F_t = \frac{4^n - 1 - (\#\text{ of missing links})}{4^n - 1},$$



# Summary

*Previous results*

- Physics enhanced machine learning in classical mechanics
- Tomography for time independent Hamiltonian

*Our results*

- Extend physics enhanced machine learning to quantum systems
- Detect the hidden structure for time dependent Hamiltonian


- **Chen-Di Han**, Bryan Glaz, Mulugeta Haile, and Ying-Cheng Lai. Tomography of time-dependent quantum spin networks with machine learning. *Phys. Rev. A* **104**, 062404 (2021).

# Publications

1. **Chen-Di, Han**, Cheng-Zhen Wang, and Ying-Cheng Lai. "Classifying and detecting quantum scars by machine learning." *To be submitted.*

2. **Chen-Di Han,** Bryan Glaz, Mulugeta Haile, and Ying-Cheng Lai. Tomography of time-dependent quantum spin networks with machine learning. *Phys. Rev. A* **104**, 062404 (2021).

3. **Chen-Di Han**, Cheng-Zhen Wang, Hong-Ya Xu, Danhong Huang and Ying-Cheng Lai. Decay of semiclassical massless Dirac fermions from integrable and chaotic cavities. *Phys. Rev. B* **98**, 104308 (2018).

4. Cheng-Zhen Wang, **Chen-Di Han**, Hong-Ya Xu, and Ying-Cheng Lai. Chaos-based Berry phase detector. *Phys. Rev. B* **99**, 144302 (2019).

5. **Chen-Di Han**, Hong-Ya Xu, Danhong Huang and Ying-Cheng Lai. Atomic collapse in pseudospin-1 systems. *Phys. Rev. B* **99**, 245413 (2019).

6. **Chen-Di Han**, Hong-Ya Xu, Liang Huang and Ying-Cheng Lai. Manifestations of chaos in relativistic quantum systems-A study based on out-of-time-order correlator. *Phys. Open* **1**,100001 (2019).

# Publications

7. **Chen-Di Han**, Hong-Ya Xu, and Ying-Cheng Lai. Electrical confinement in a spectrum of two-dimensional Dirac materials with classically integrable, mixed, and chaotic dynamics. *Phys. Rev. Res.* **2**, 013116 (2020).

8. **Chen-Di Han**, Hong-Ya Xu, and Ying-Cheng Lai. Pseudospin modulation in coupled graphene systems. *Phys. Rev. Res.* **2**, 033406 (2020).

9. **Chen-Di Han**, Bryan Glaz, Mulugeta Haile and Ying-Cheng Lai. Adaptable Hamiltonian neural networks. *Phys. Rev. Res.* **3**, 023156 (2021).

10. **Chen-Di Han** and Ying-Cheng Lai. Optical response of two-dimensional Dirac materials with a flat band. *Phys. Rev. B.* **105**, 155405 (2022).

11. Li-Li Ye, **Chen-Di Han**, Liang Huang and Ying-Cheng Lai. Geometry-induced wave-function collapse. *Phys. Rev. A.* **106**, 022207 (2022).

12. **Chen-Di Han** and Ying-Cheng Lai. Generating extreme quantum scattering in graphene with machine learning. *Under review by Phys. Rev. B.*

13. **Chen-Di Han** and Ying-Cheng Lai. Deep learning for graphene metasurface design. *In preparation.*

# Thanks for your attention !