Happy new year of

Quantum topology identification with deep neural networks and quantum walks

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3. arXiv:1811.12630 (2018);

Introduction

- Aim: To get a general and efficient method to identify topological materials.
- Claim: Deep neural networks and quantum walks together can efficiently identify topological phases and phase transitions, and assist engineering new topological materials.
- Importance: Our approach is generally applicable and suitable for different experimental setups.

Topology in quantum systems

Topologically protected matter	Topologically ordered matter
• Interactions are ignored	• Interactions are important
• Unique topologically protected ground state	• Topologically protected degeneracy of ground states
• Momentum space analysis	• Lattice/spatial space analysis
• Topological invariant: Chern number, Z_2-index…	• Topology of higher-genus manifolds;
• Short-range quantum entanglement	• Long-range quantum entanglement
• Quantum Hall effect; topological insulators…	• Fractional quantum Hall effect; topological codes…

Chern number

• The Chern number is a topological invariant. It is very reminiscent of the Euler characteristic (Gauss-Bonnet theorem):

$$\chi = \frac{1}{2\pi}\int_S dA\; K = 2 - 2g$$

for an orientable surface, where K is the Gaussian curvature and g is the genus (easy to check for sphere where $K = 1/R^2$).

• The topology comes from the geometric phase integral of the ground state in FBZ.

$$C_{n'n} = \frac{1}{2\pi}\int d\mathbf{k}\;\Omega(\mathbf{k})_{n'n}$$

$$\Omega(\mathbf{k})_{n'n} = i\left\langle \frac{\partial}{\partial k_x} u_{n',\mathbf{k}} \middle| \frac{\partial}{\partial k_y} u_{n,\mathbf{k}} \right\rangle - i\left\langle \frac{\partial}{\partial k_y} u_{n',\mathbf{k}} \middle| \frac{\partial}{\partial k_x} u_{n,\mathbf{k}} \right\rangle$$

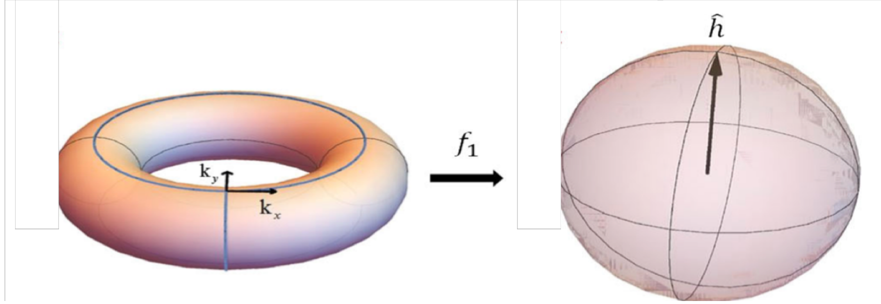
Chern number

• Consider a 2-band Chern insulator Hamiltonian

$$H(\mathbf{k}) = \mathbf{h}(\mathbf{k}) \cdot \vec{\sigma} = \begin{pmatrix} h_z & h_x - ih_y \\ h_x + ih_y & -h_z \end{pmatrix}$$

where $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$ is an array of Pauli matrices. The energies are $\pm|\mathbf{h}(\mathbf{k})|$ so we can define the unit vector $\hat{\mathbf{h}} \equiv \frac{\mathbf{h}}{|\mathbf{h}|}$

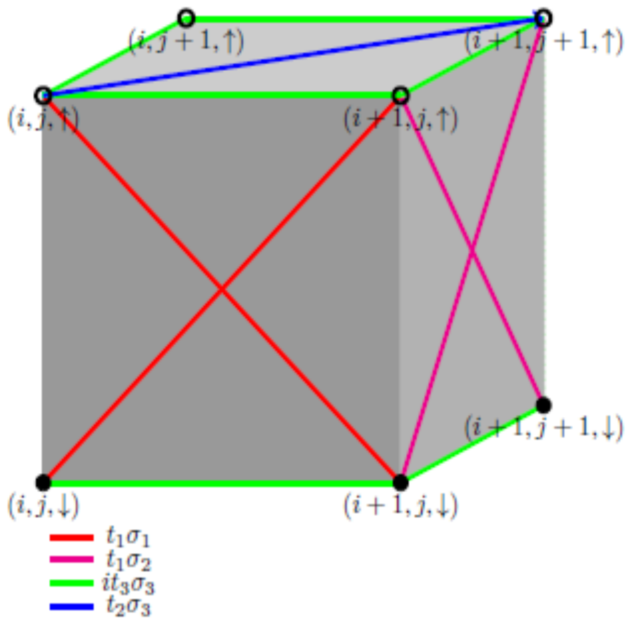
• For a closed contour over the energy surface (now defined on the 2-sphere), the (lower-band) Chern number is equal to the number of times the unit vector $\hat{\mathbf{h}}$ wraps around the origin as a function of **k** (important fact that we will need later)



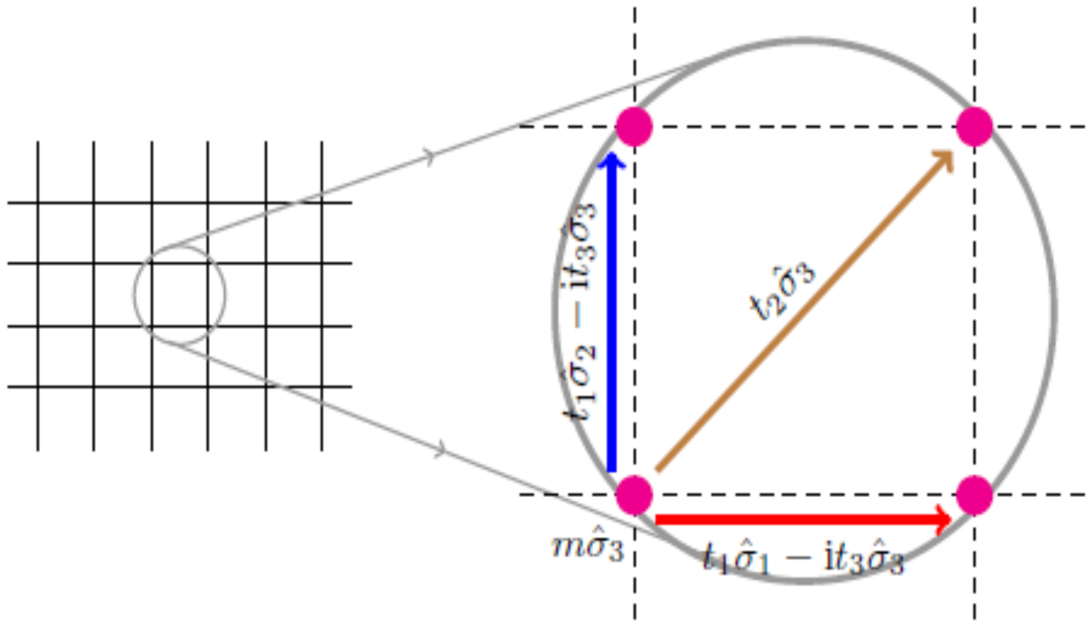
Model

$$\hat{H} = \sum_{i,j}[c^{\dagger}_{i,j}\frac{m}{2}\hat{\sigma}_3 c_{i,j} + c^{\dagger}_{i+1,j}(t_1\hat{\sigma}_1 - \mathrm{i}t_3\hat{\sigma}_3)c_{i,j}$$

$$+ c^{\dagger}_{i,j+1}(t_1\hat{\sigma}_2 - \mathrm{i}t_3\hat{\sigma}_3)c_{i,j} + c^{\dagger}_{i+1,j+1}t_2\hat{\sigma}_3 c_{i,j} + H.c.]$$



(a)



(b)

Model

- In momentum space:

$$H(\mathbf{k}) = \mathbf{h}(\mathbf{k}) \cdot \vec{\sigma} = \begin{pmatrix} h_z & h_x - ih_y \\ h_x + ih_y & -h_z \end{pmatrix}$$

- In the tight-binding model, the entries become:

$$h_x = 2t_1 \cos(k_x);$$
$$h_y = 2t_1 \cos(k_y);$$
$$h_z = m + 2t_2 \cos(k_x + k_y) + 2t_3 [\sin(k_x) + \sin(k_y)]$$

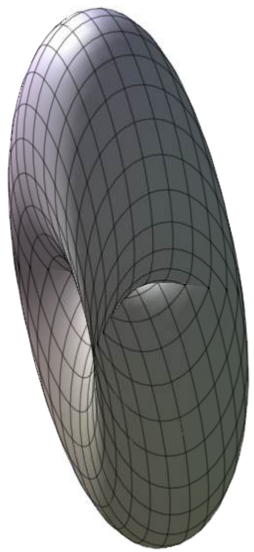
'hopping' amplitudes

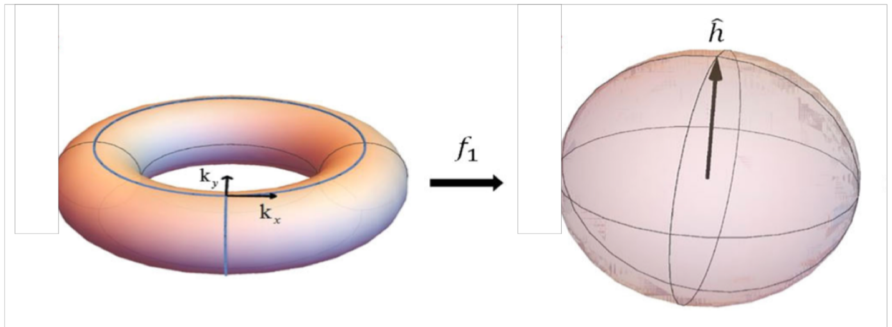
- This 'mass' term comes from the energy difference between hopping in the upper and lower planes.

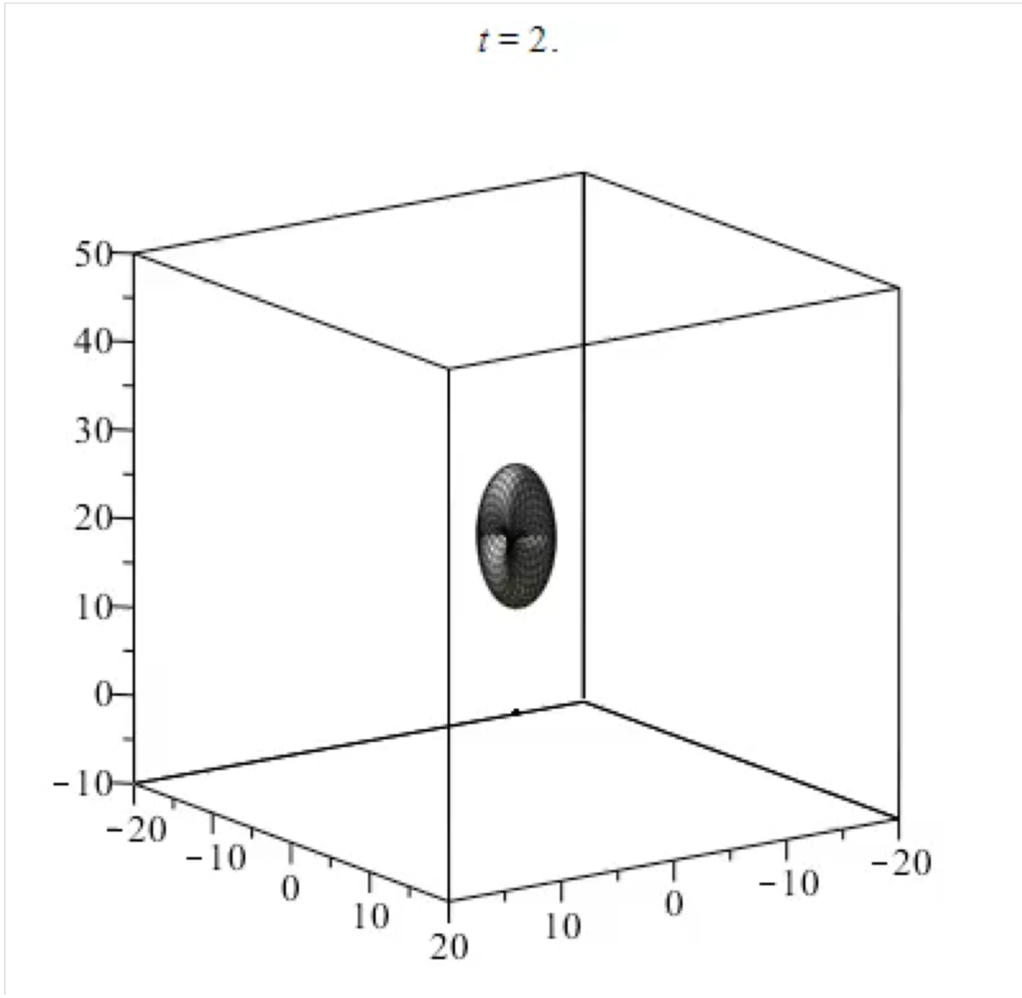
Geometric picture of the topology

- Recall that the Chern number is defined by the number of times the surface of the Hamiltonian (h_x, h_y, h_z) wraps around the origin:

t_2=0

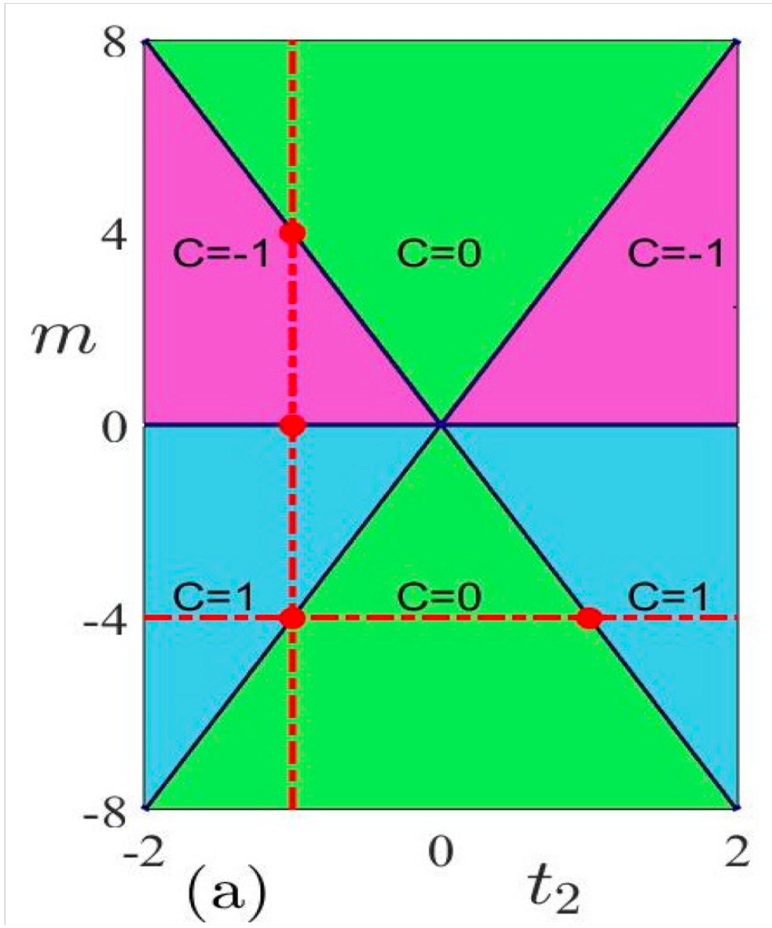






Topological phase diagram

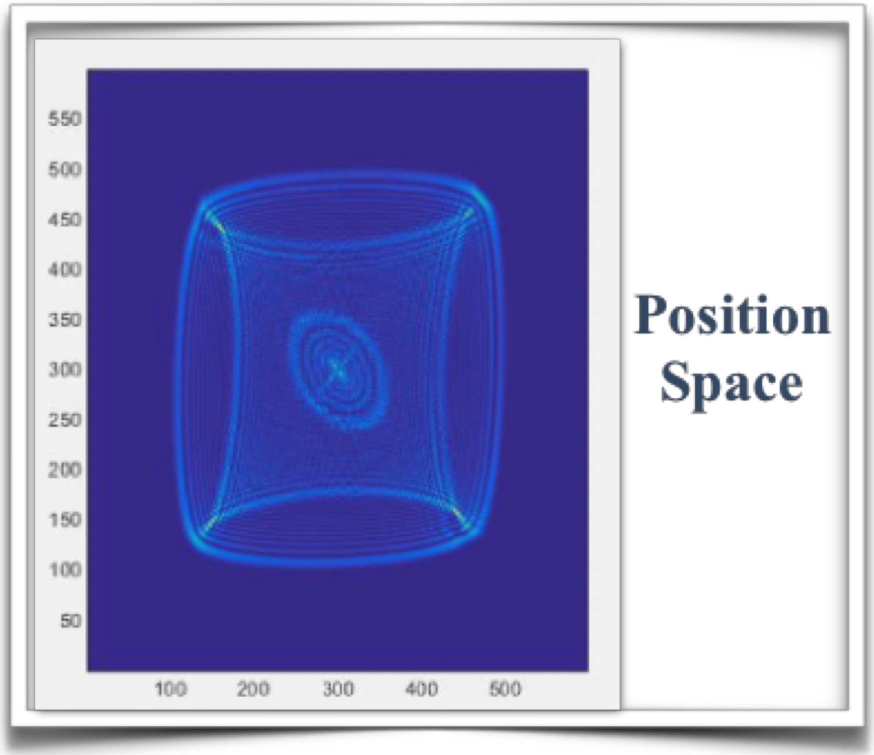
- Chern number distributions in parameters plane



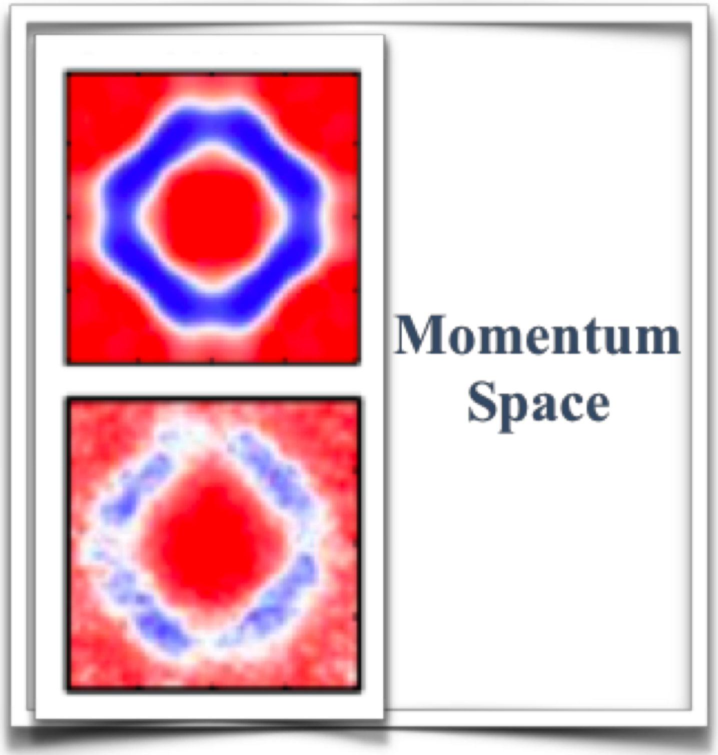
Zhang et al. PRL 119, 197401 (2017);

Continuous-time quantum walks(CTQW)

- One particle dynamical evolutions governed with H
- Described with Schrödinger equation



Zhang et al. PRL **119**, 197401 (2017);



Sun, Yi, Wang, ***Zhang***, et al. PRL **121, 250403** (2018);

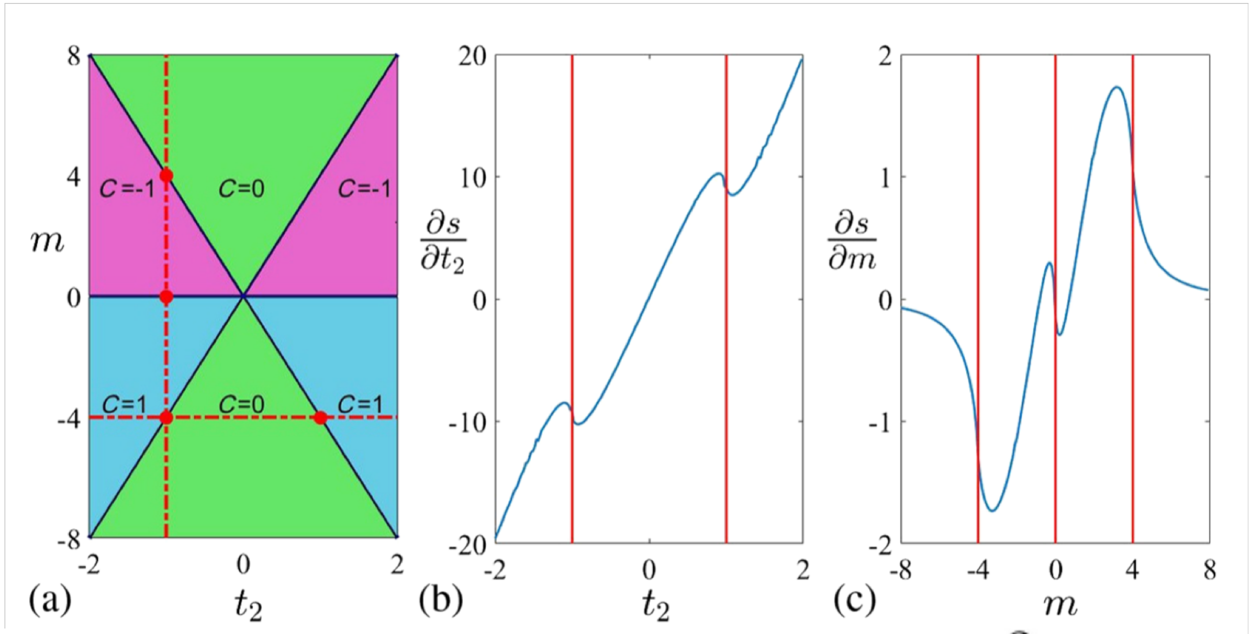
CTQW with Chern number ±1, 0

$$\hat{H} = \sum_{i,j} [c_{i,j}^{\dagger} \frac{m}{2} \hat{\sigma}_3 c_{i,j} + c_{i+1,j}^{\dagger} (t_1 \hat{\sigma}_1 - \mathrm{i} t_3 \hat{\sigma}_3) c_{i,j} + c_{i,j+1}^{\dagger} (t_1 \hat{\sigma}_2 - \mathrm{i} t_3 \hat{\sigma}_3) c_{i,j} + c_{i+1,j+1}^{\dagger} t_2 \hat{\sigma}_3 c_{i,j} + H.c.]$$

- With $t_2=0$

$$v \equiv \frac{\partial}{\partial t} \left(\langle r^2 \rangle - \langle r \rangle^2 \right)$$

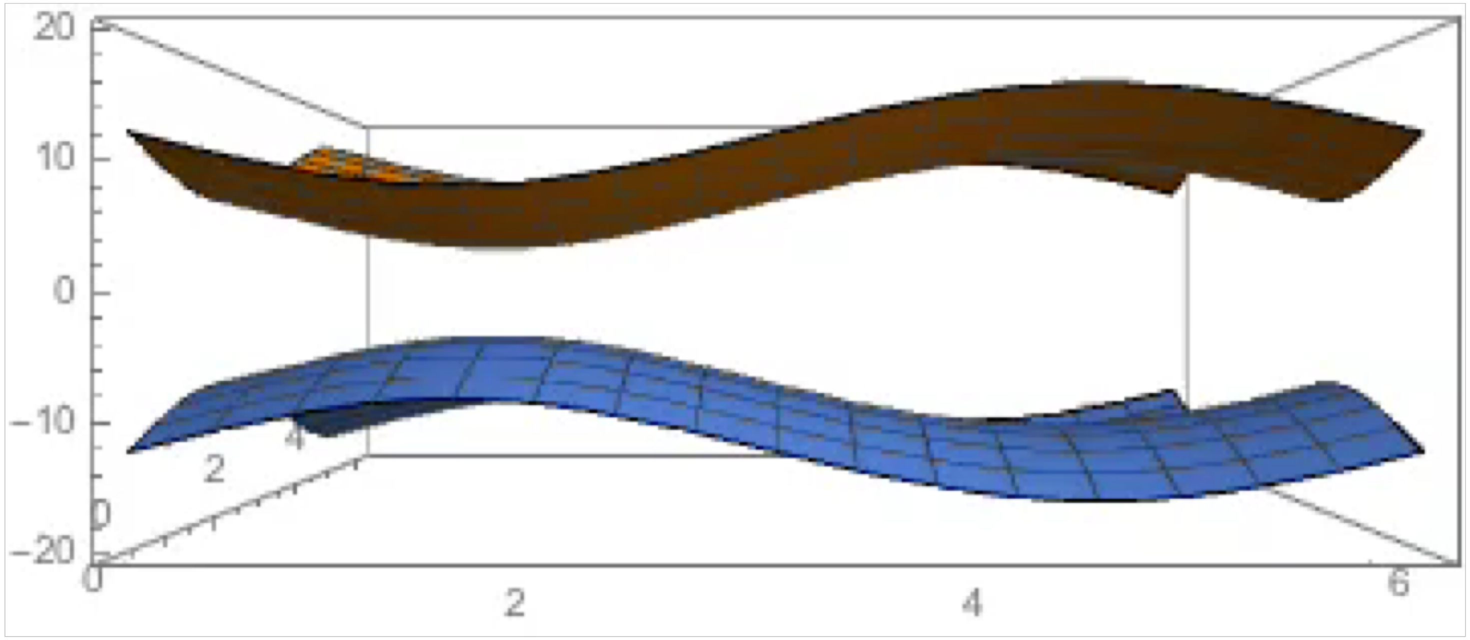
$$s = \left(\frac{\hbar}{t}\right) \frac{\partial v}{\partial t_2}$$



$$\left(\frac{\hbar^2}{t}\right) v \approx \int \frac{d\mathbf{k}}{(2\pi)^2} \left[\nabla_{\mathbf{k}} h(\mathbf{k})\right]^2 = \int \frac{d\mathbf{k}}{(4\pi)^2} \frac{\left[\nabla_{\mathbf{k}} h(\mathbf{k})^2\right]^2}{h(\mathbf{k})^2}$$

Energy bands

- The energy bands as a function of t_3 through the phase transition from C = 0 to C = 1 (m = -12 t_1):

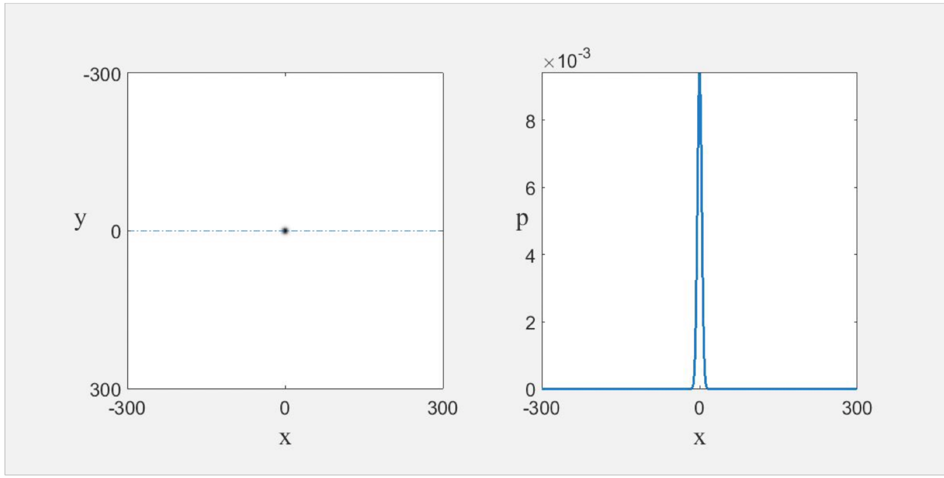


$$C = \frac{t_1^2}{\pi} \int d\mathbf{k} \frac{2t_3 \left(\sin k_x + \sin k_y\right) + m \sin k_x \sin k_y}{h(\mathbf{k})^3}$$

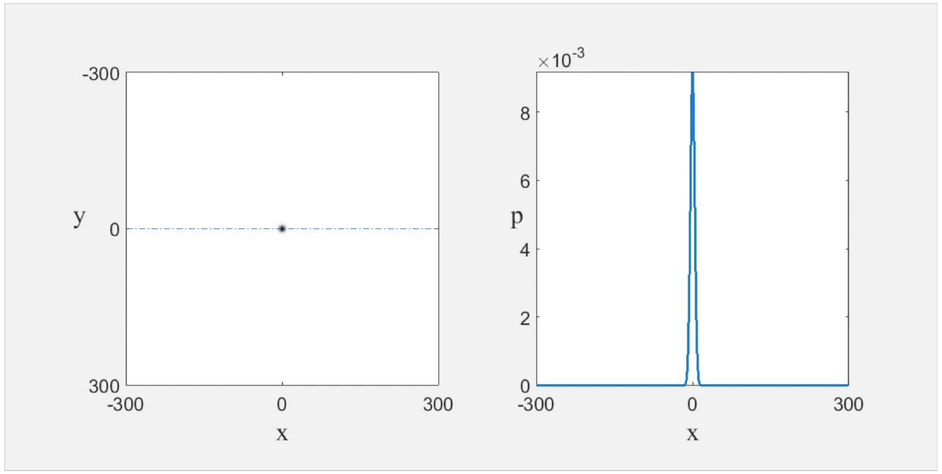
CTQW with Chern number ±1, 0

$$\hat{H} = \sum_{i,j} [c^{\dagger}_{i,j} \frac{m}{2} \hat{\sigma}_3 c_{i,j} + c^{\dagger}_{i+1,j} (t_1 \hat{\sigma}_1 - \mathrm{i} t_3 \hat{\sigma}_3) c_{i,j} + c^{\dagger}_{i,j+1} (t_1 \hat{\sigma}_2 - \mathrm{i} t_3 \hat{\sigma}_3) c_{i,j} + c^{\dagger}_{i+1,j+1} t_2 \hat{\sigma}_3 c_{i,j} + H.c.]$$

- Density profiles in positon space, with $t_2 = 0$



C=0

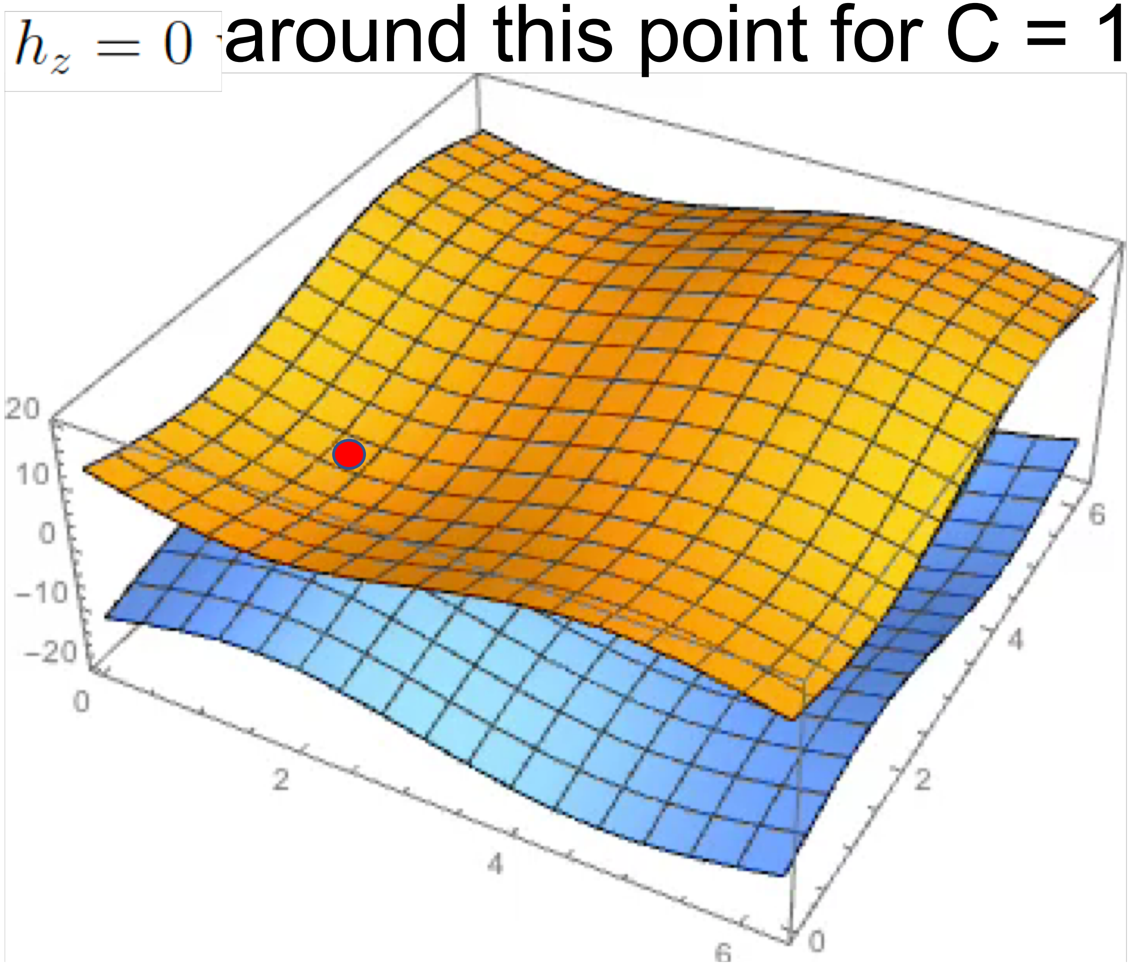


C=1

Zhang et al. PRL 119, 197401 (2017);

Energy bands

- Looking more top-wise, the band energies are minimized (maximized) at the point $(k_x, k_y) = (\pi/2, \pi/2)$ for C = 0, but in a ring around this point for C = 1:



CTQW with Chern number ±1, 0

- The wave function in position space

$$|\psi(t)\rangle = \sum_{\boldsymbol{k}} \begin{pmatrix} \frac{h_z(-\mathrm{i}\sin(E_{\boldsymbol{k}}t))}{E_{\boldsymbol{k}}} - \cos\left(E_{\boldsymbol{k}}t\right) \\ \frac{(h_x+\mathrm{i}h_y)(-\mathrm{i}\sin(E_{\boldsymbol{k}}t))}{E_{\boldsymbol{k}}} \end{pmatrix} |\boldsymbol{k}\rangle ,$$

- Around $E_k = \pm\sqrt{h_x^2 + h_y^2 + h_z^2} = 0$

$$\psi_{\downarrow}(r,t) \sim \int_0^{\infty} \frac{k^2 dk J_1\left[r\left(\frac{\pi}{2}+k\right)\right]}{\sqrt{a+bk^2+ck^4}} \sim \begin{cases} \text{const.} & \mathrm{C}=0 \\ J_1(r) & \mathrm{C}=1 \end{cases}$$

so that there is a ring of peaks near the spatial origin for non-zero Chern number, but no feature for topological trivial systems.

CTQW with Chern number ±1, 0

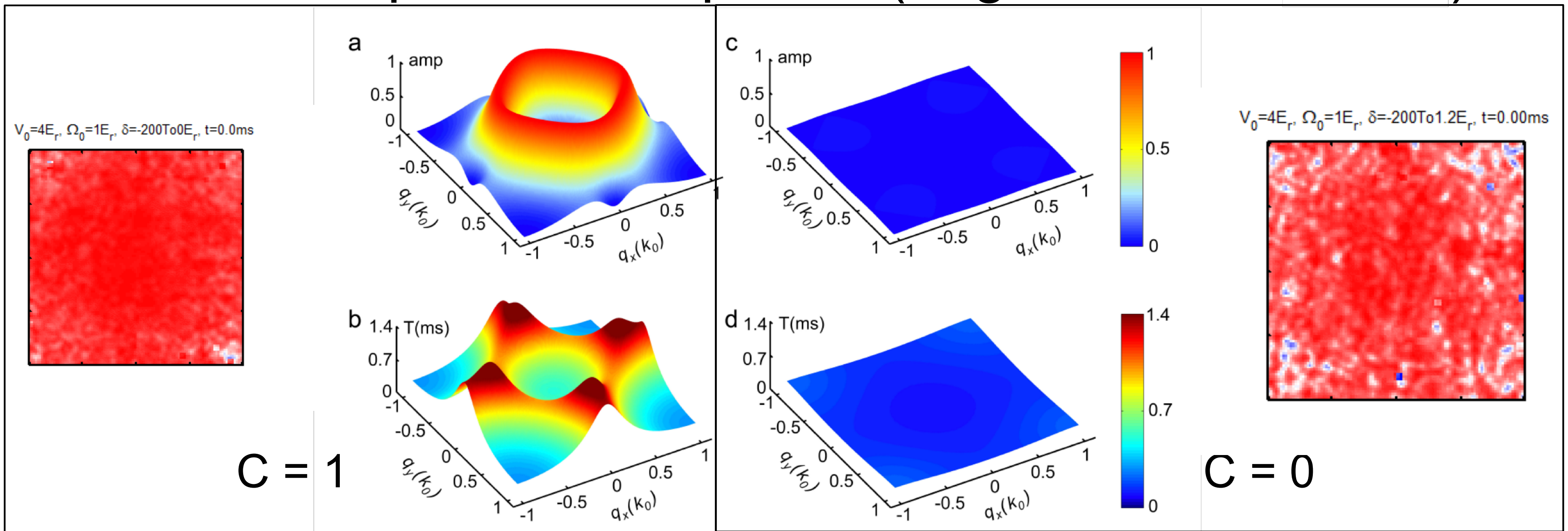
- Dynamical observation in momentum space:

$$|\psi(t)\rangle = \sum_{\boldsymbol{k}} \begin{pmatrix} \frac{h_z(-\mathrm{i}\sin(E_{\boldsymbol{k}}t))}{E_{\boldsymbol{k}}} - \cos\left(E_{\boldsymbol{k}}t\right) \\ \frac{(h_x+\mathrm{i}h_y)(-\mathrm{i}\sin(E_{\boldsymbol{k}}t))}{E_{\boldsymbol{k}}} \end{pmatrix} |\boldsymbol{k}\rangle\,,$$

$$P(\boldsymbol{k}) = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow},$$

$$= \frac{h_z^2 + \cos\left(2E_k t\right)\left(h_x^2 + h_y^2\right)}{E_k^2},$$

- Oscillation amplitude and period (ring locations $h_z = 0$)



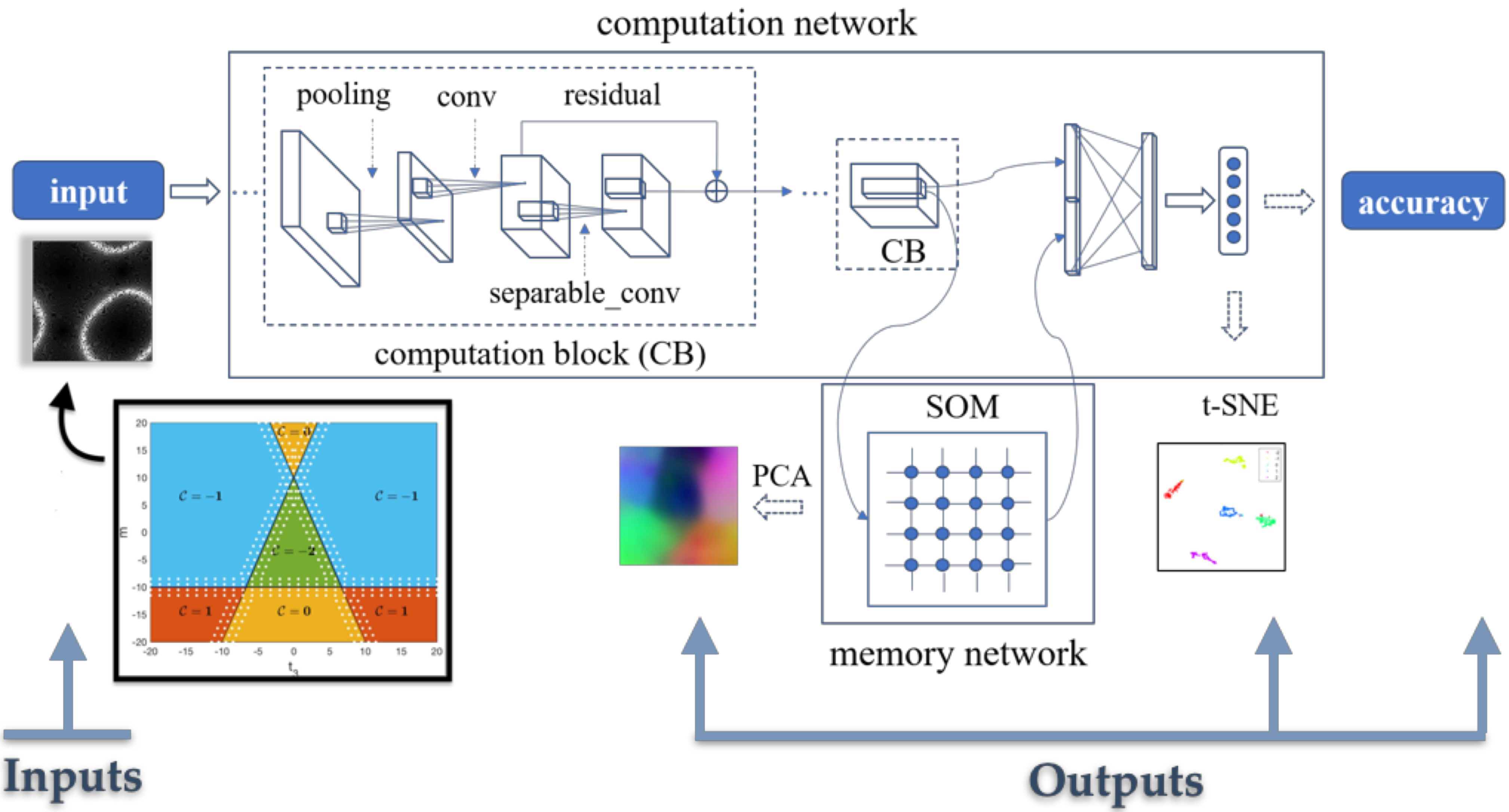
Sun, Yi, Wang, Zhang, et al. PRL 121, 250403 (2018);

Higher C ?

perturbations?

Conjecture:
CTQW contain all information on topology of the Hamiltonian.
Problem:
How do we identify the topology

Solution: Deep Neural Networks & CTQW

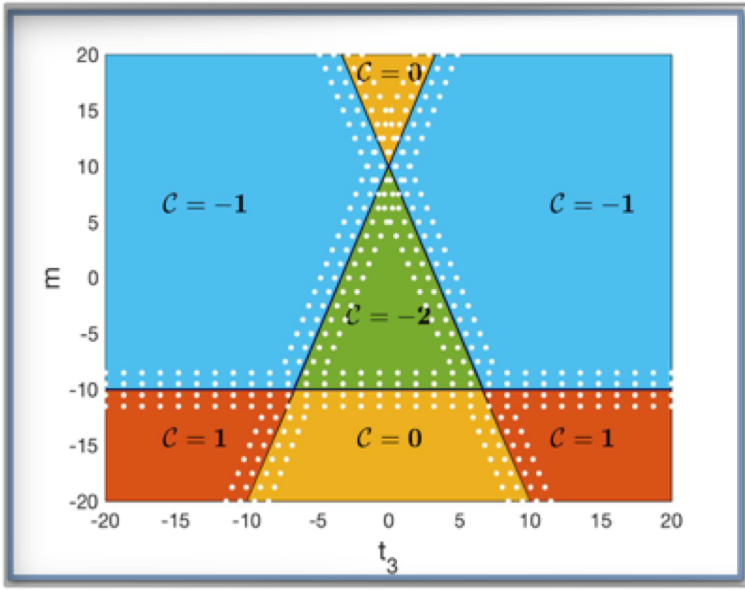


Ming, Lin, Bartlett, Zhang, arXiv 1811.12630 (2018);

Input data: CTQW

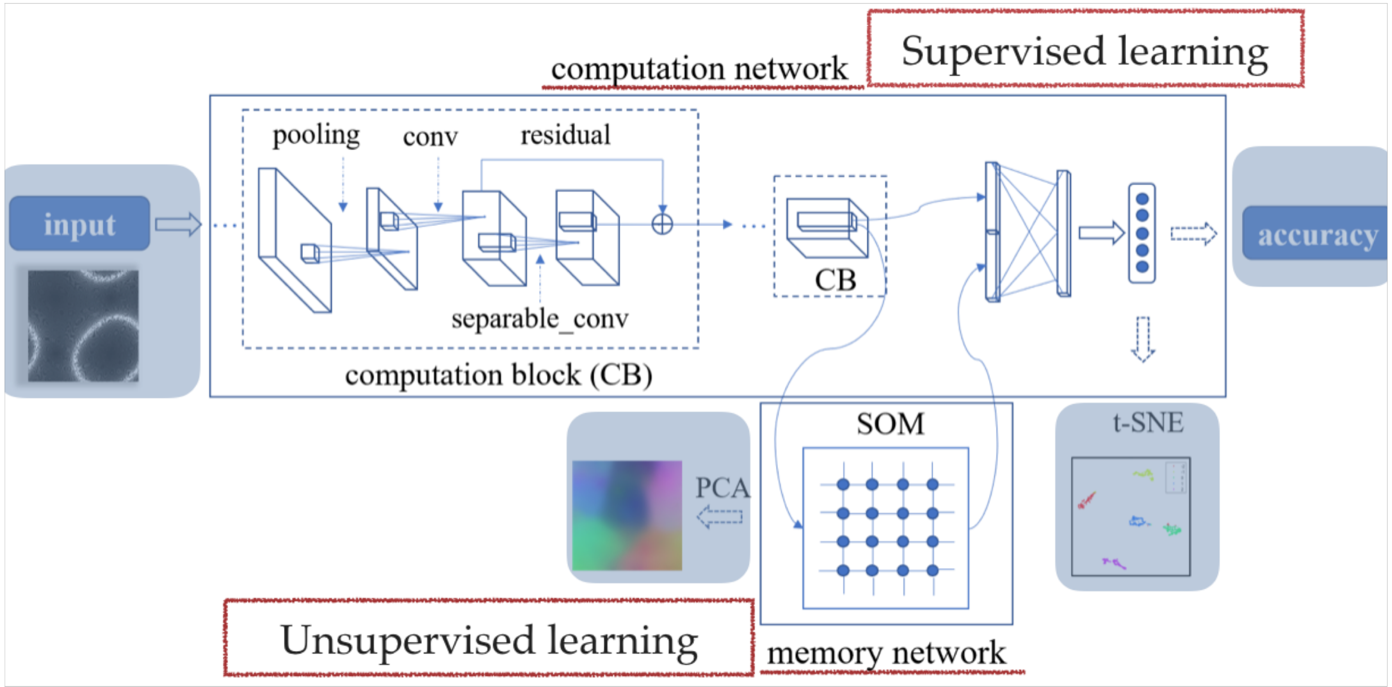
- 2D Spin-orbit coupling Hamiltonian with strength {m, t_3}
- Chern number of our simulated system C={0, ±1, ±2}

$$\hat{H} = \sum_{x,y} \Big[c^\dagger_{x,y} \frac{m}{2} \hat{\sigma}_3 c_{x,y} + c^\dagger_{x+1,y} (t_{1x} \hat{\sigma}_1 - \mathrm{i} \frac{3t_3}{4} \hat{\sigma}_3) c_{x,y} + c^\dagger_{x,y+1} (t_{1y} \hat{\sigma}_2 - \mathrm{i} \frac{3t_3}{4} \hat{\sigma}_3) c_{x,y} + c^\dagger_{x+1,y+1} t_2 \hat{\sigma}_3 c_{x,y} + h.c. \Big]$$



- "whole": all the coloured area;
- "Transition": all the dotted area;
- Density profiles in both momentum and position space
- Noisy data

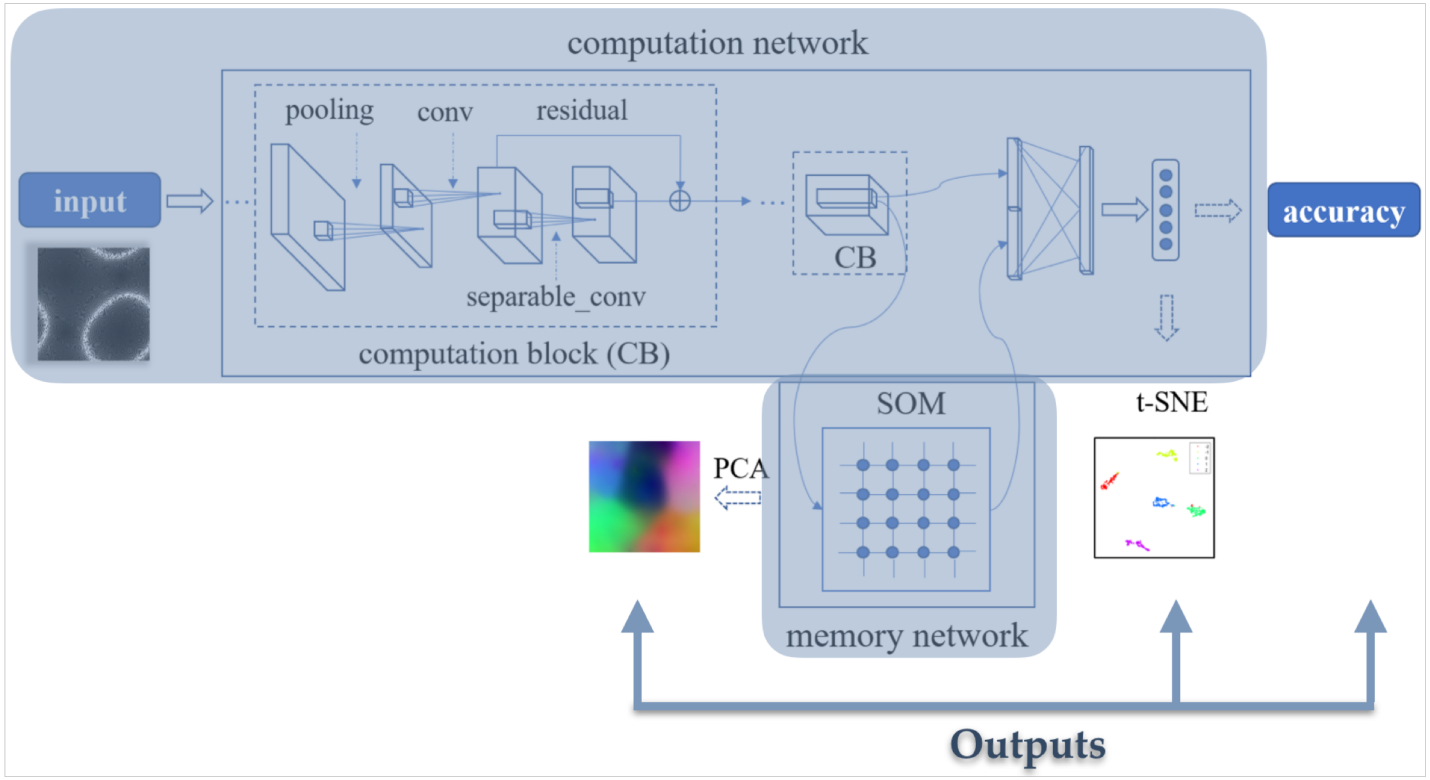
DNN: hybrid learning paradigm



- **Computation network:** Error correction learning, such as back-propagation with gradient descent. **Supervised learning**: reduce the difference between trained output and the target vectors.
- **Memory network:** Self-organising map (SOM) reveals the hidden correlations; **Unsupervised learning**

Outputs:

- **Computation network:** Statistical accuracy and T-distributed stochastic neighbour embedding (t-SNE)
- **Memory network:** Principal component analysis (PCA)



Results-I:

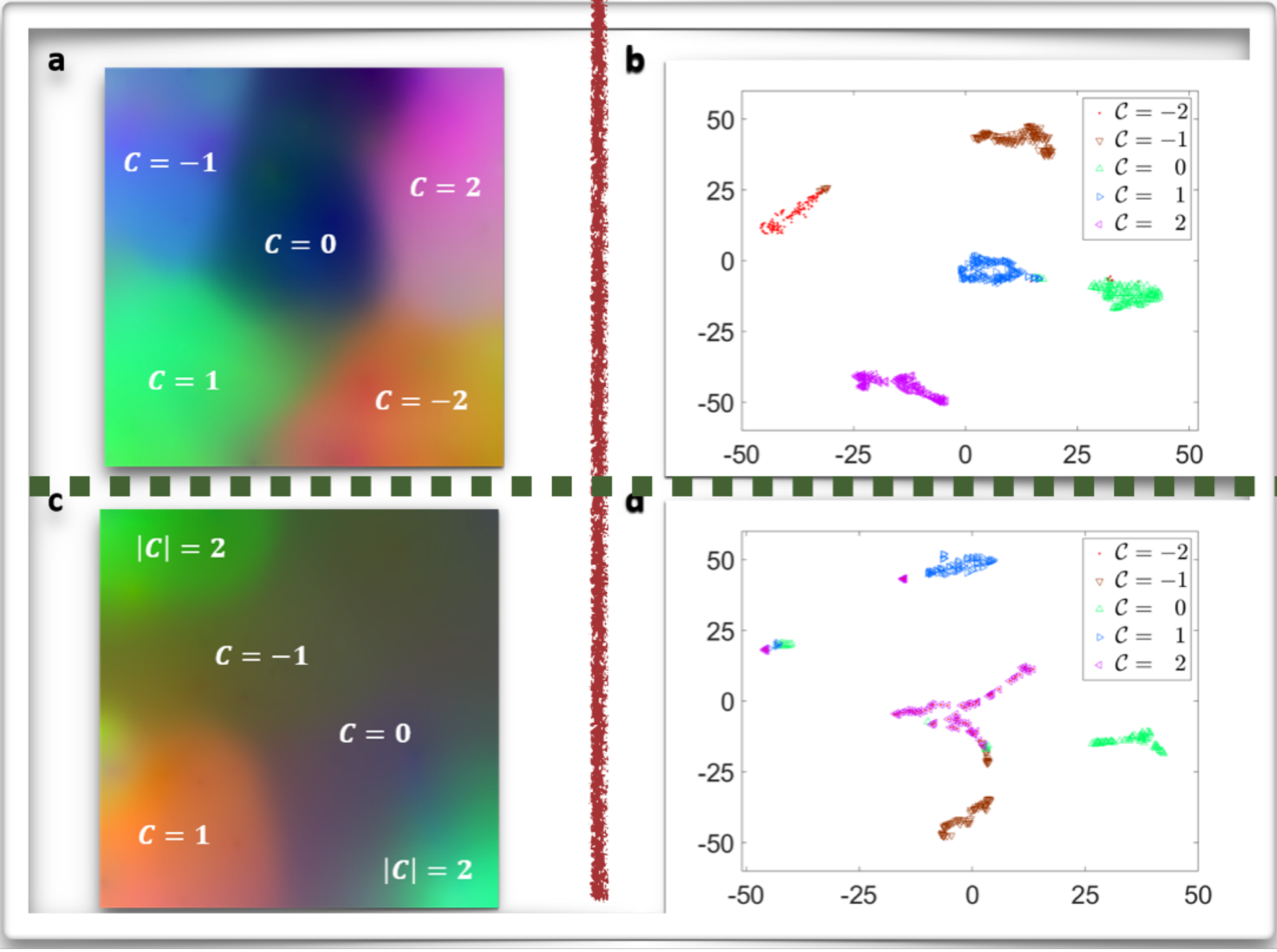
The statistical accuracy with ideal input data							
Density Profile Data		$\mathcal{C}$					Overall
Phase Diagram Area	Measurement Domain	-2	-1	0	1	2	
Whole	Momentum	0.979	0.954	0.965	0.952	1.000	0.970
	Position	0.726	0.961	0.692	0.931	0.195	0.703
Transition	Momentum	0.994	0.869	0.965	0.647	1.000	0.917
	Position	0.94	0.672	0.748	0.587	0.566	0.714

The statistical accuracy with noisy input data							
Density Profile Data		$\mathcal{C}$					Overall
Phase Diagram Area	Measurement Domain	-2	-1	0	1	2	
Whole	Momentum	0.952	0.960	0.955	0.919	1.000	0.957
	Position	0.290	0.955	0.832	0.909	0.554	0.711
Transition	Momentum	0.959	0.880	0.882	0.625	1.000	0.891
	Position	0.924	0.843	0.805	0.648	0.541	0.744

Results-II:

Principal component analysis (PCA)

T-distributed stochastic neighbour embedding (t-SNE)

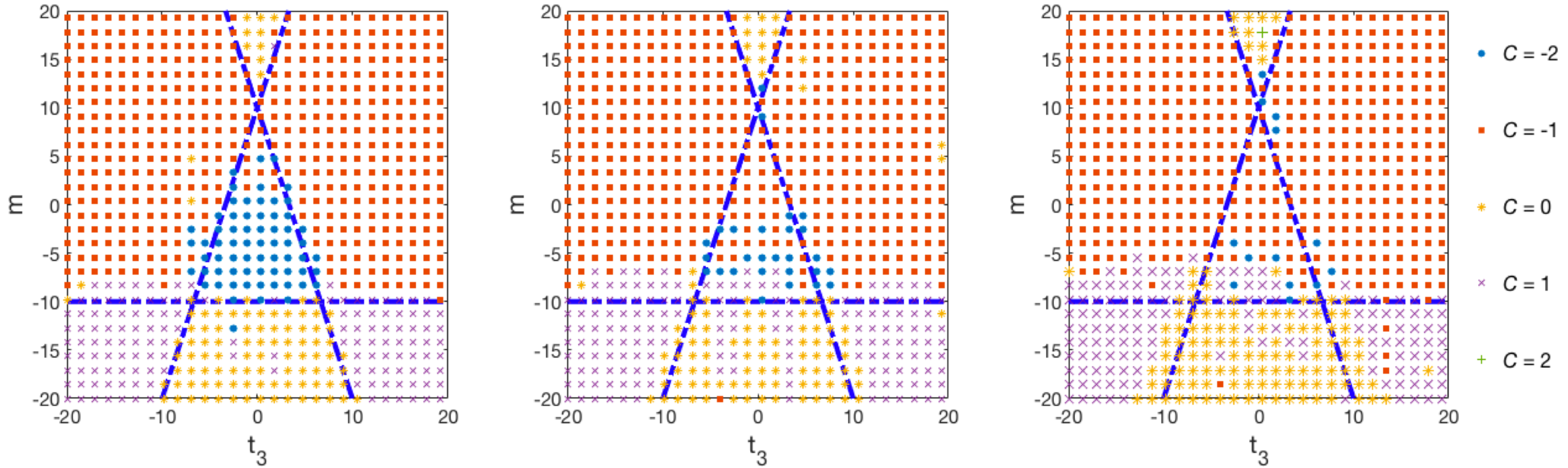


Momentum

Position

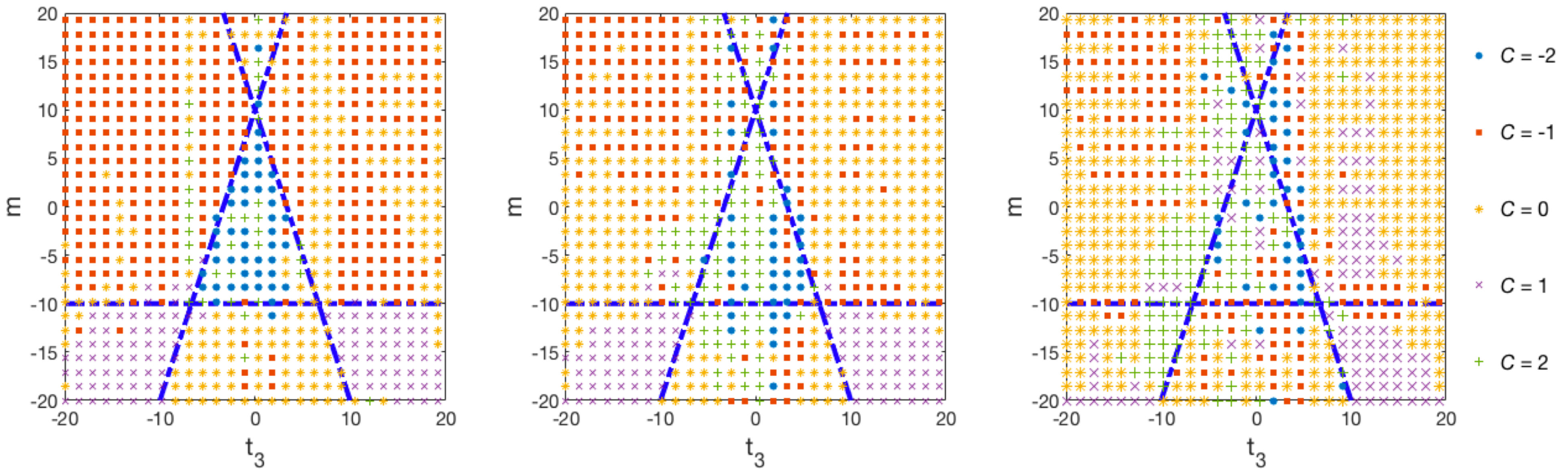
Identify the effects of perturbation-I

- Long-range interactions: Next-nearest neighbour coupling in x direction: $h^x_{nnn} = tt^* \cos(2k_x)\sigma_z$
- *tt* is taking 3,6,9
- With trained DNN, we obtain the phase diagram

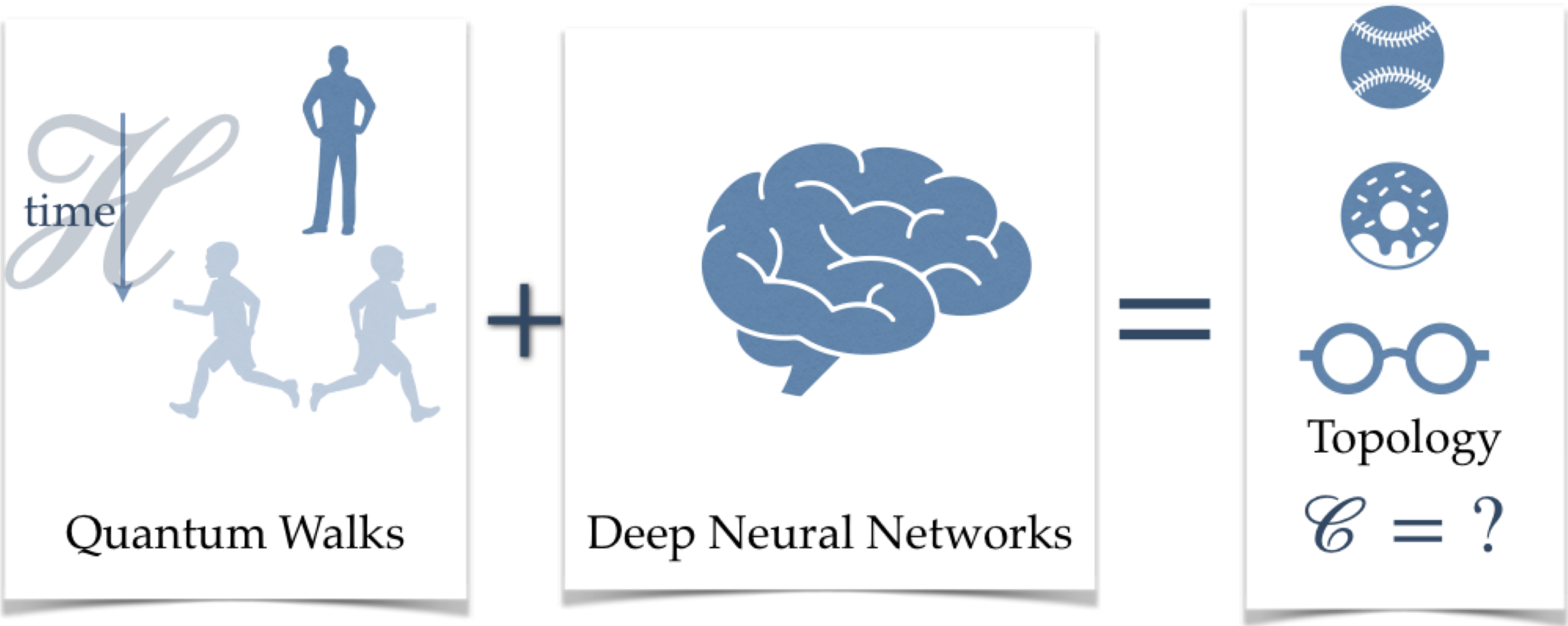


Identify the effects of perturbation-II

- External magnetic field in y direction $h^{y}_{m}=\varphi Y\sigma_z$
- φ is taking from 0.001, 0.005, 0.01
- With trained DNN, we obtain the phase diagram



Summary



A universal automated method for quantum topology identification, the efficient discovery and analysis of novel quantum material, the design of robust quantum technologies.

Thanks!

*Ming, Lin, Bartlett, **Zhang**, arXiv 1811.12630 (2018);*