

# Scalable quantum simulation for topological quantum phases on noisy quantum devices



Seiji Yunoki (RIKEN)



Tomonori Shirakawa (RIKEN)

## Rong-Yang Sun (RIKEN)

*Computational Materials Science Research Team  
RIKEN Center for Computational Science (R-CCS)*

*and*

*RIKEN Center for Quantum Computing (RQC)*

*and*

*RIKEN iTHEMS*



**QIMG2023**  
**2023/09/25**

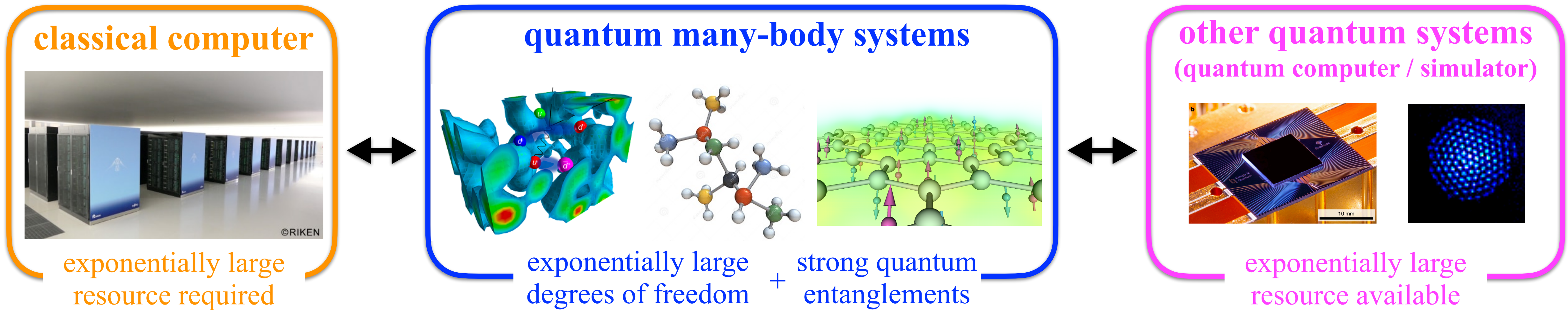
- Quantum simulation in NISQ era & its scalability
- Scalable quantum simulation of symmetry-protected topological (SPT) states  
[arXiv:**2303.17187**]
- Scalable quantum simulation of intrinsic topologically ordered (TO) states  
[arXiv:**2210.14662**]
- Summary

“...Nature isn’t classical, dammit, and **if you want to make a simulation of nature, you’d better make it quantum mechanical**, and by golly it’s a wonderful problem, because it doesn’t look so easy...”

— R. P. Feynman, *Int. J. Theor. Phys.* **21**, 467 (1982)

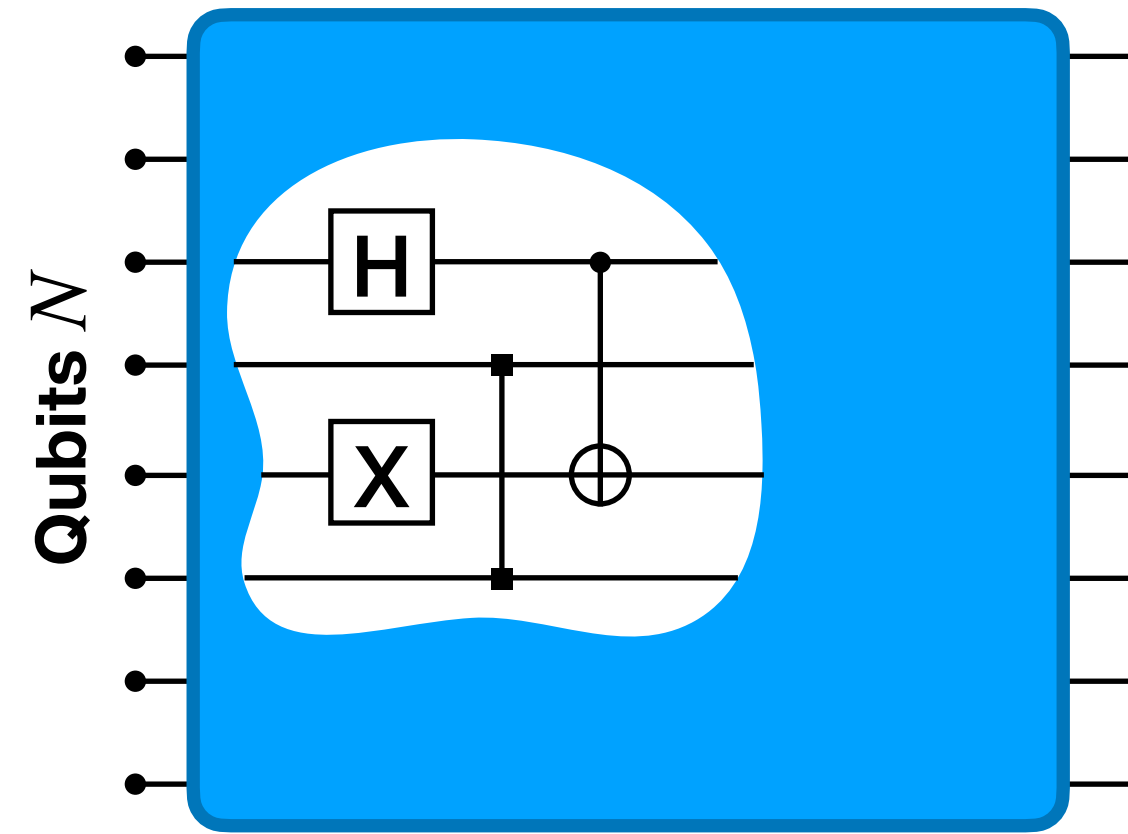


R. P. Feynman



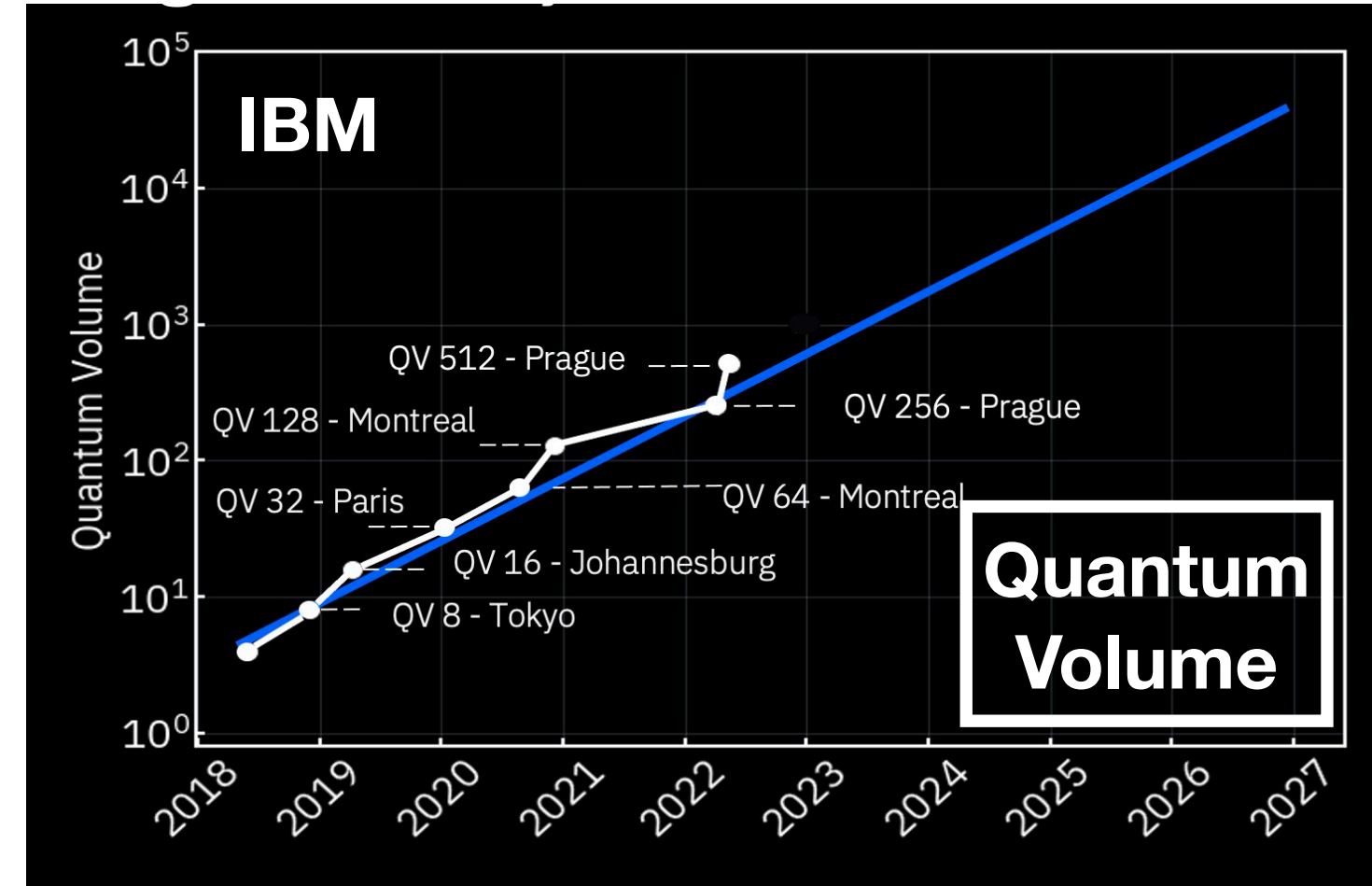
Simulating a quantum system by using other quantum systems (i.e. **controllable** quantum devices)

## Quantum circuit

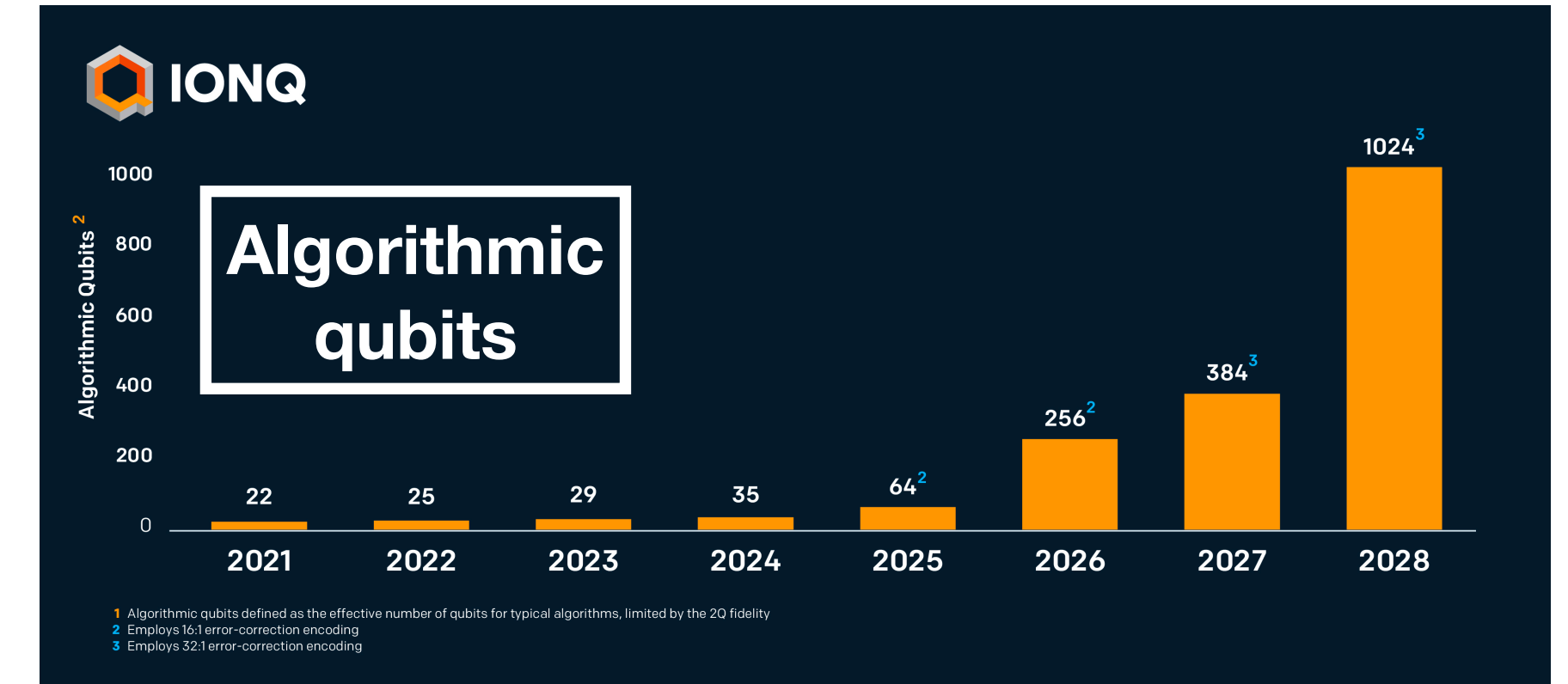


Circuit Depth  $D$

## Capacity metrics of NISQ devices



$$\log_2 V_Q = \arg \max \{ \min[N, D(N)] \}$$

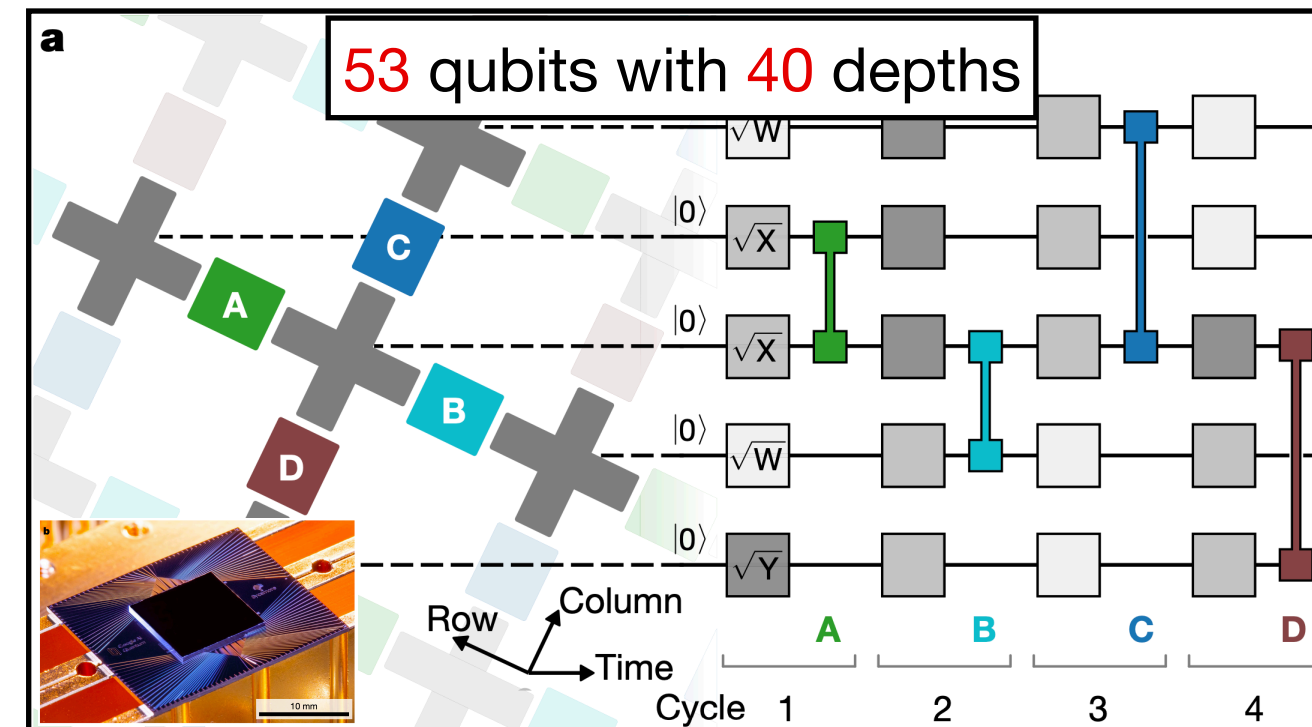


$$\#AQ = N: \text{successful performing } N^2 \text{ two-site gates}$$

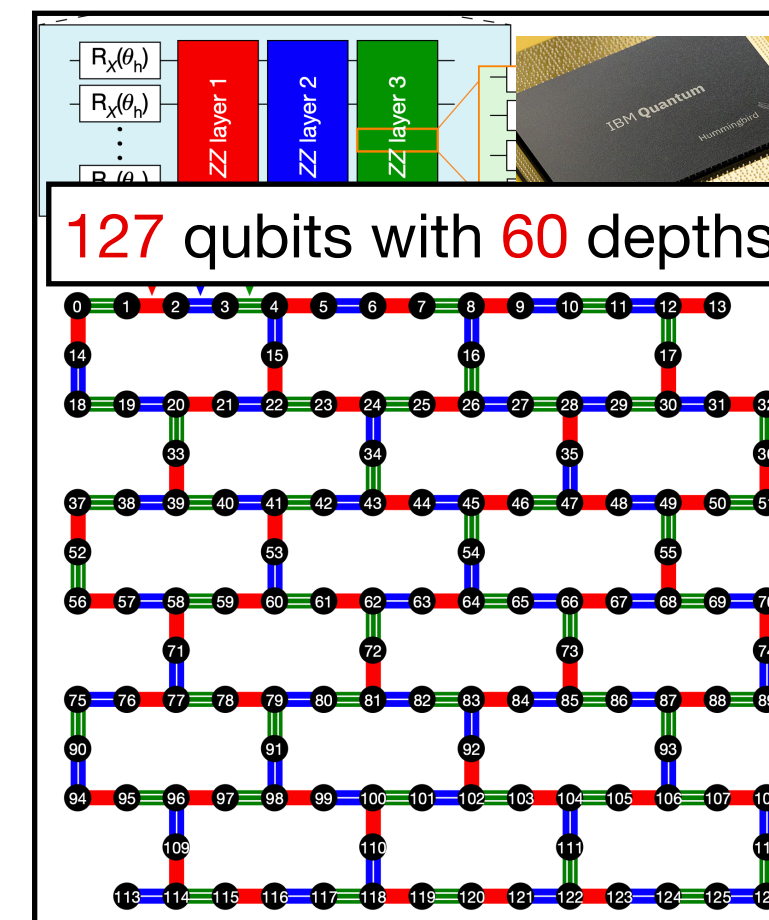
## Noisy intermediate-scale quantum (NISQ) device

A few  $\mathcal{O}(10^1 \sim 10^2)$  qubits **without** error correction

A few  $\mathcal{O}(10^0 \sim 10^1)$  circuit depths

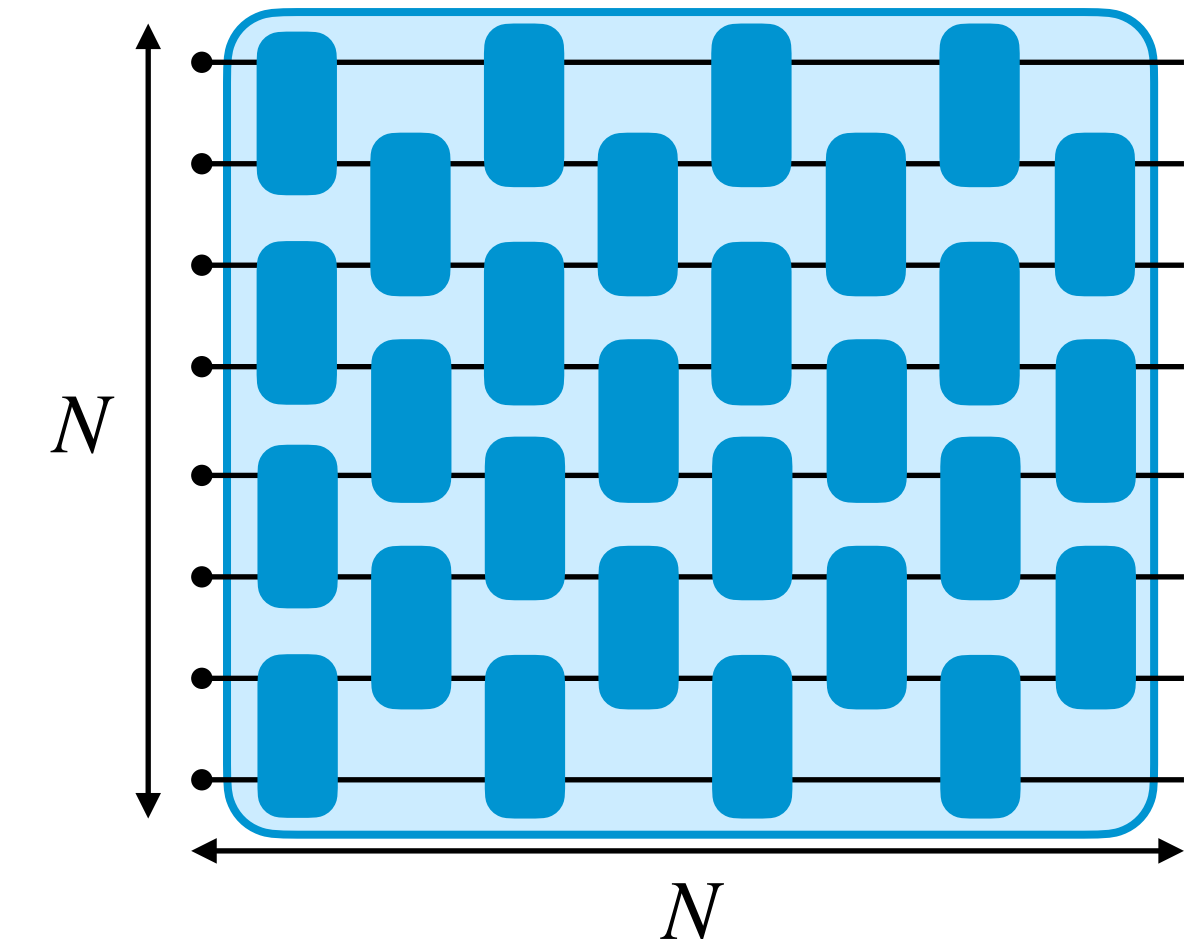


Nature **574**, 7779 (2019)



Nature **618**, 7965 (2023)

## NISQ device scalability

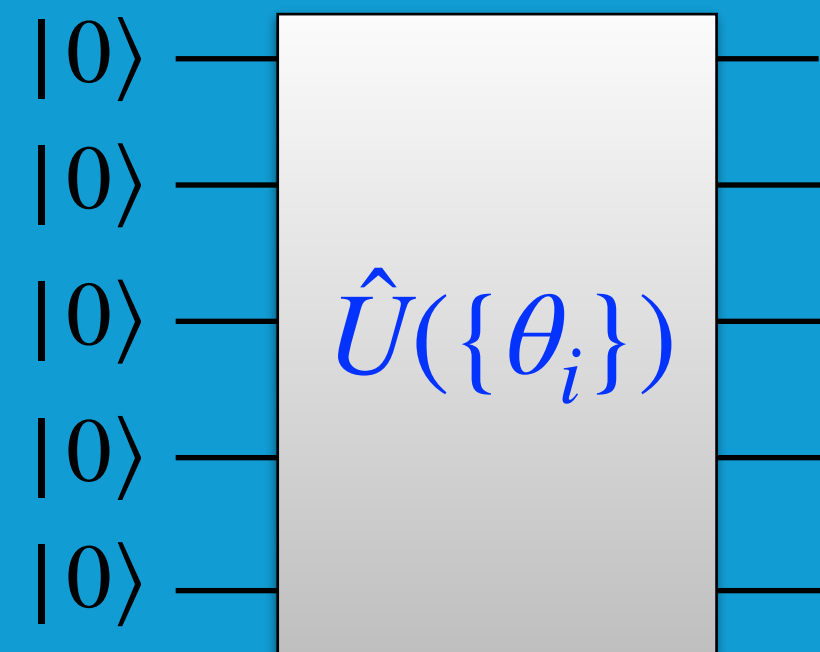


## VQE & its scalabilities

$$\hat{H} |\Psi_G\rangle = E_G |\Psi_G\rangle$$

quantum computer

Parametrized quantum circuit (PQC)



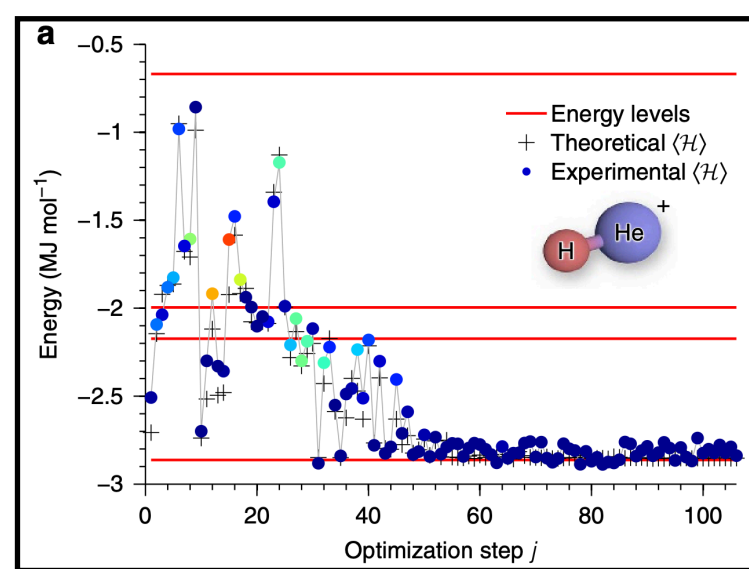
expectation value of energy

$$E(\{\theta_i\}) = \sum_k \langle \hat{H}_k \rangle_{\{\theta_i\}}$$

variational quantum state:

**PQC Ansatz**

$$|\Psi(\{\theta_i\})\rangle = \hat{U}(\{\theta_i\}) |0\rangle = \text{unitary operator}$$



classical computer

optimization of variational parameters  $\{\theta_i\}$

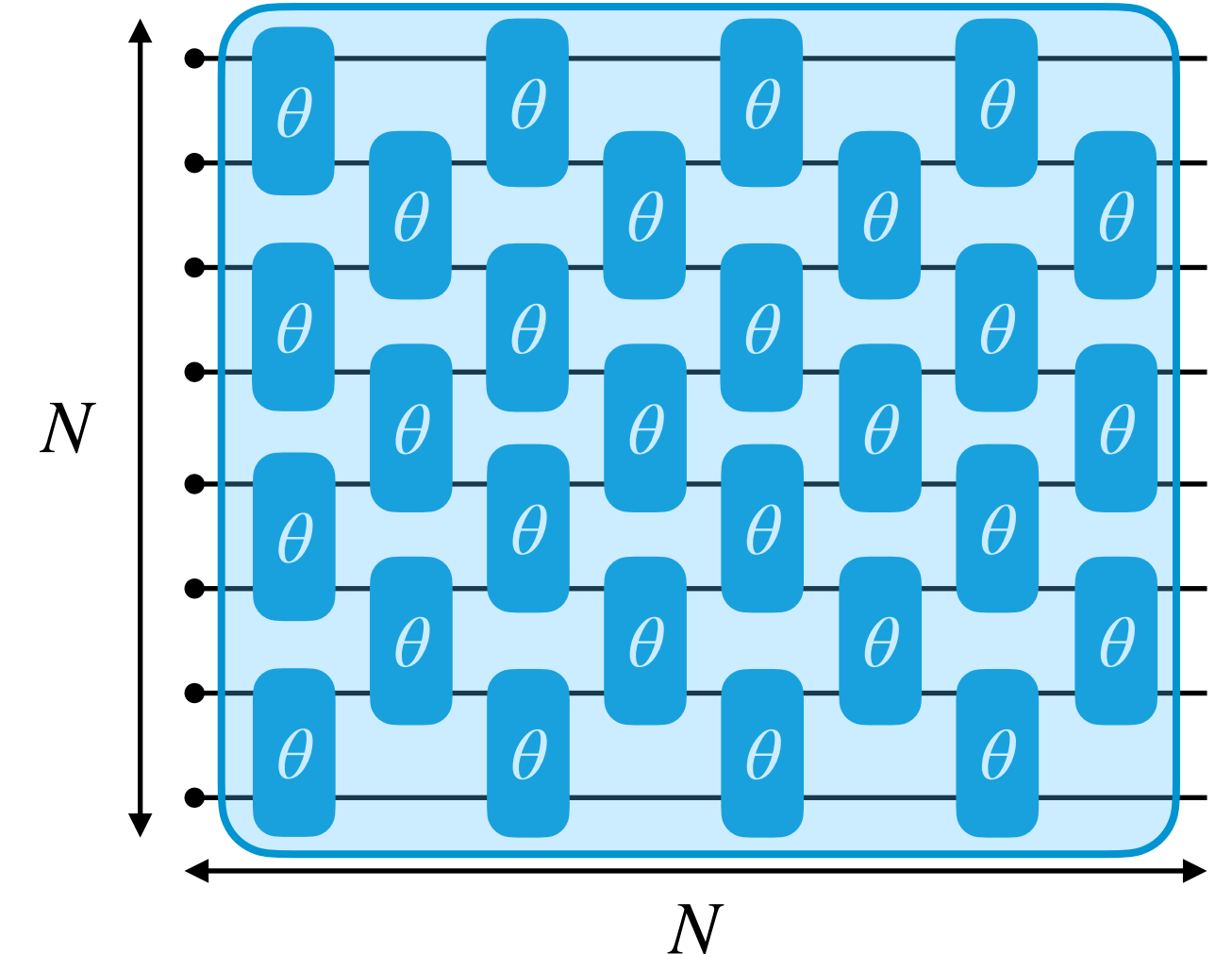
$$\theta_i \leftarrow \theta_i - \lambda \partial E(\{\theta_i\}) / \partial \theta_i$$

Gradient Descent,  
SPSA, COBYLA, ...

$$|\Psi(\{\theta_i\}_{\text{opt}})\rangle \approx |\Psi_G\rangle$$

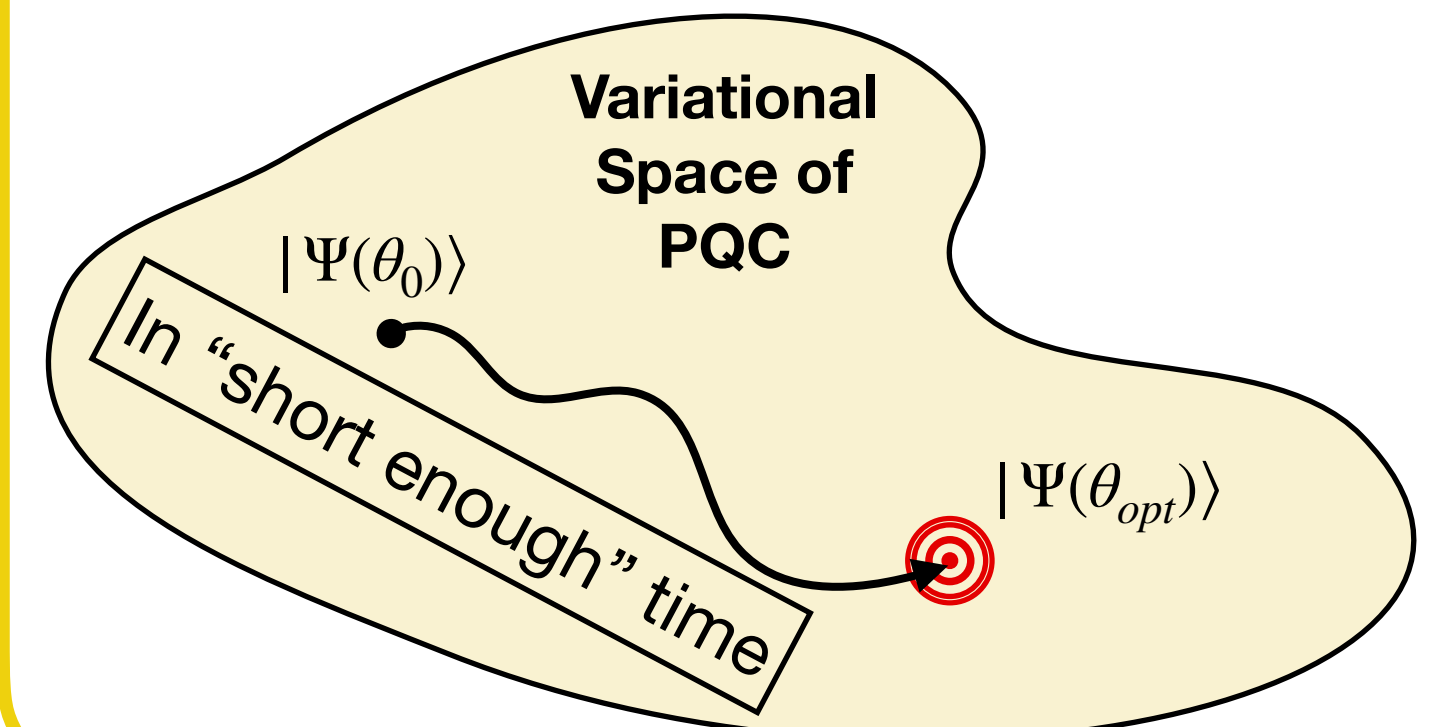
Peruzzo et. al., Nat. Commun. 5, 4213 (2014)

**Scalable PQC Ansatz**



$$\text{Volume of PQC} \leq O(N^2)$$

**Scalable classical optimizer**



# Scalable quantum simulation of symmetry-protected topological states

*R.-Y. Sun, T. Shirakawa, and S. Yunoki, Phys. Rev. B **108**, 075127 (2023) [arXiv:2303.17187]*

## Quantum circuit definition of topological phases

Topological phases: Symmetry-protected topological (SPT) state & intrinsic topological order (TO)

PHYSICAL REVIEW B **82**, 155138 (2010)



**Local unitary transformation, long-range quantum entanglement, wave function renormalization, and topological order**

Xie Chen,<sup>1</sup> Zheng-Cheng Gu,<sup>2</sup> and Xiao-Gang Wen<sup>1</sup>

<sup>1</sup>Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

<sup>2</sup>Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA

(Received 28 July 2010; revised manuscript received 21 September 2010; published 26 October 2010)

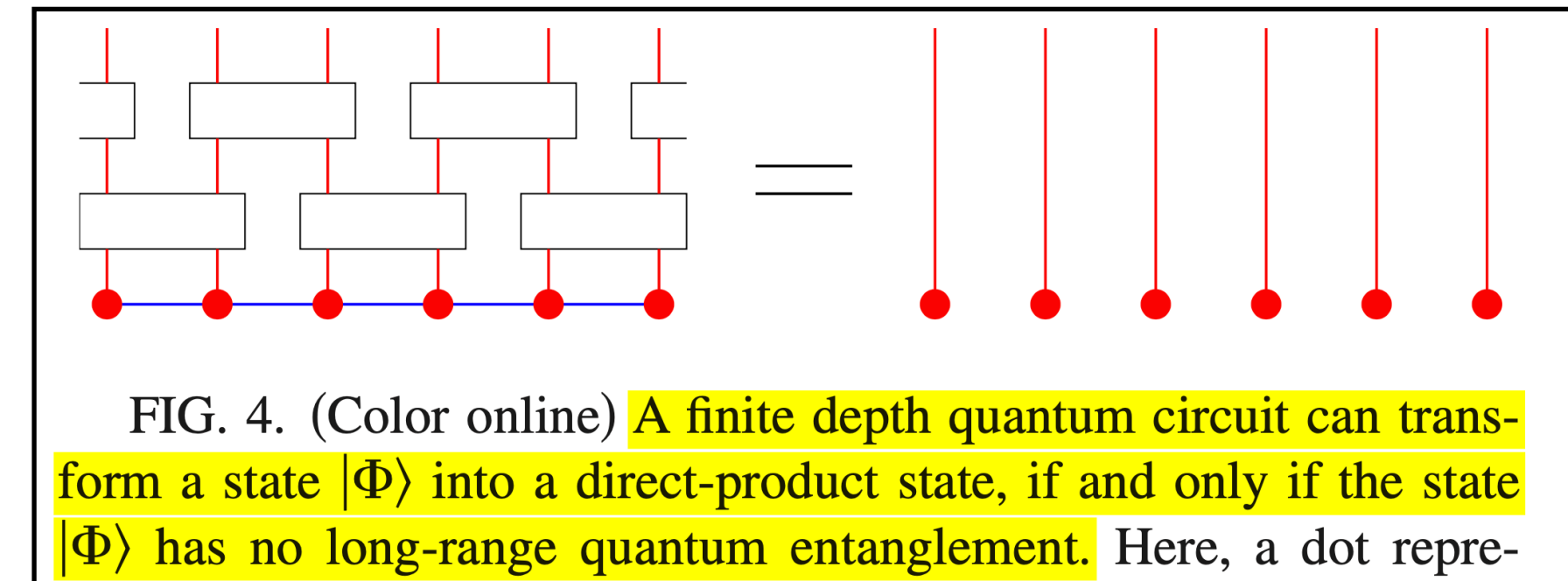
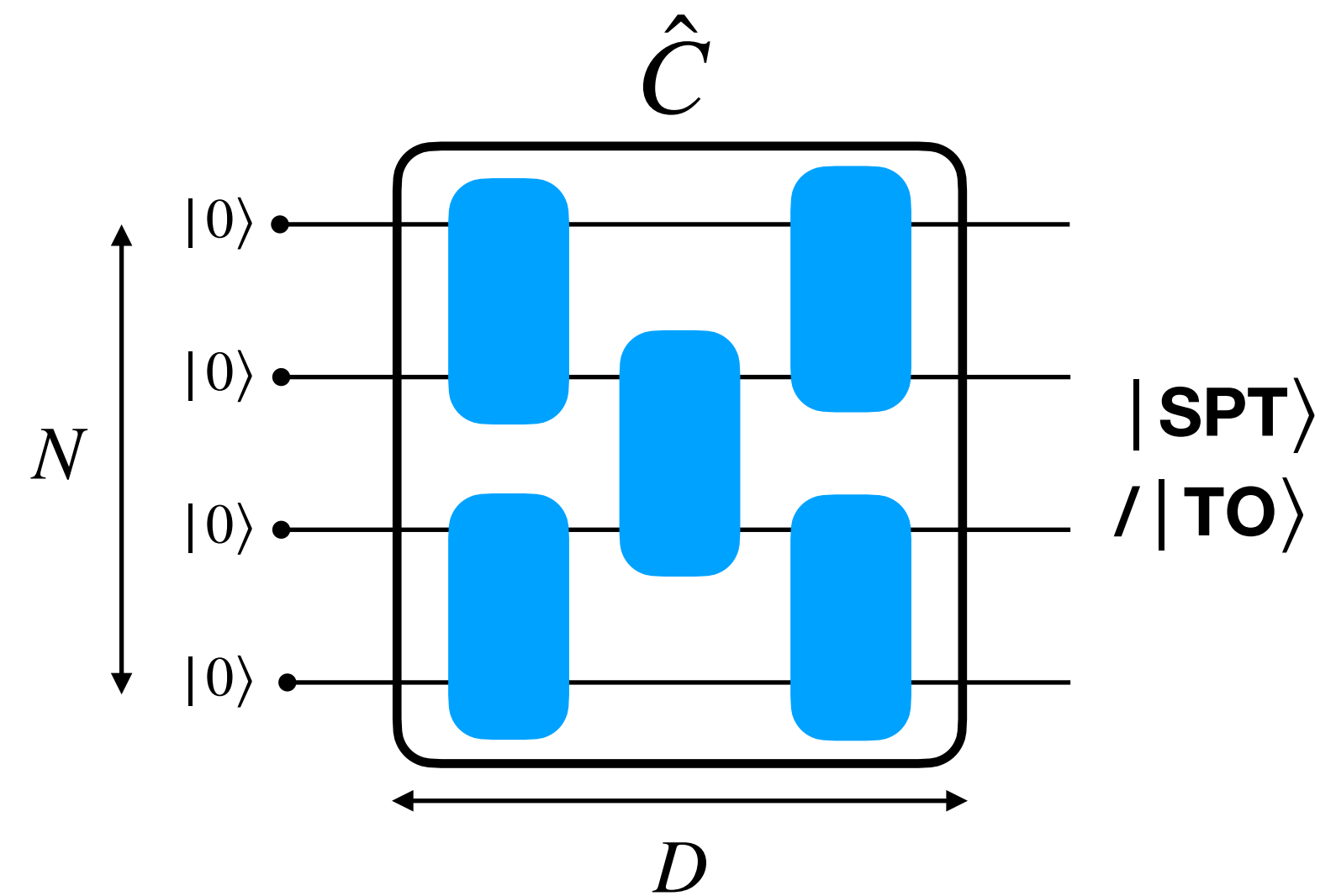


FIG. 4. (Color online) A finite depth quantum circuit can transform a state  $|\Phi\rangle$  into a direct-product state, if and only if the state  $|\Phi\rangle$  has no long-range quantum entanglement. Here, a dot represents a qubit.

would like to show that *two gapped states*  $|\Phi(0)\rangle$  and  $|\Phi(1)\rangle$  are in the same phase, if and only if they are related by a local unitary (LU) evolution. We define a LU evolution as a



- SPT (short-range entangled)**
  - $D \propto N$  for symmetric  $\hat{C}$
  - Exist constant  $D$  for unsymmetric  $\hat{C}$
- TO (long-range entangled)**
  - $D \propto N$  for any  $\hat{C}$

- $\hat{C}$  is NISQ **scalable**
- In the same phase  $\Leftrightarrow$  connected by **finite** depth quantum circuit

## Two-layer structured PQC Ansatz

$$|\Psi(\theta)\rangle = \hat{C}(\theta)\hat{C}_0|0\rangle$$

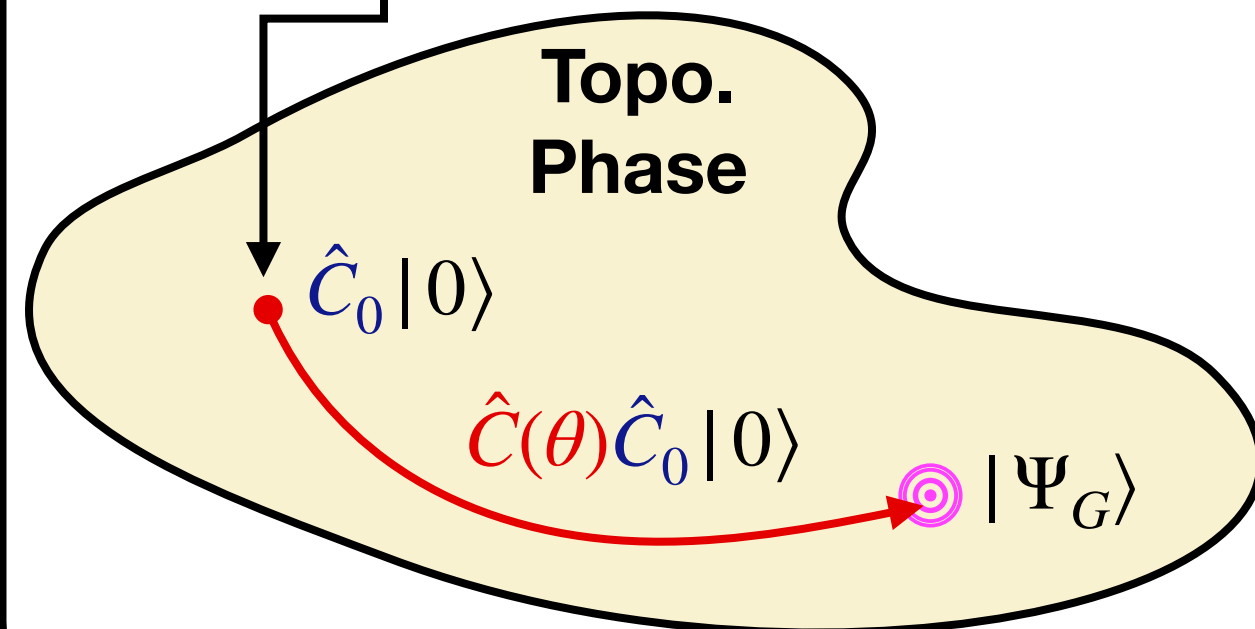
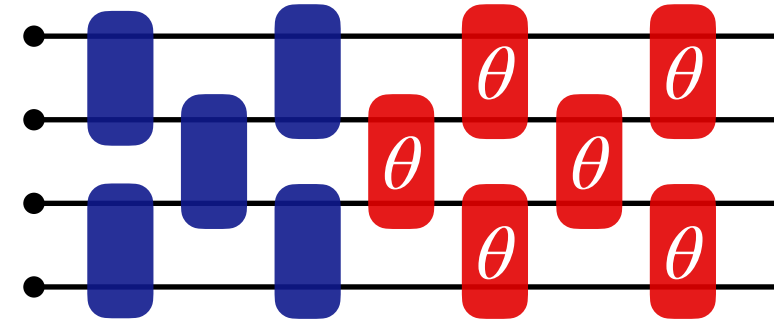
**Scalable initialization layer  $\hat{C}_0$**

- Constant** depth for SPT
- Linear** depth for TO

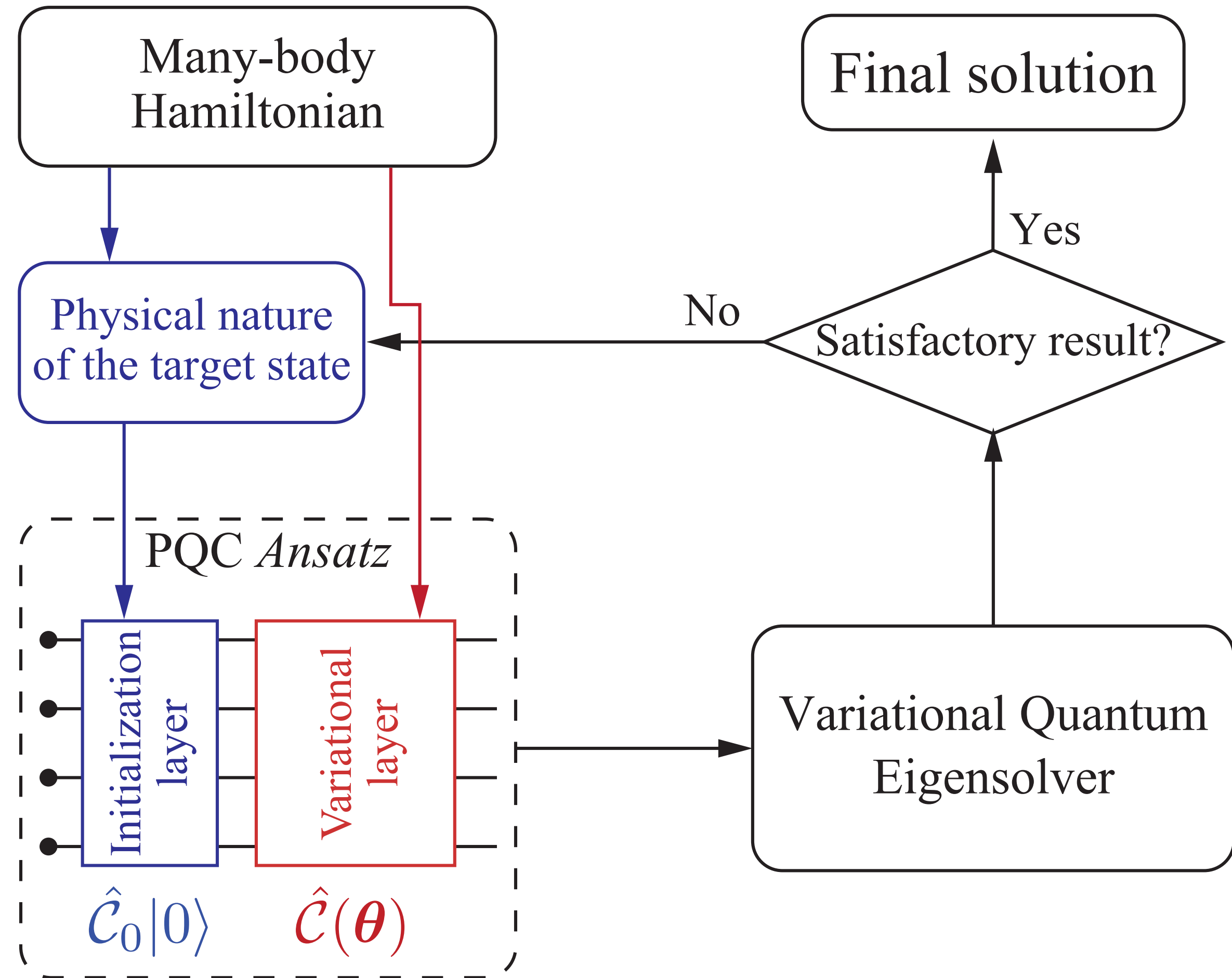
**Scalable variational layer  $\hat{C}(\theta)$**

- Constant** depth

**Possible choice:  
fixed point state**



### Computation scheme



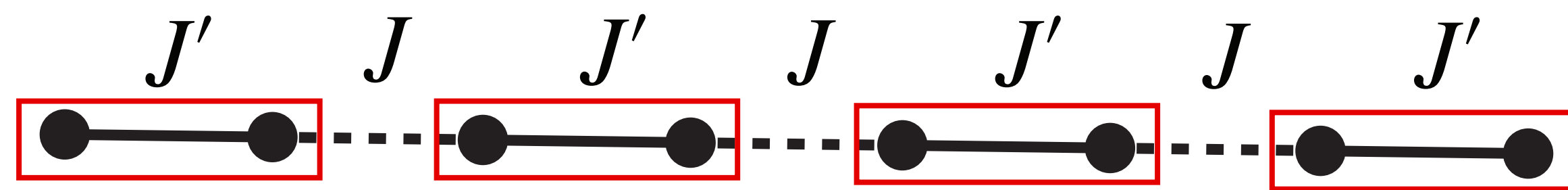


## $S = 1/2$ alternating Heisenberg chain (AHC)

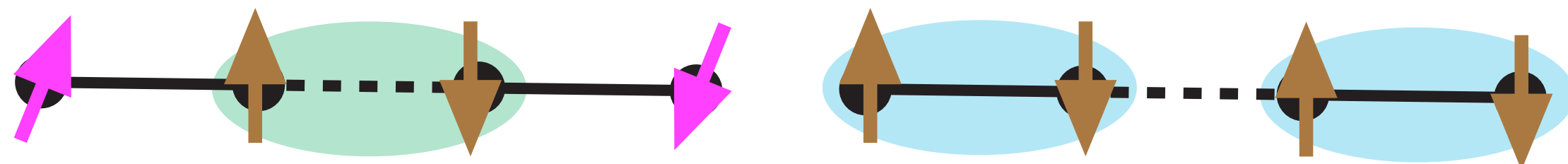
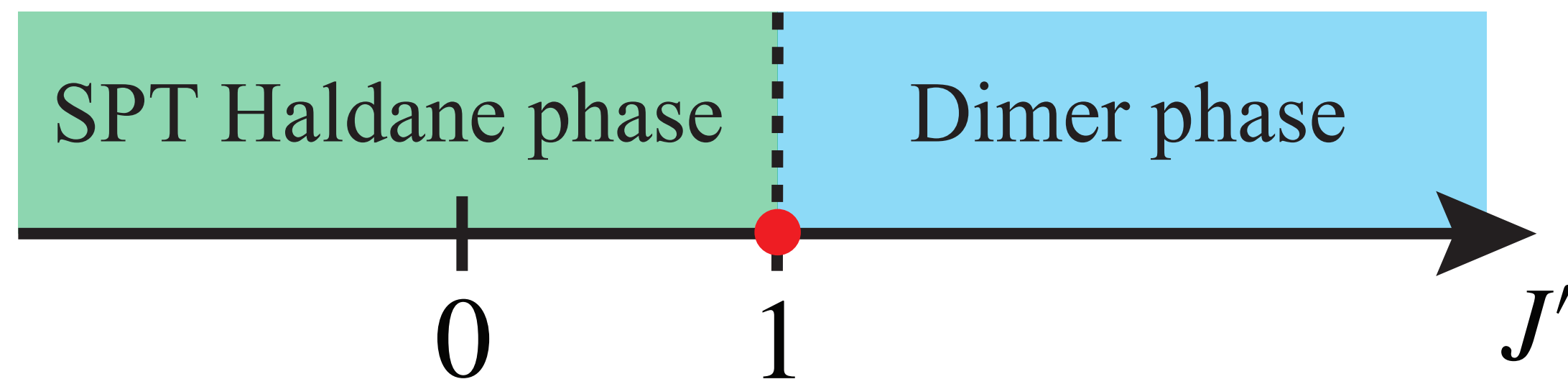
Hida, PRB 45, 5 (1992)

$$H = \sum_{i=0}^{L/2-1} \left( J' \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1} + J \mathbf{S}_{2i+1} \cdot \mathbf{S}_{2(i+1)} \right)$$

$$J = 1$$



Unitcell



$J' < 1$  SPT Haldane phase

Fixed point:  $J' = 0$

$S = 1$  Haldane chain:  $J' = -\infty$

$J' > 1$  trivial dimer phase

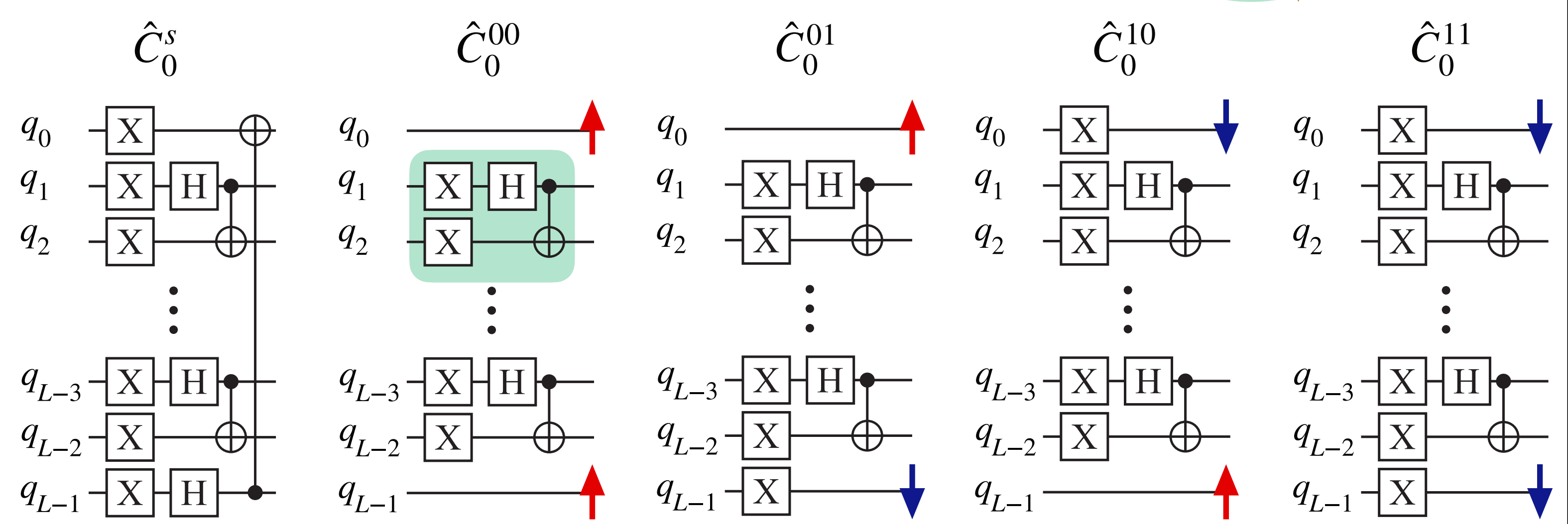
Fixed point:  $J' = \infty$

In general, non-exactly solvable

## PQC Ansatz for AHC

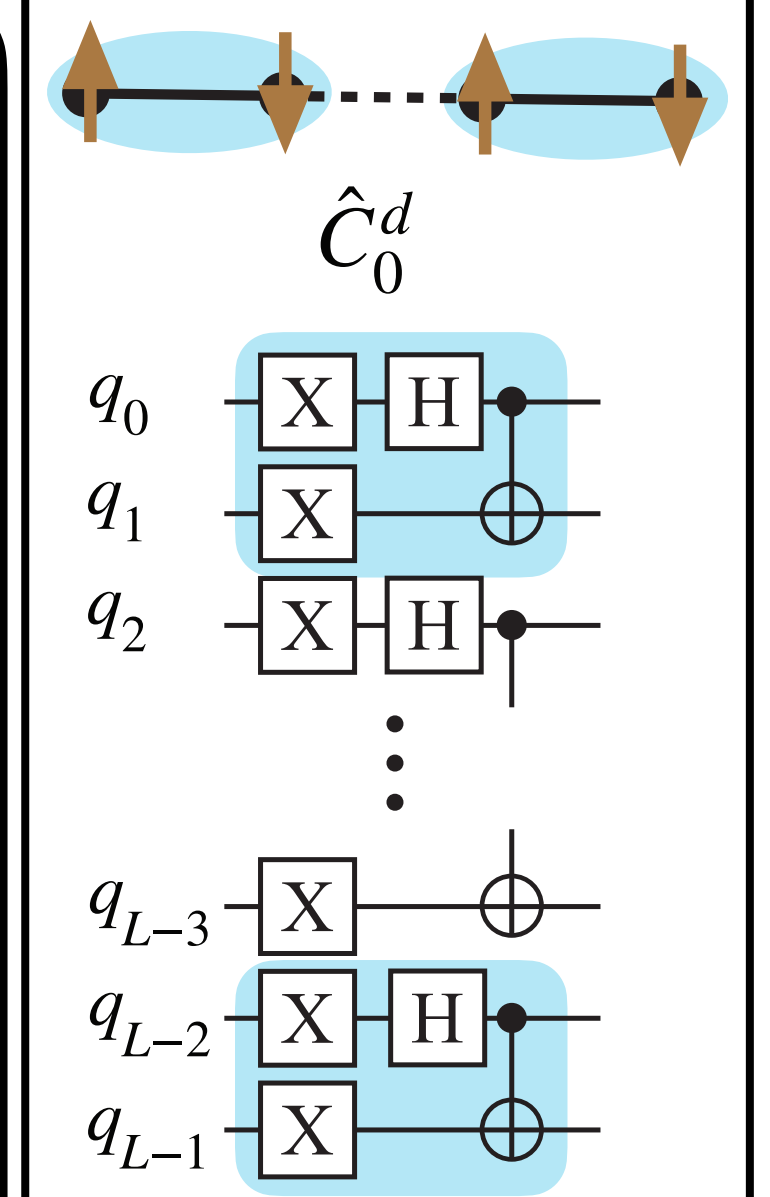
### Initialization layer

#### For SPT



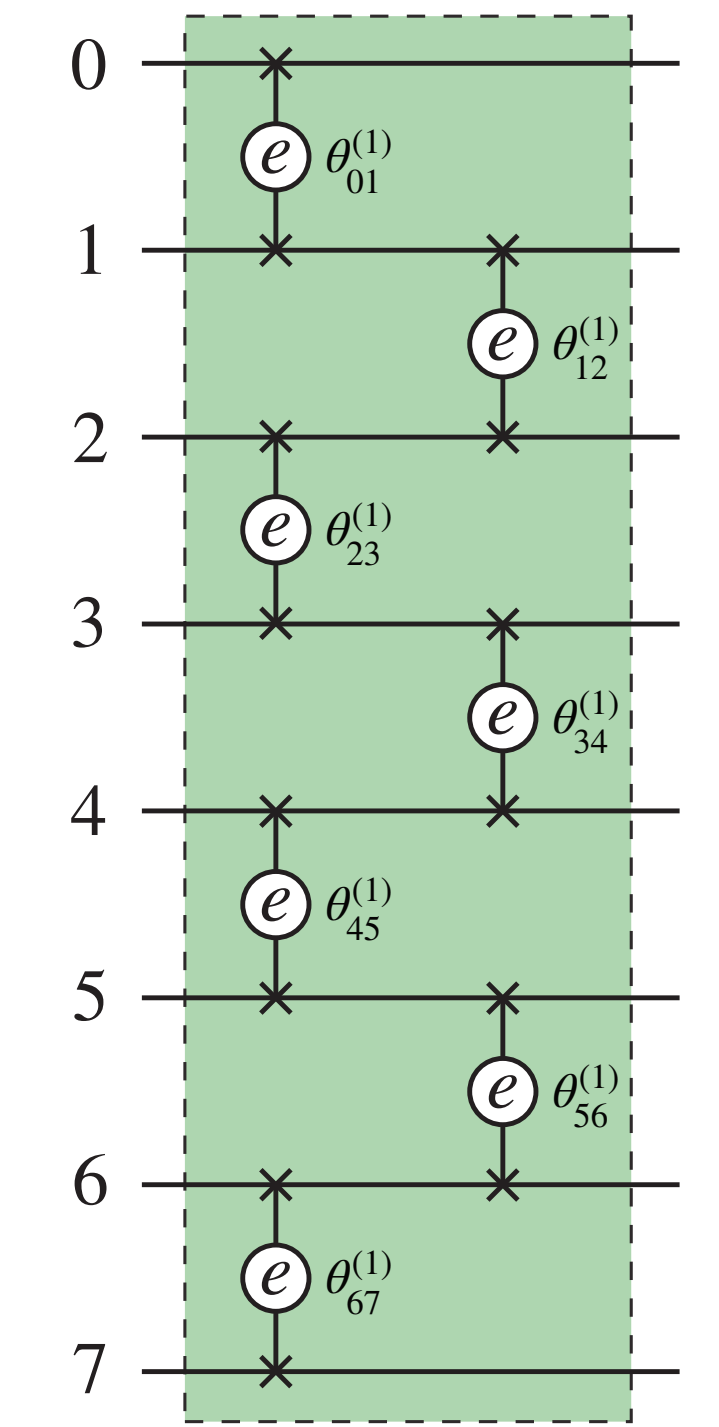
Fixed point at  $J' = 0$

#### For dimer



at  $J' = \infty$

### Variational layer: eSWAP brick wall

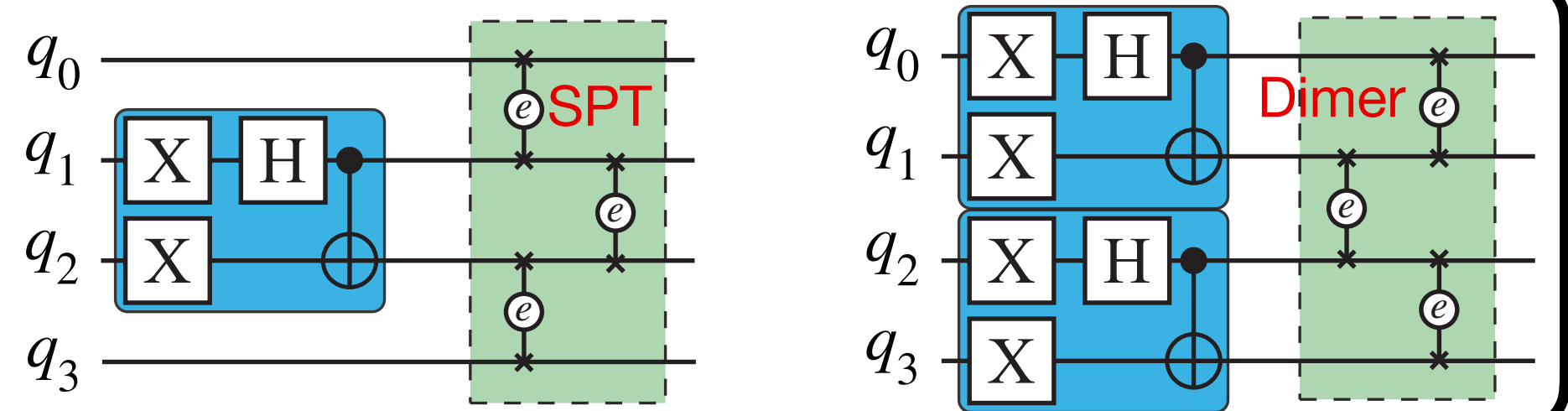


$\times D$

$$e^{\theta_{ij}} \propto e^{-i\theta S_i S_j}$$

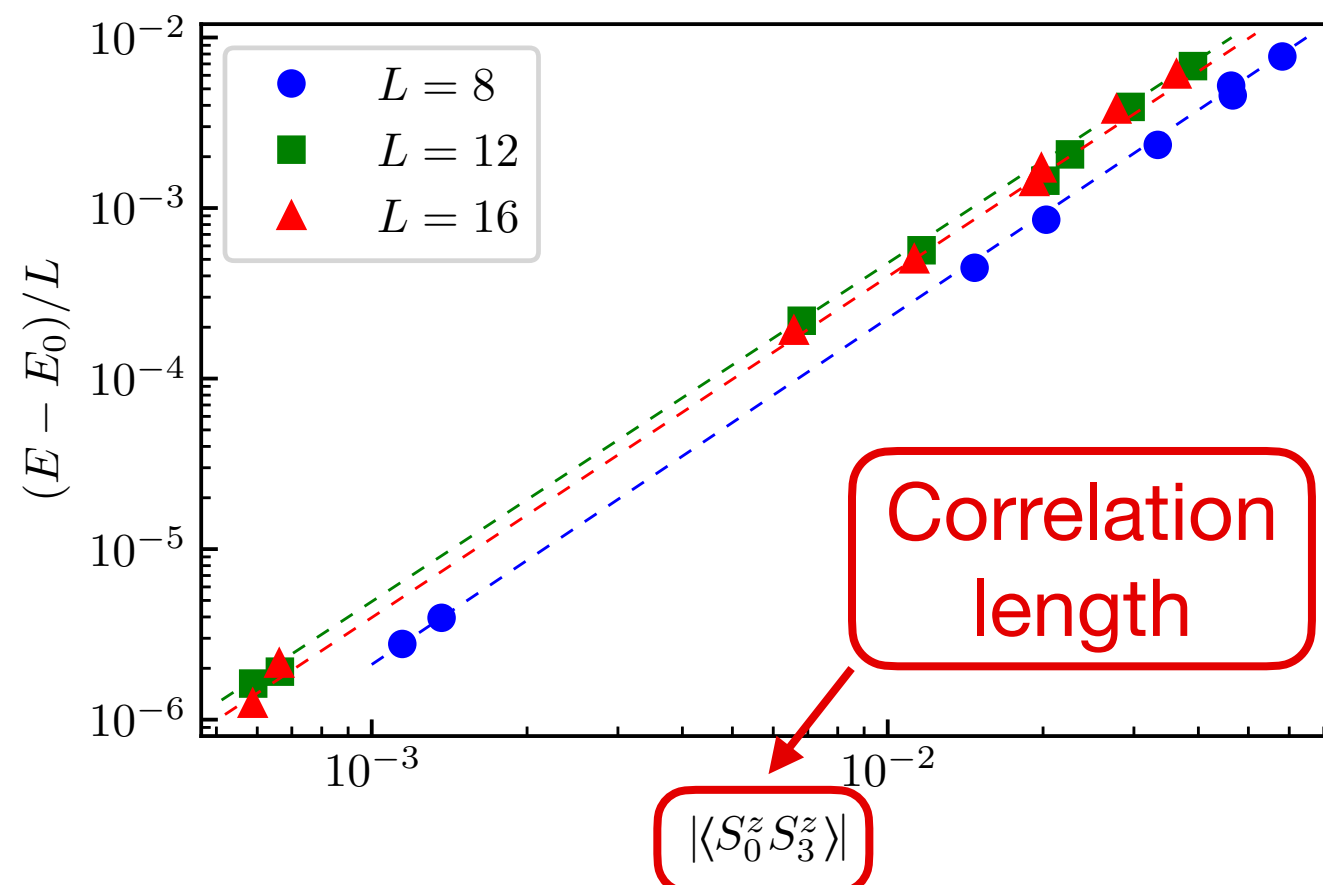
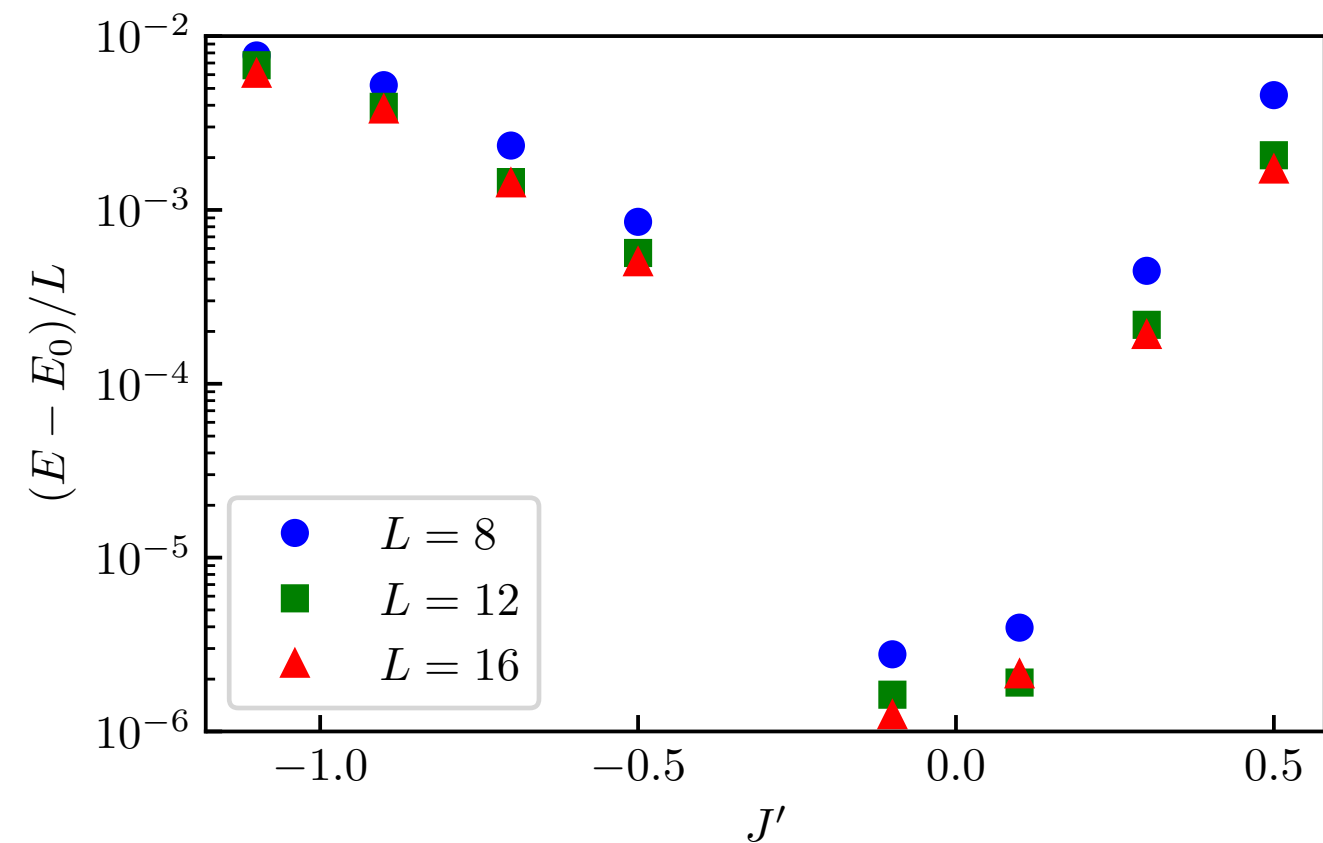
Complete examples:

$N = 4$   
 $D = 1$



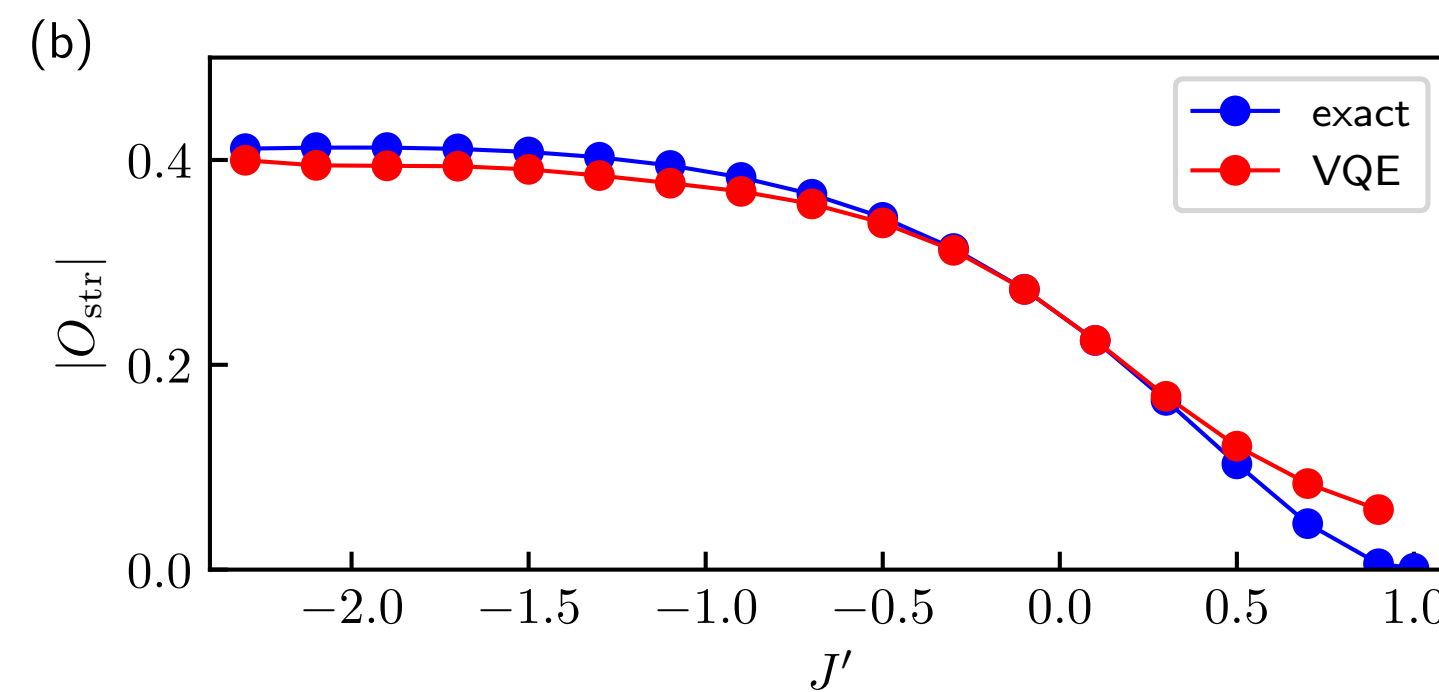
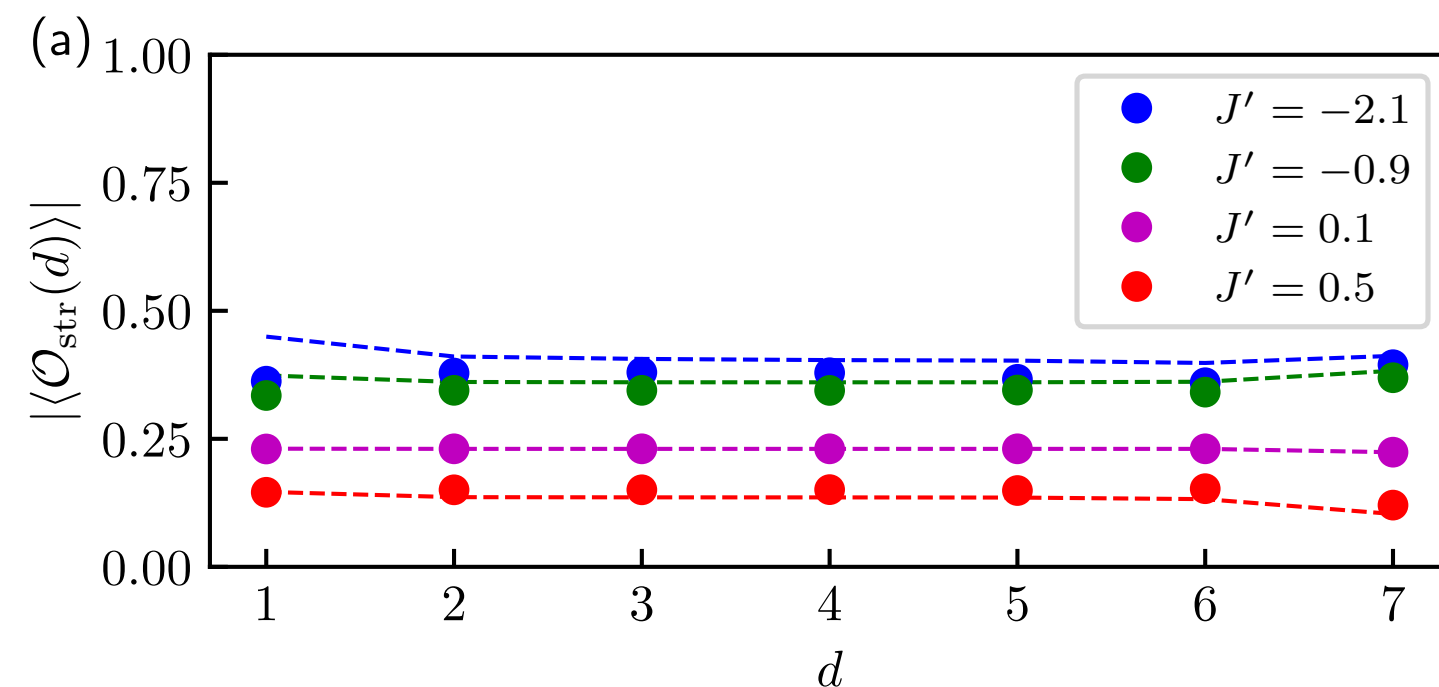
## VQE simulation of AHC using $D = 1$ shallow circuit Ansatz

### Ground state energy in SPT

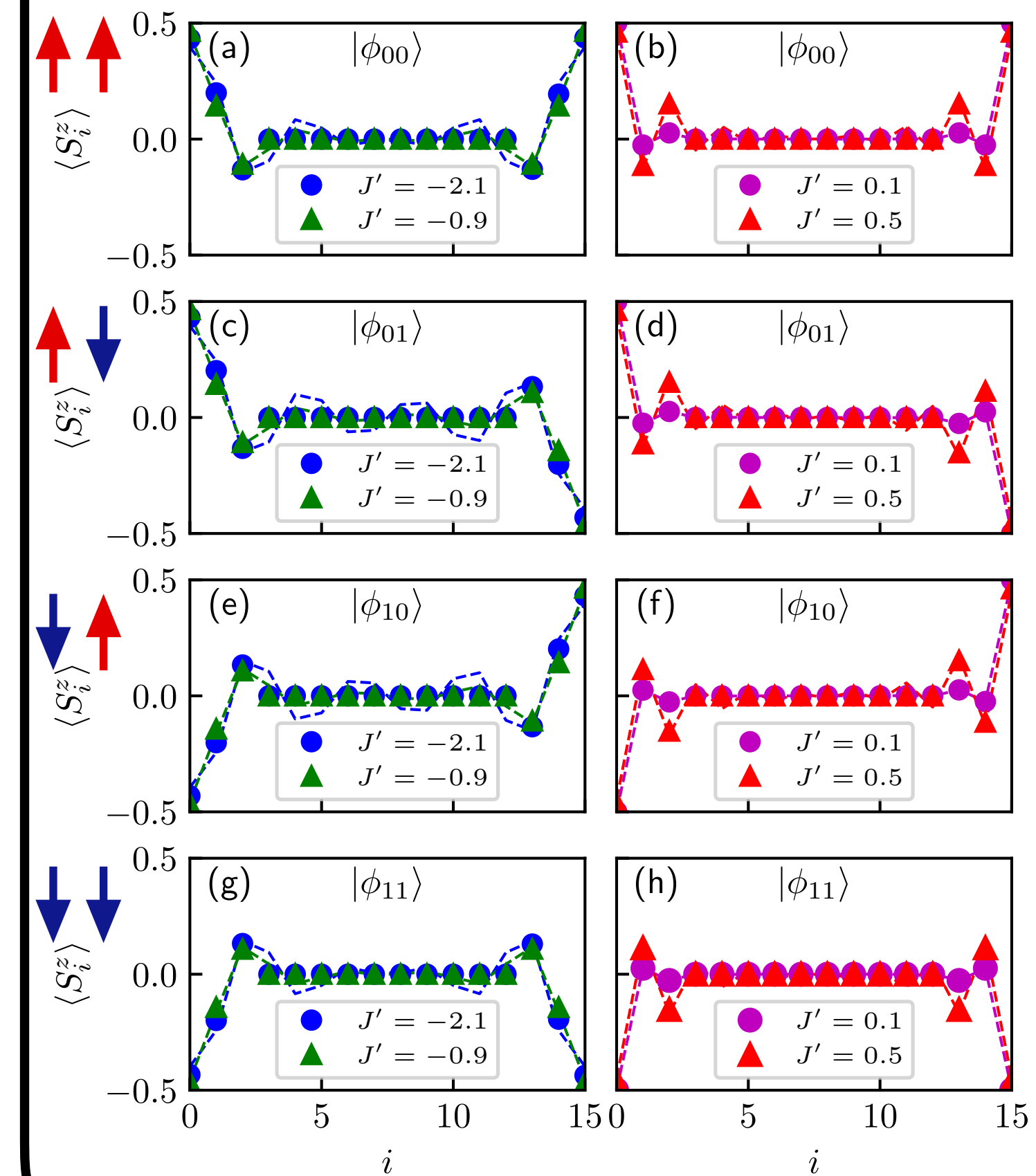


### String order in SPT

$$\mathcal{O}_{\text{str}}(d) = \mathcal{S}_k^z \left( \prod_{l=k+1}^{k+d-1} \exp(i\pi \mathcal{S}_l^z) \right) \mathcal{S}_{k+d}^z$$



### Edge spin patterns in SPT

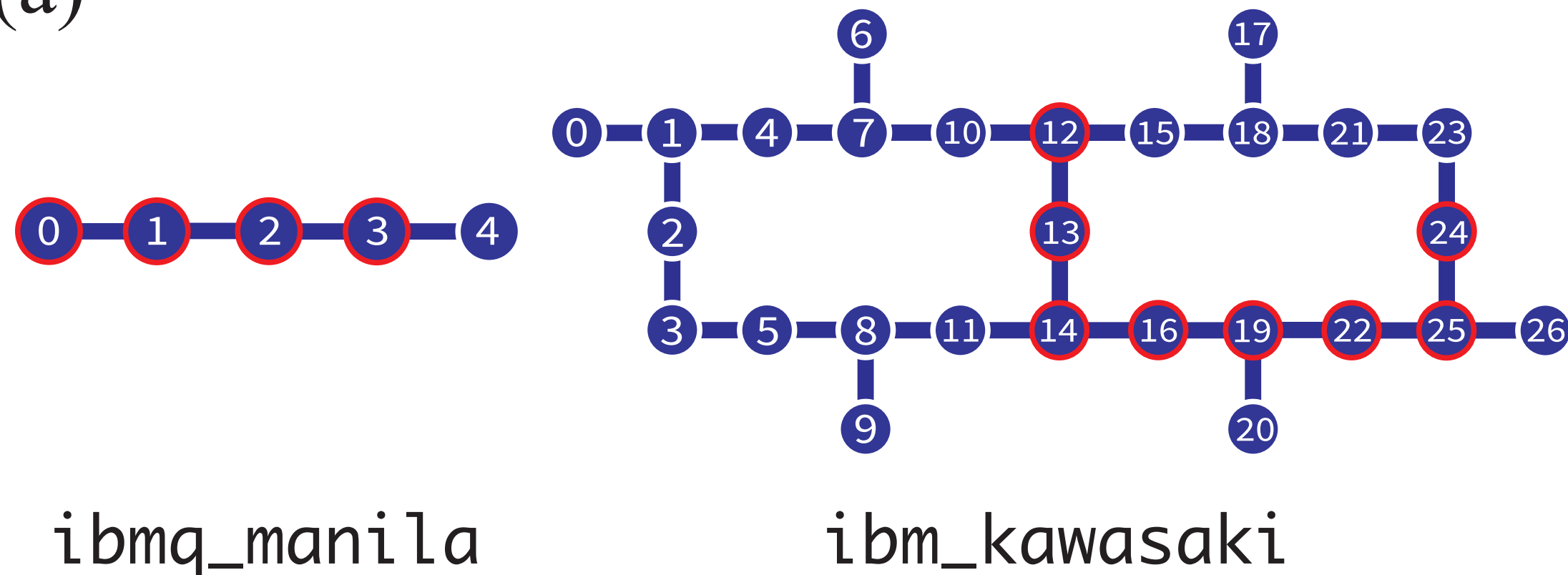


**Scalable:** Keeping accuracy with increasing system size

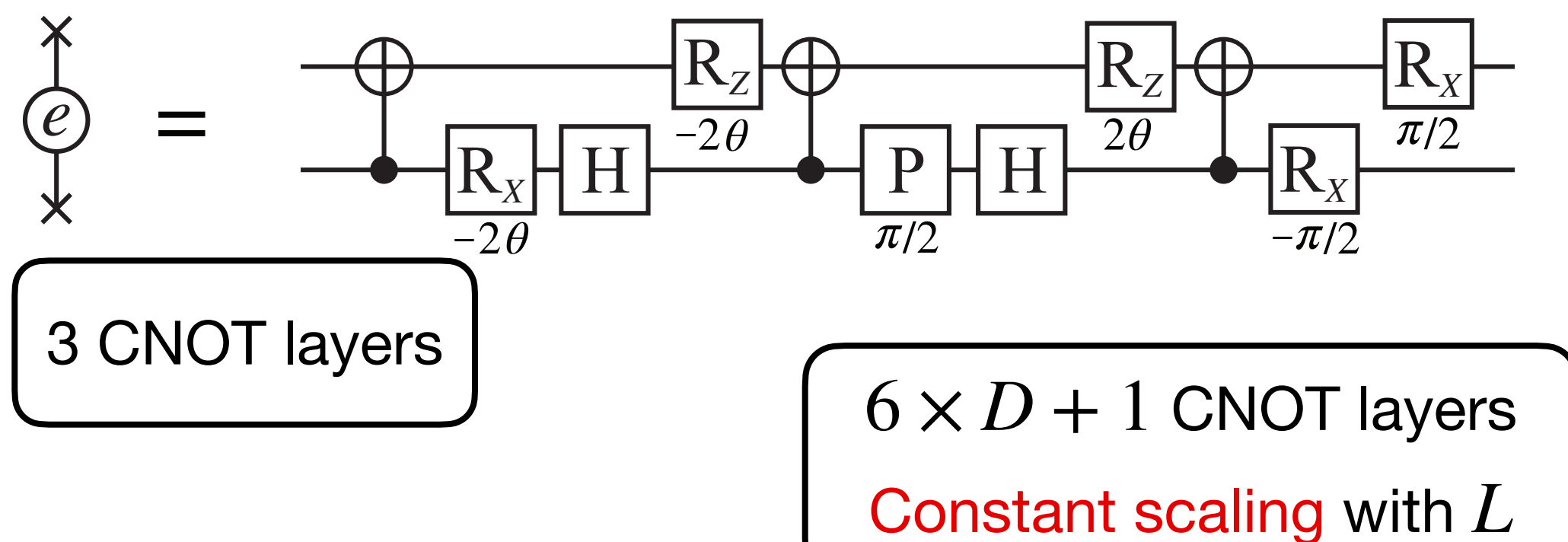
## Realize SPT state on real quantum computer

### Quantum devices & gate realization

(a)

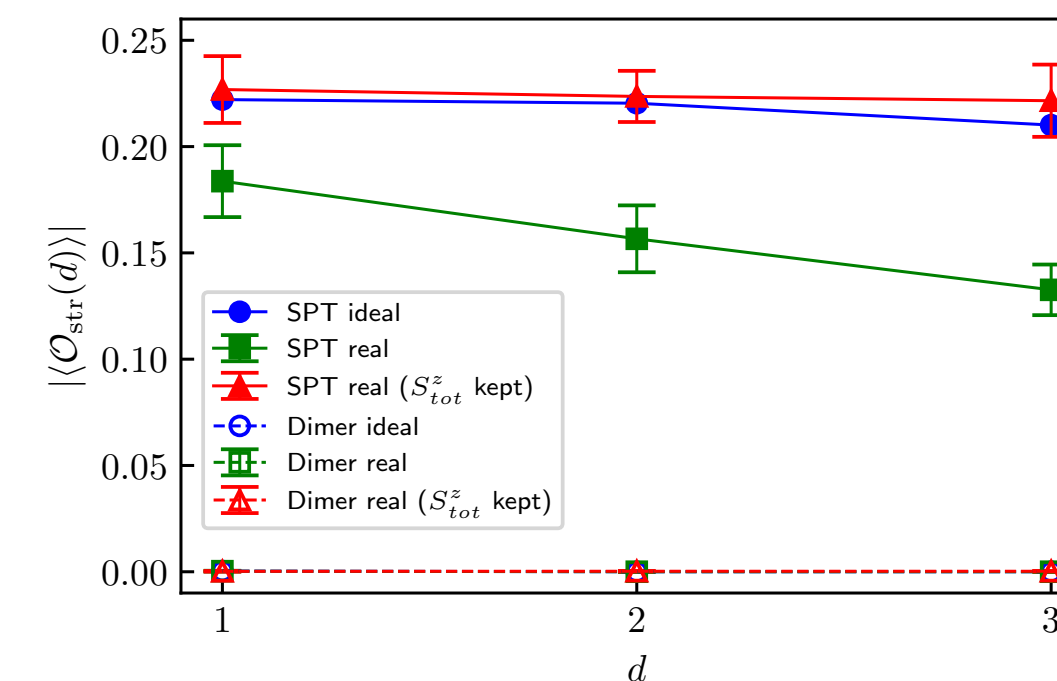


(b)

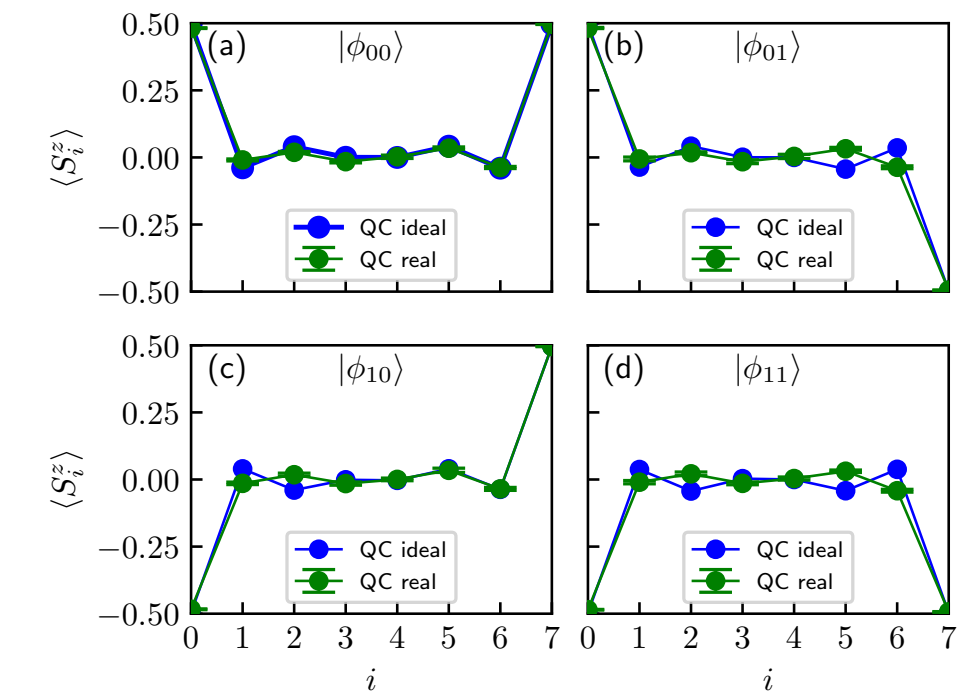


### Real quantum experiments with $D = 1$ Ansatz

String order



Edge spins

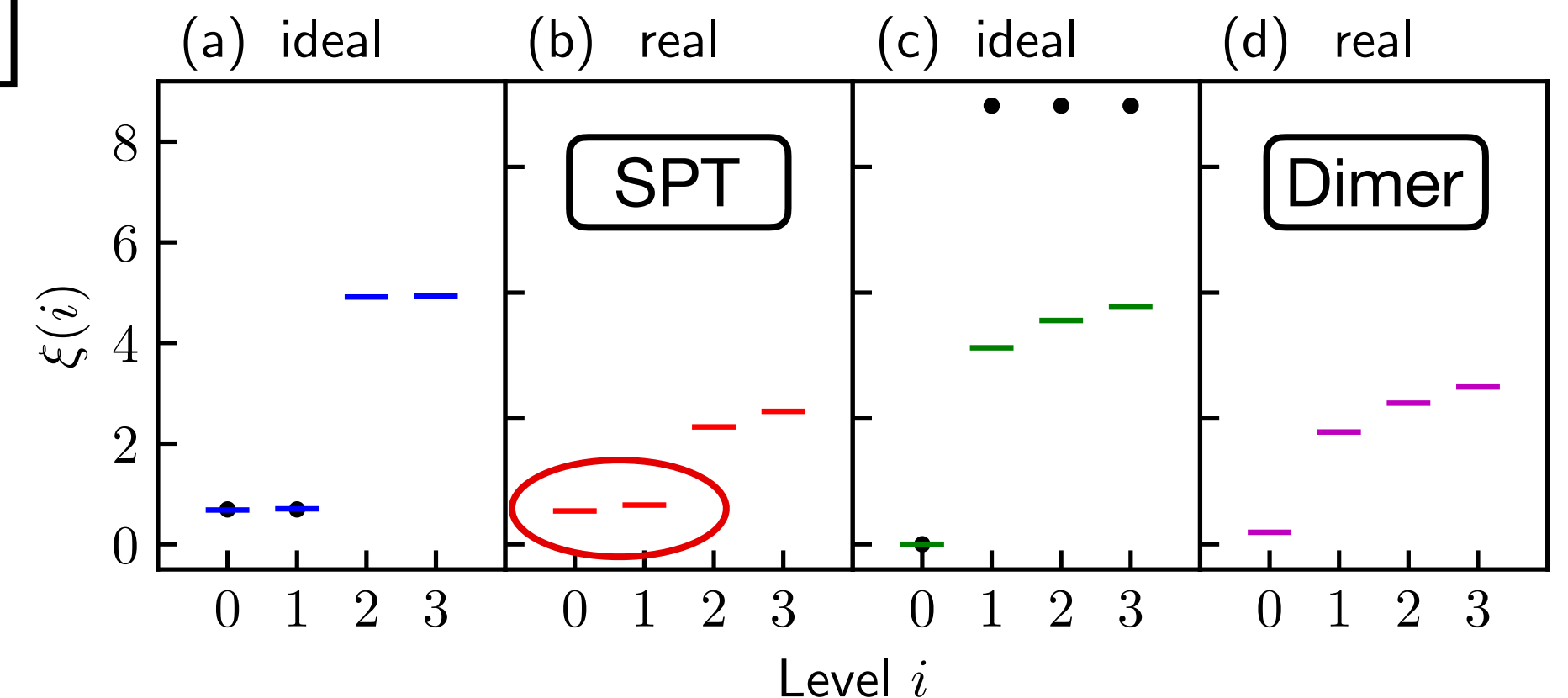


SPT Haldane phase

0 1

$J' = 0.15$

Entanglement spectrum



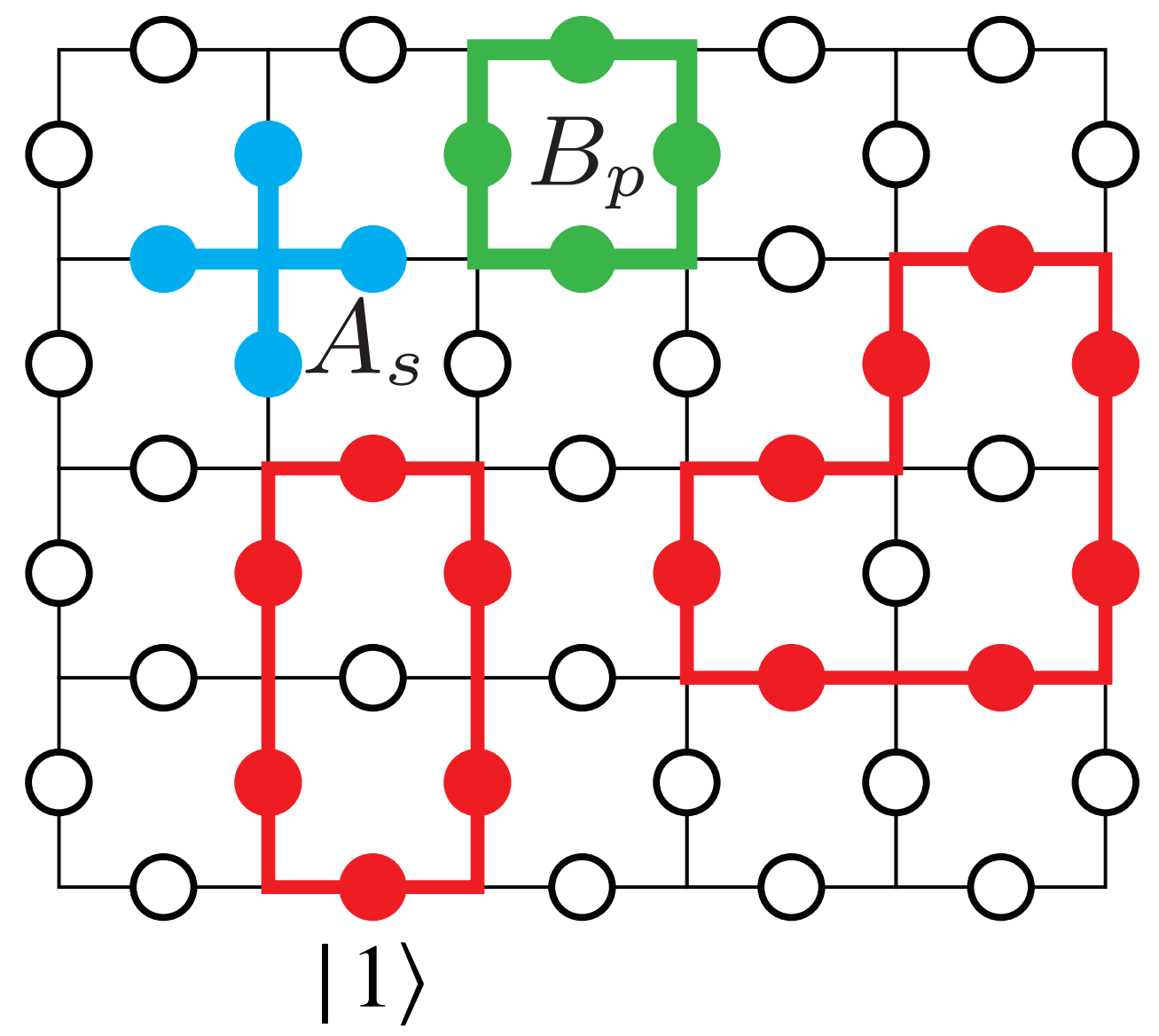
# Scalable quantum simulation of intrinsic topologically ordered states

*R.-Y. Sun, T. Shirakawa, and S. Yunoki, Phys. Rev. B **107**, L041109 (2023) [arXiv:2210.14662]*

## Toric code model and its realization on NISQ device

### Toric code model

$$H_{TC} = - \sum_s A_s - \sum_p B_p$$

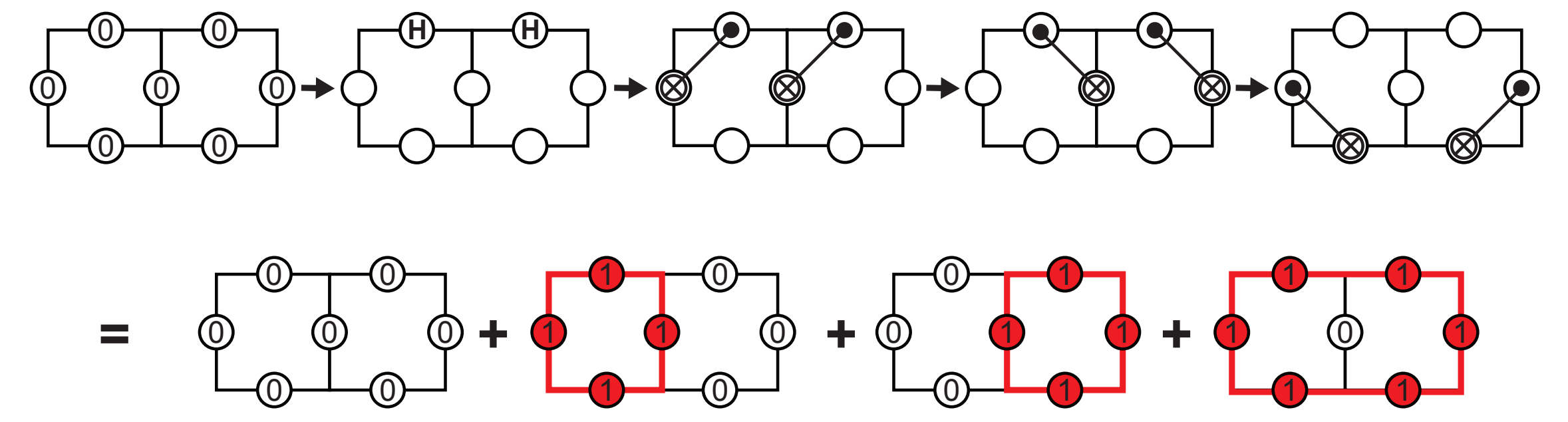


$$A_s = \prod_{i \in s} \sigma_i^z \quad B_p = \prod_{i \in p} \sigma_i^x$$

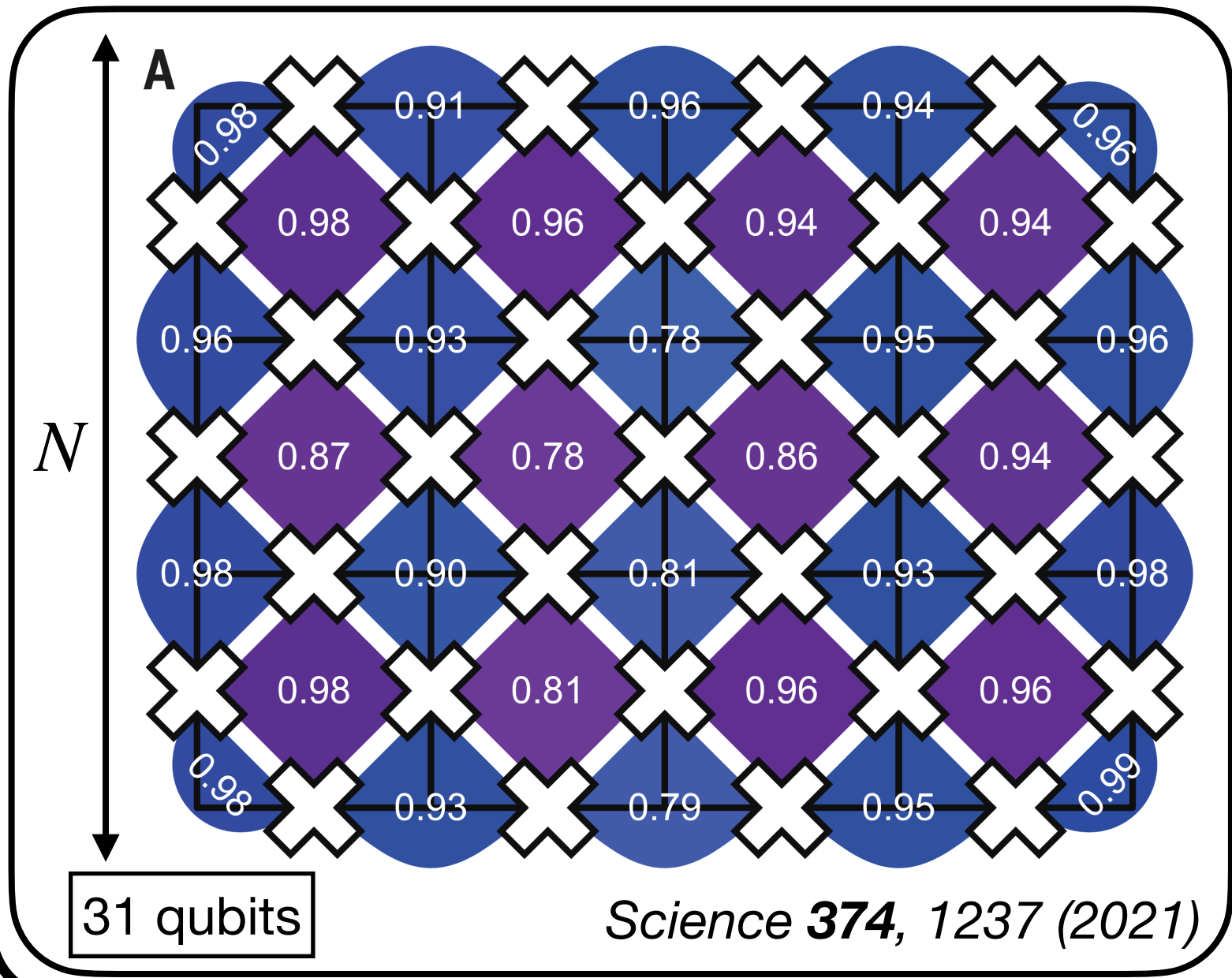
- Intrinsic topological order
- Quantum loop gas with **equal** weights

$$|\Psi_G\rangle = |\text{grid}\rangle + |\text{loop}\rangle + |\text{loop}\rangle + \dots$$

### NISQ realization of toric code state



PRX Quantum **3**, 040315 (2022)



31 qubits

Science **374**, 1237 (2021)

● — ⊕ CNOT

Hadamard gate

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

NISQ **scalable**:

$$3 + 2[(N - 1)/2]$$

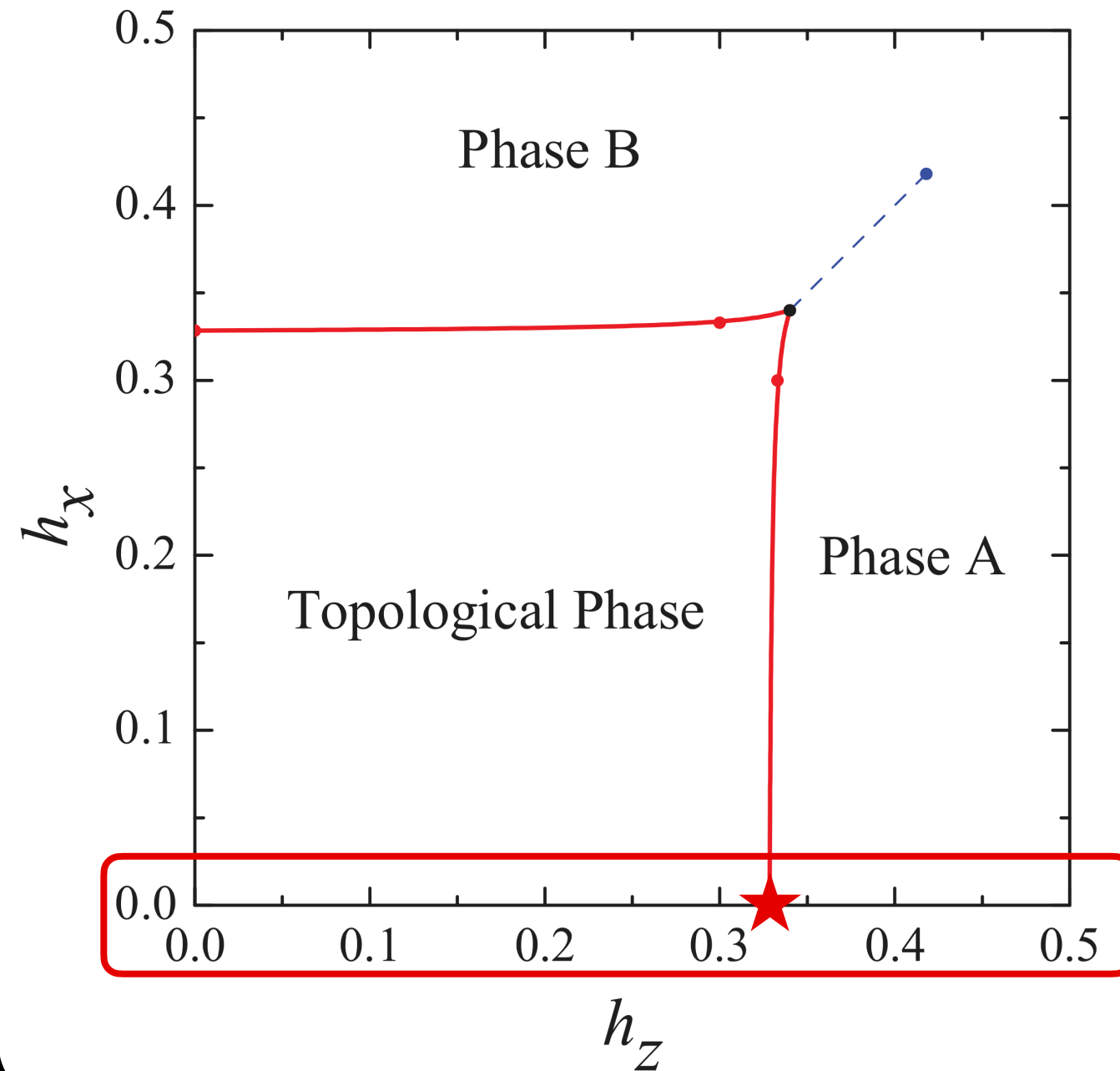
CNOT layers

## Toric code model in a magnetic field

$$H_{\text{TCM}}(x) = (1 - x)H_{\text{TC}} - x \sum_{i=1}^N \sigma_i^z \quad x \in [0,1]$$

Non-exactly solvable

QMC phase diagram



$$h_z = \frac{x}{1-x}$$

Topological order to ferromagnetic order:  $x_c \sim 0.25$

PRB 85, 195104 (2012)

Goal: simulate  $H_{\text{TCM}}(x)$  on quantum computer

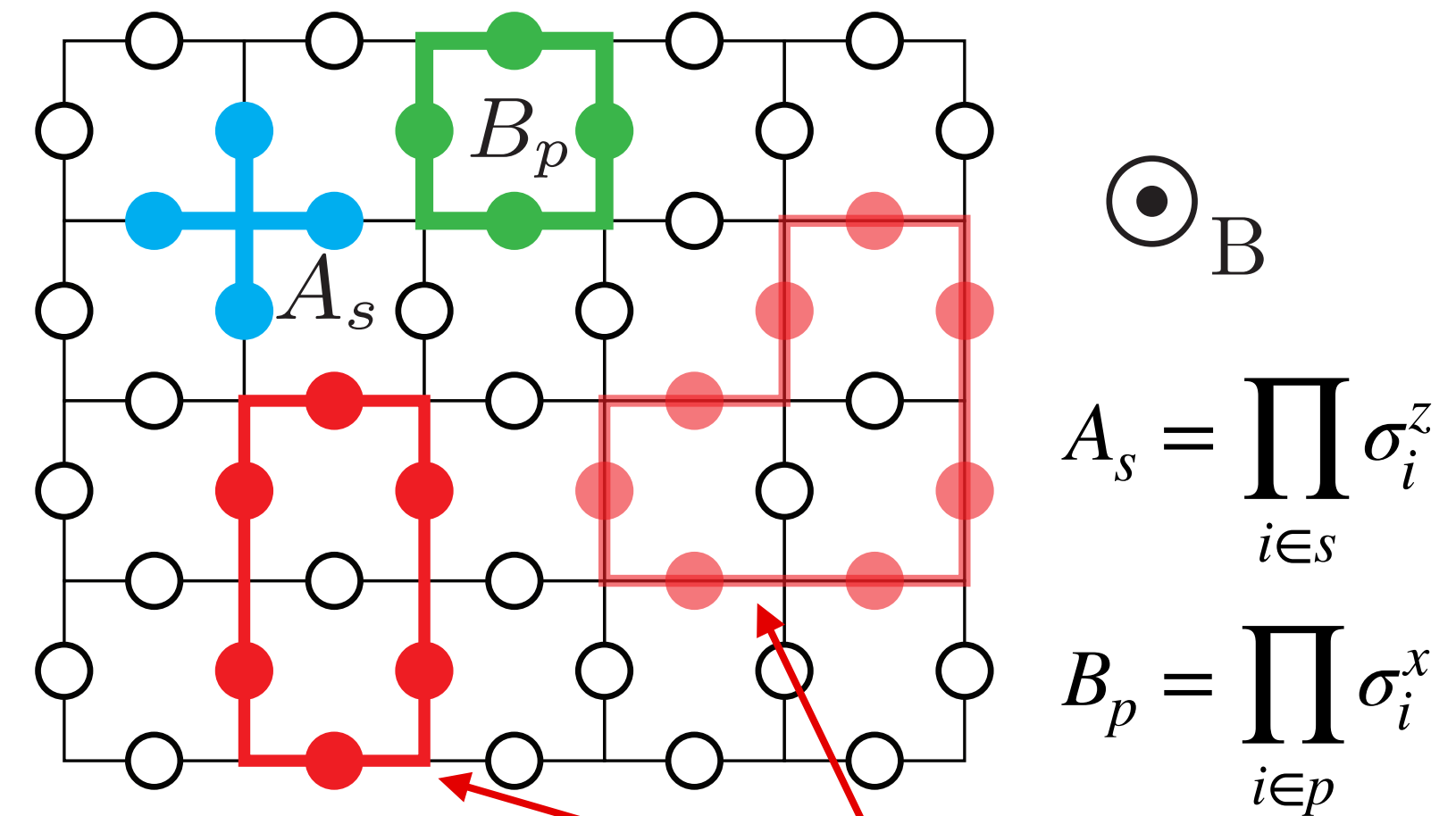
PRL 98, 070602 (2007)

PHYSICAL REVIEW LETTERS

week ending  
16 FEBRUARY 2007

### Breakdown of a Topological Phase: Quantum Phase Transition in a Loop Gas Model with Tension

Simon Trebst,<sup>1</sup> Philipp Werner,<sup>2</sup> Matthias Troyer,<sup>3</sup> Kirill Shtengel,<sup>4</sup> and Chetan Nayak<sup>1,5</sup>



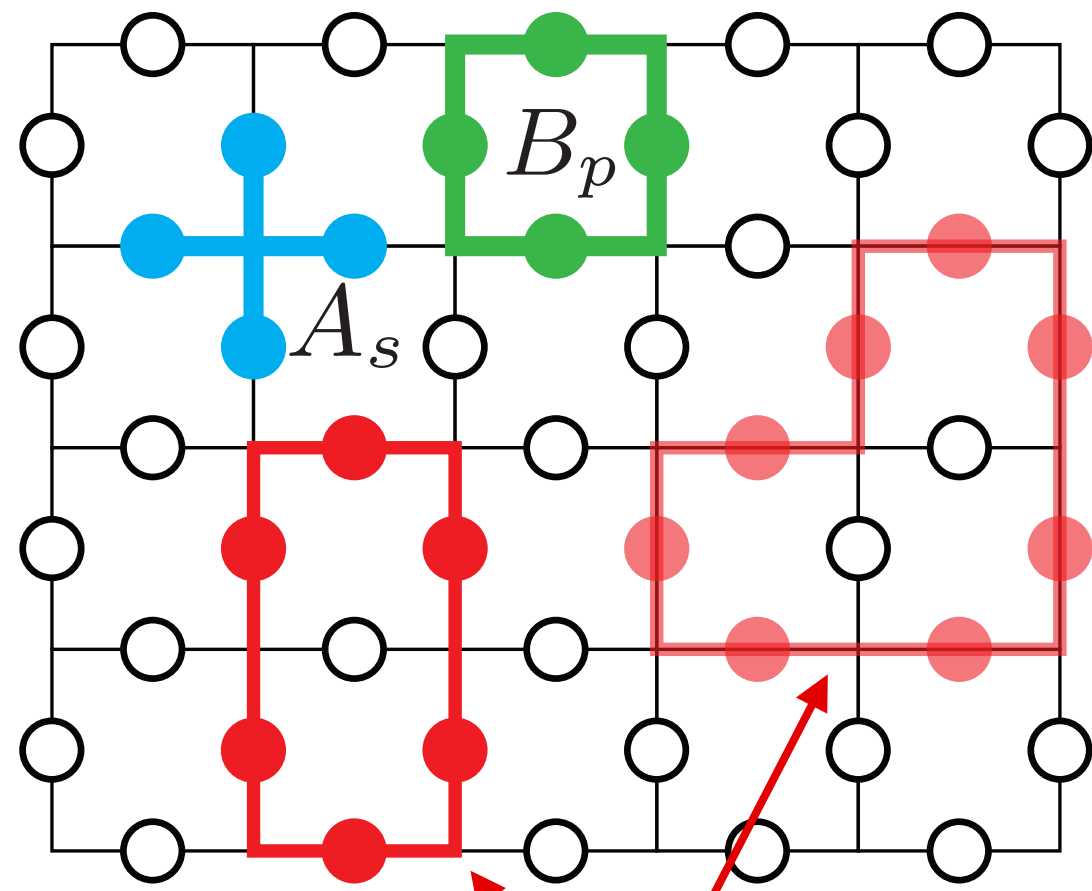
Loop weights

$$|\Psi_G\rangle = | \text{grid} \rangle + | \text{loop 1} \rangle + | \text{loop 2} \rangle + \dots$$

## Parametrized loop gas circuit (PLGC)

$$H_{\text{TCM}}(x) = (1 - x)H_{\text{TC}} - x \sum_{i=1}^N \sigma_i^z$$

$$x \in [0, 1]$$


 $\odot_B$ 

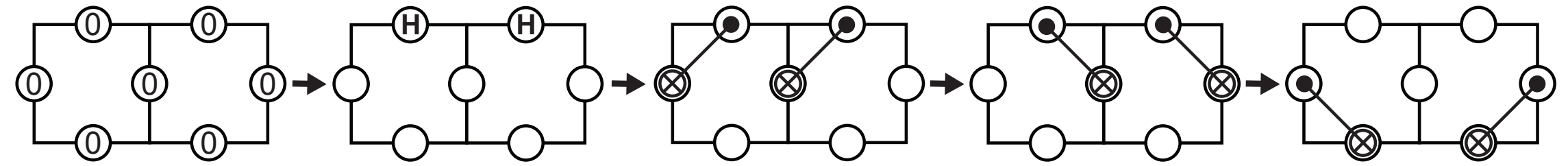
$$A_s = \prod_{i \in s} \sigma_i^z$$

$$B_p = \prod_{i \in p} \sigma_i^x$$

Loop weights

GS: Quantum loop gas with **non-equal** weights

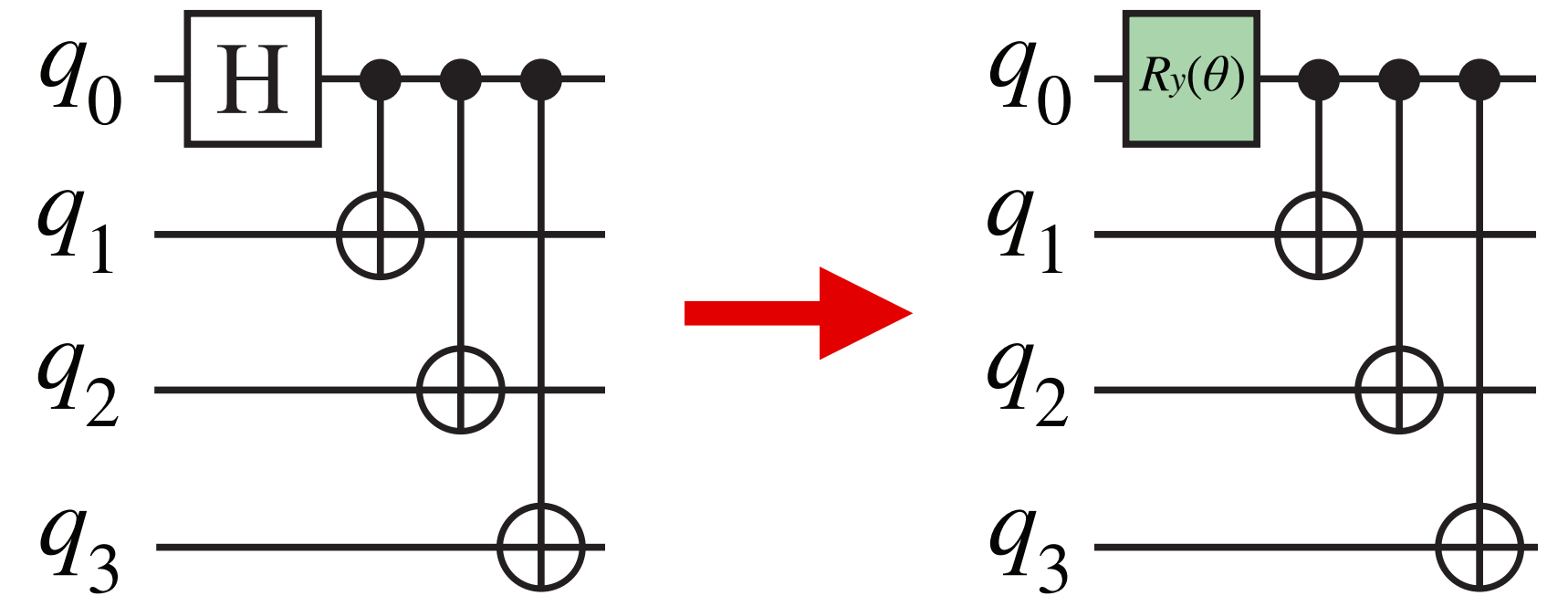
### PLGC Ansatz: weight-adjustable loop gas



$$= \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4}$$

$$H|0\rangle = R_y(\pi/2)|0\rangle$$

$$R_y(\theta) = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix}$$



# of parameters = # of plaquettes

$$|\Psi(\theta)\rangle = \prod_{p=1}^{N_p} \left( \cos(\theta_p/2)I + \sin(\theta_p/2)B_p \right) |00\dots 0\rangle$$

$$= | \text{Grid 1} \rangle + | \text{Grid 2} \rangle + | \text{Grid 3} \rangle + \dots$$

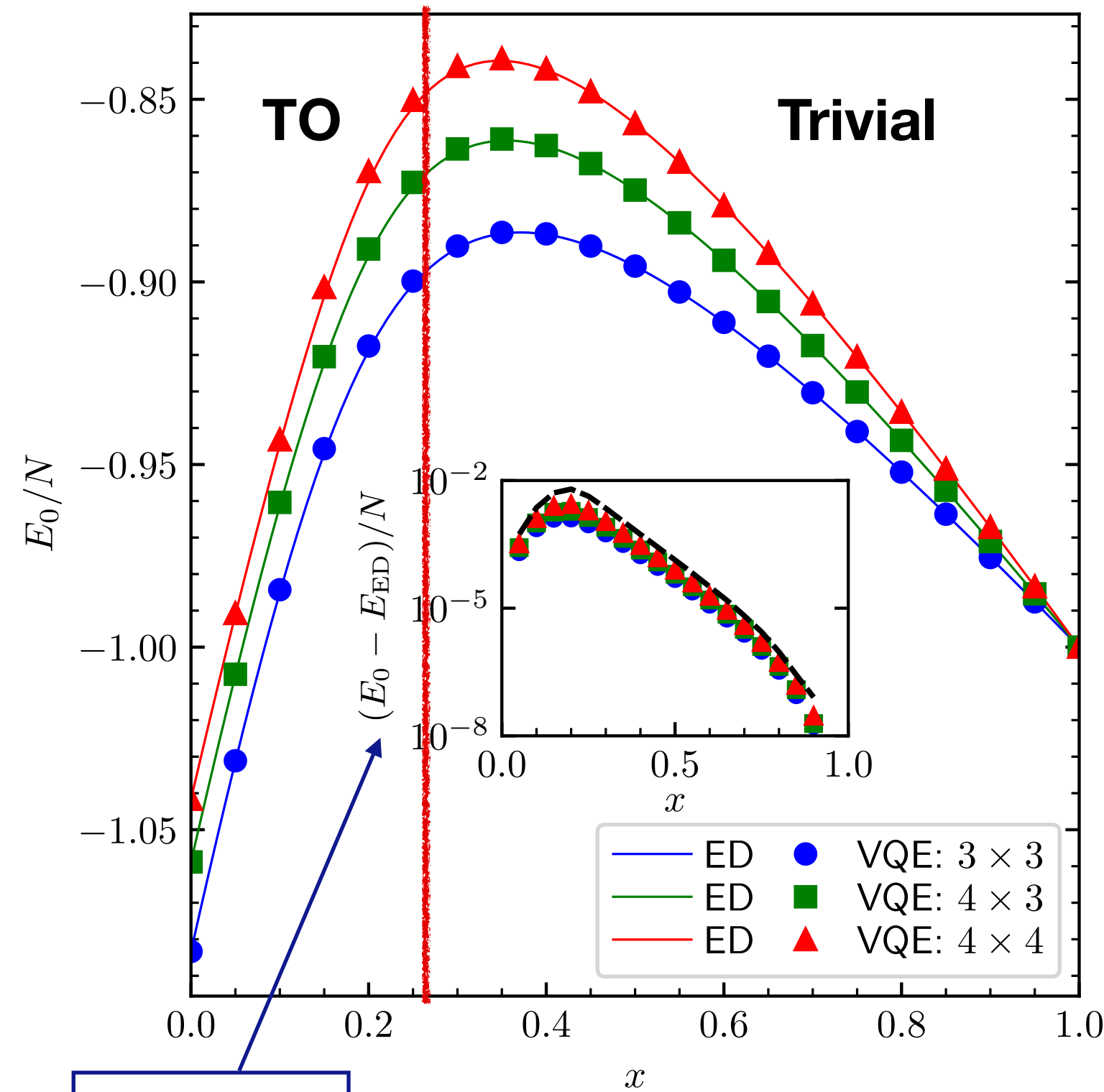
**Scalable on NISQ devices**  
No additional complexity



## VQE simulation of $H_{\text{TCM}}(x)$ using PLGC Ansatz

### Ground state energy

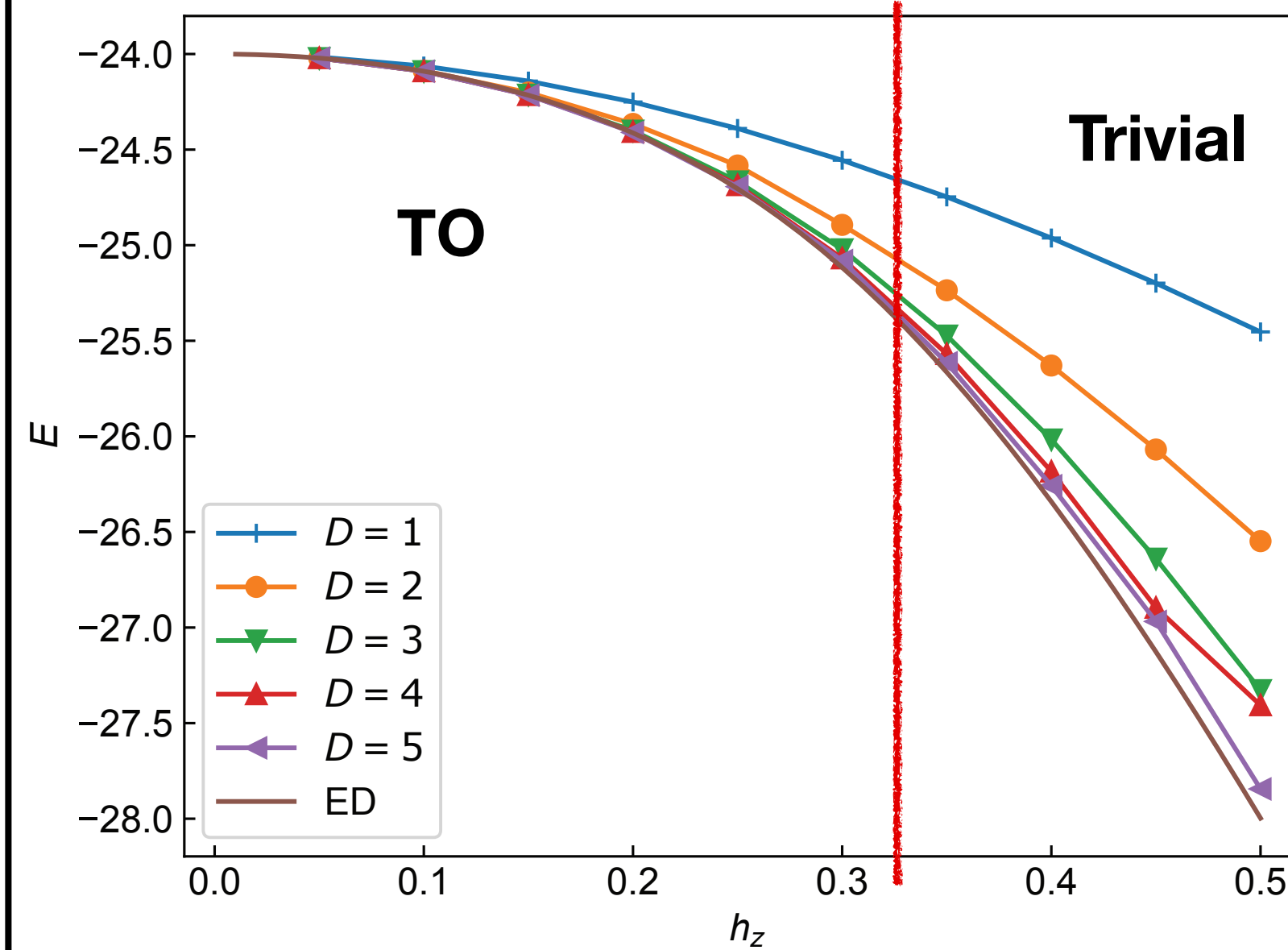
PLGC (our work)



Energy difference

QAOA-type (previous result)

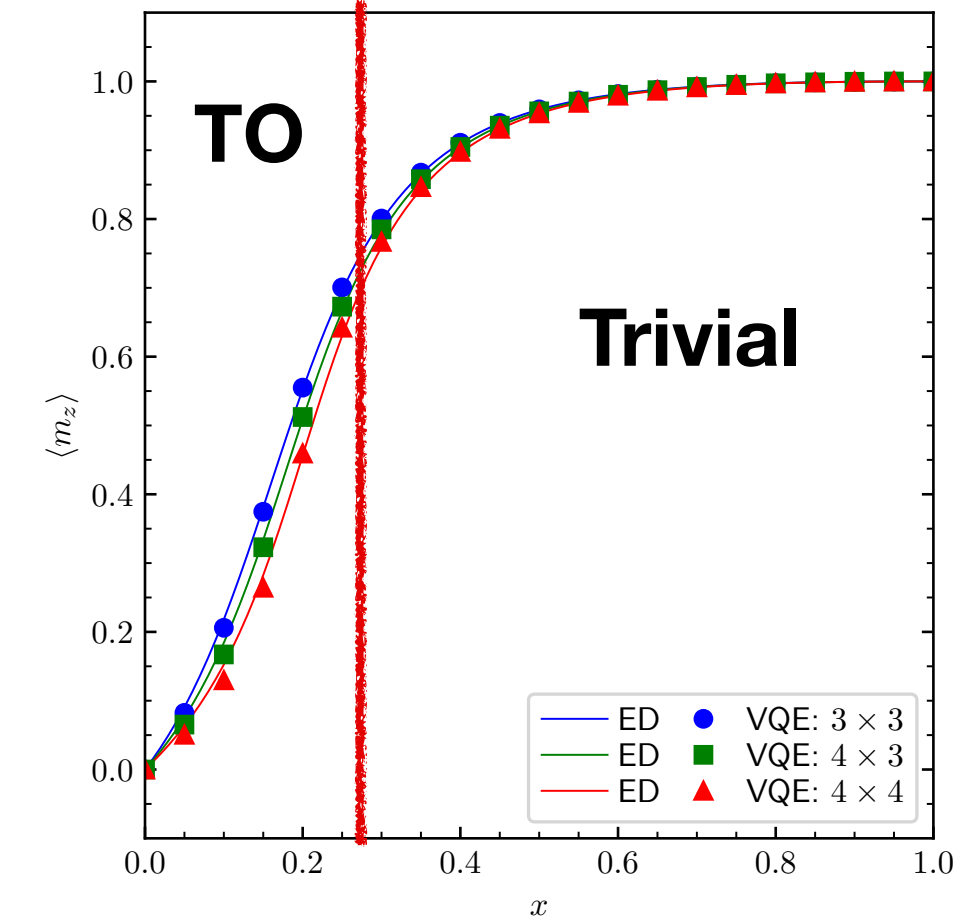
$$|\Psi(\theta_l^0, \theta_l^1)\rangle = \prod_{l=1}^D \left[ e^{-i\theta_l^0 H_{\text{TC}}} e^{-i\theta_l^1 H_h} \right] |\Psi_0\rangle$$



arXiv:2202.02909

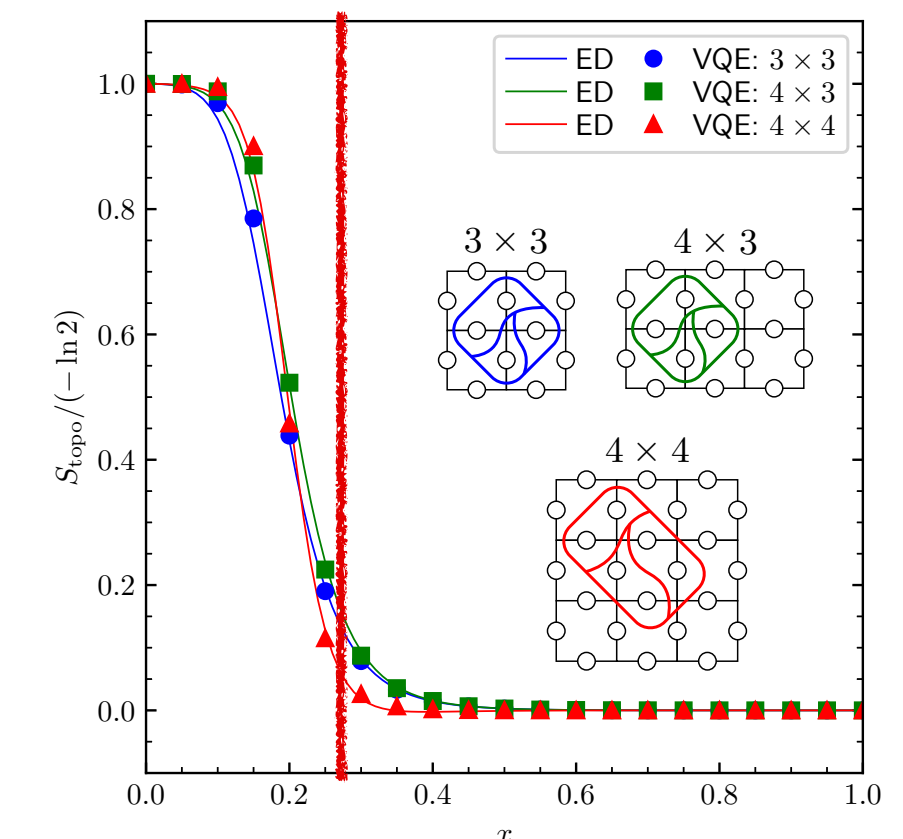
### Magnetization

$$\langle m_z \rangle = \frac{1}{N} \sum_{i=1}^N \langle \sigma_i^z \rangle$$



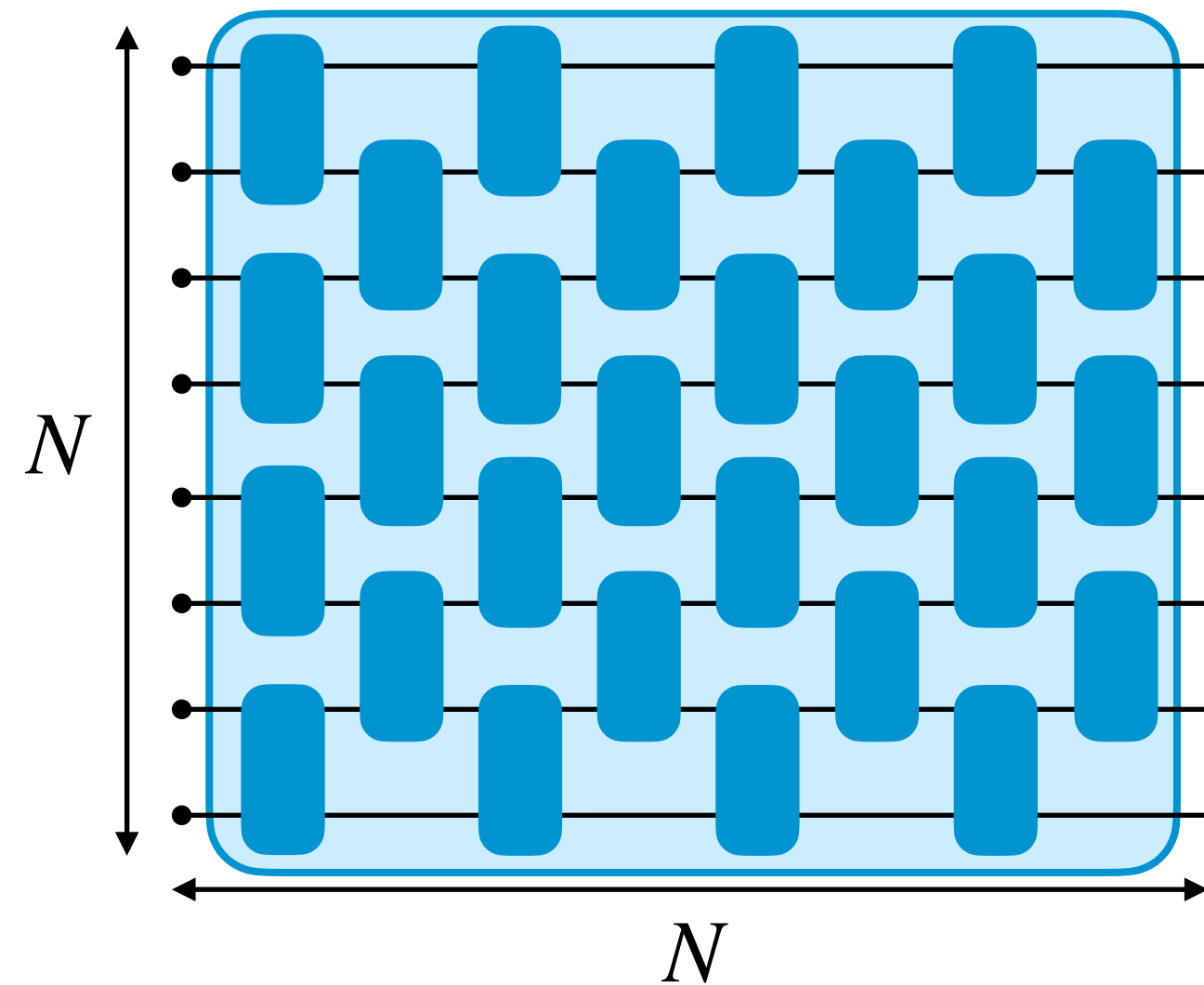
### Topological entanglement entropy

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



Realize **scalable** VQE simulations

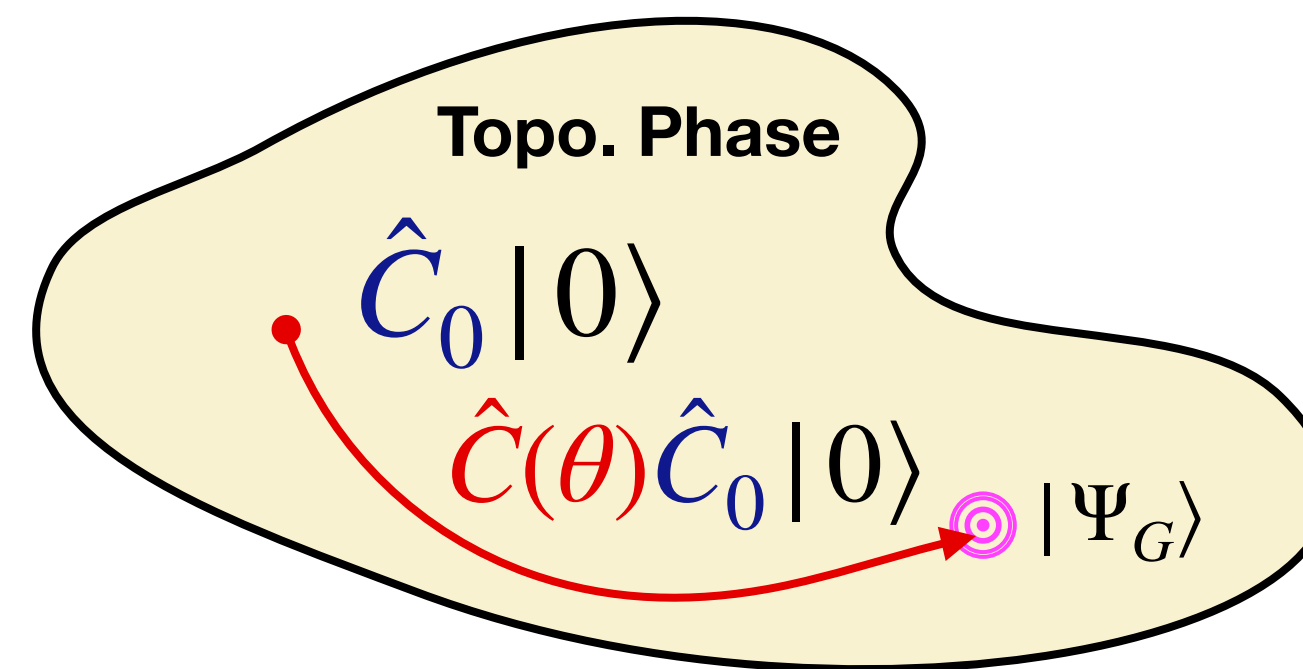
## $N \times N$ NISQ playground



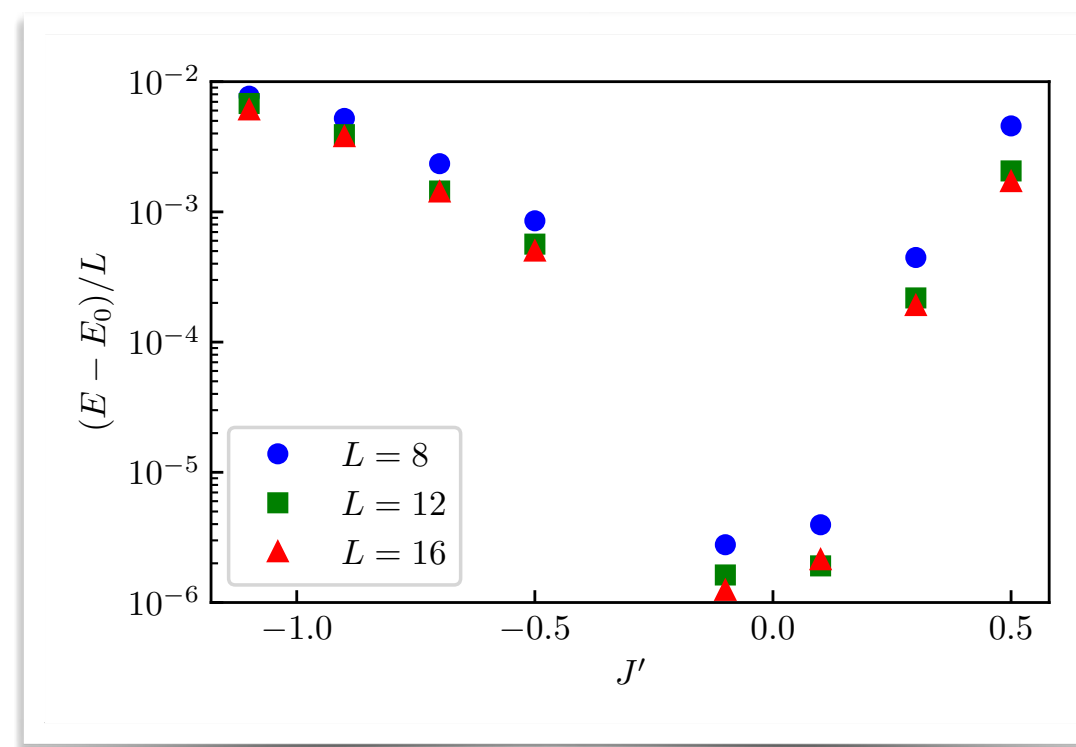
- NISQ scalability:  $N \times N$  circuit
- Scalable PQC: Volume  $\leq O(N^2)$
- Enough for topological states
- Promising in the near future

## Two-layer structured PQC Ansatz

$$|\Psi(\theta)\rangle = \hat{C}(\theta)\hat{C}_0|0\rangle$$

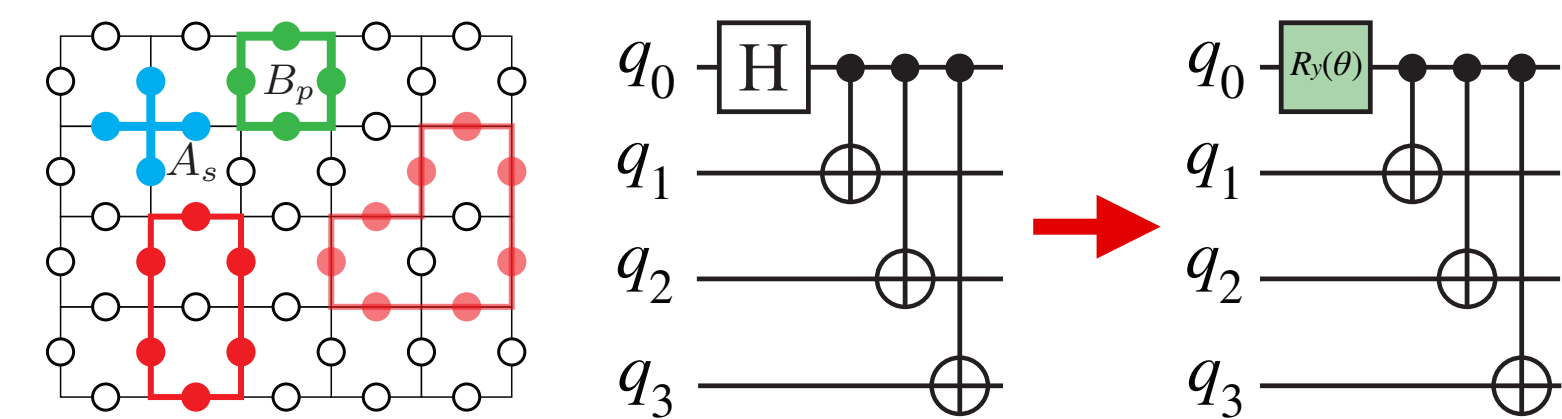


## Scalable VQE for 1D SPT



R.-Y. Sun et. al., arXiv:2303.17187

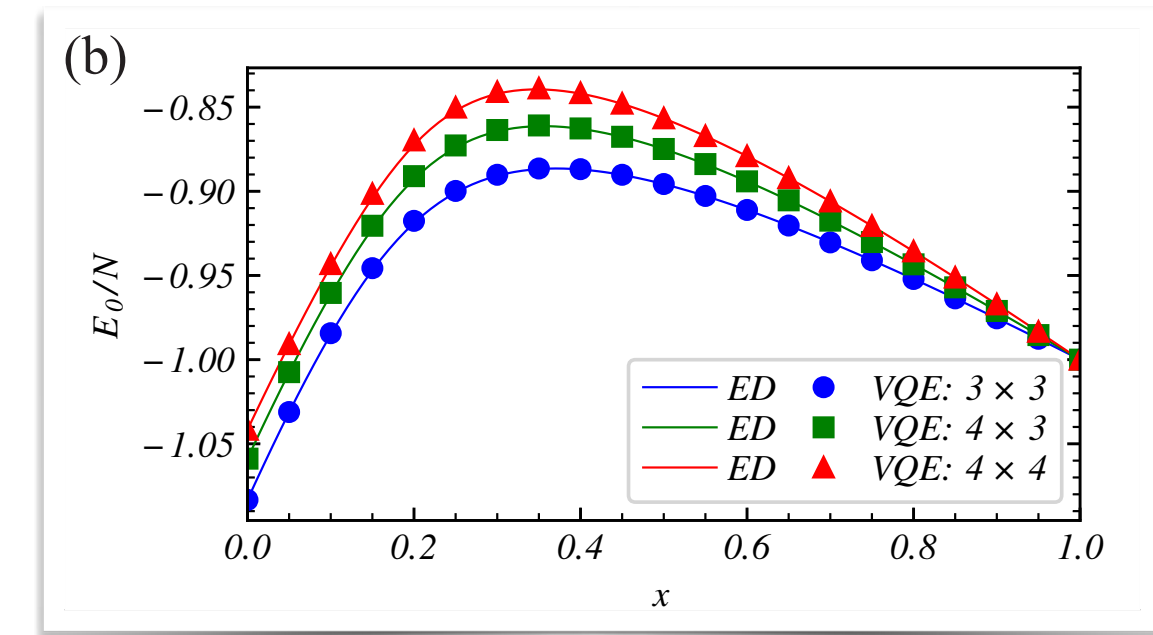
## Parametrized loop gas circuit (PLGC)



$$|\Psi(\theta)\rangle = \prod_{p=1}^{N_p} \left( \cos(\theta_p/2)I + \sin(\theta_p/2)B_p \right) |00\dots 0\rangle$$

$$= \left| \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \end{array} \right\rangle + \left| \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \end{array} \right\rangle + \left| \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \end{array} \right\rangle + \dots$$

## Scalable VQE for TC + magnetic field



R.-Y. Sun et. al., arXiv:2210.14662

**Thank you for your attention!**