Phase transition in Parametrized quantum circuits

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RIKEN-iTHEMS

collaborate with

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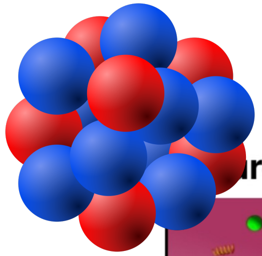
[arXiv:2603.27532]

QuantHEP, Queen Mary University of London, Jul. 16

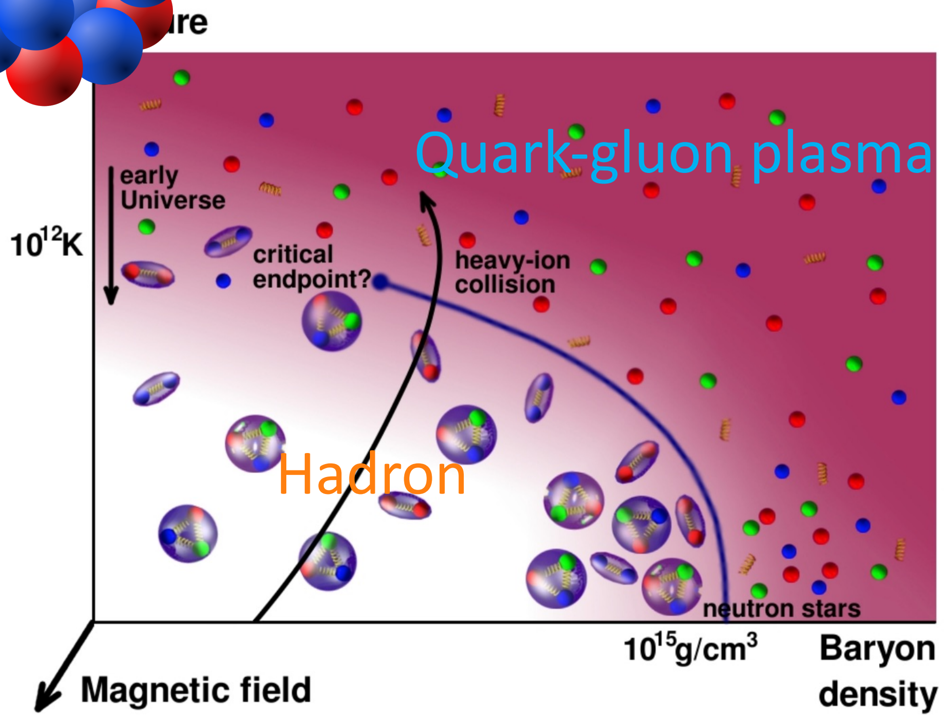
Main Content

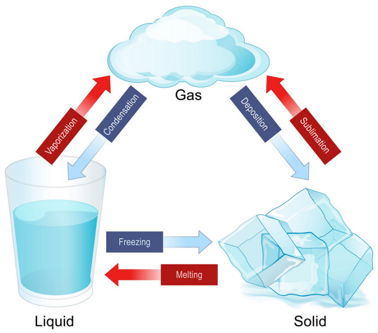
- ❑Why quantum computer for phase transition?
- ❑Phase transition mechanism
- ❑Phase transition in Ising whip circuit
- ❑Towards quantum advantage
- ❑Conclusion

Why quantum computer?

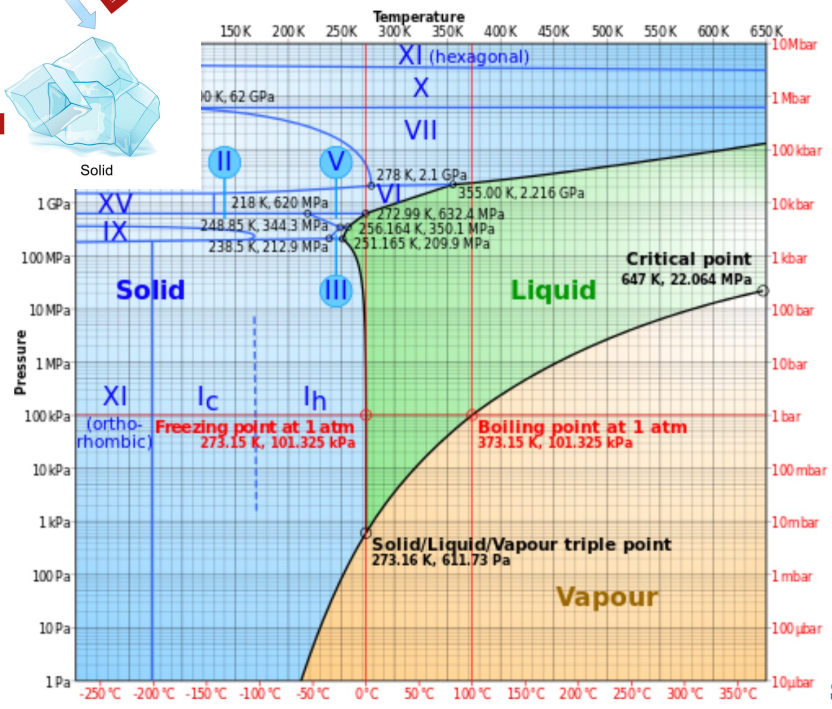


Phase diagram of QCD





Phase diagram of H_2O



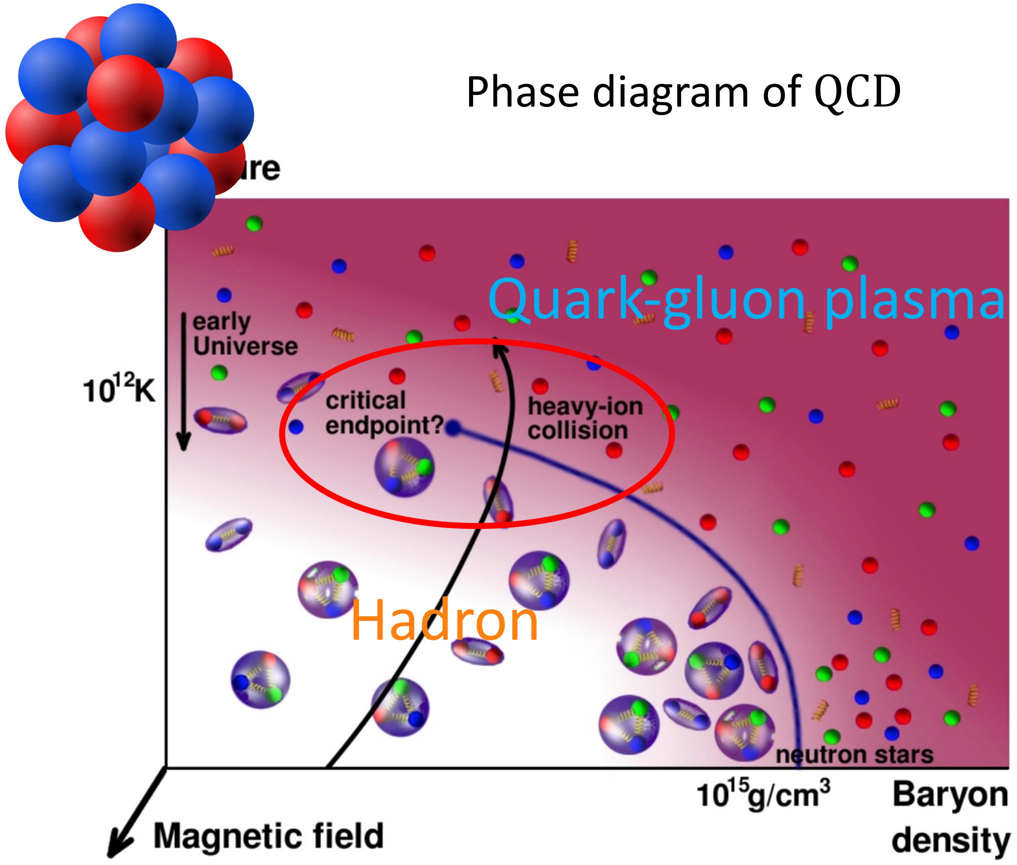
Source

- Phase transition plays a fundamental role to study many-body systems.
- Classical algorithms often fail near the critical point.

[See talks by Elisa Ercolessi, Simon Jonathan Williams, Zlatko Papic, Lena Funcke, James Hancock, Max McGinley …]

Why quantum computer?

Phase diagram of QCD



Monte-Carlo algorithm: Critical slowing down problem.

$$\tau \sim \xi^z$$

Tensor network: critical states have larger entanglement (S).

$$\chi \sim e^S$$

Mean-field method: critical states have larger fluctuation.

$$\langle s_i s_j \rangle \neq \langle s_i \rangle \langle s_j \rangle$$

- Phase transition plays a fundamental role to study many-body systems.
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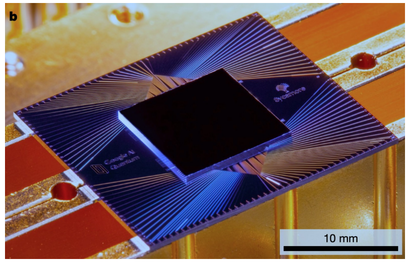

Quantum computer:

- No configuration sampling, and no critical slowing down.
- Large entanglement can be obtained.
- Quantum fluctuation in the exponential Hilbert space.

Monte-Carlo algorithm: Critical slowing down problem.

$$\tau \sim \xi^{z}$$

Tensor network: critical states have larger entanglement (S).

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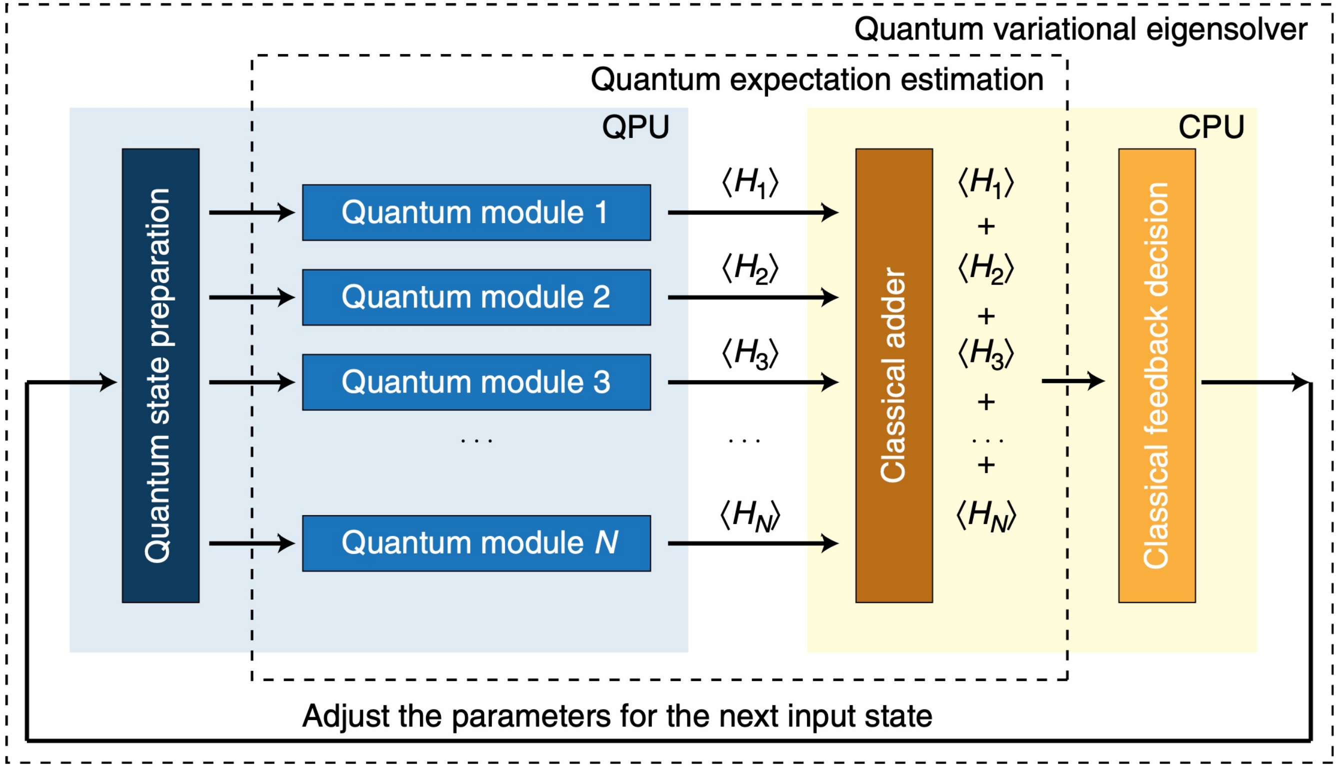
Parametrized quantum circuits in VQE

Variational quantum eigensolver (VQE)

[Peruzzo et. al. (2014), and talks by Nico Dichter, James Hancock…]



Hamiltonian expectation on quantum computers

optimization performed on classical computers

- To prepare the ground state (thermal state) of Hamiltonian

$$H = \sum_i a_i \sigma_i \qquad \text{eg. } H_{\text{Ising}} = \sum_{\langle i,j \rangle} Z_i Z_j$$

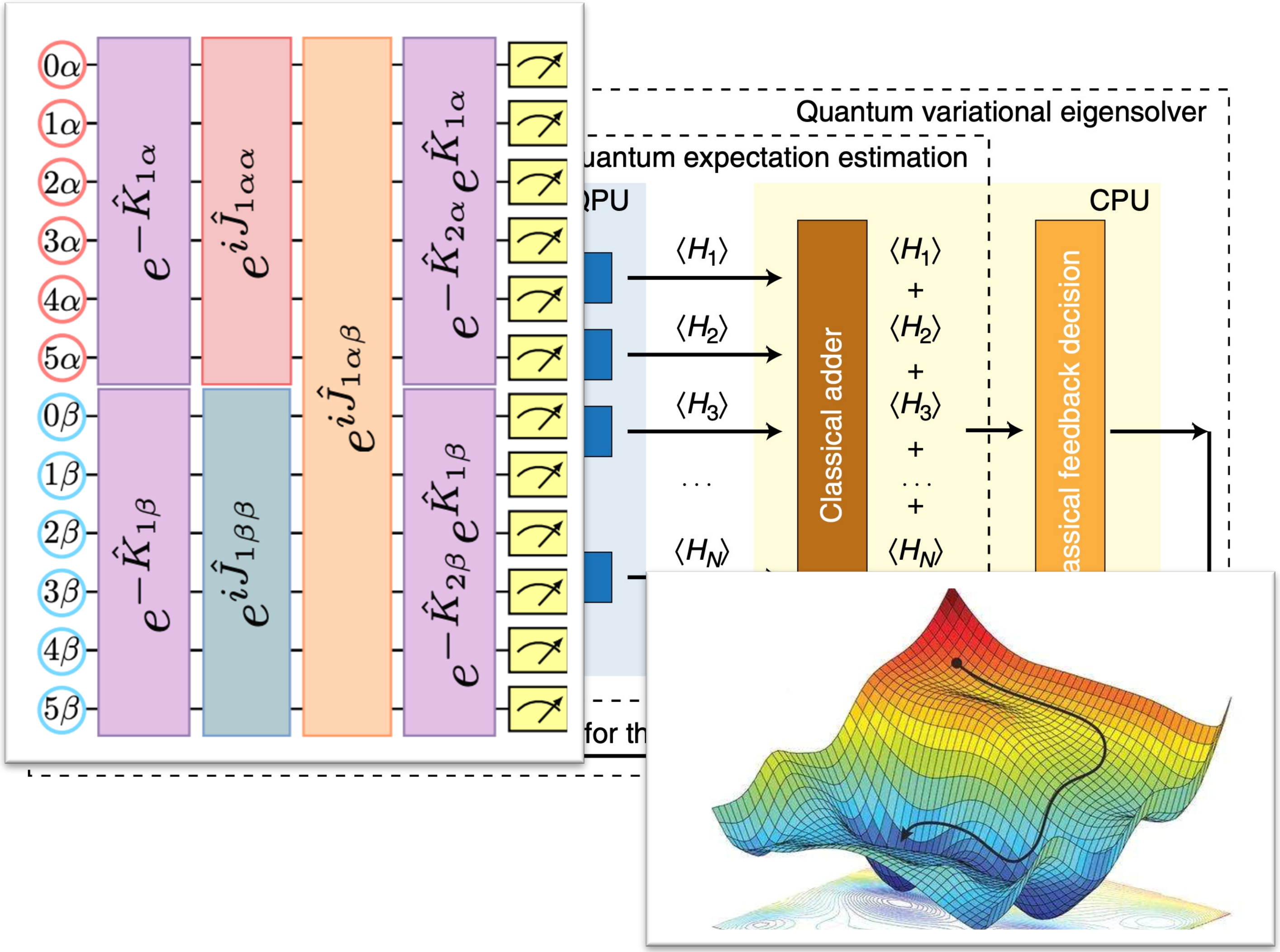
- The energy (free energy) is minimized variationally.

$$E_0 = \min_{\boldsymbol{\theta}} \langle \phi(\boldsymbol{\theta}) | H | \phi(\boldsymbol{\theta}) \rangle$$

$$F_0 = \min_{\boldsymbol{\theta}} \left(\langle \phi(\boldsymbol{\theta}) | H | \phi(\boldsymbol{\theta}) \rangle - T S_{\boldsymbol{\theta}} \right)$$

Parametrized quantum circuits in VQE

Parametrized quantum circuit(PQC)



classical optimization

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- The success of VQE highly rely on the choice of parametrized quantum circuits (PQC).

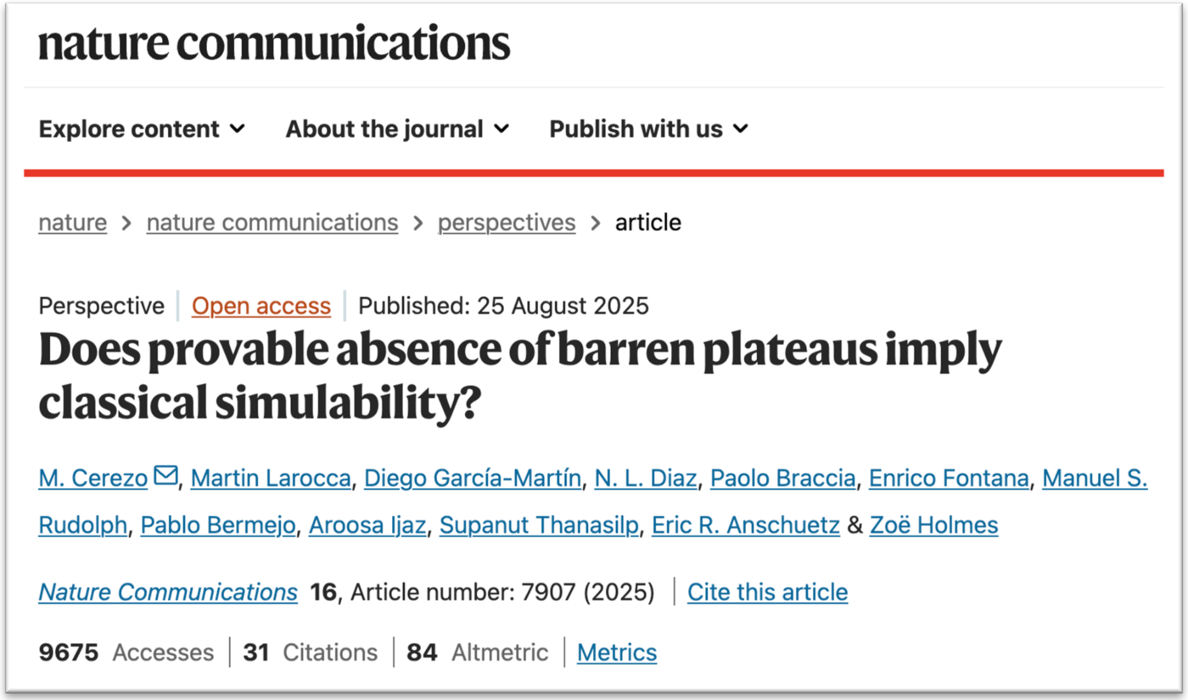
$$|\phi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta}) |\bar{0}\rangle$$

Challenges for Parametrized quantum circuits

- The accuracy of PQC is not high enough, especially at the phase transition point.

- The classical simulability-trainability conjecture:

  VQE might have no quantum advantage.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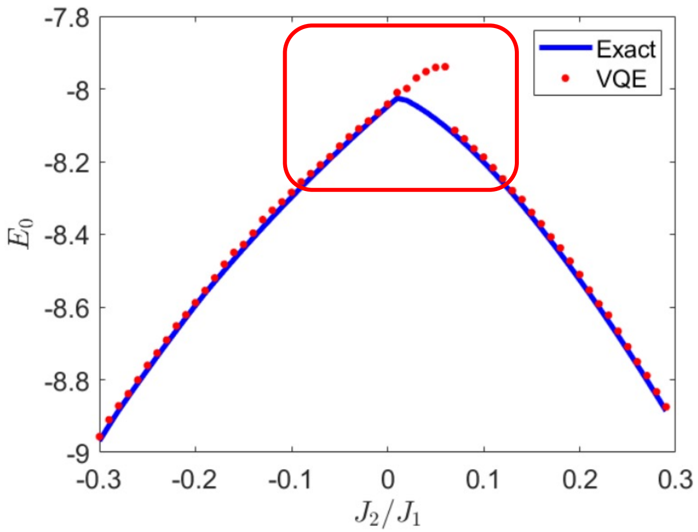
Does provable absence of barren plateaus imply classical simulability?

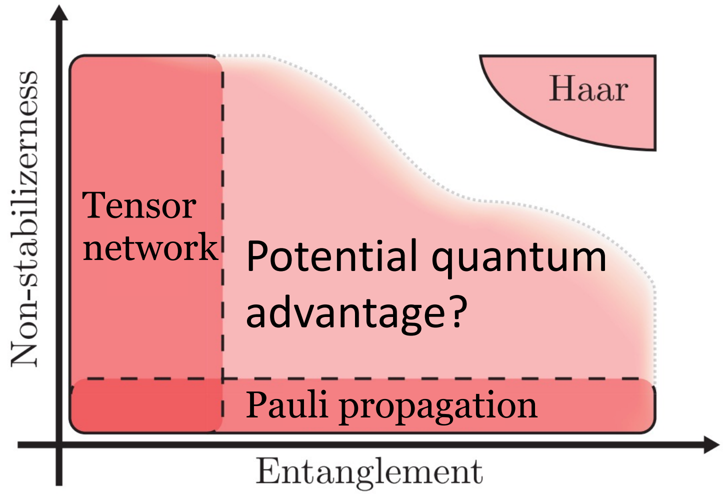
M. Cerezo, Martin Larocca, Diego García-Martín, N. L. Diaz, Paolo Braccia, Enrico Fontana, Manuel S. Rudolph, Pablo Bermejo, Aroosa Ijaz, Supanut Thanasilp, Eric R. Anschuetz & Zoë Holmes

Nature Communications 16, Article number: 7907 (2025) | Cite this article

9675 Accesses | 31 Citations | 84 Altmetric | Metrics



[Y. Guo, M. Qin (2023)]



[A. Sinibaldi et. al. PRR (2025)]

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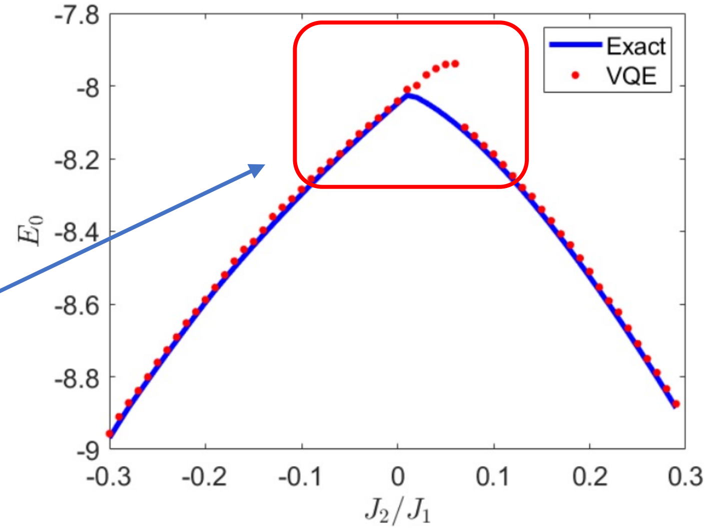


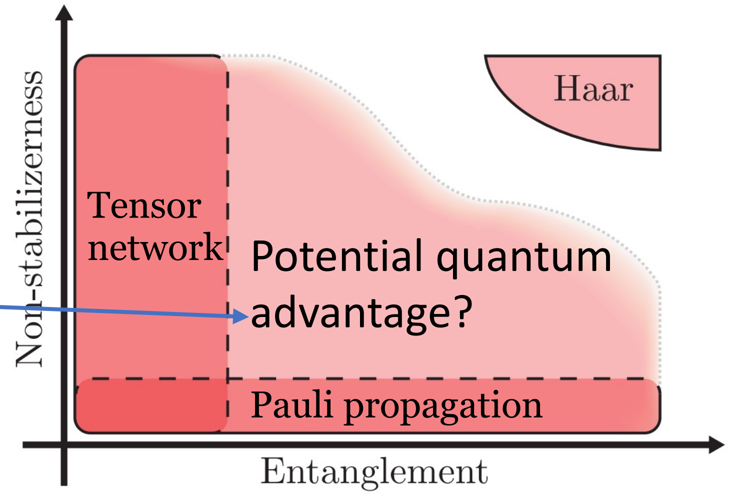
[Y. Guo, M. Qin (2023)]

- The classical simulability-trainability conjecture:

  VQE might have no quantum advantage.

➢ Does the phase structure exist in principle in PQCs ?

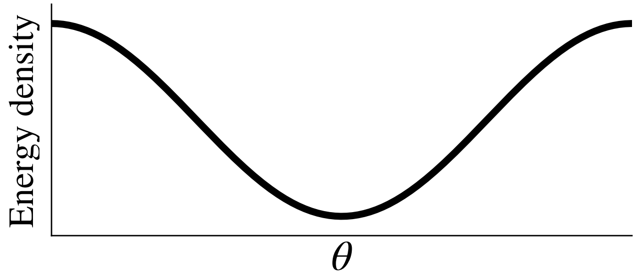
➢ Possible quantum advantage using PQCs?

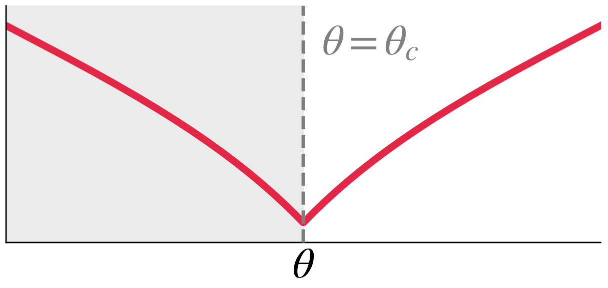


[A. Sinibaldi et. al. PRR (2025)]

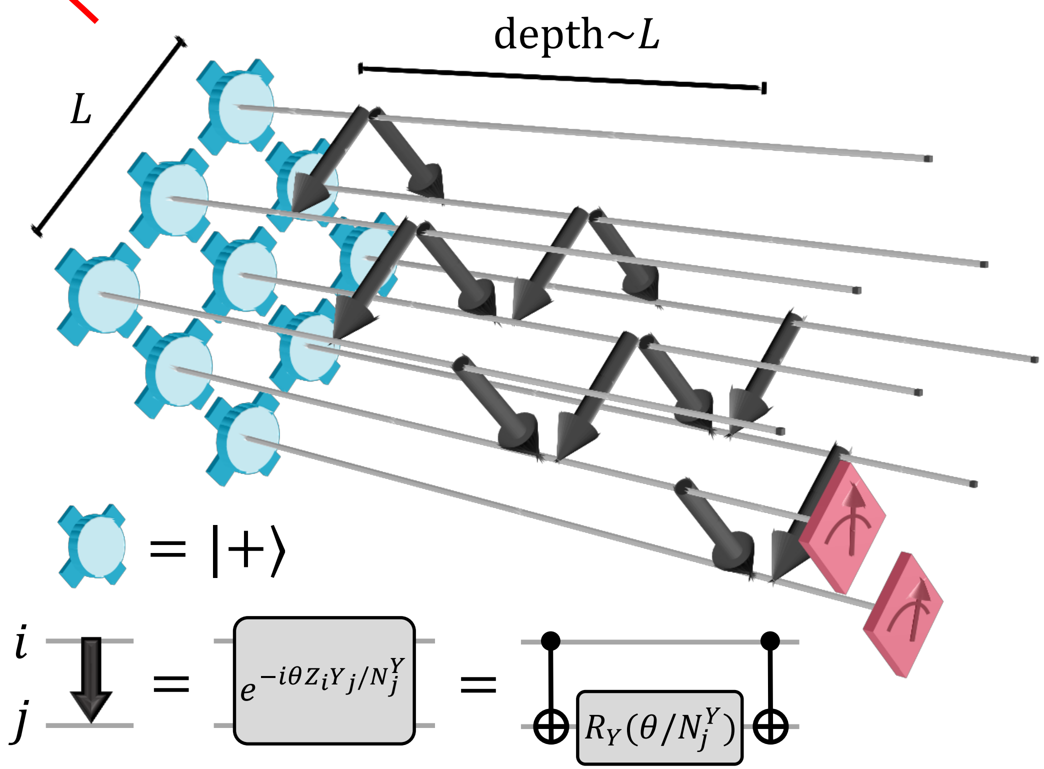
Challenges for Parametrized quantum circuits

$$\frac{\partial \langle O \rangle_{\theta(J)}}{\partial J} = \frac{\partial \theta}{\partial J} \boxed{\frac{\partial \langle O \rangle_{\theta(J)}}{\partial \theta}}$$





- PQC without phase transition.
- PQC with phase transition.



- Deep PQC with phase transition, and is provably barren-plateau free.

✓ Does the phase structure exist in principle in PQCs ?

Yes, only if the PQC is deep enough.

✓ Possible quantum advantage using PQCs?

More possible to be observed near the phase transition point of PQC.

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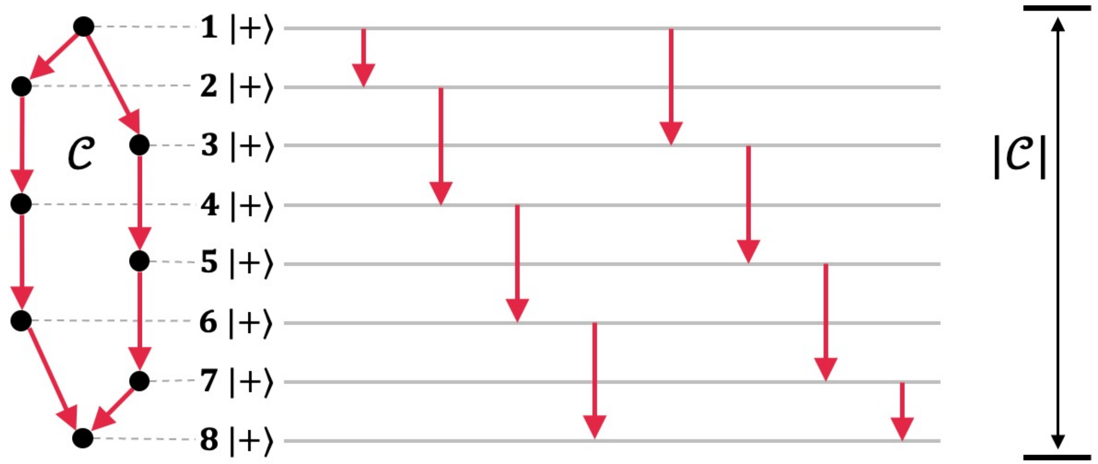
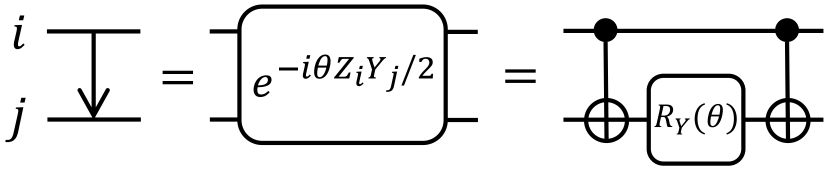
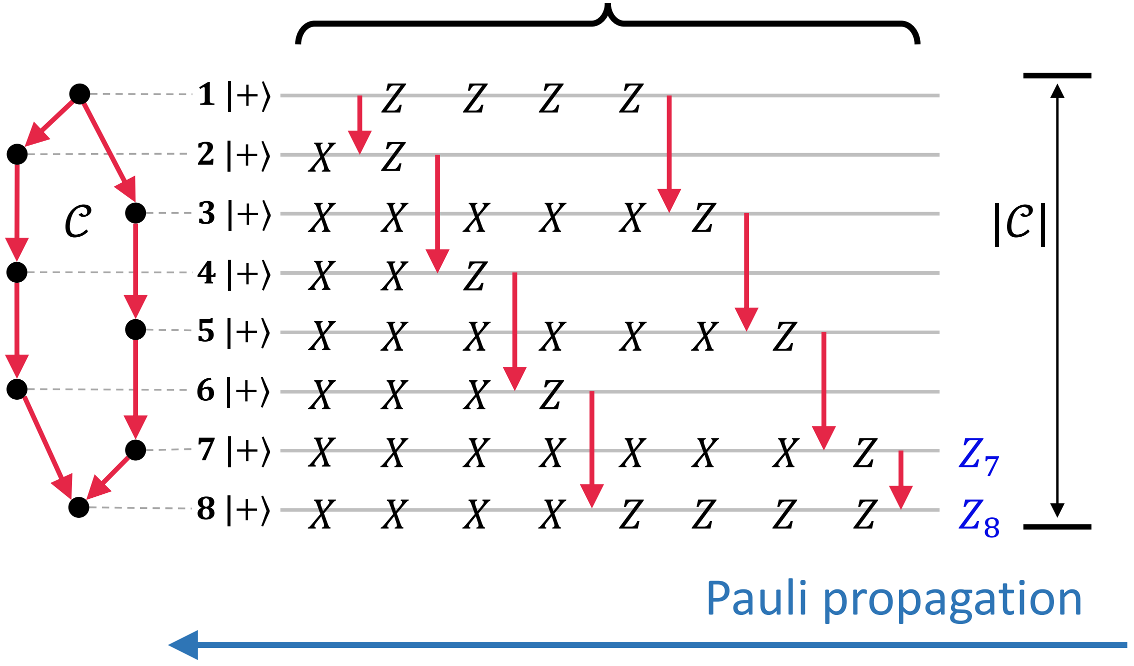
Emergence of singularity in PQC





Emergence of singularity in PQC

Non-local Pauli path



$$U_{ZY}\, ZZ\, U_{ZY}^{\dagger} = \cos\theta\, ZZ - \sin\theta\, IX$$

- Each ZY-rotation transformation gives a $\sin\theta/\cos\theta$ to the Pauli path.

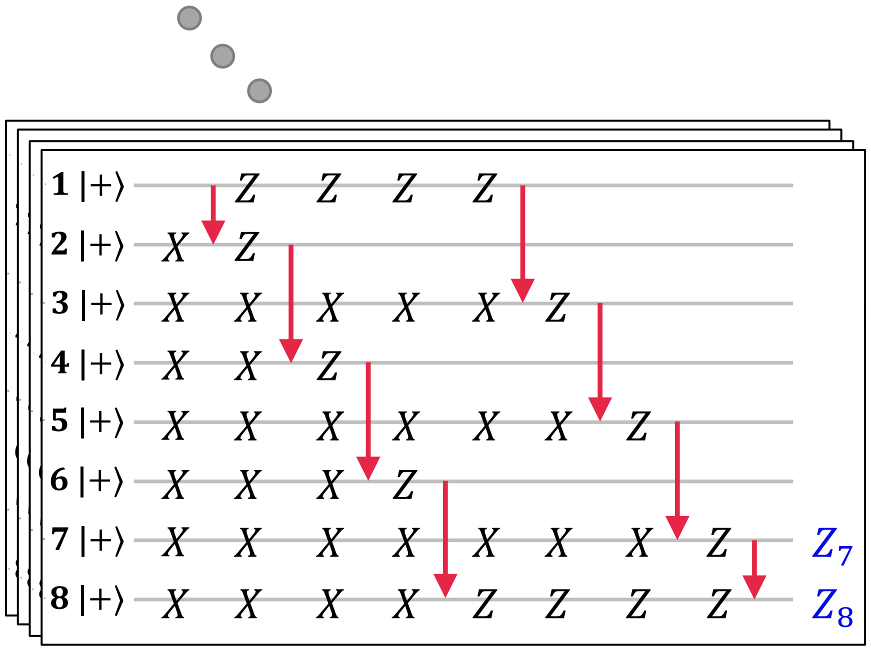
(1) Non-local Pauli path leads to divergent derivatives:

$$\langle\phi(\theta)|ZZ|\phi(\theta)\rangle = -\sin\theta\cos\theta + (-\sin\theta)^{|\mathcal{C}|-1}\cos\theta$$

$$\frac{\partial\langle ZZ\rangle_\theta}{\partial\theta} = -|\mathcal{C}|(-\sin\theta)^{|\mathcal{C}|-2}\cos^2\theta + \mathcal{O}(1)$$

$$\frac{\partial^2\langle ZZ\rangle_\theta}{\partial\theta^2} = \underbrace{|\mathcal{C}|^2(-\sin\theta)^{|\mathcal{C}|-3}}_{\text{leads to divergence at } |\mathcal{C}| \to \infty}\cos^3\theta + \mathcal{O}(|\mathcal{C}|)$$

Emergence of singularity in PQC



$$\times\mathcal{O}\left(\frac{1}{|\mathcal{C}|(\sin\theta)^{|\mathcal{C}|}}\right)$$

(1) Non-local Pauli path leads to divergent derivatives:

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(2) The number of Pauli paths should be exponentially large to the cycle length $|\mathcal{C}|$.

$$|\mathcal{C}|^2(-\sin\theta)^{|\mathcal{C}|-3}\times\mathcal{O}\left(\frac{1}{|\mathcal{C}|(\sin\theta)^{|\mathcal{C}|}}\right) = \mathcal{O}(|\mathcal{C}|)$$

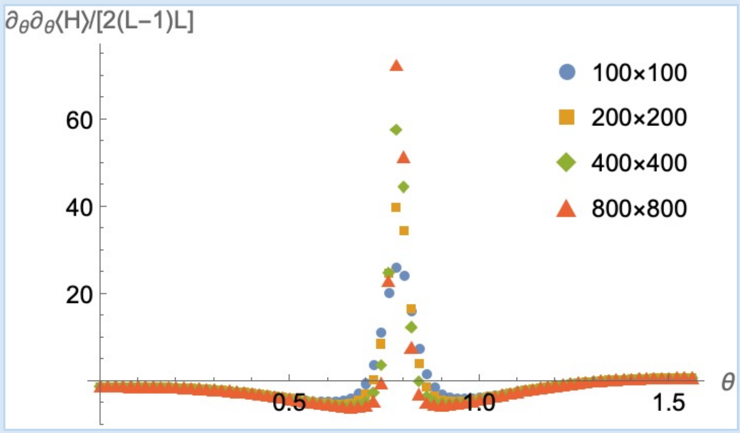
Phase transition mechanism

A large number of non-local Pauli paths.

$\partial_\theta^2\langle ZZ\rangle$: divergence

$\partial_\theta\langle ZZ\rangle$: discontinuity

$\langle ZZ\rangle$: cusp



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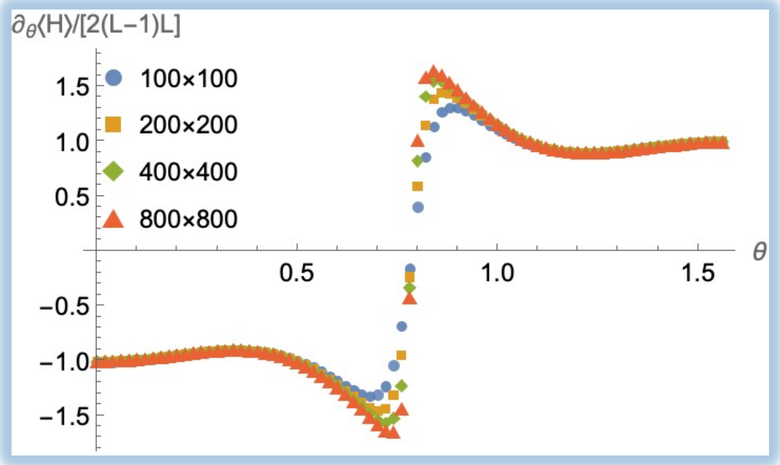

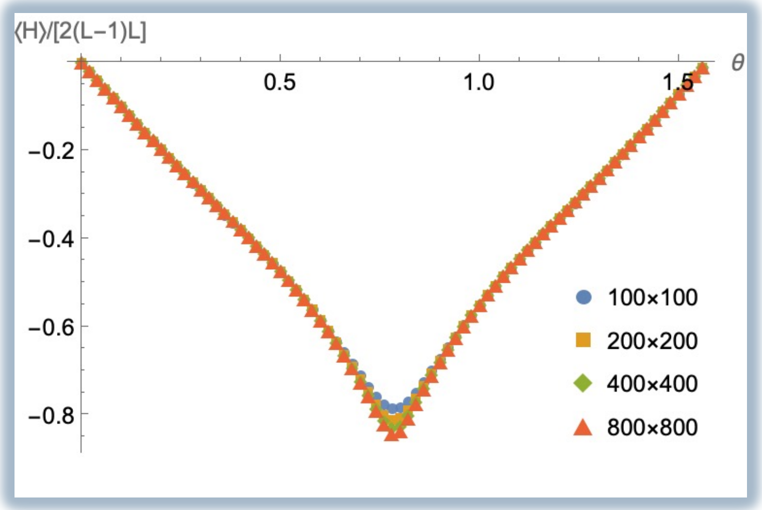

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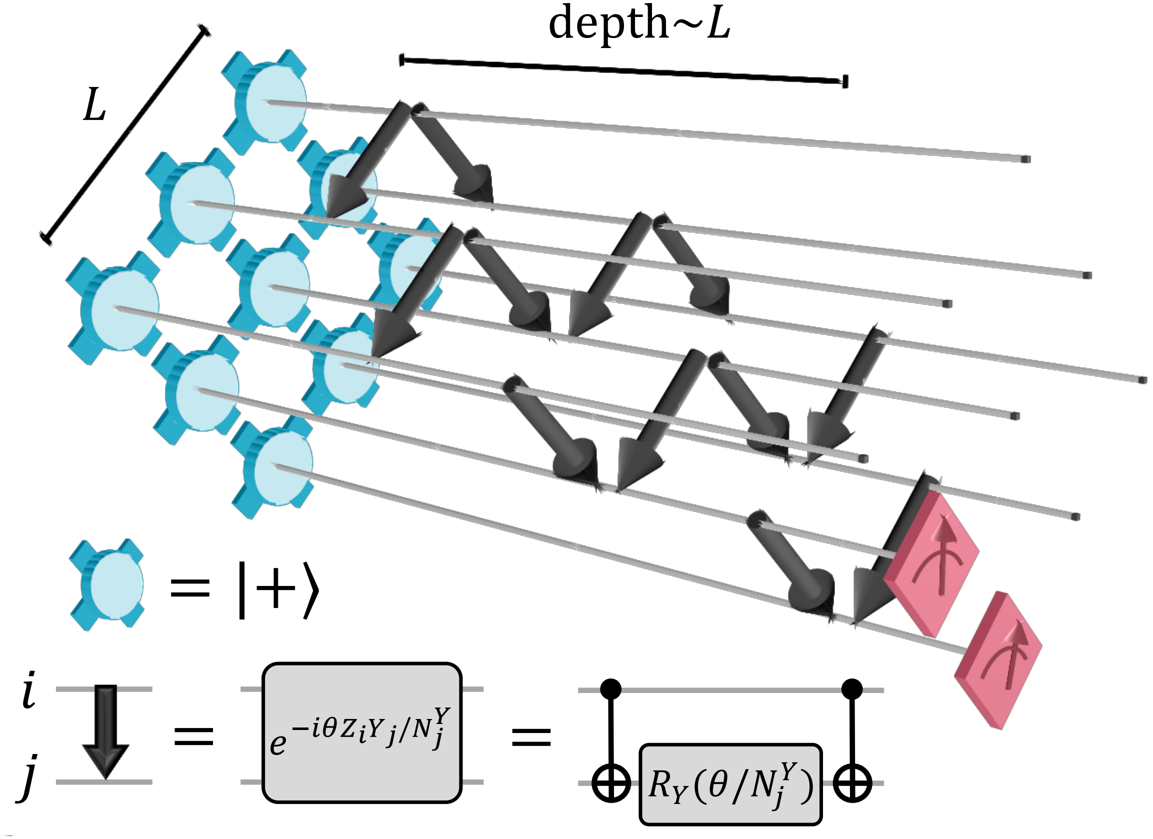
Ising whip circuit

2-d whip circuit

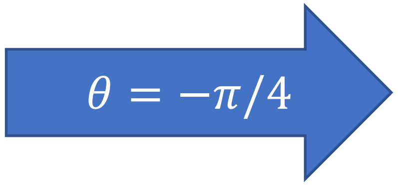


N_j^Y : The total number of arrows pointing to qubit j

- Ising whip circuit prepares the ground state of the Ising model:

$$\bar{H} = -\frac{1}{2N}\sum_{\langle i,j\rangle} Z_i Z_j$$

- The ground state is the GHZ-state:

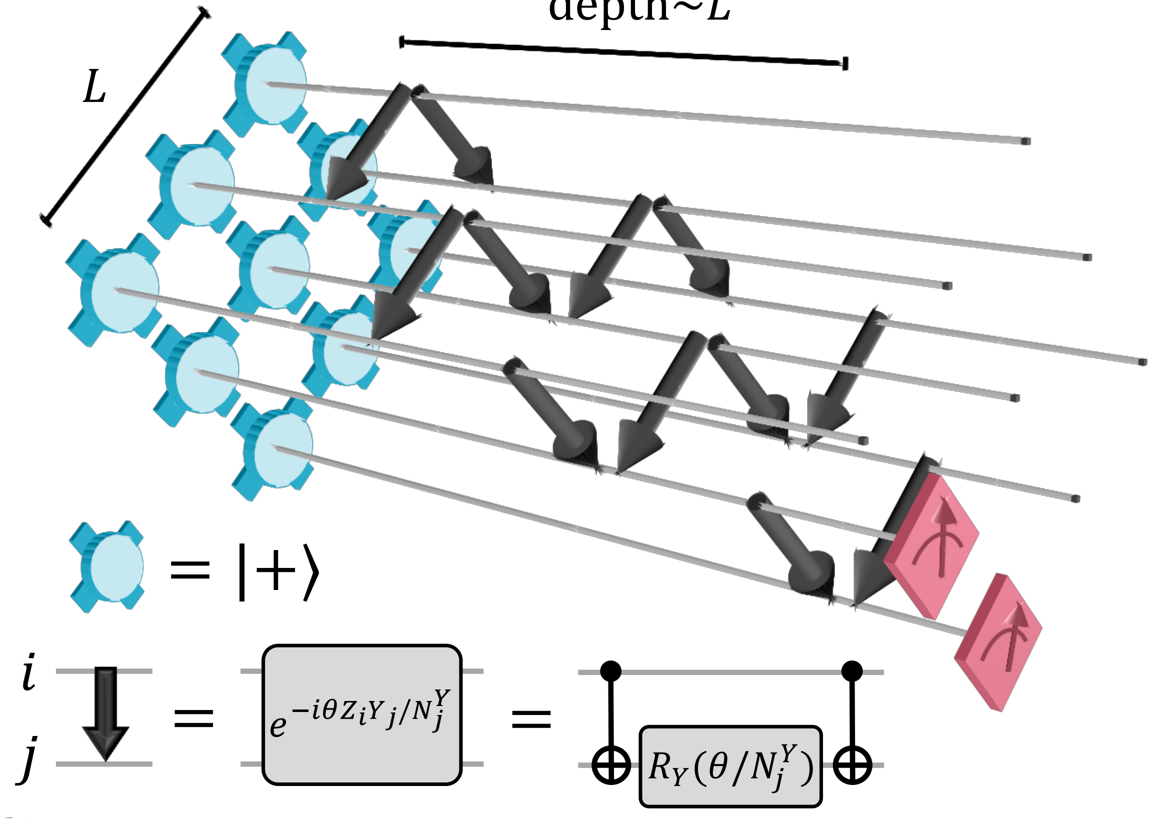


$$|\phi_{\mathrm{w}}(\theta)\rangle \equiv \prod_{\langle i,j\rangle} e^{-i\theta Z_i Y_j / N_j^Y} \, |+\rangle^{\otimes N}\Big|_{\theta=-\pi/4}$$
$$= \frac{1}{\sqrt{2}}(|0\rangle^{\otimes N} + |1\rangle^{\otimes N}).$$

Similar sequential circuits can be designed for other models like $\mathbb{Z}_2$ gauge theory.

[XW, X. Feng, T. Hartung, K. Jansen, P. Stornati PRA (2023)]
[XW, Y. Chai, X. Feng, Y. Guo, K. Jansen, C. Tüysüz PRA (2025)]

2-d whip circuit



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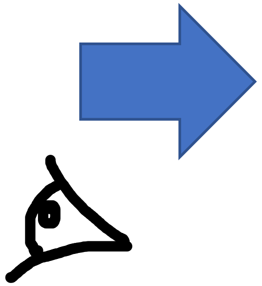
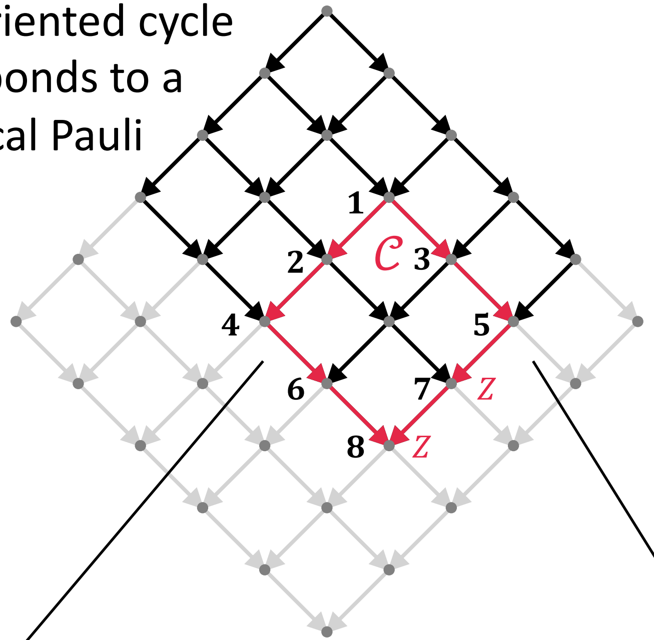
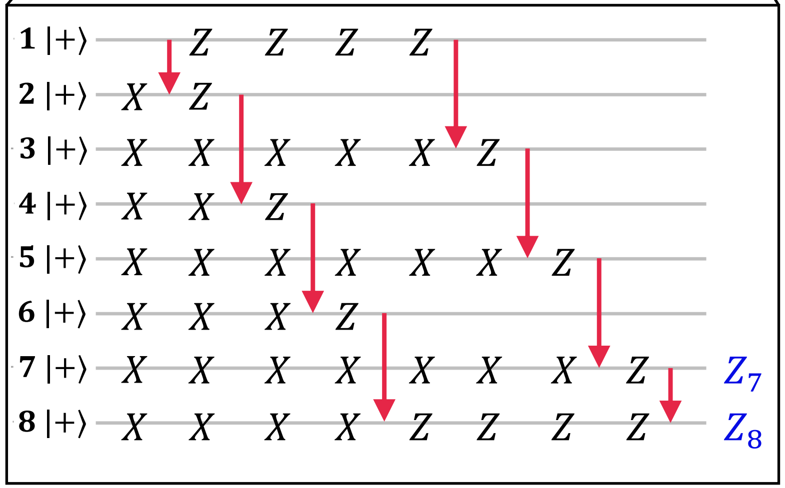


- Each oriented cycle corresponds to a non-local Pauli path.





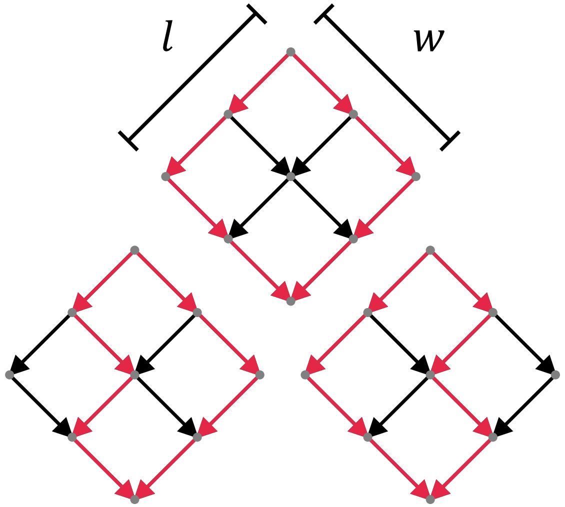
Phase transition in Ising whip circuit

- Count **the number of non-crossing cycles** within the length-l width-w rectangle by the **Lindström-Gessel-Viennot (LGV) lemma**:

$$N_{\mathcal{C}}(l,w) = \frac{lw}{(l+w-1)(l+w)^2}\left[\binom{l+w}{l}\right]^2$$

with the scaling behavior:

$$\lim_{l=w\to\infty} N_{\mathcal{C}}(l,w) = \frac{2}{\pi|\mathcal{C}|^2}2^{|\mathcal{C}|}$$



$N_{\mathcal{C}}(2,2) = 3$ non-crossing cycles contributed to $\langle ZZ\rangle_\theta$

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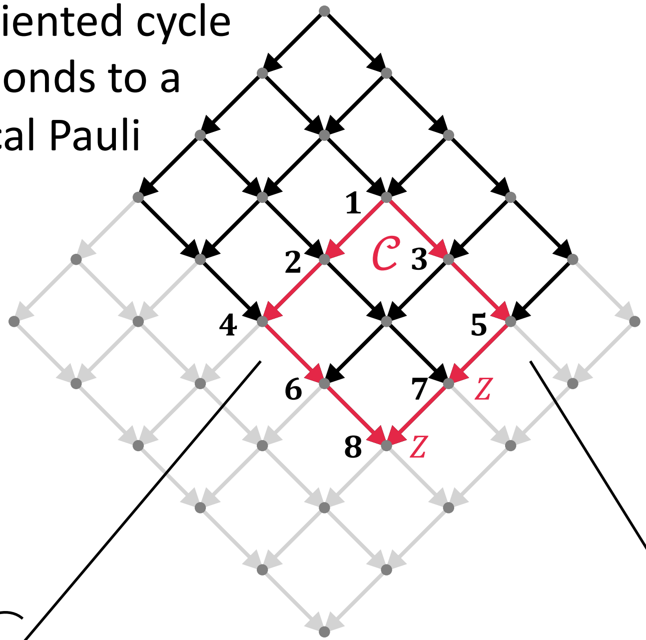
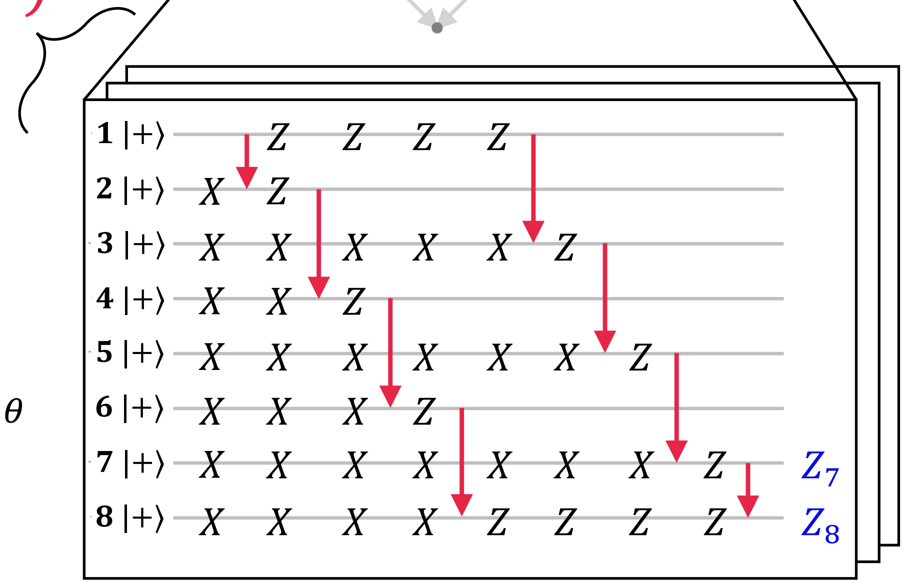


$\mathcal{O}(2^{|\mathcal{C}|})$



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- Collect cycles with the same length $|\mathcal{C}|$ into **layers** indexed by $\mathcal{L}$. Their contributions are summed over using **Chu-Vandermonde identity**:

$$\sum_{k=0}^{r}\binom{m}{k}\binom{n}{r-k} = \binom{m+n}{r}$$

- All layers are summed over as a series:

$$\langle Z_i Z_j\rangle_\theta = -\sum_{\mathcal{L}=1}^{\infty}\frac{4^{\mathcal{L}-1}\Gamma\left(\mathcal{L}-\frac{1}{2}\right)}{\sqrt{\pi}\,\mathcal{L}!}(\cos\theta\sin\theta)^{2\mathcal{L}-1}$$

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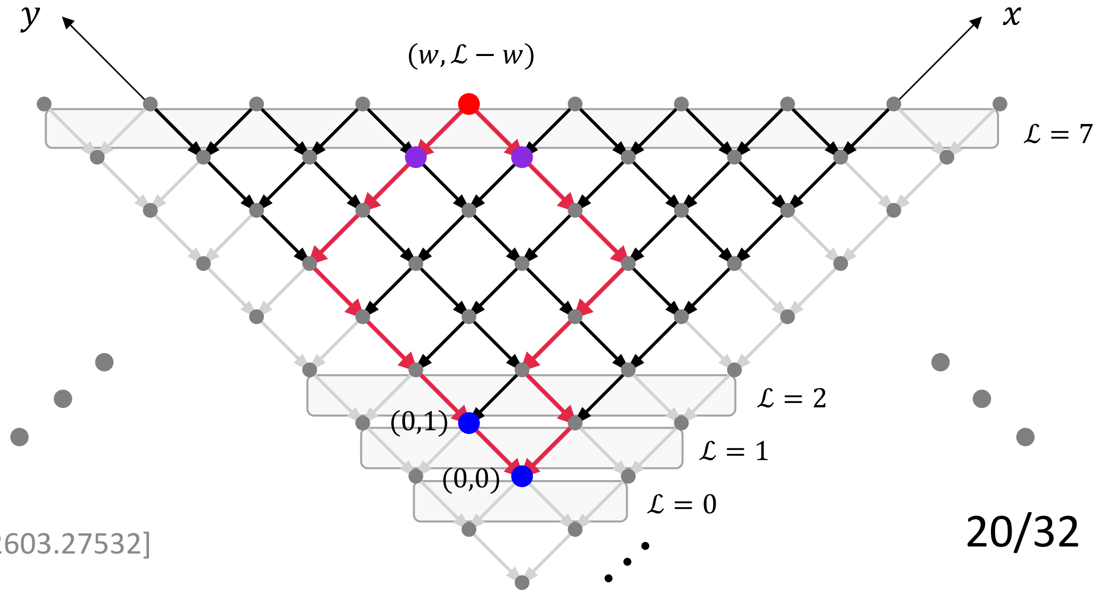
$$\bar{H} = -\frac{1}{2N}\sum_{\langle i,j\rangle} Z_i Z_j$$



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- In the infinite volume limit $N\to\infty$, non-analyticity is emerged from the analytic quantum gates:

$$\langle\phi_{\mathrm{w}}(\theta)|\bar{H}|\phi_{\mathrm{w}}(\theta)\rangle = \frac{1-|\cos 2\theta|}{\sin 2\theta} \quad \text{as } N\to\infty.$$

- $\cos 2\theta$ periodically change its sign at $\theta_c \equiv \pi\left(-\frac{1}{4}+\frac{k}{2}\right), k\in\mathbb{Z}$.

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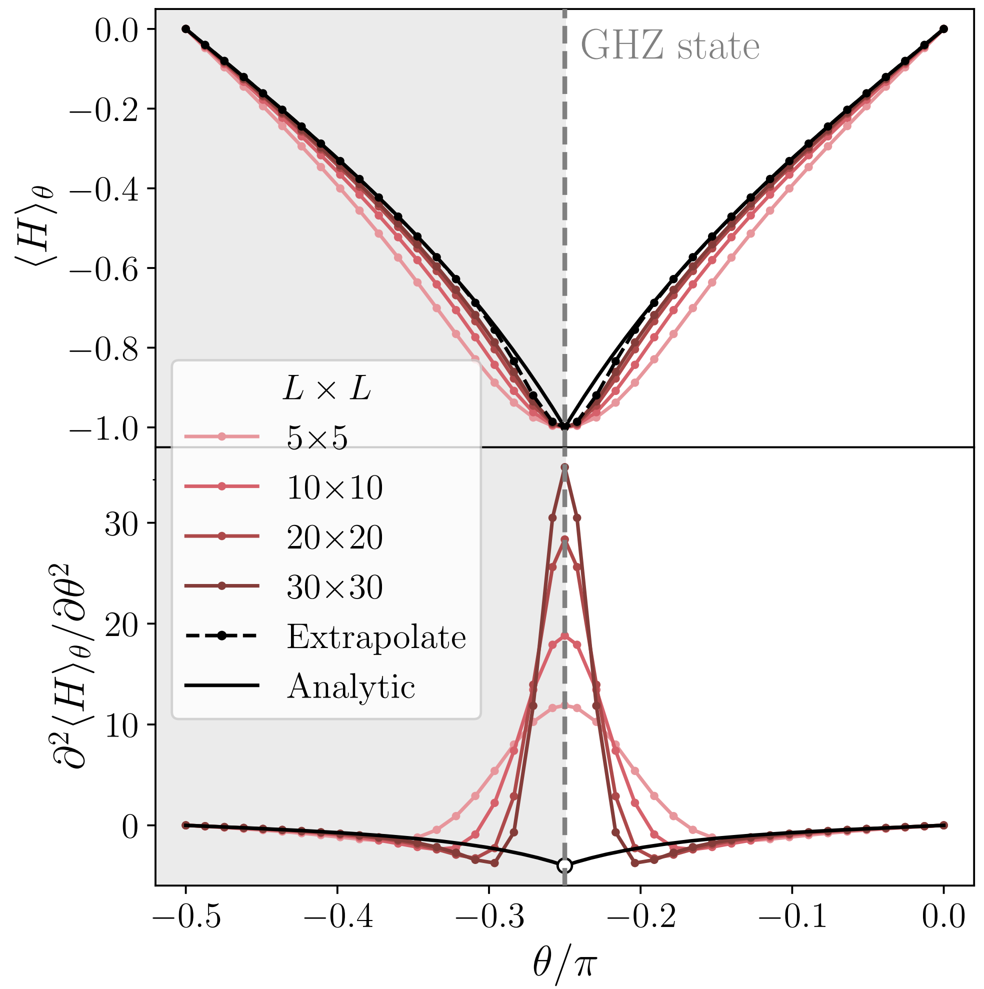
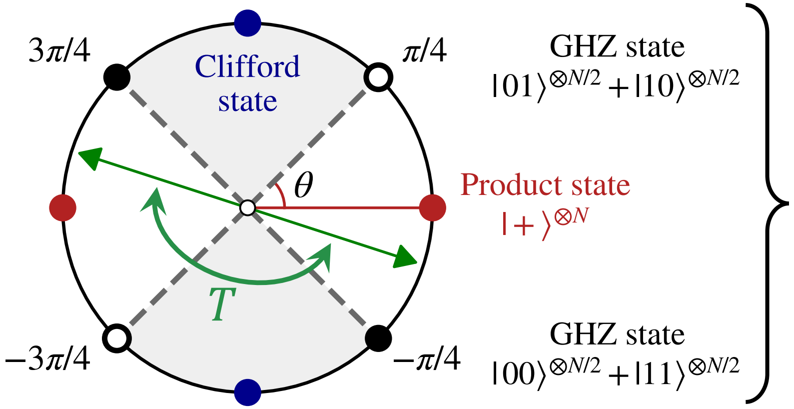


- Non-analyticity in the Ising whip circuit at $\theta_c = -\pi/4$.

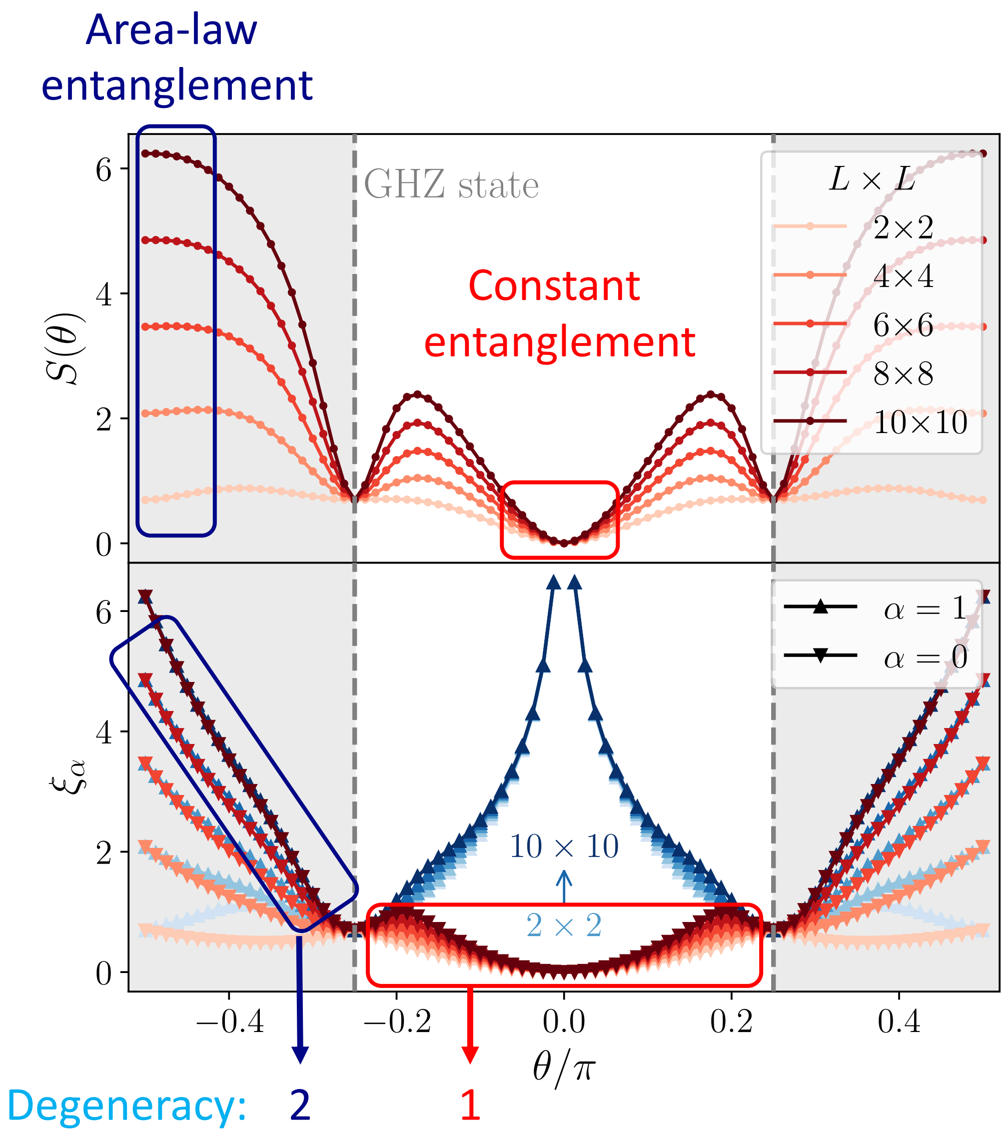
Phase transition in Ising whip circuit

- Phase diagram of the circuit-based "phase transition".



Are these two regions in different phases?

Yes, with two evidences.



Evidence 1:

Different entanglement entropy and the degeneracy of the entanglement spectrum.

- entanglement entropy:

$$S(\theta) = -\mathrm{Tr}(\rho_A \log \rho_A)$$

- entanglement spectrum:

$$|\phi_{\mathrm{w}}(\theta)\rangle = \sum_j e^{-\xi_j(\theta)/2} |\phi_j^A\rangle \otimes |\phi_j^{\bar{A}}\rangle$$

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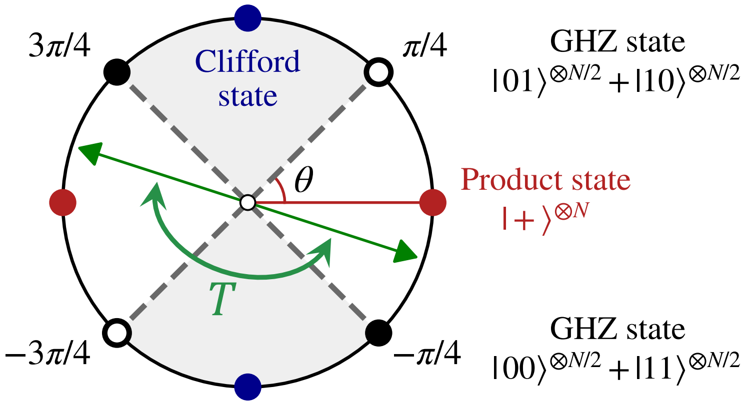
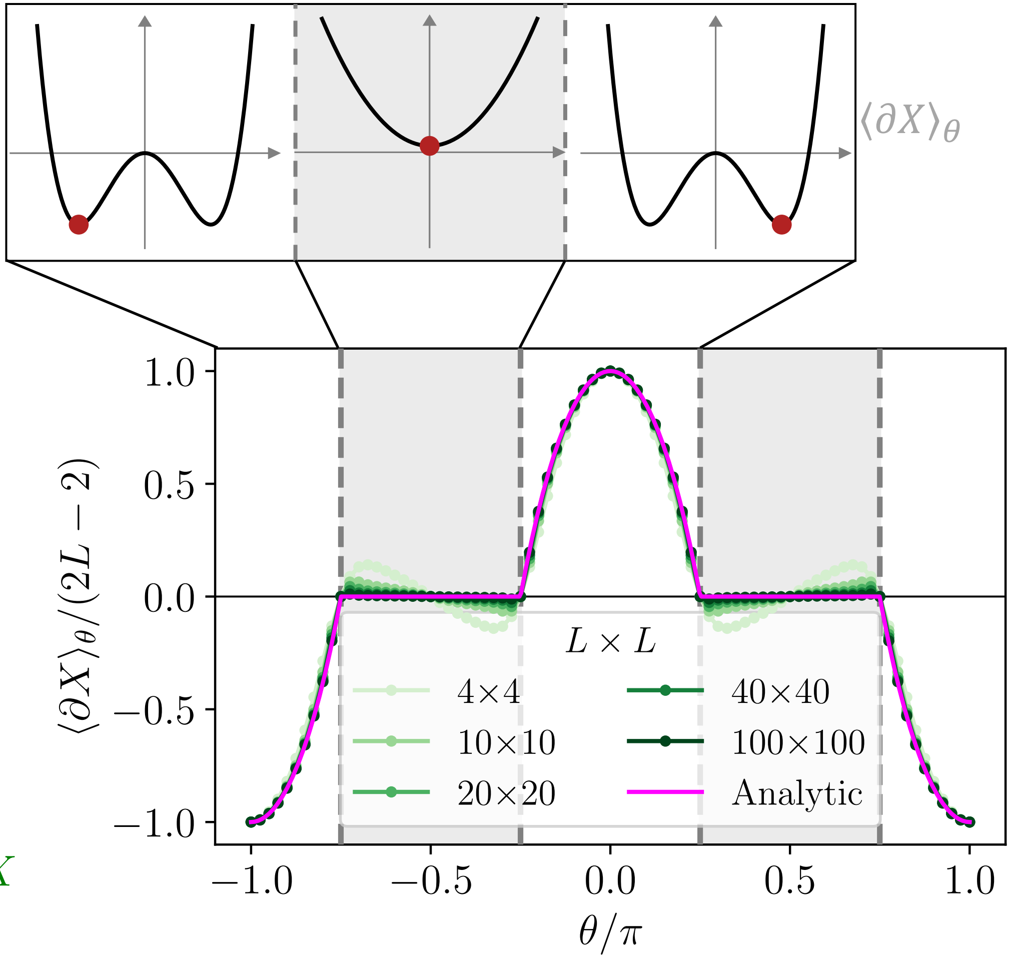


Are these two regions in different phases?

Yes, with two evidences.



Evidence 2:

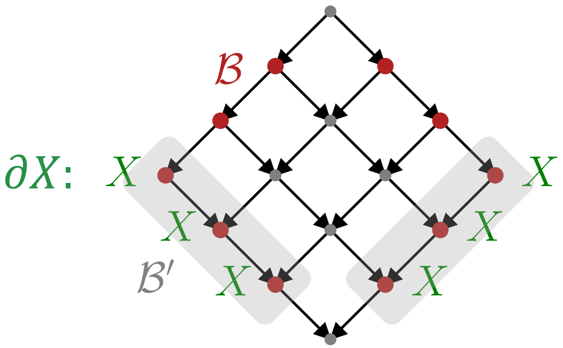
The identified order parameter of the Ising whip circuit

$$\partial X \equiv \sum_{i\in\mathcal{B}'} X_i$$

which anti-commute with the symmetry operator $\hat{T}$

$$\{\partial X, \hat{T}\} = 0,$$

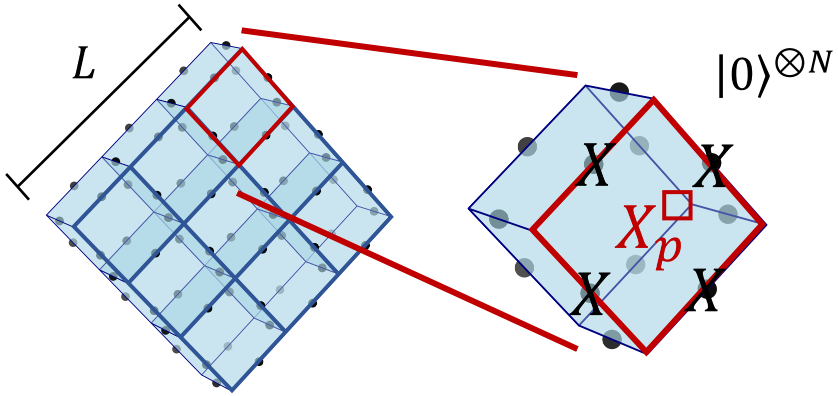
$$\hat{T} \equiv \prod\nolimits_{i\in\mathcal{B}} Z_i$$



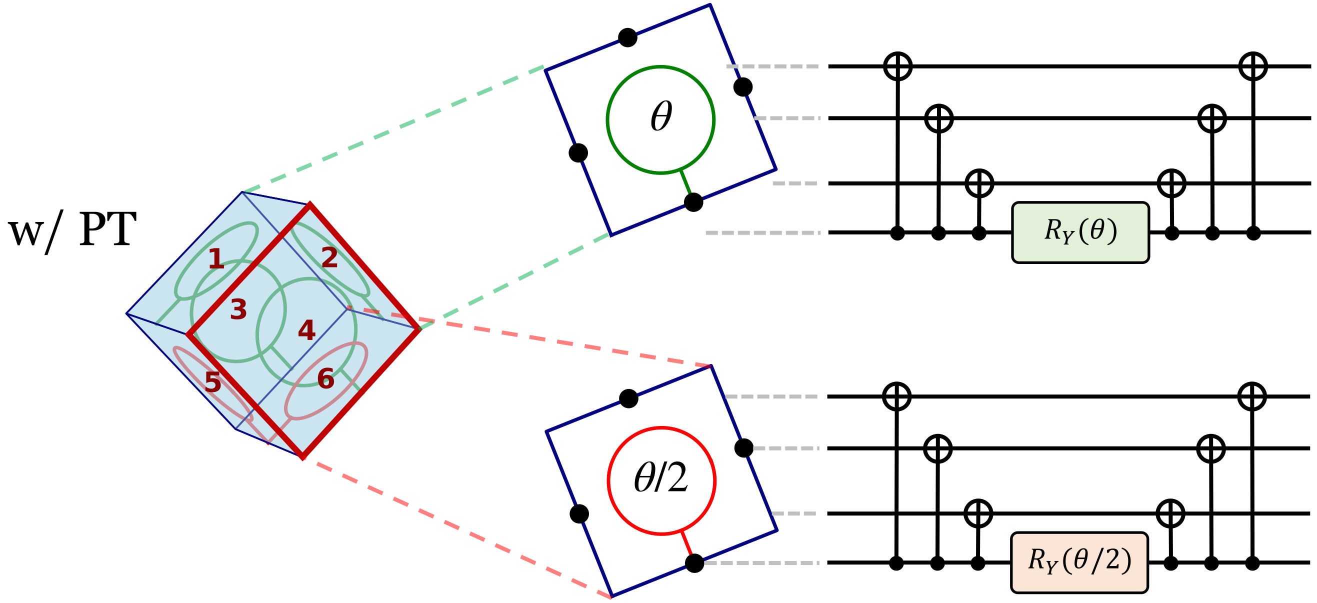
➢ The grey and blank regions correspond to the symmetry breaking and preserving phase, respectively.

Phase transition in $\mathbb{Z}_2$ weight-adjustable loop ansatz

- Lattice of $\mathbb{Z}_2$ weight-adjustable loop ansatz (WALA)



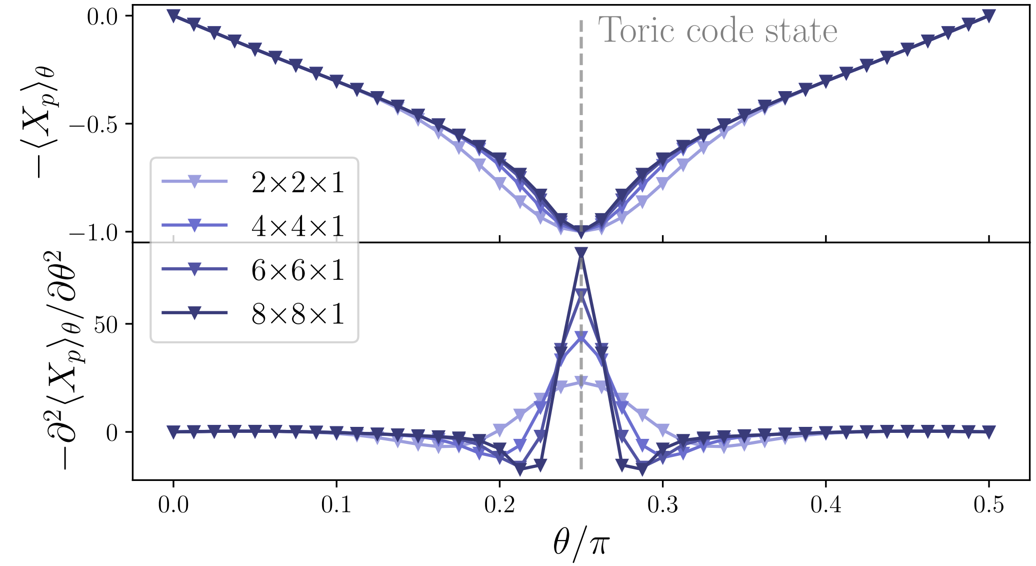
- WALA with phase transition:



- WALA exactly prepares the Toric code state, i.e., the ground state of the $\mathbb{Z}_2$ gauge theory

$$H_{\mathrm{TC}} = -\sum_{\text{plaquette}} X_p^{\square}$$

$$-X_p^{\square}\left|\phi_{\mathbb{Z}_2}\left(\frac{\pi}{4}\right)\right\rangle = -\left|\phi_{\mathbb{Z}_2}\left(\frac{\pi}{4}\right)\right\rangle, \qquad \forall\, p \in \Lambda$$



➢ Phase transition can be observed in the 3-d WALA at $\theta = \frac{\pi}{4}$.

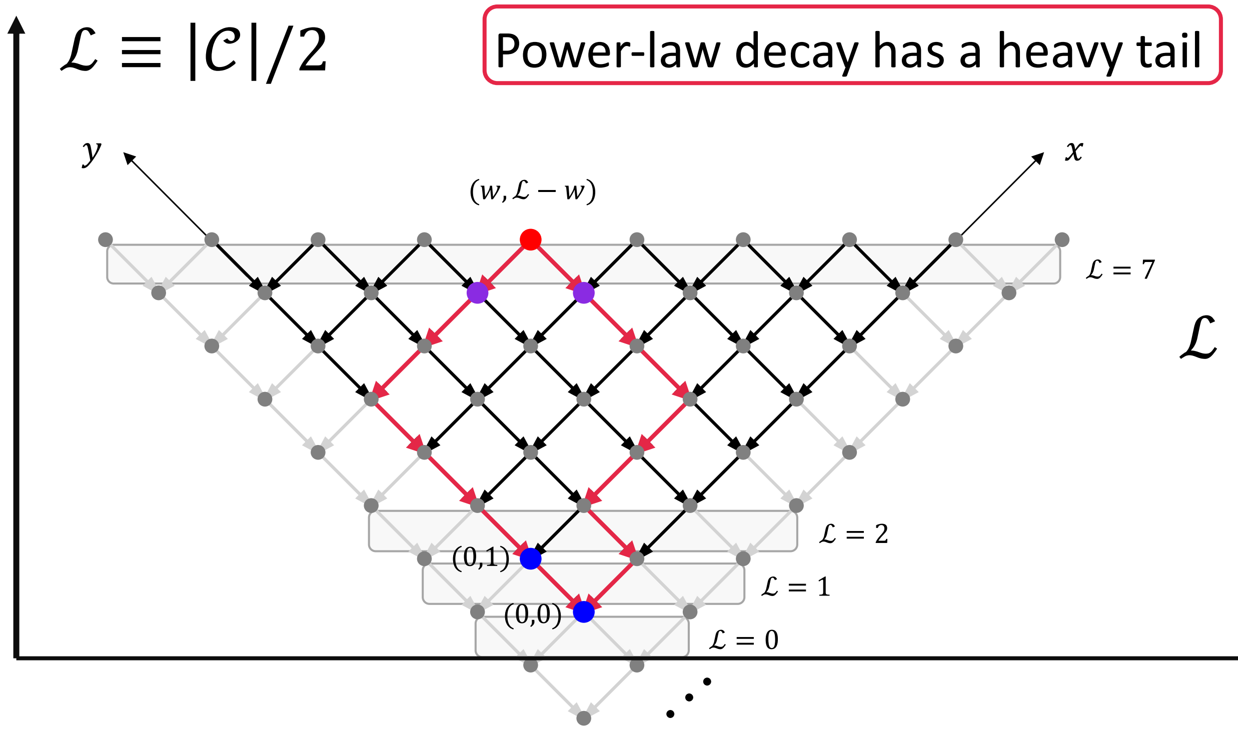
Main Content

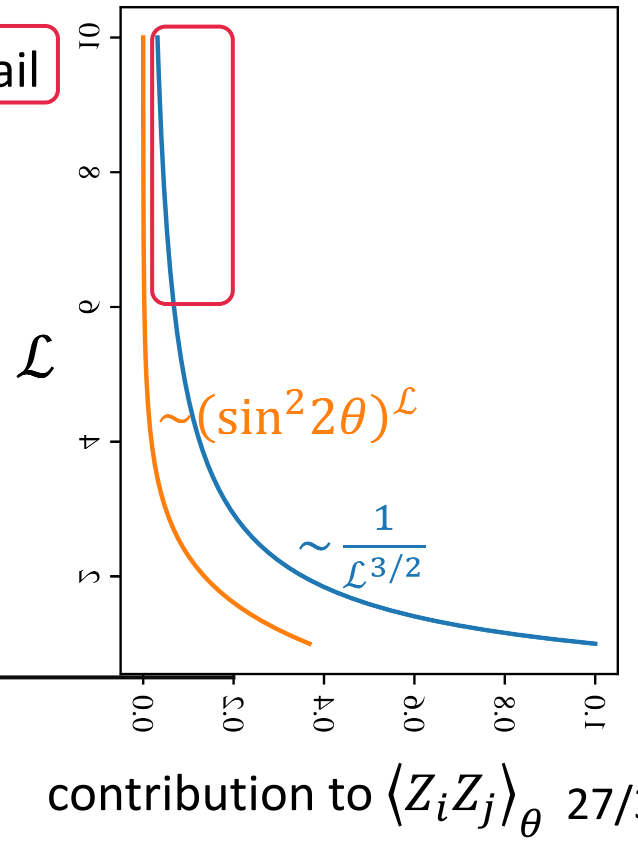
- ❑ Why quantum computer for phase transition?
- ❑ Phase transition mechanism
- ❑ Phase transition in Ising whip circuit
- ❑ Towards quantum advantage
- ❑ Conclusion

Hardness of classical simulation at $\boldsymbol{\theta_c}$

➢ Circuit-based phase transition has exponential to power-law transformation:

$$\langle Z_i Z_j \rangle_\theta = -\sum_{\mathcal{L}=1}^{\infty} \frac{4^{\mathcal{L}-1}\Gamma\left(\mathcal{L}-\frac{1}{2}\right)}{\sqrt{\pi}\,\mathcal{L}!}(\cos\theta\sin\theta)^{2\mathcal{L}-1} \sim \sum_{\mathcal{L}\gg 1}^{\infty} \frac{1}{\mathcal{L}^{3/2}}(\sin 2\theta)^{2\mathcal{L}-1} \begin{cases} \text{Exponential decay at } \theta \neq \theta_c = \pi\left(\frac{1}{4}+\frac{k}{2}\right), k \in \mathbb{Z} \\ \text{Power-law decay at } \theta = \theta_c \end{cases}$$





Hardness of classical simulation at $\boldsymbol{\theta_c}$

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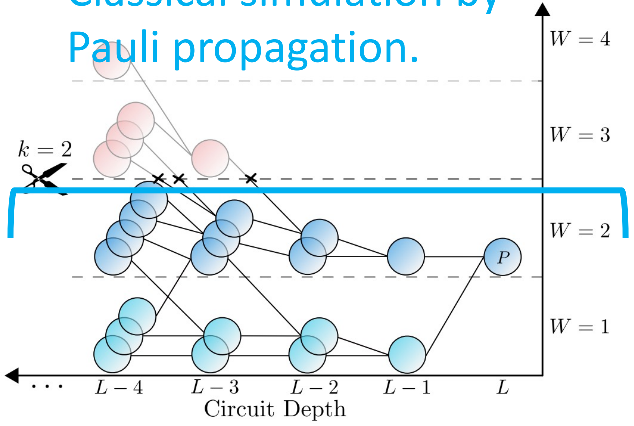
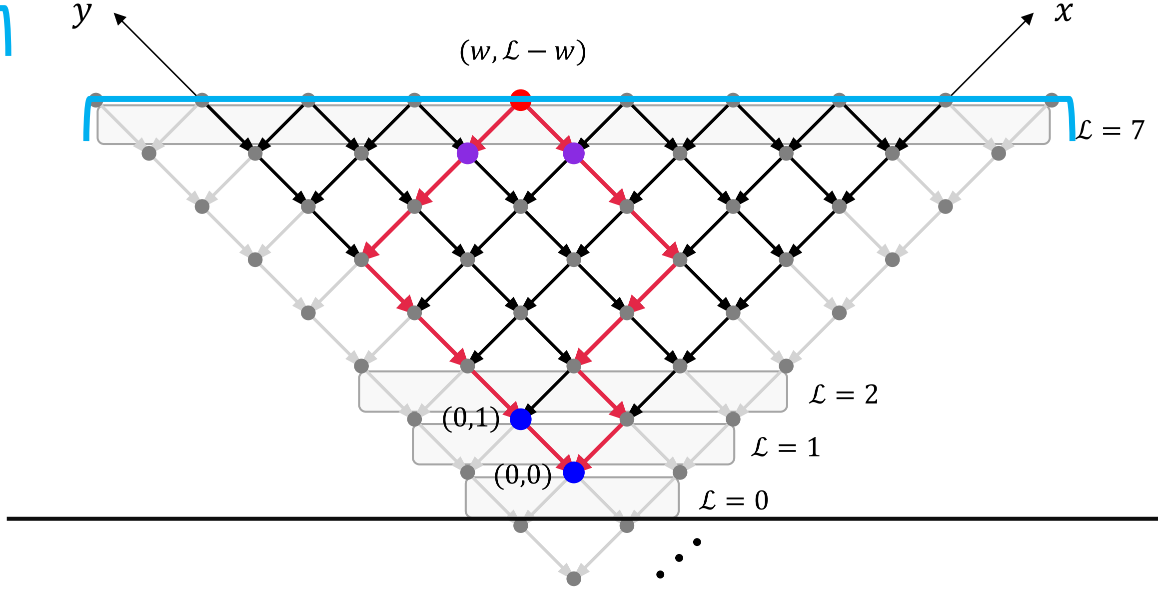
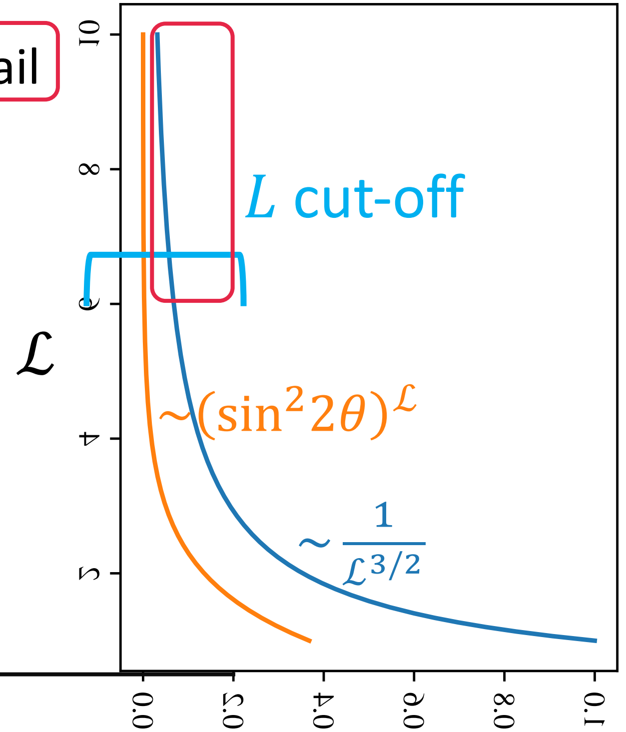
Classical simulation by Pauli propagation.



[A. Angrisani, et. al. PRL (2025)]

Power-law decay has a heavy tail





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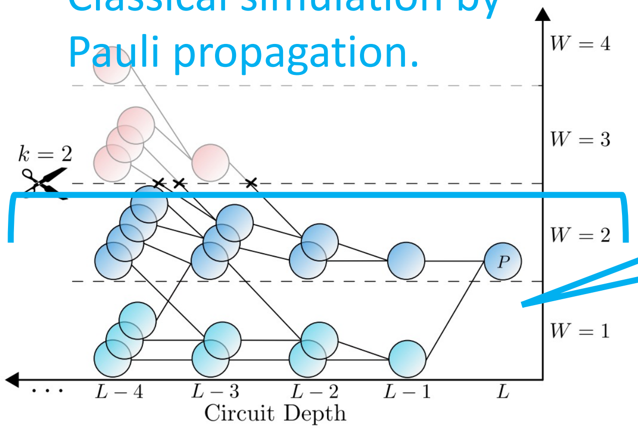
Exponential decay at $\theta \neq \theta_c = \pi\left(\frac{1}{4}+\frac{k}{2}\right), k \in \mathbb{Z}$

Power-law decay at $\theta = \theta_c$

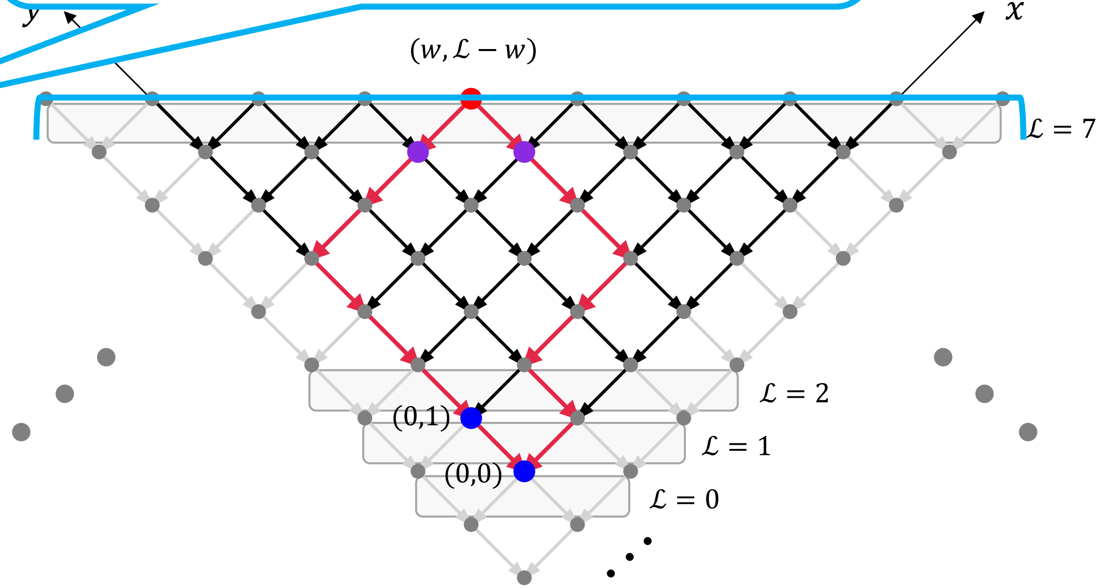
Classical simulation by Pauli propagation.

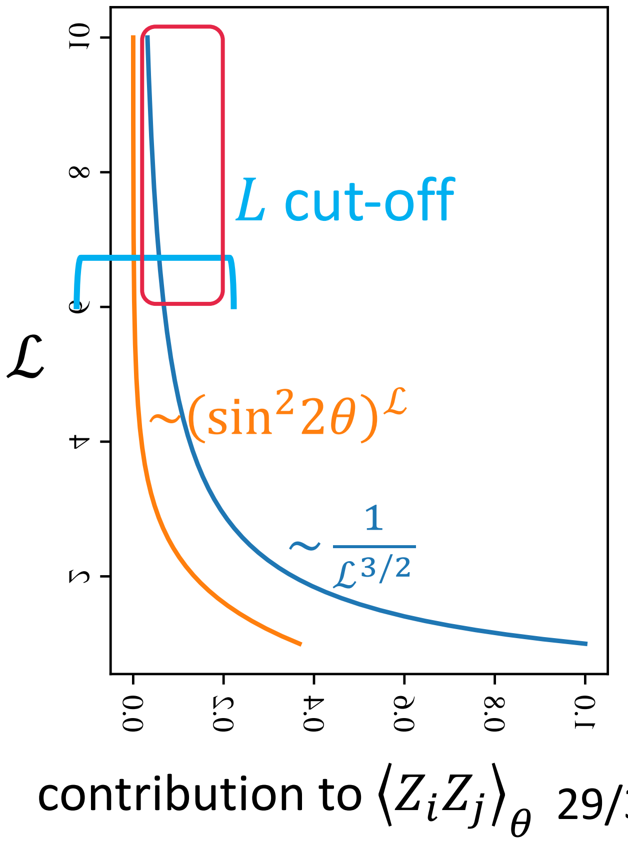


[A. Angrisani, et. al. PRL (2025)]

Pauli propagation evaluates $\langle Z_i Z_j \rangle_\theta$ within an error $\epsilon \sim 1/\mathrm{poly}(L)$:

$T_{\text{naive PP}} \sim \mathcal{O}(4^{\mathrm{poly}(L)})$ at θ_c

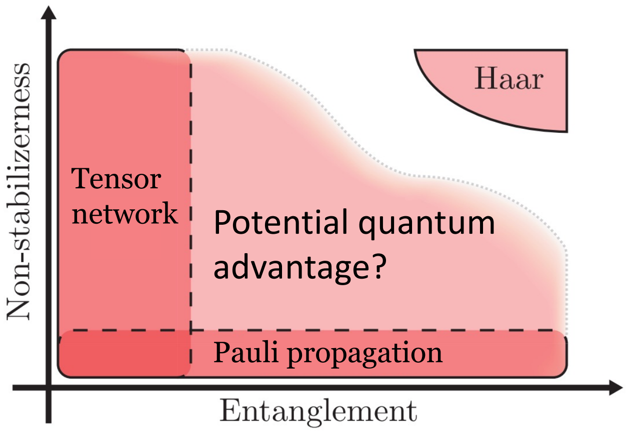




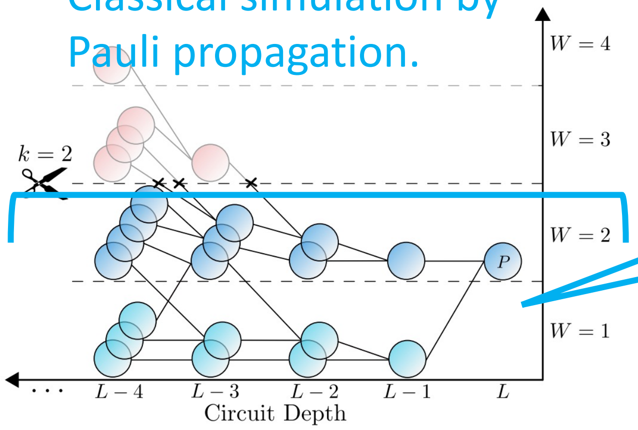
Hardness of classical simulation at $\boldsymbol{\theta_c}$

- Circuit-based phase transition has exponential to power-law transformation:

$$\langle Z_i Z_j \rangle_\theta = -\sum_{\mathcal{L}=1}^{\infty} \frac{4^{\mathcal{L}-1}\Gamma\left(\mathcal{L}-\frac{1}{2}\right)}{\sqrt{\pi}\,\mathcal{L}!} (\cos\theta\sin\theta)^{2\mathcal{L}-1} \sim \sum_{\mathcal{L}=1}^{\infty} \frac{1}{\mathcal{L}^{3/2}} (\sin 2\theta)^{2\mathcal{L}-1}$$



Classical simulation by Pauli propagation.



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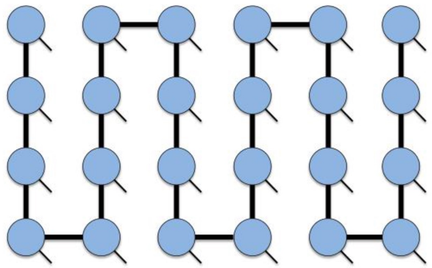
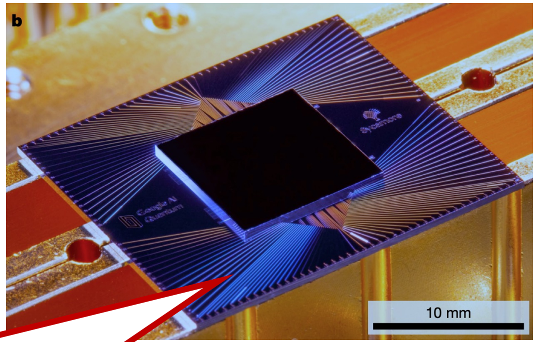
Pauli propagation evaluates $\langle Z_i Z_j \rangle_\theta$ within an error $\epsilon \sim 1/\mathrm{poly}(L)$: $T_{\text{naive PP}} \sim \mathcal{O}(4^{\mathrm{poly}(L)})$ at θ_c

Matrix product state (MPS) fails due to the area law entanglement

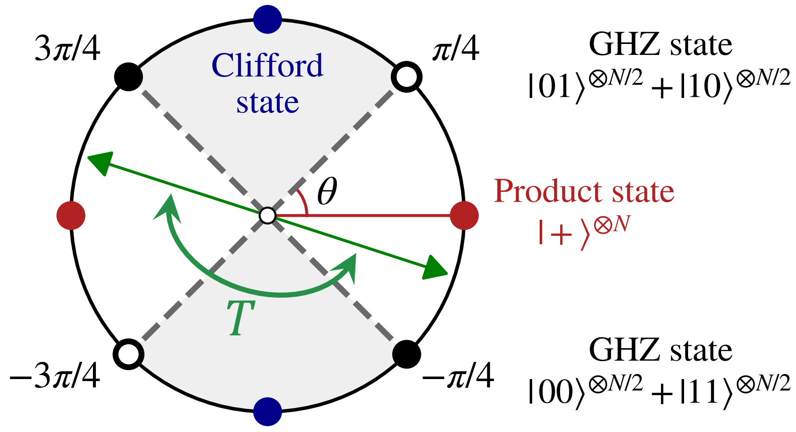


And more classical simulation methods?



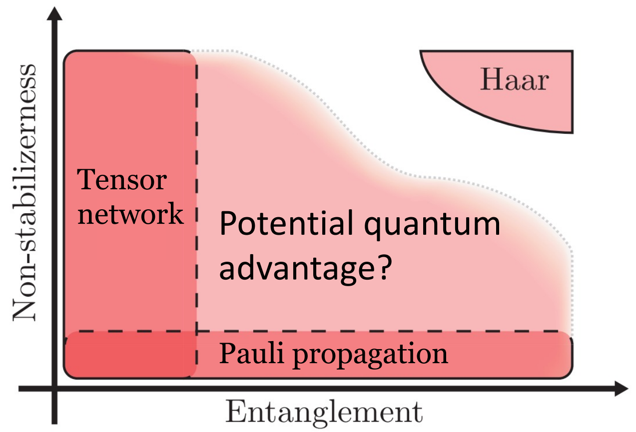
Quantum computer evaluates $\langle Z_i Z_j \rangle_\theta$ within an error $\epsilon \sim 1/\mathrm{poly}(L)$: $T_{\mathrm{QC}} \sim \mathcal{O}(\mathrm{poly}(L))$

Conclusion and outlook



Conclusion

- We propose a mechanism of **circuit-based phase transition**.
  👉 Phase transition can be studied directly on quantum circuits.
- We derive the **phase diagram** of the Ising whip circuit.
- PQC near the critical region can potentially demonstrate **quantum advantage.**



Outlook

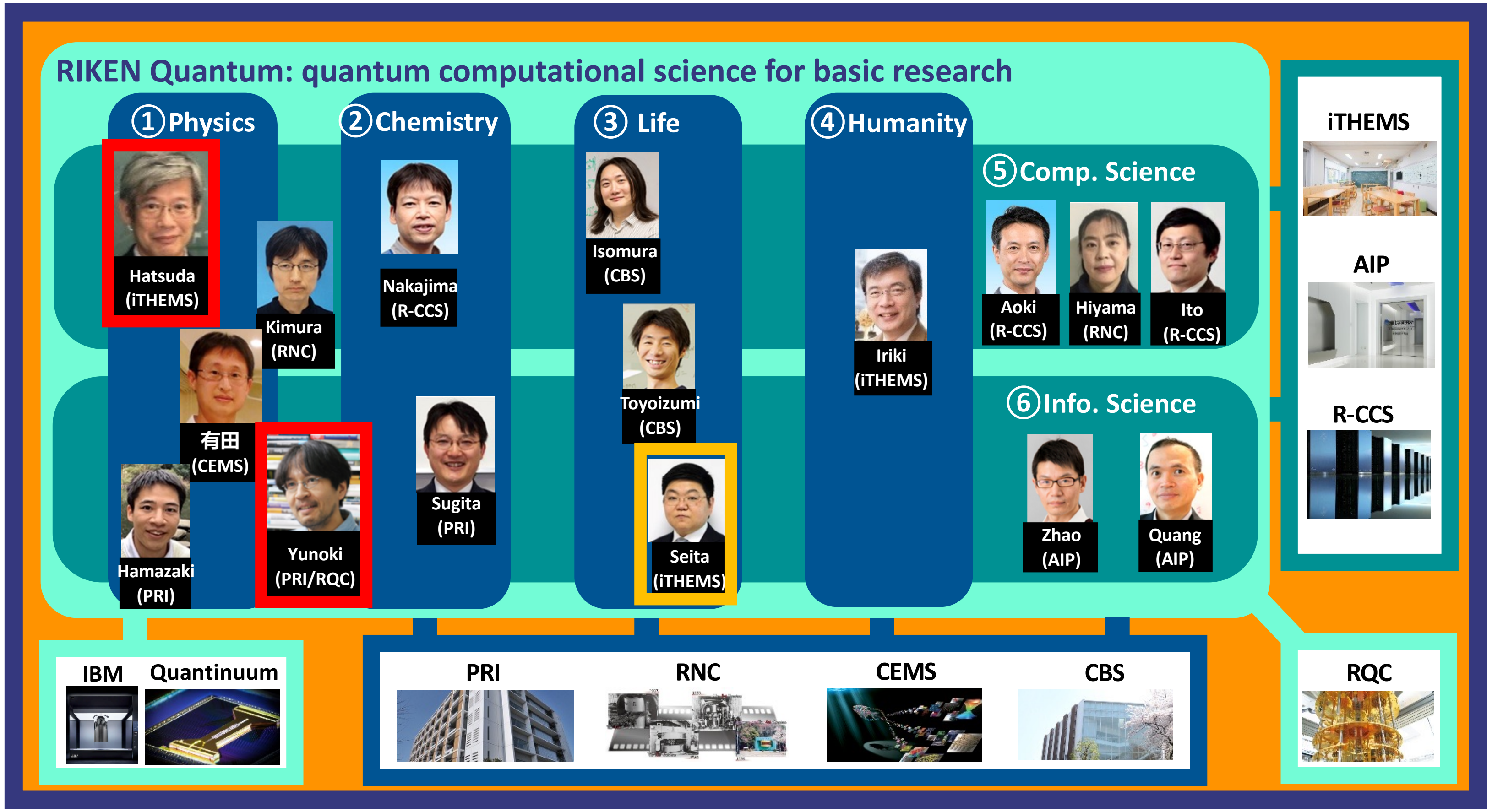
- State preparation accuracy of PQCs with phase transition ?
- The effect of quantum noise to the singularity in PQC ?
- Correspondence to the conventional phase transition ?

RIKEN Quantum

https://rq.riken.jp/en/

<u>All-RIKEN activity</u> to foster breakthroughs in quantum computational science including people from

- physics,
- chemistry,
- life sciences,
- humanities,
- computational science,
- information science…



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Abe (Keio)

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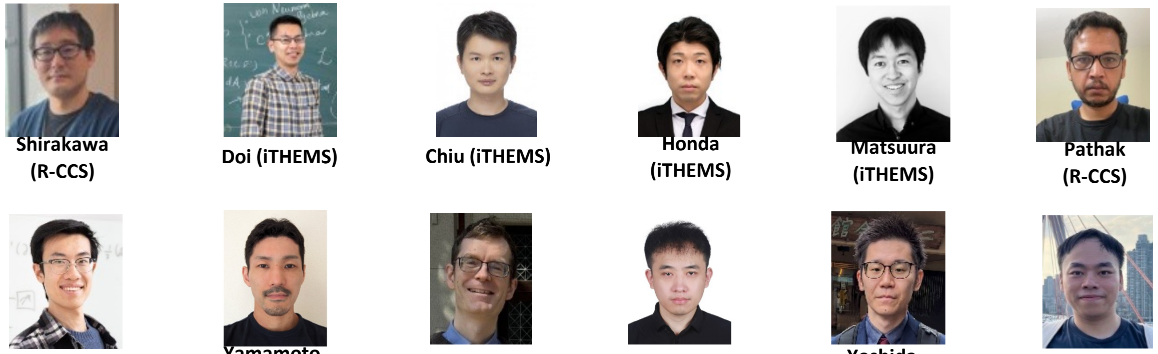
S. Iso (iTHEMS)

Scientific Advisor

Participating researchers



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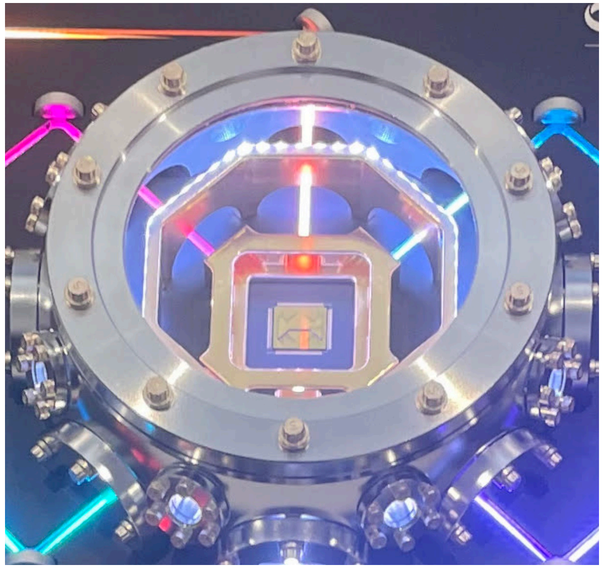
Chiu (iTHEMS)
Honda (iTHEMS)
Matsuura (iTHEMS)
Pathak (R-CCS)
Wang (iTHEMS)
Yamamoto (iTHEMS)
Loetstedt (PRI)
Xu (iTHEMS)
Yoshida (RNC)
Li (iTHEMS)

Quantum Facilities at RIKEN

IBM Heron R2 “ibm_Kobe”*
(156 qubits)

RIKEN & Fujitsu QC **
(256 qubits)



Quantinuum H2 “黎明” ***
(20 qubits)

* https://www.riken.jp/pr/news/2025/20250624_1/index.html
** https://www.riken.jp/en/news_pubs/news/2025/20250422_1/index.html
*** https://www.quantinuum.com/press-releases/quantinuums-reimei-quantum-computer-now-fully-operational-at-riken-ushering-in-a-new-era-of-hybrid-quantum-high-performance-computing

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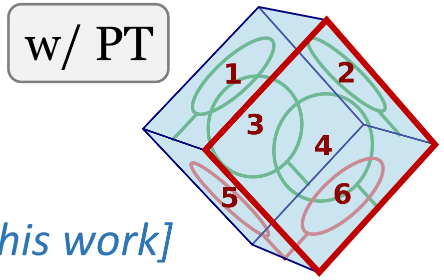
Thanks for listening!

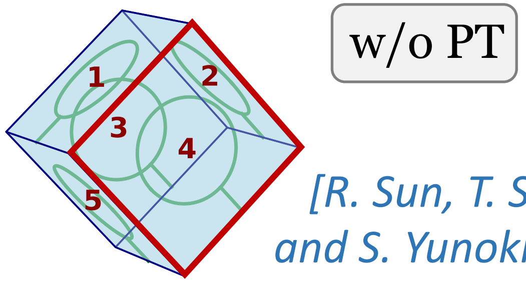
Backup: $\mathbb{Z}_2$ weight-adjustable loop ansatz

- Use VQE to prepare the ground state of $H_{\mathbb{Z}_2}(x)$ using WALA w/ and w/o phase transition.

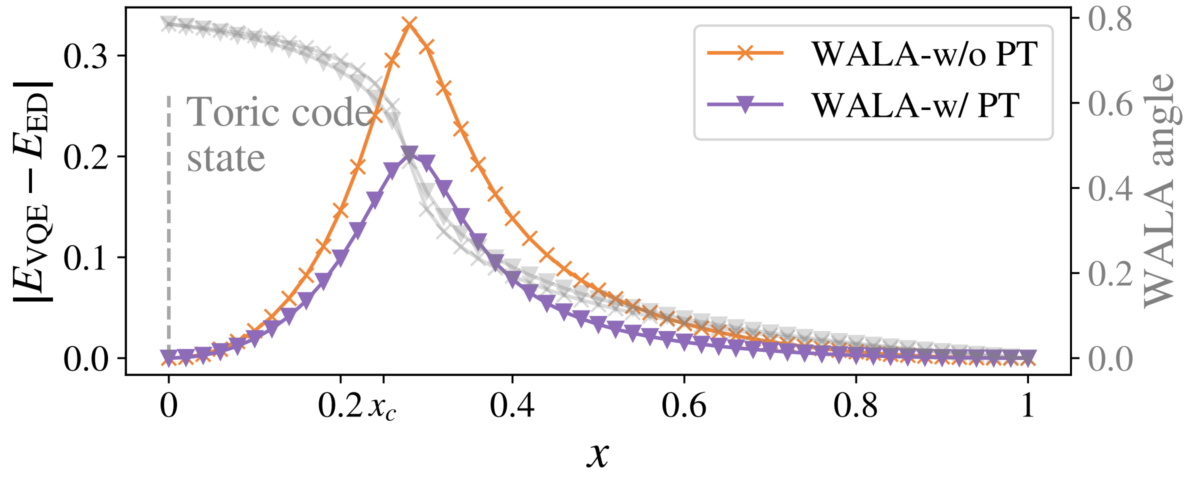
$$H_{\mathbb{Z}_2}(x) = -(1-x)\sum_{\text{plaquette}} X_p - x\sum_{\text{links}} Z_l - \sum_{\text{vertex}} Z_v^+$$



[This work]



[R. Sun, T. Shirakawa, and S. Yunoki PRB (2023)]

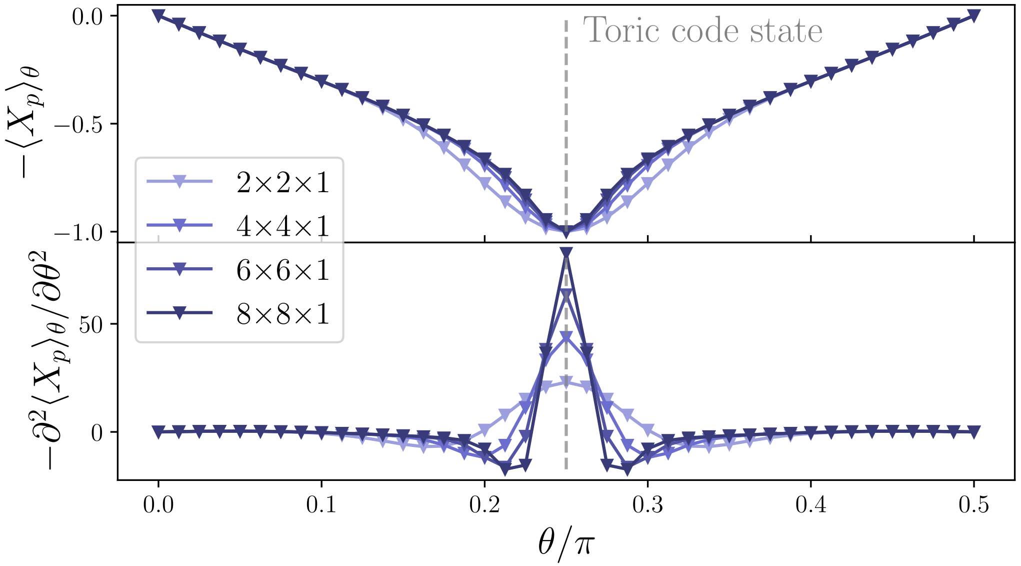


- WALA with PT prepares the ground state with higher accuracy.

- WALA exactly prepares the Toric code state, i.e., the ground state of the $\mathbb{Z}_2$ gauge theory

$$H_{\mathrm{TC}} = -\sum_{\text{plaquette}} X_p^{\square}$$

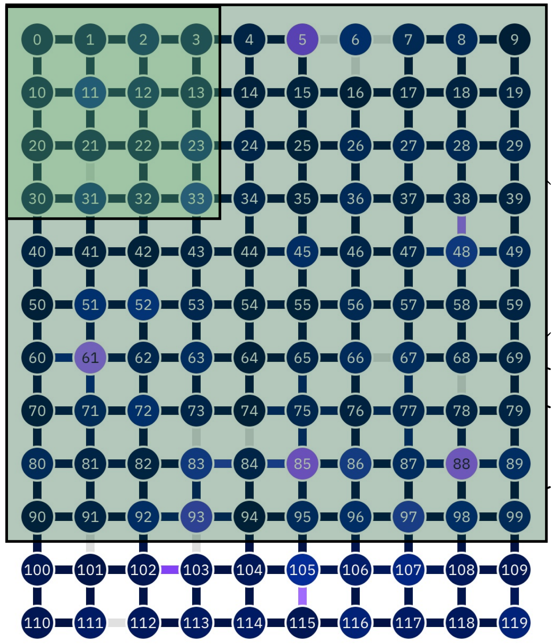
$$-X_p^{\square}\left|\phi_{\mathbb{Z}_2}\left(\frac{\pi}{4}\right)\right\rangle = -\left|\phi_{\mathbb{Z}_2}\left(\frac{\pi}{4}\right)\right\rangle, \qquad \forall\, p \in \Lambda$$

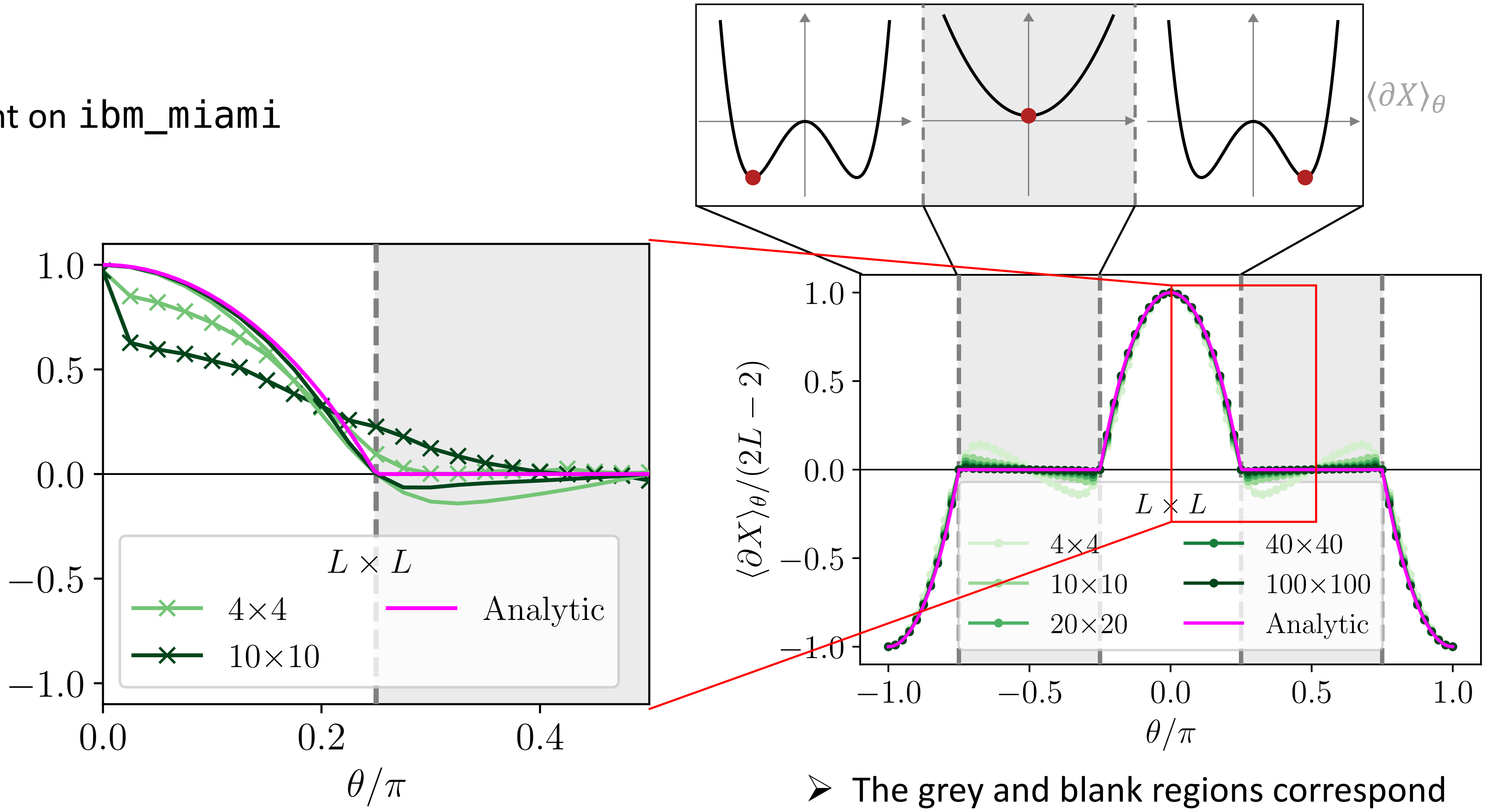


- Phase transition can be observed in the 3-d WALA at $\theta = \frac{\pi}{4}$.

Backup: Phase transition in Ising whip circuit

- hardware measurement on `ibm_miami`





➢ Quantum noise destroy the non-analyticity in the whip circuit

➢ The grey and blank regions correspond to the symmetry breaking and preserving phase, respectively.

Backup: Divergent correlation length in Ising whip circuit

- Correlation length ξ is given by

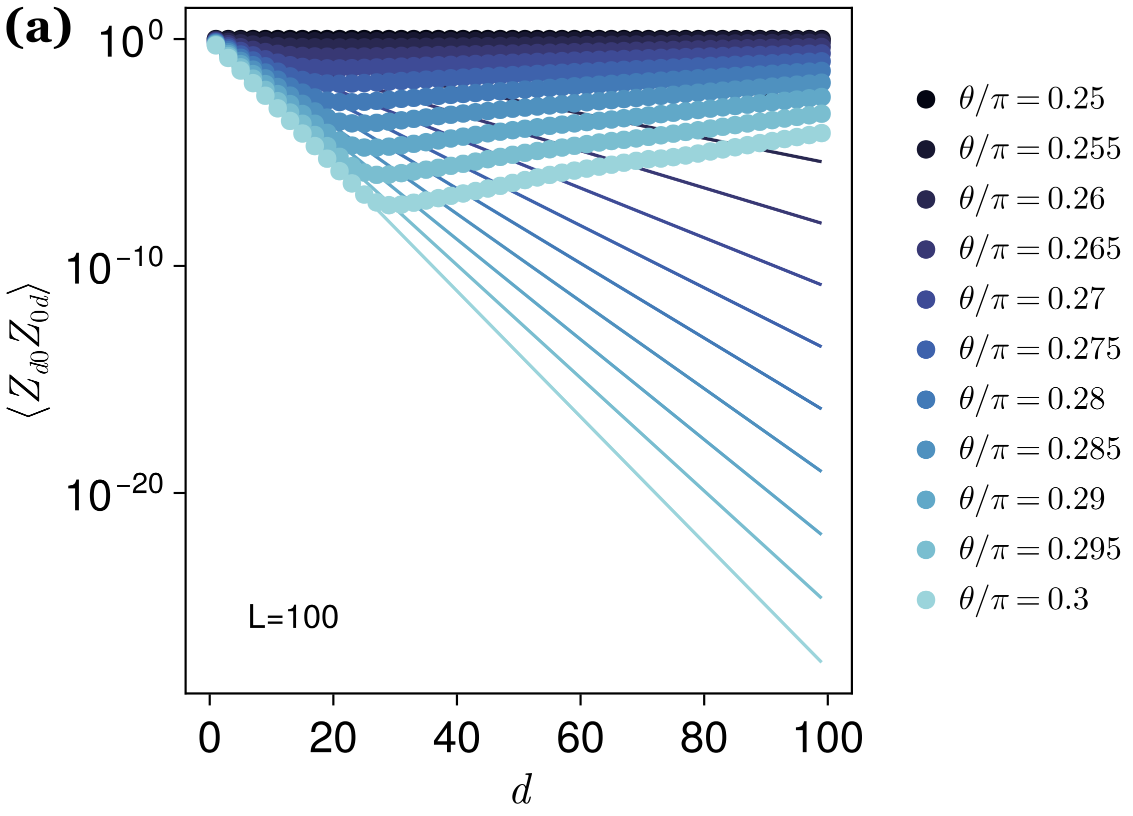
$$\langle Z_{(d,0)} Z_{(0,d)} \rangle \sim e^{-d/\xi}$$

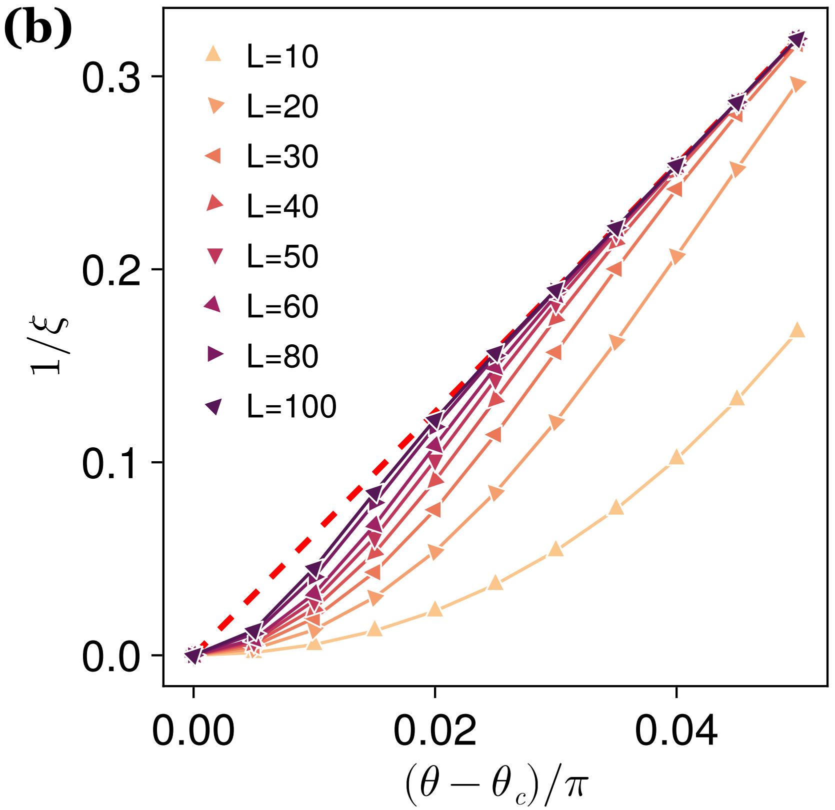
- The critical exponent is defined as

$$\xi \sim |\theta - \theta_c|^{-\nu}$$

We prove that

$$\nu = 1$$





- ➢ Exponential decay of the correlation length
- ➢ Correlation length diverged at $\theta = \theta_c = \pi\left(\frac{1}{4} + \frac{k}{2}\right), k \in \mathbb{Z}$