

Title: Quantum Advantages in Energy Minimization - VIRTUAL ONLY

Speakers: Leo Zhou

Series: Perimeter Institute Quantum Discussions

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Abstract: Minimizing the energy of a many-body system is a fundamental problem in many fields. Although we hope a quantum computer can help us solve this problem better than classical computers, we have a very limited understanding of where a quantum advantage may be found. In this talk, I will present some recent theoretical advances that shed light on quantum advantages in this domain. First, I describe rigorous analyses of the Quantum Approximate Optimization Algorithm applied to minimizing energies of classical spin glasses. For certain families of spin glasses, we find the QAOA has a quantum advantage over the best known classical algorithms. Second, we study the problem of finding a local minimum of the energy of quantum systems. While local minima are much easier to find than ground states, we show that finding a local minimum under thermal perturbations is computationally hard for classical computers, but easy for quantum computers.

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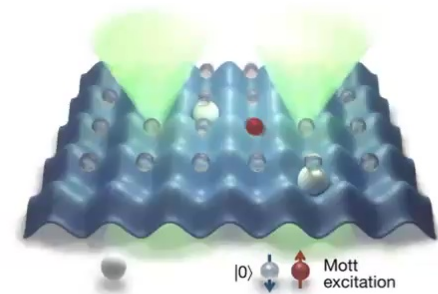
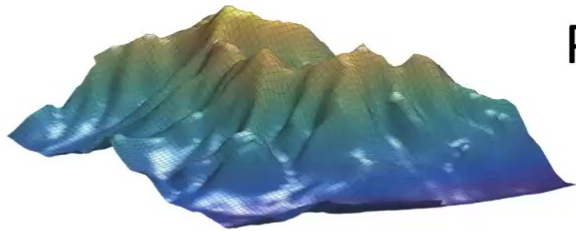
Zoom link TBA

# Quantum Advantages in Energy Minimization

**Leo Zhou**

Perimeter Institute Seminar

Feb 28, 2024



# Energy minimization: a fundamental problem

Energy function

$$C(\mathbf{x}) : \mathcal{X} \rightarrow \mathbb{R}$$

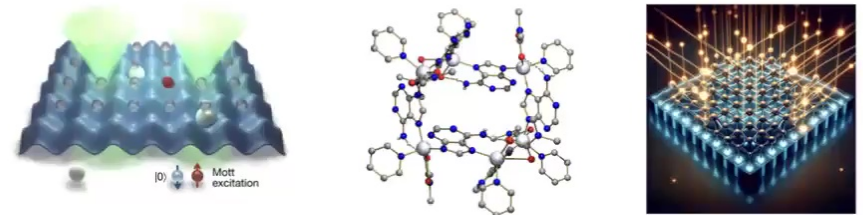
Want  $\mathbf{x}^* \in \mathcal{X}$   
so  $C(\mathbf{x}^*)$  is minimized

## Classical systems



$$\mathcal{X} = \{\pm 1\}^n \text{ or } \mathbb{R}^n$$

## Quantum systems



$$\mathcal{X} = \{|\psi\rangle\} \subseteq \mathbb{C}^{2^n} \text{ or } \{\rho\}$$

# Minimize energy *better* with *quantum computers*?

Classical computers are already (surprisingly) successful...

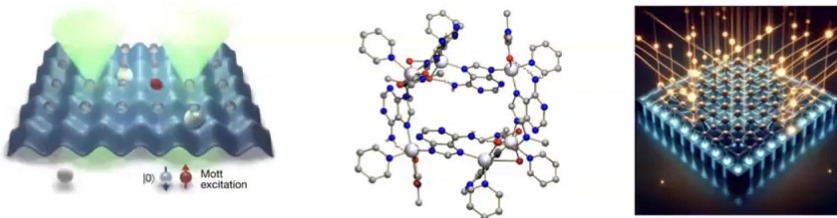
Classical systems  $\{\pm 1\}^n$  or  $\mathbb{R}^n$



## **Classical algorithms:**

Linear Programming, SDP relaxation, Stochastic gradient descent, Bayesian optimization, Simulated annealing, ...

Quantum systems  $\mathbb{C}^{2^n}$



## **Classical algorithms:**

Tensor network, DMRG, Quantum Monte-Carlo, Density Functional Theory, Neural network ansatz, ...

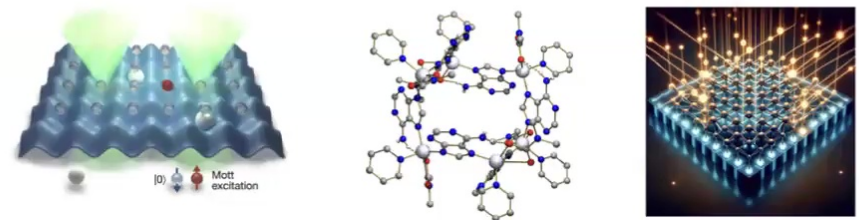


**Today:** Rigorous evidence of quantum advantages for minimizing energy of both classical and quantum systems!

**Classical systems**  $\{\pm 1\}^n$  or  $\mathbb{R}^n$



**Quantum systems**  $\mathbb{C}^{2^n}$



1

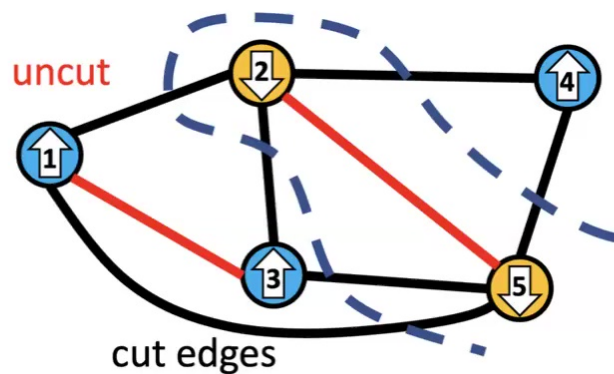
**qAdvantage** for finding near-ground states of spin glasses

2

**qAdvantage** for find local minima of quantum systems

# A Classical Problem: MaxCut (diluted spin glass)

**Goal:** Find a **bipartition** of vertices that cuts the most edges



**Random Guessing or Greedy Search** guarantees for any graph,

$$C(\mathbf{z})/C_{\max} \geq 0.5$$

**Semidefinite Programming (SDP)** algorithm improves worst-case guarantee

$$C(\mathbf{z})/C_{\max} \geq 0.878$$

[Goemans Williamson 1995]

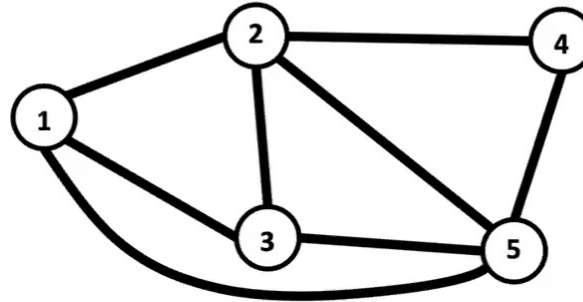
$$C = \sum_{\langle i,j \rangle} \frac{1}{2} (1 - z_i z_j)$$

Equivalent to minimizing  $\tilde{C} = \sum_{\langle i,j \rangle} z_i z_j$

# Quantum Approximate Optimization Algorithm (QAOA)

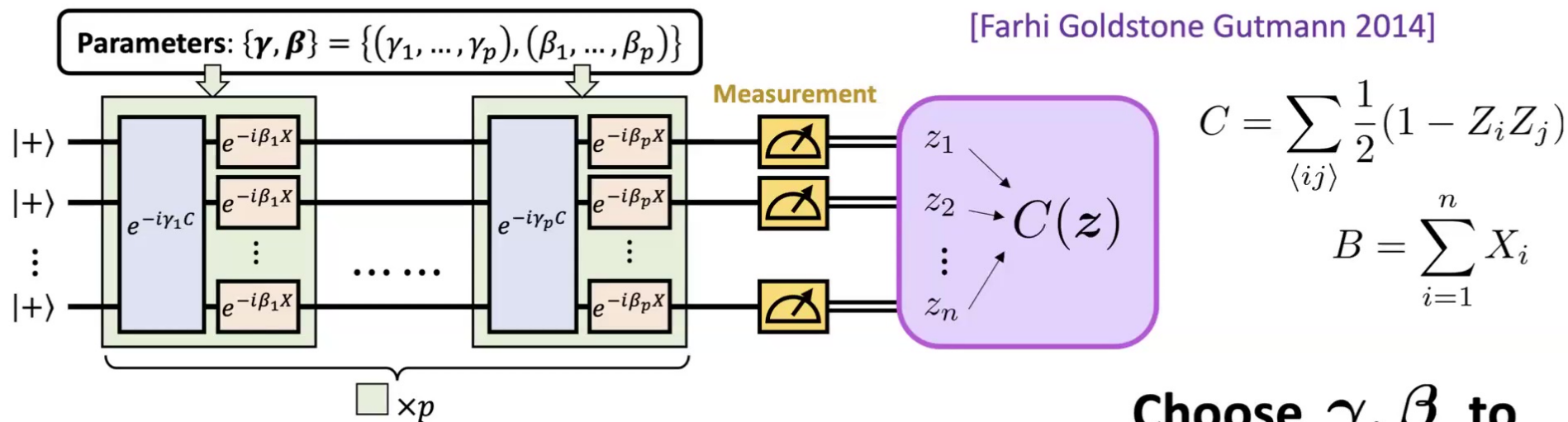
[Farhi Goldstone Gutmann 2014]

$$C(\mathbf{z}) = \sum_{\langle ij \rangle} \frac{1}{2} (1 - z_i z_j)$$



# Quantum Approximate Optimization Algorithm (QAOA)

[Farhi Goldstone Gutmann 2014]



$$C = \sum_{\langle ij \rangle} \frac{1}{2} (1 - Z_i Z_j)$$

$$B = \sum_{i=1}^n X_i$$

$$|\boldsymbol{\gamma}, \boldsymbol{\beta}\rangle = e^{-i\beta_p B} e^{-i\gamma_p C} \dots e^{-i\beta_1 B} e^{-i\gamma_1 C} |+\rangle^{\otimes n}$$

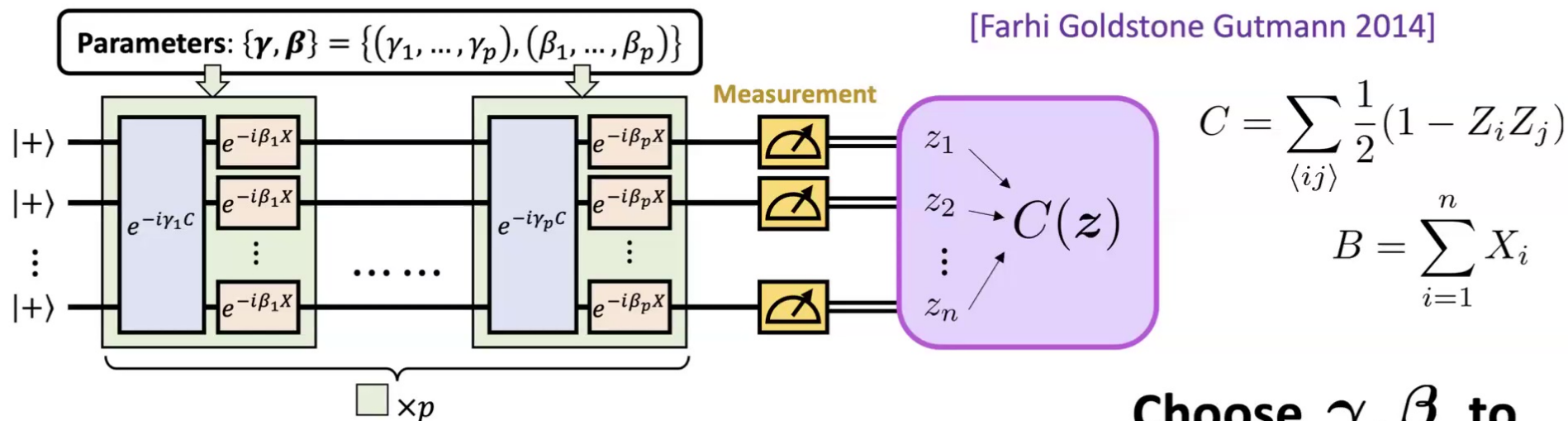
**Choose  $\boldsymbol{\gamma}, \boldsymbol{\beta}$  to maximize  $\langle C \rangle$**

Various **heuristics** exist to efficiently choose good parameters

- Parameter pattern & interpolation between depths [LZ Wang Choi Pichler Lukin 2018, PRX 2020]

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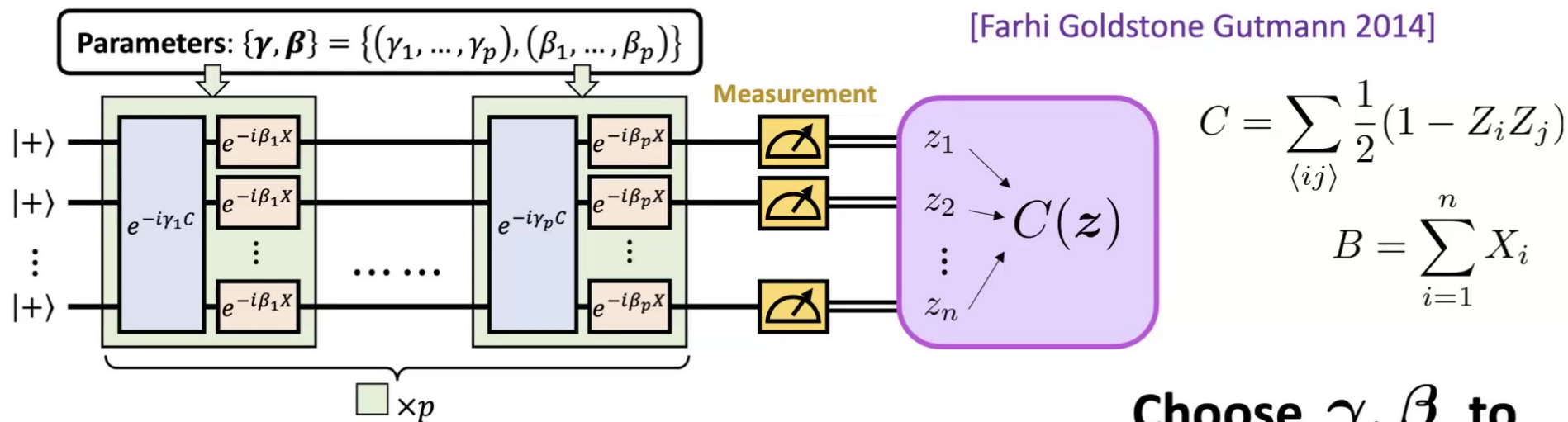
Various **heuristics** exist to efficiently choose good parameters

- Parameter pattern & interpolation between depths [LZ Wang Choi Pichler Lukin 2018, PRX 2020]
- Classical Warm Start [Egger et al 2020], Annealing-inspired [Sacks Serbyn 2021], Parameter Transfers [Galda et al 2021], Graph Neural Network [Jain et al 2022] .....



# Quantum Approximate Optimization Algorithm (QAOA)

[Farhi Goldstone Gutmann 2014]



$$|\boldsymbol{\gamma}, \boldsymbol{\beta}\rangle = e^{-i\beta_p B} e^{-i\gamma_p C} \dots e^{-i\beta_1 B} e^{-i\gamma_1 C} |+\rangle^{\otimes n}$$

**Choose  $\boldsymbol{\gamma}, \boldsymbol{\beta}$  to maximize  $\langle C \rangle$**

- Simple & easy implementation (e.g. ions (2019), superconductors (2020) and atoms (2022))
- Cannot classically sample (“supremacy”) even @  $p=1$  [Farhi Harrow 2016] [Krovi 2022]
- **Guaranteed to get  $C_{\max}$  as depth  $p \rightarrow \infty!$**

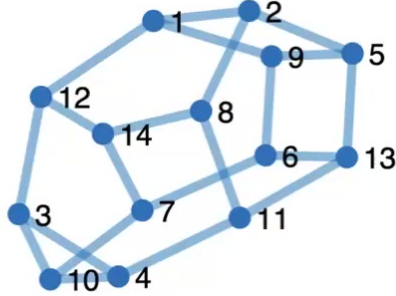


# Performance guarantee of the QAOA

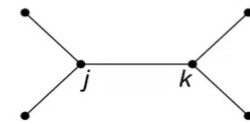
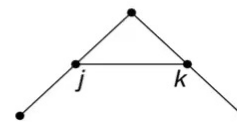
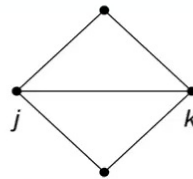
- Early approach: Analyze performance via “subgraphs”

$$|s\rangle = |+\rangle^{\otimes n}$$

**Example: MaxCut on 3-regular graphs**



$$p = 1 \quad \langle s | \underbrace{e^{i\gamma C} e^{i\beta B} Z_j Z_k e^{-i\beta B} e^{-i\gamma C}}_{\text{supported on 3 types of subgraphs}} | s \rangle$$



**Worst case guarantee:** [Farhi Goldstone Gutmann 2014]

$$\langle C \rangle / C_{\max} \geq 0.6924$$

$$C(z_{\text{Greedy}}) / C_{\max} \geq 0.5$$

$$C(z_{\text{SDP}}) / C_{\max} \geq 0.878$$

**Difficult for higher  $p$  as (classical) analysis complexity grow as  $2^{2^{O(p)}}$  !**

# How about average case?



For a large random  $D$ -regular graph, statistical theory predicts the maximum “cut fraction” is (w.h.p.)

$$\frac{C_{\max}}{\# \text{ edges}} = \frac{1}{2} + \frac{V_{\max}(D)}{\sqrt{D}}$$

$$C = \sum_{\langle i,j \rangle} \frac{1}{2} (1 - z_i z_j)$$

$$\lim_{D \rightarrow \infty} V_{\max}(D) = \Pi_* = 0.7631 \dots$$

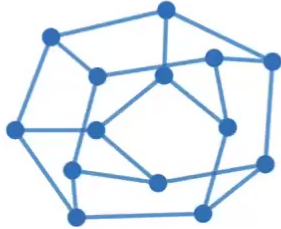
**(Parisi value)**

[Parisi 1979] [Dembo Montanari Sen 2017]



Nobel Physics 2021

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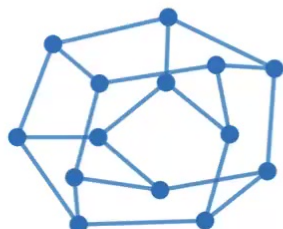
[Parisi 1979] [Dembo Montanari Sen 2017]

We know the ground energy... BUT no algorithm to find the ground state bit string!



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[Dembo Montanari Sen 2017]

Best *assumption-free* classical algorithms get:

$$V^{\text{SDP}}(D) = 2/\pi + o_D(1)$$

↪ 0.6366...

[Montanari Sen 2015]

[Barak Marwaha 2021]

[Thompson Parekh Marwaha 2021]

Assuming a “No OGP” conjecture, a **Local Message Passing algorithm** with  $p$  rounds gets:

$$V_p^{\text{LMP}}(D) \geq \Pi_* - O_D(1/\sqrt{p})$$

↪ 0.7631...

[Alaoui Montanari Sellke 2021]

# QAOA on MaxCut of $D$ -regular graphs



- Let the **cut fraction** achieved by the QAOA be

$$\frac{\langle \gamma, \beta | C | \gamma, \beta \rangle}{\# \text{ edges}} = \frac{1}{2} + \frac{V_p^{\text{QAOA}}(D, \gamma, \beta)}{\sqrt{D}}$$

and let  $\bar{V}_p^{\text{QAOA}}(D) := \max_{\gamma, \beta} V_p^{\text{QAOA}}(D, \gamma, \beta)$

- At  $p = 1$ , for triangle-free graphs, we know  $\lim_{D \rightarrow \infty} \bar{V}_1^{\text{QAOA}}(D) \simeq 0.3033$   
[Wang Hadfield Jiang Rieffel 2018]
- At  $p = 2$ , for graphs with girth  $> 5$ , we know  $\lim_{D \rightarrow \infty} \bar{V}_2^{\text{QAOA}}(D) \simeq 0.4075$   
[Marwaha 2021]

**Note: Large girth  $\cong$  Random / Average case**



# Performance of the QAOA on MaxCut for random or large-girth regular graphs

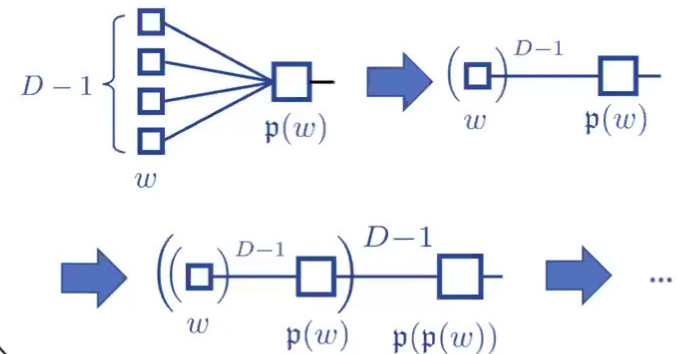
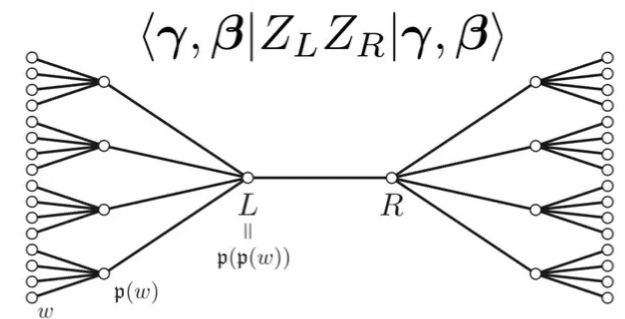
- For any  $D$ -regular graph with girth  $> 2p + 1$ , we give an  $\tilde{O}(16^p)$  time iteration using  $O(4^p)$  memory to exactly compute

$$V_p^{\text{QAOA}}(D, \gamma, \beta)$$

- In the  $D \rightarrow \infty$  limit, we give an  $\tilde{O}(4^p)$  time iteration using  $O(p^2)$  memory for

$$V_p^{\text{QAOA}}(\gamma, \beta) := \lim_{D \rightarrow \infty} V_p^{\text{QAOA}}(D, \gamma, \beta)$$

**Key idea: efficient analytical contraction of a tree tensor network**



[Basso Farhi Marwaha Villalonga LZ, TQC 2022]



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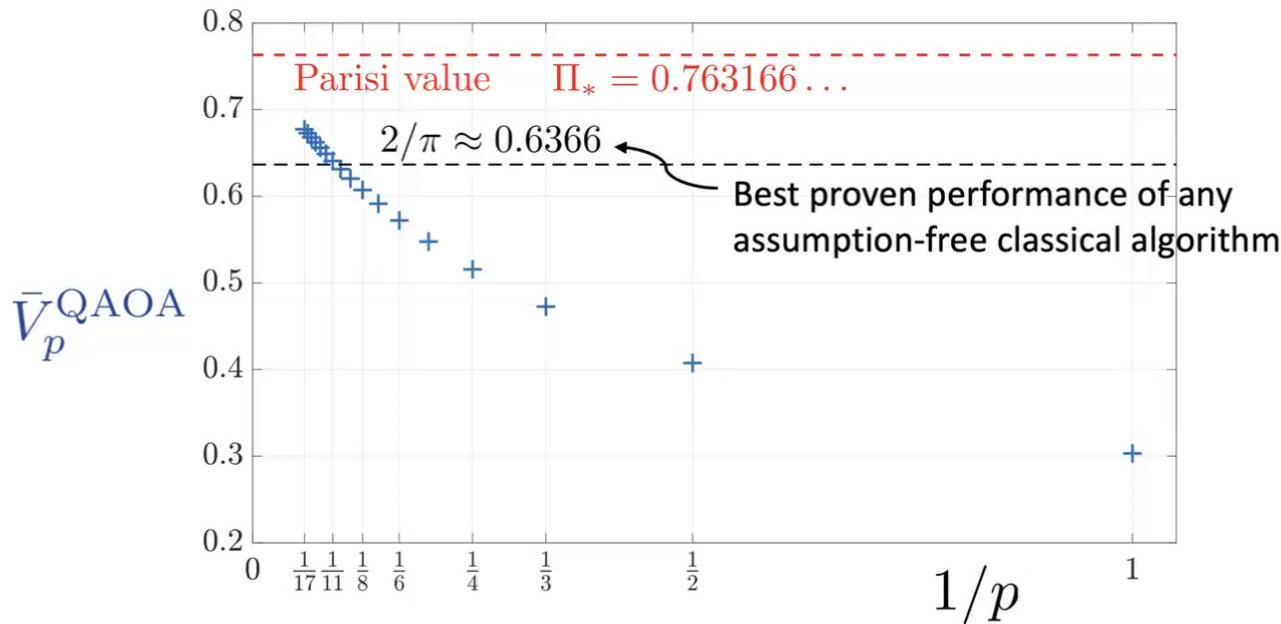
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$p$	Best $V_p^{\text{QAOA}}$
1	0.3033
2	0.4075
⋮	⋮
17	0.6773
18	0.6813
19	0.6848
20	0.6879

optimized  
lower bounds

[Basso Farhi Marwaha Villalonga LZ, TQC 2022]

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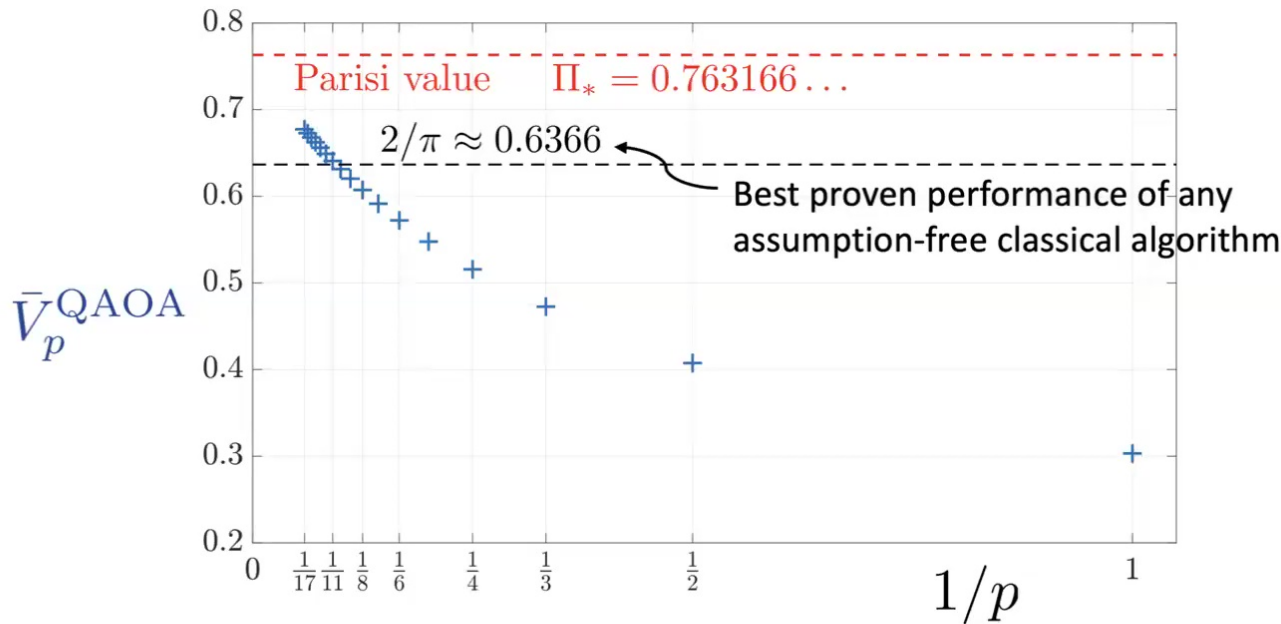


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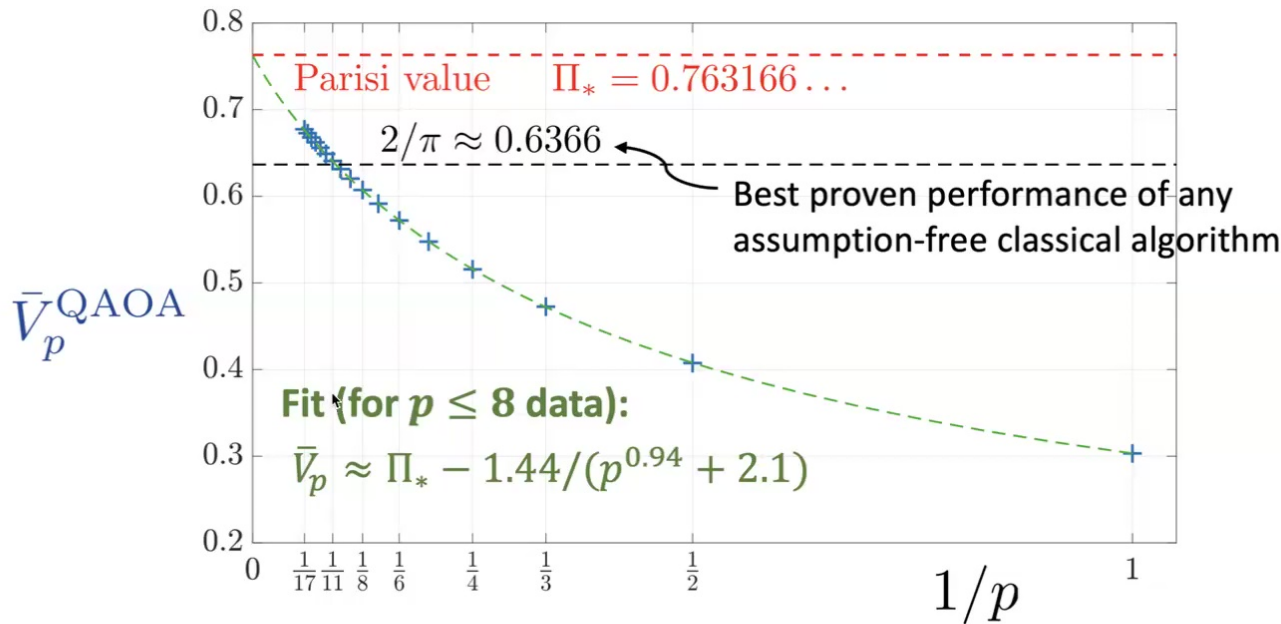
**Classical state-of-the-art:** Assuming “No OGP” conjecture, the [AMS21] Local Message Passing algorithm after  $p$  rounds gets

$$V_p^{\text{LMP}} \geq \Pi_* - O(1/\sqrt{p})$$

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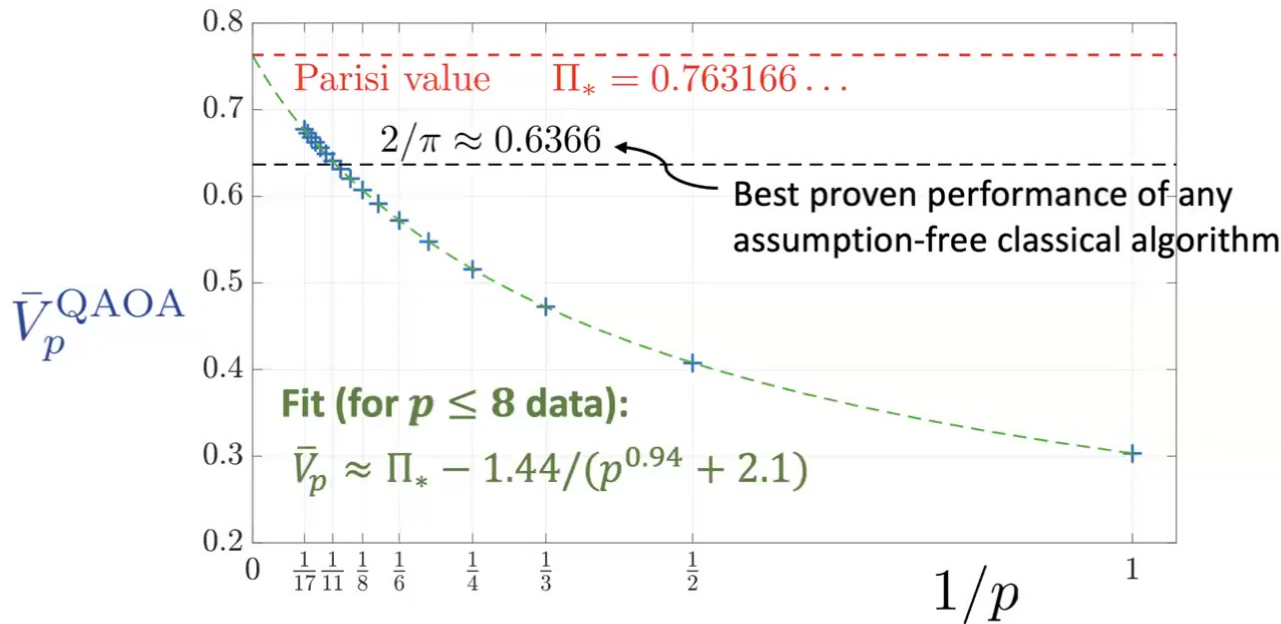
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Quadratic  
Quantum  
Advantage

[Basso Farhi Marwaha Villalonga LZ, TQC 2022]

# More general problems

$$C_J(\mathbf{z}) = \sum_{i_1, \dots, i_q=1}^n J_{i_1, i_2, \dots, i_q} z_{i_1} z_{i_2} \cdots z_{i_q}$$

- Example: fully connected Gaussian spin glasses  $J_{i_1, \dots, i_q} \sim \mathcal{N}(0, 1/n^{q+1})$
- For  $J$  drawn from any “reasonable” distribution with mean zero, we give an exact formula for

$$\lim_{n \rightarrow \infty} \mathbb{E}_J [ \langle \gamma, \beta | C_J | \gamma, \beta \rangle ] = V_p^{\text{QAOA}}(\gamma, \beta)$$

- Based on proving a “**generalized multinomial theorem**”, a rigorous version of a “path integral” calculation

$$\begin{aligned} \langle \hat{F} \rangle &= \sum_{\text{paths } \mathbf{y}} \langle s | e^{i\gamma_1 C_J} | y_1 \rangle \langle y_1 | e^{i\beta_1 B} | y_2 \rangle \langle y_2 | \cdots = \sum_{\{m_j\}} \binom{n}{\{m_j\}} \prod_j Q_j^{m_j} e^{nP(\mathbf{m}/n)} f(\mathbf{m}/n) \\ &\approx \int d\boldsymbol{\mu} e^{nS(\boldsymbol{\mu})} f(\boldsymbol{\mu}) \xrightarrow{n \rightarrow \infty} f(\boldsymbol{\mu}^*) \end{aligned}$$

[Basso Gamarnik Mei LZ, FOCS 2022]



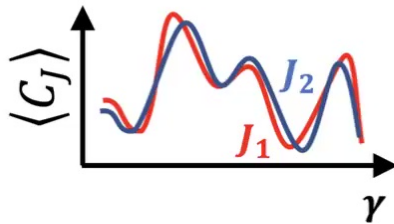
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$$C_J(\mathbf{z}) = \sum_{i_1, \dots, i_q=1}^n J_{i_1, i_2, \dots, i_q} z_{i_1} z_{i_2} \cdots z_{i_q}$$

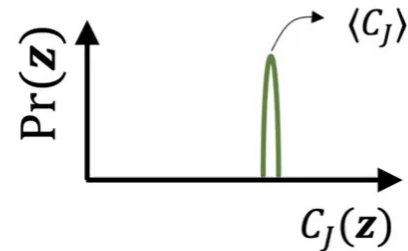
- Can also show **concentration** via second moment calculation

$$\lim_{n \rightarrow \infty} \mathbb{E}_J [\langle \gamma, \beta | C_J^2 | \gamma, \beta \rangle] = \lim_{n \rightarrow \infty} \left( \mathbb{E}_J [\langle \gamma, \beta | C_J | \gamma, \beta \rangle] \right)^2$$

## Concentrate over instances



## Concentrate over measurements



- Can reuse optimized parameters for similar instances!
- This is true even in nonlocal regime (e.g. all-to-all connected graph)!!

[Basso Gamarnik Mei LZ, FOCS 2022]

# Summary: Minimizing classical spin glasses

- Rigorous average-case analysis of QAOA to high depths is possible
  - $2^{O(p)}$  vs previous  $2^{2^{O(p)}}$  cost for worst-case analysis
- **A quantum advantage** in solving MaxCut on random graph



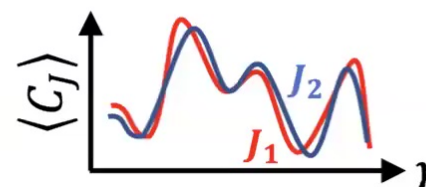
	Best Classical	QAOA
Proven Performance	$2/\pi \approx 0.6366$	$\geq 0.6879$
Conjectured	$0.763166 - 1/\sqrt{p}$	$0.763166 - 1/p$

[Basso Farhi Marwaha Villalonga LZ, TQC 2022]

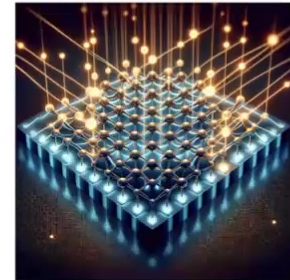
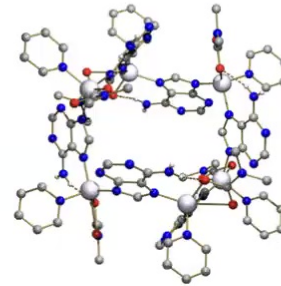
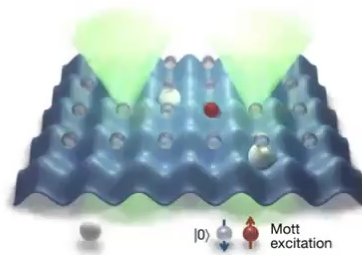
- Can analyze harder general problems with path integrals

$$C_J(\mathbf{z}) = \sum_{i_1, \dots, i_k=1}^n J_{i_1, i_2, \dots, i_k} z_{i_1} z_{i_2} \cdots z_{i_k}$$

Concentrate over instances



[Basso Gamarnik Mei LZ, FOCS 2022]



## Part 2

# Minimizing Energy of *Quantum* Systems

Based on [Chen Huang Preskill LZ, STOC 2024] [arXiv:2204.10306](https://arxiv.org/abs/2204.10306)



Anthony Chen



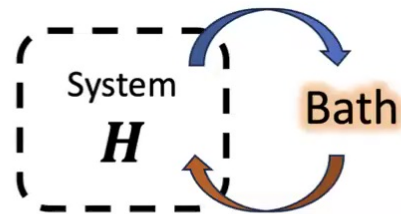
Robert Huang



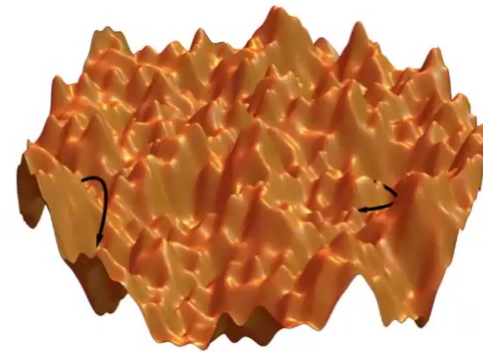
John Preskill



Ground states (global minima) of quantum systems are hard to find in general, even for Nature!



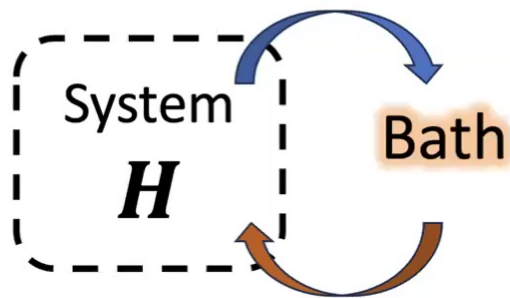
Nature cools system  
to a *local minimum*



e.g., spin glass

**Local minima are more physical than global minima**

*How tractable is the problem of **finding a local minimum** using classical and quantum computers?*



[Chen Huang Preskill LZ, STOC 2024]

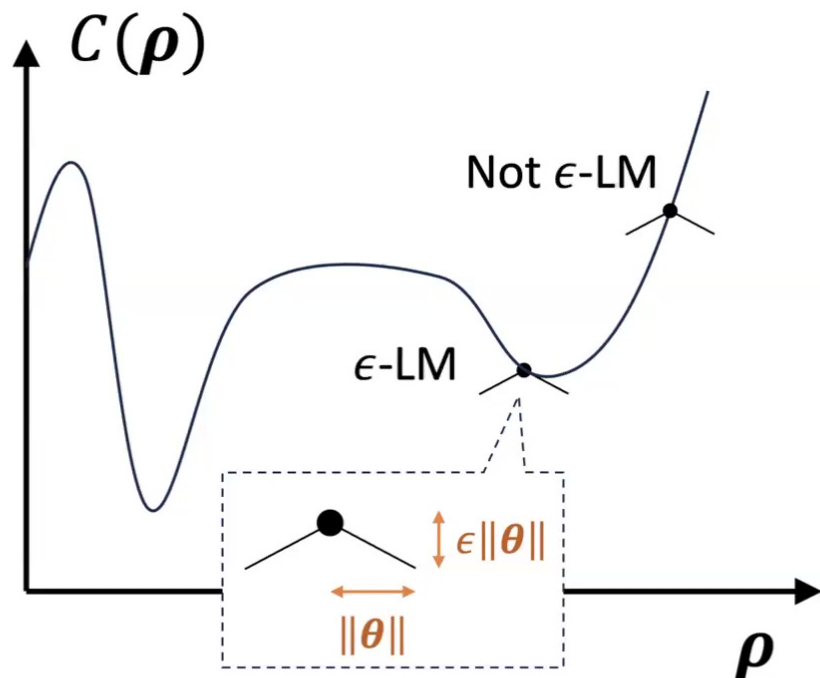
## Our Main Result

Cooling to a local minimum is universal for quantum computation.

⇒ Finding a local minimum of quantum system is **classically HARD** and **quantumly EASY!**



# What is a local minimum?



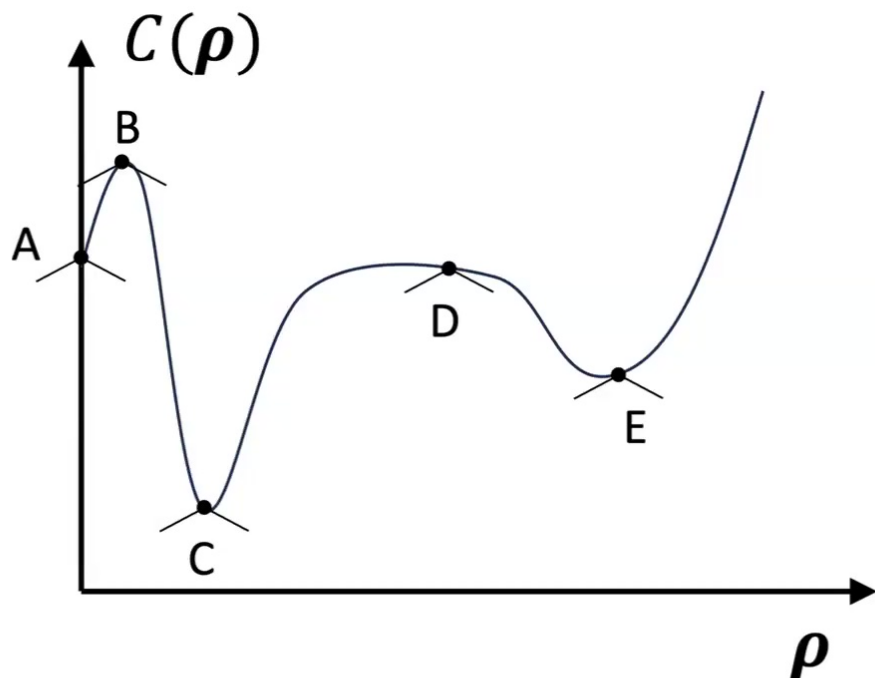
- Domain:  $n$ -qubit state  $\rho$
- Energy function:  $C(\rho) = \text{tr}(\mathbf{H}\rho)$
- A family of perturbations:  $\rho \rightarrow \mathcal{P}_\theta[\rho]$
- $\rho$  is an  **$\epsilon$ -approximate local minimum** if

$$C(\rho) \leq C(\mathcal{P}_\theta[\rho]) + \epsilon \|\theta\|$$

for all small enough  $\theta$



# What is a local minimum?



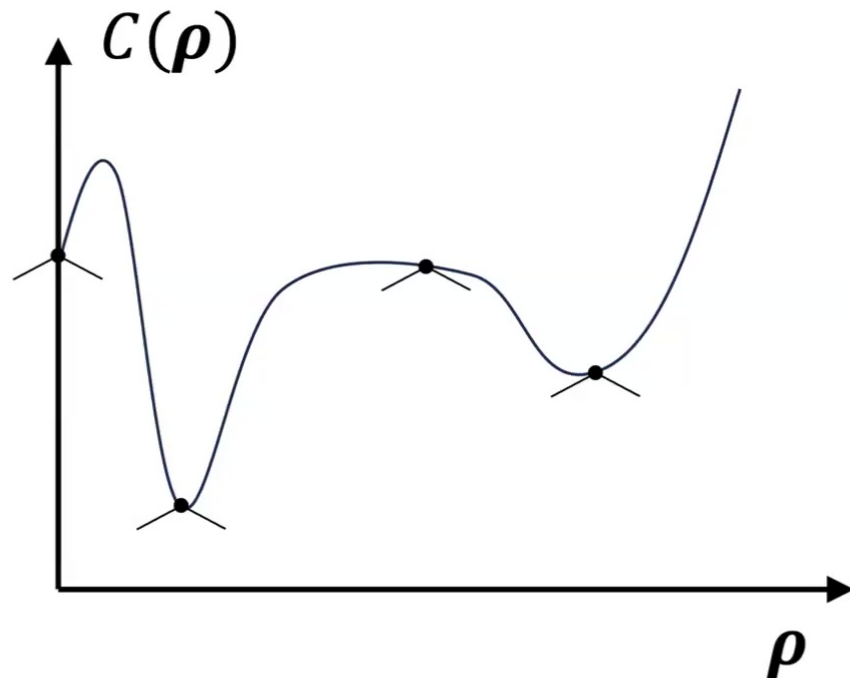
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for all small enough  $\theta$

A, C, D, E are  $\epsilon$ -approx LM  
B is not

# The problem of finding a local minimum

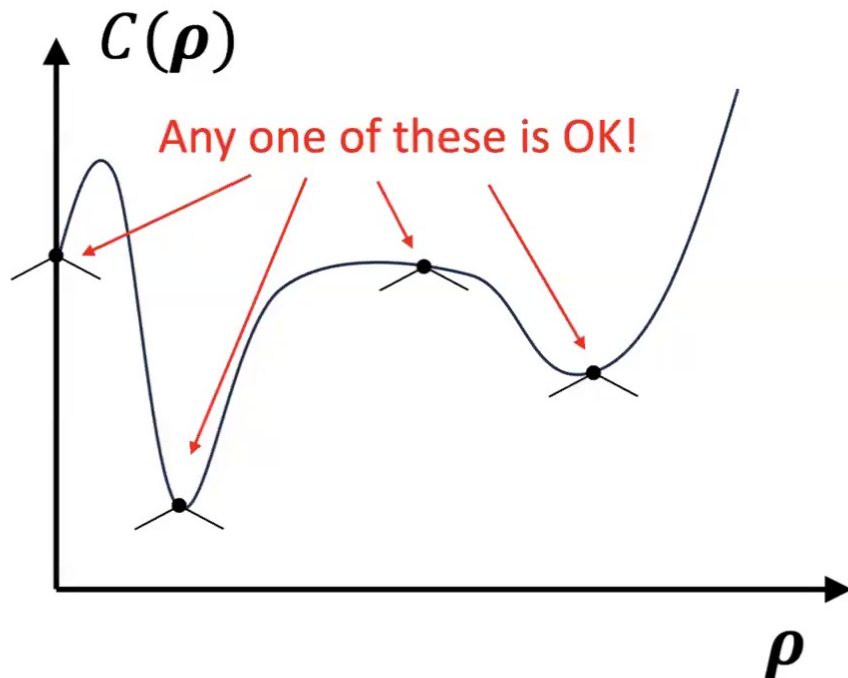


- **Input:**

1.  $\mathbf{H}$ , where  $\|\mathbf{H}\| = \text{poly}(n)$
2. a family of perturbation  $\{\mathcal{P}_\theta\}_\theta$
3. some  $\epsilon > 1/\text{poly}(n)$
4. a (local) observable  $\mathbf{O}$

- **Problem:** Output estimated  $\text{Tr}(\mathbf{O}\rho^*)$  within  $\epsilon$  error for any  $\epsilon$ -approx local minimum  $\rho^*$  under the perturbations.

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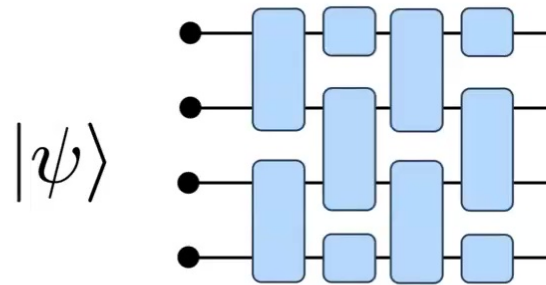
- **Problem:** Output estimated  $\text{Tr}(O\rho^*)$  within  $\epsilon$  error for any  $\epsilon$ -approx local minimum  $\rho^*$  under the perturbations.

Note: purely classical input + output

# Example: Local unitary perturbations

$$|\psi\rangle \rightarrow \mathcal{P}_{\boldsymbol{\theta}}[|\psi\rangle] = e^{-i \sum_a \theta_a \mathbf{h}_a} |\psi\rangle \quad \theta_a \in \mathbb{R}$$

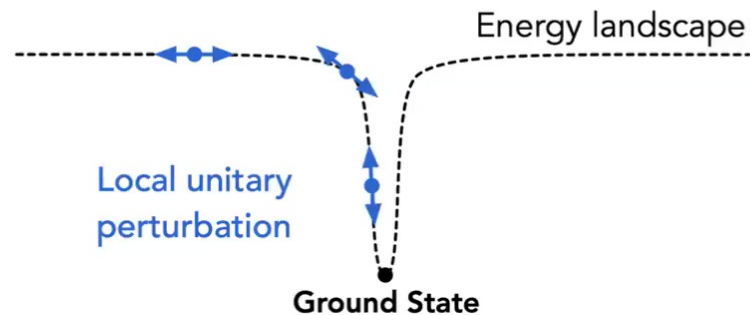
where  $\{\mathbf{h}_a\}_a = \{\text{one- and two-qubit Pauli operators}\}$ .



e.g., Adapt-VQE,  
QC as geometry

# Finding a local minimum under **local unitary perturbations** is classically easy

“Barren plateau”



- For any local Hamiltonian  $H$ , any random state is a local minima for any  $\epsilon \geq 1/\text{poly}(n)$ .
- There are  $\exp(\exp(n))$  such local minima!
- The local minimum problem becomes **TOO EASY!** Classically just output  $\text{Tr}(\mathbf{O}\rho^*) = \text{Tr}(\mathbf{O})/2^n$

# Nature-inspired **Thermal perturbations**

$$\rho \rightarrow \mathcal{P}_\theta[\rho] = e^{\sum_a \theta_a \mathcal{L}_a}[\rho] \quad \theta_a \in \mathbb{R}_{\geq 0}$$

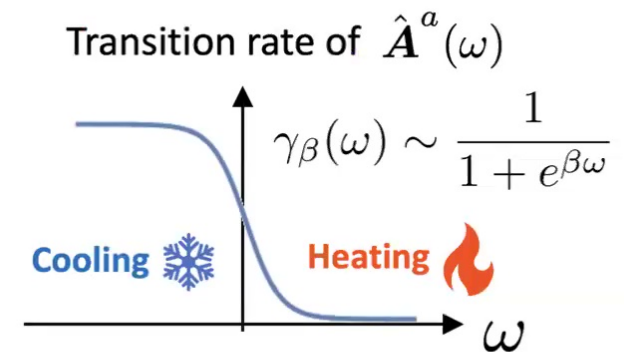
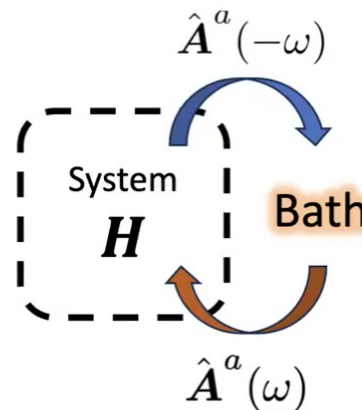
where  $\mathcal{L}_a$  is a thermal Lindbladian for the system weakly coupled to a bath

**Parameters**

$\beta$  inverse temperature

$\mathcal{T}$  coarse-grain timescale

$\{\hat{A}^a\}_a$  local jump operators



Based on rigorous version of Davies equation [Mozgunov Lidar 2020]



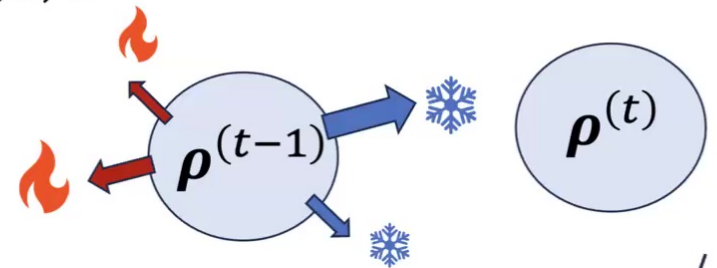
# Quantum Thermal Gradient Descent can find local minima under **thermal perturbations**

- Consider any  $n$ -qubit Hamiltonian  $\mathbf{H}$  where  $\|\mathbf{H}\| \leq B$
- To find an  $\epsilon$ -local minimum under thermal perturbations by  $\{\mathcal{L}_a\}_{a=1}^m$ :

Initialize at any state  $\rho^{(0)}$ , and for each step  $t = 1, 2, 3, \dots$

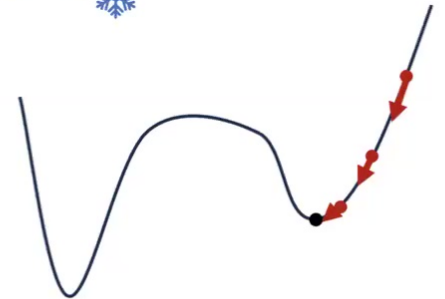
① Estimate  $g_a = \partial_a \langle \mathbf{H} \rangle = \text{tr}(\rho \mathcal{L}_a^\dagger [\mathbf{H}])$  to  $0.01\epsilon$  precision

② If all  $g_a > -0.99\epsilon$ , STOP. Otherwise evolve  $\rho^{(t)} = \exp(\sum_a \theta_a \mathcal{L}_a) [\rho^{(t-1)}]$  where  $\theta_a = -\min(0, g_a)/9B^2$



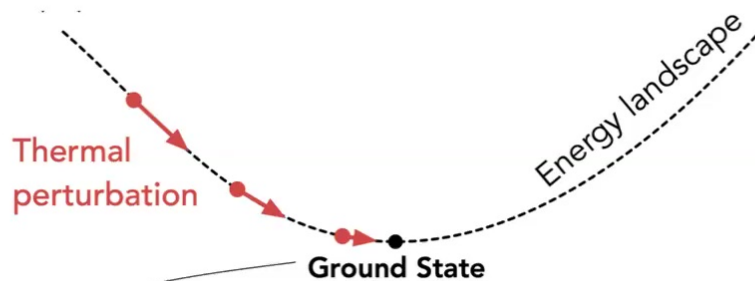
This **provably converges** within  $O(B^3/\epsilon^2)$  steps!

Finding a local minimum is **quantumly easy!**



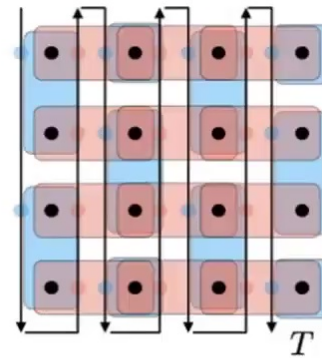
# Finding a local minimum under **thermal perturbations** is classically hard

For any circuit  $U_C = U_T \cdots U_1$



$$|\text{GS}\rangle = \sum_{t=0}^T \sqrt{\xi_t} (U_t \cdots U_2 U_1 |0^n\rangle) \otimes |t\rangle$$

- **Theorem:** Certain 2D Hamiltonians whose ground states encode universal quantum computation have ***no suboptimal local minima*** when  $\epsilon^{-1}, \beta, \tau \geq \text{poly}(n)$ .



$$H_C = \sum_t U_t \otimes |011\rangle\langle 001| + \cdots$$

# BQP-hard Hamiltonian

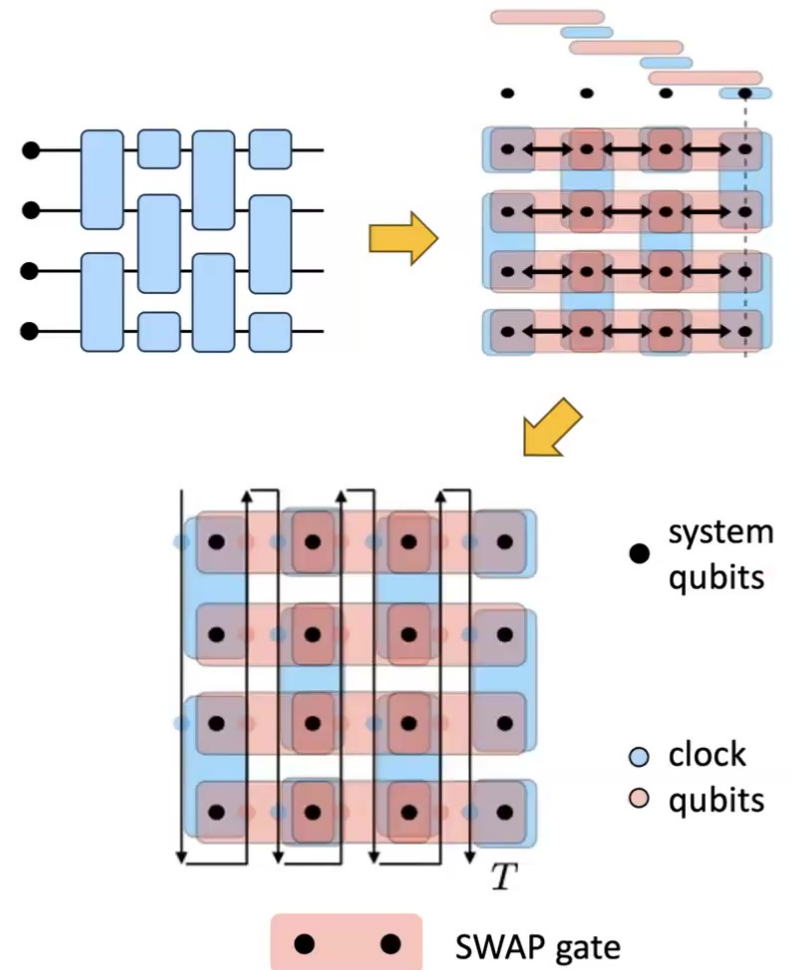
- Write any circuit as a sparse 2D circuit  

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- BQP-hard Hamiltonian on  $n + T$  qubits:

$$H_C = H_{\text{clock}} + H_{\text{in}} + H_{\text{prop}}$$

- $H_{\text{clock}} = \sum_t f_t \cdot I \otimes |01\rangle\langle 01|_{t,t+1}$   
 $\rightarrow$  clock qubits are in states  $|t\rangle = |1^t 0^{T-t}\rangle$
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See e.g. [Kitaev Shen Yu 2002] [Oliveira Terhal 2008]



# BQP-hard Hamiltonians have good gradients

- Goal: show  $\mathbf{H}_C$  has no suboptimal local minima
- Negative gradient condition:

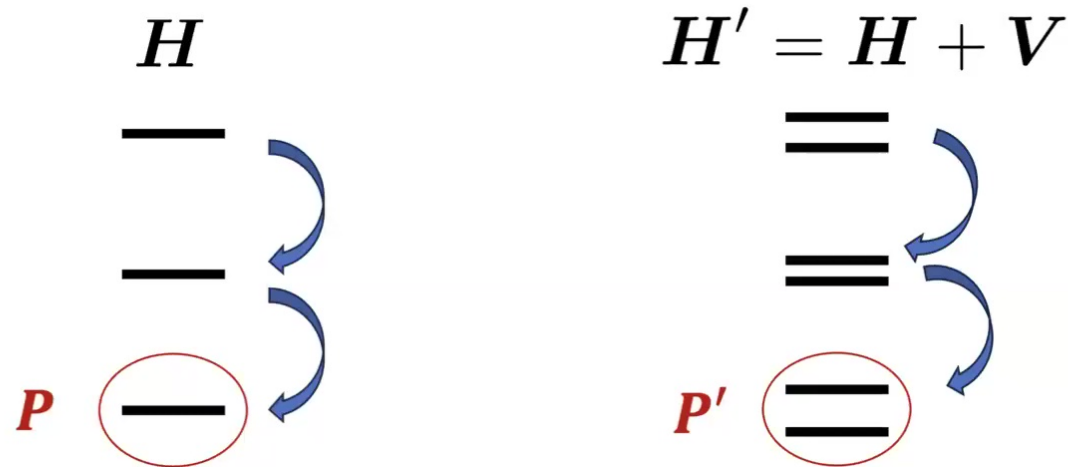
$$\mathcal{L}^\dagger[\mathbf{H}] \preceq -r(\mathbf{I} - \mathbf{P}_{\text{GS}})$$

“any excited state must have good gradients”

$$\frac{d}{dt} \langle \mathbf{H} \rangle = \langle \mathcal{L}^\dagger[\mathbf{H}] \rangle \leq -r(1 - \langle \mathbf{P}_{\text{GS}} \rangle)$$

- Proving this for all arbitrary superposition of excited states of  $\mathbf{H}_C$  seems daunting... how?

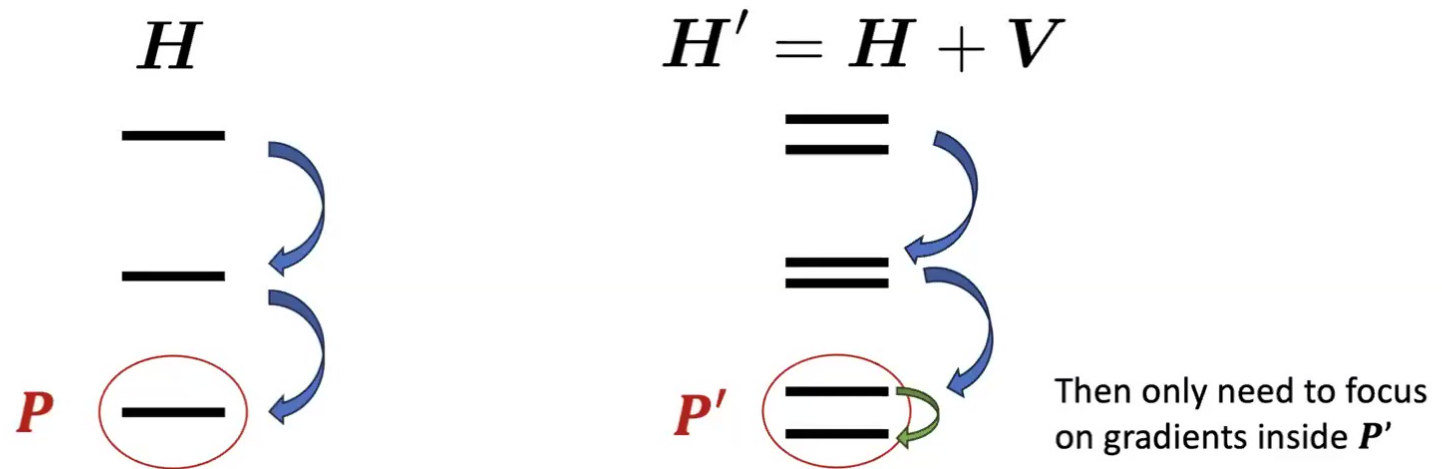
Key proof idea: Gradient of excited states robust under perturbation



**Lemma**

$$\mathcal{L}^\dagger[H] \preceq -r(I - P) \implies \mathcal{L}'^\dagger[H'] \preceq -r(I - P')$$

# Key proof idea: Gradient of excited states robust under perturbation



**Lemma**

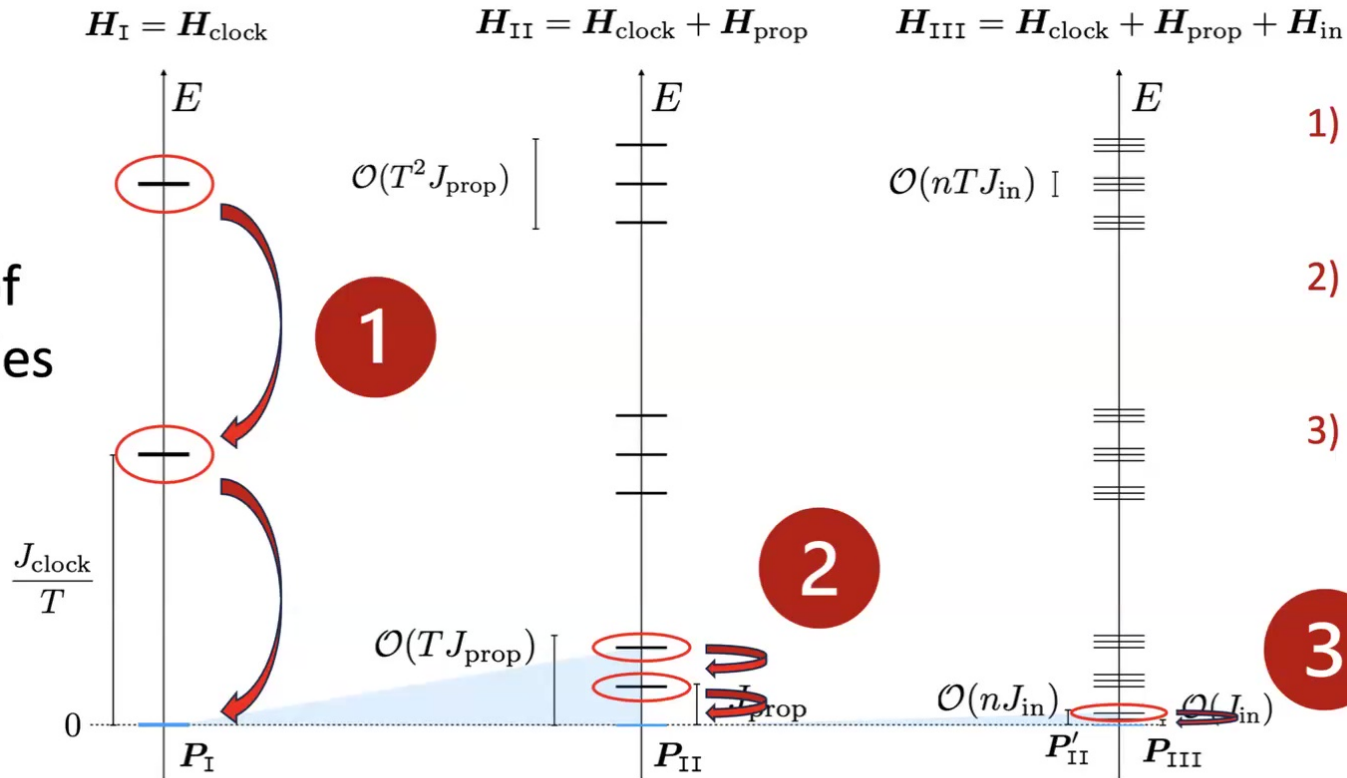
$$\mathcal{L}^\dagger[H] \preceq -r(I - P) \implies \mathcal{L}'^\dagger[H'] \preceq -r(I - P')$$

\*Standard perturbative argument doesn't work – Errors in thermal Lindbladians are suppressed *not* by **spectral gap** ( $\min |E_i - E_j|$ ) but by “**Bohr frequency gap**” ( $\min |E_i - E_j| - |E_k - E_l|$ )



# No local minima in excited states

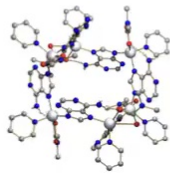
Exploit a hierarchy of energy scales



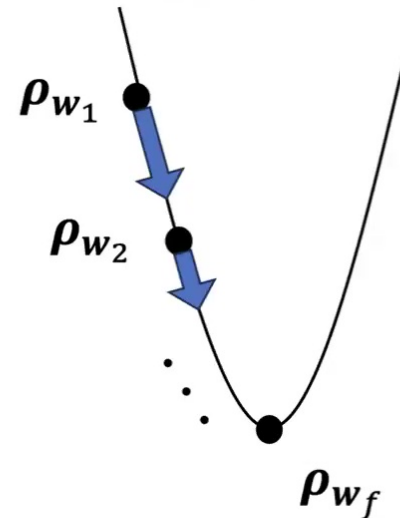
- 1) Large gradients in excited states of  $H_I$
- 2) Large gradients in excited states of  $P_I H_{II} P_I$
- 3) Large gradients in excited states of  $P_{II} H_{III} P_{II}$

# Quantum advantage in cooling to local minima

A possible method to detect quantum advantage



Energy landscape of *classical ansatz*



Evaluate gradient

$$g_a = \text{tr} \left( \mathcal{L}_a^\dagger[H] \rho_{w_f} \right)$$

$\mathcal{L}_a^\dagger[H]$  is often quasi-local  
→ can evaluate classically

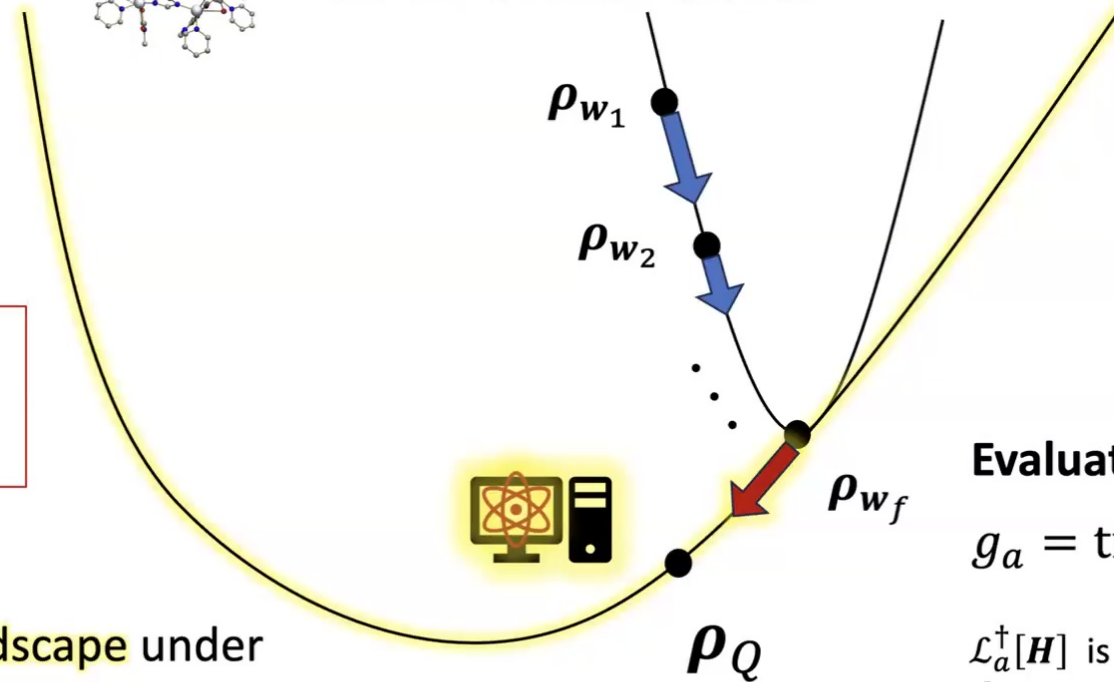
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$g_a < -\epsilon \rightarrow$   
quantum advantage!



Energy landscape of *classical ansatz*



Energy landscape under **thermal (quantum) perturbations**

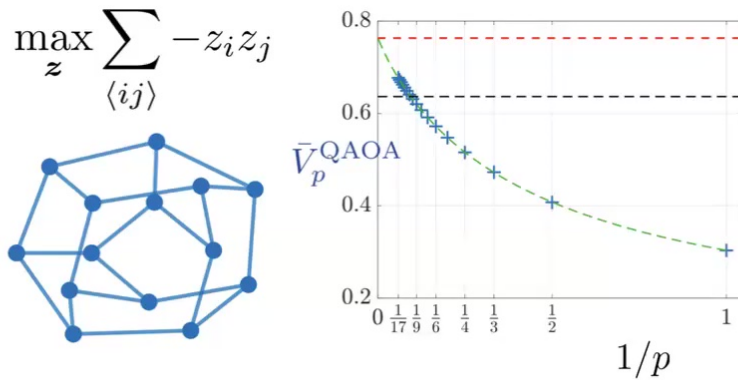
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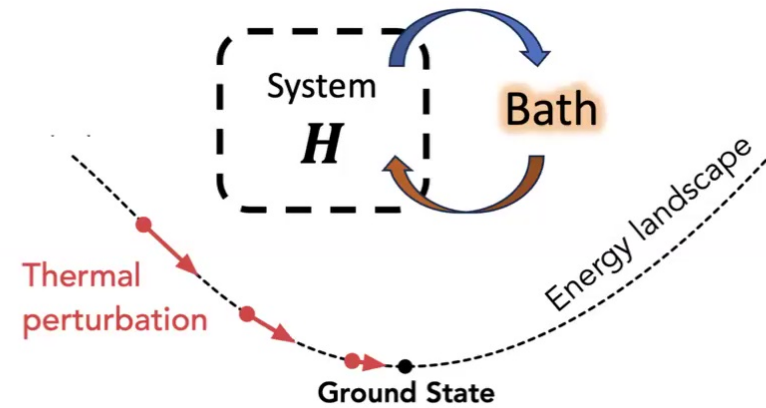
# Summary: Quantum Advantages in Energy Minimization

## Classical systems



	Best Classical	QAOA
Proven	$2/\pi \approx 0.6366$	$\geq 0.6879$
Conjectured	$0.763166$ $- 1/\sqrt{p}$	$0.763166$ $- 1/p$

## Quantum systems



$$\langle \text{GS} | \mathbf{Z}_j | \text{GS} \rangle \approx \langle 0^n | \mathbf{U}_C^\dagger \mathbf{Z}_j \mathbf{U}_C | 0^n \rangle$$

- No suboptimal local minima
- Finding a local minimum is **classically HARD** and **quantumly EASY!**

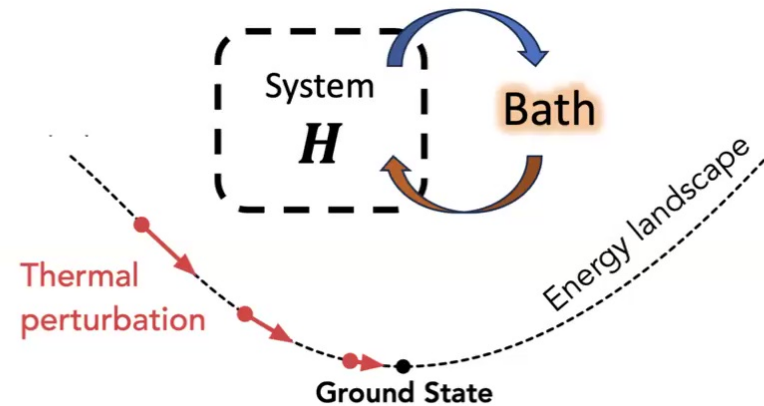
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### Outlook

- Prove convergence to the Parisi value
- Can we analyze QAOA when  $p > \log n$ ?
- Quantum algorithms for classical problems over random structure

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# BQP-hard Hamiltonian

- Write any circuit as a sparse 2D circuit  

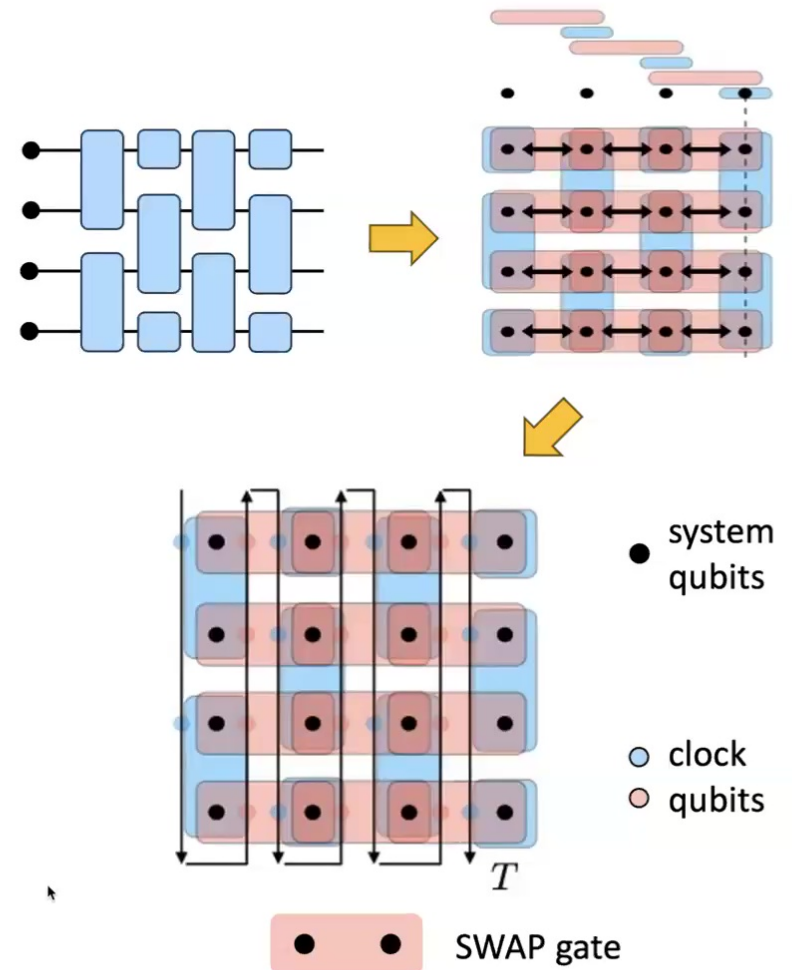
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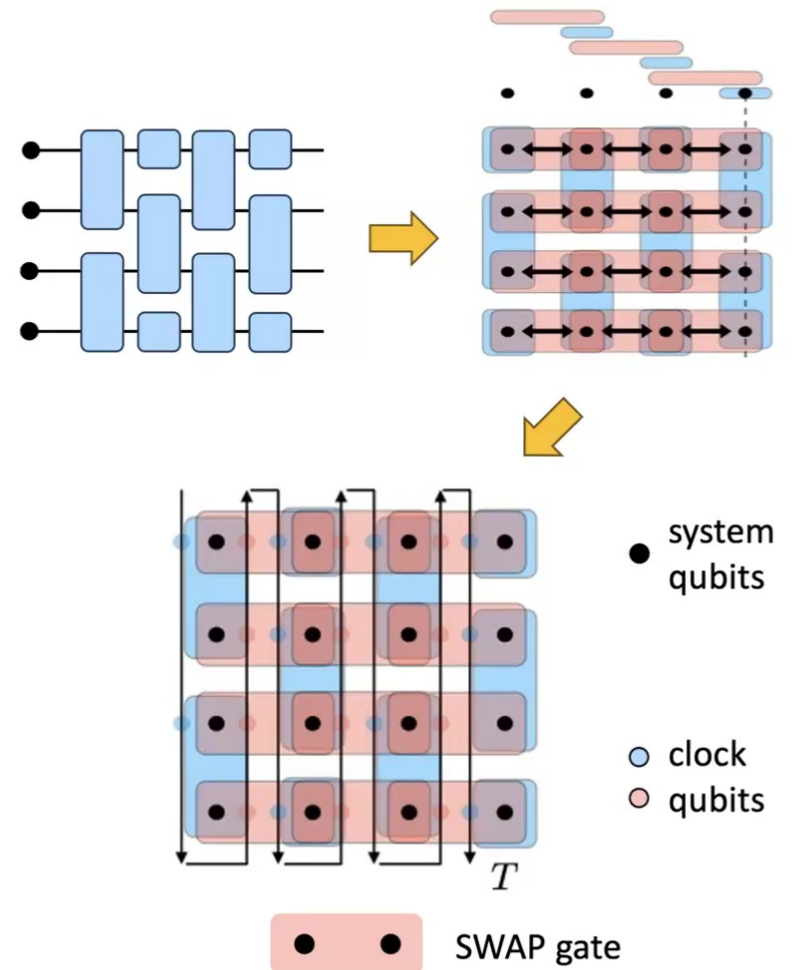
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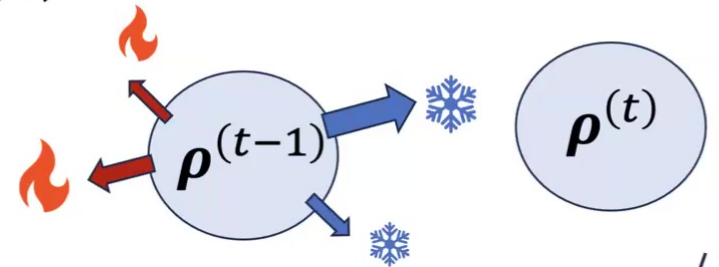


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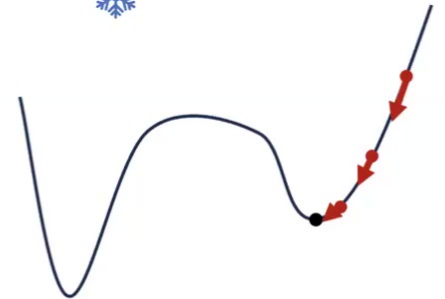
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