量子计算机制备Gibbs态研究Ising模型的临界行为和跑动耦合

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Content

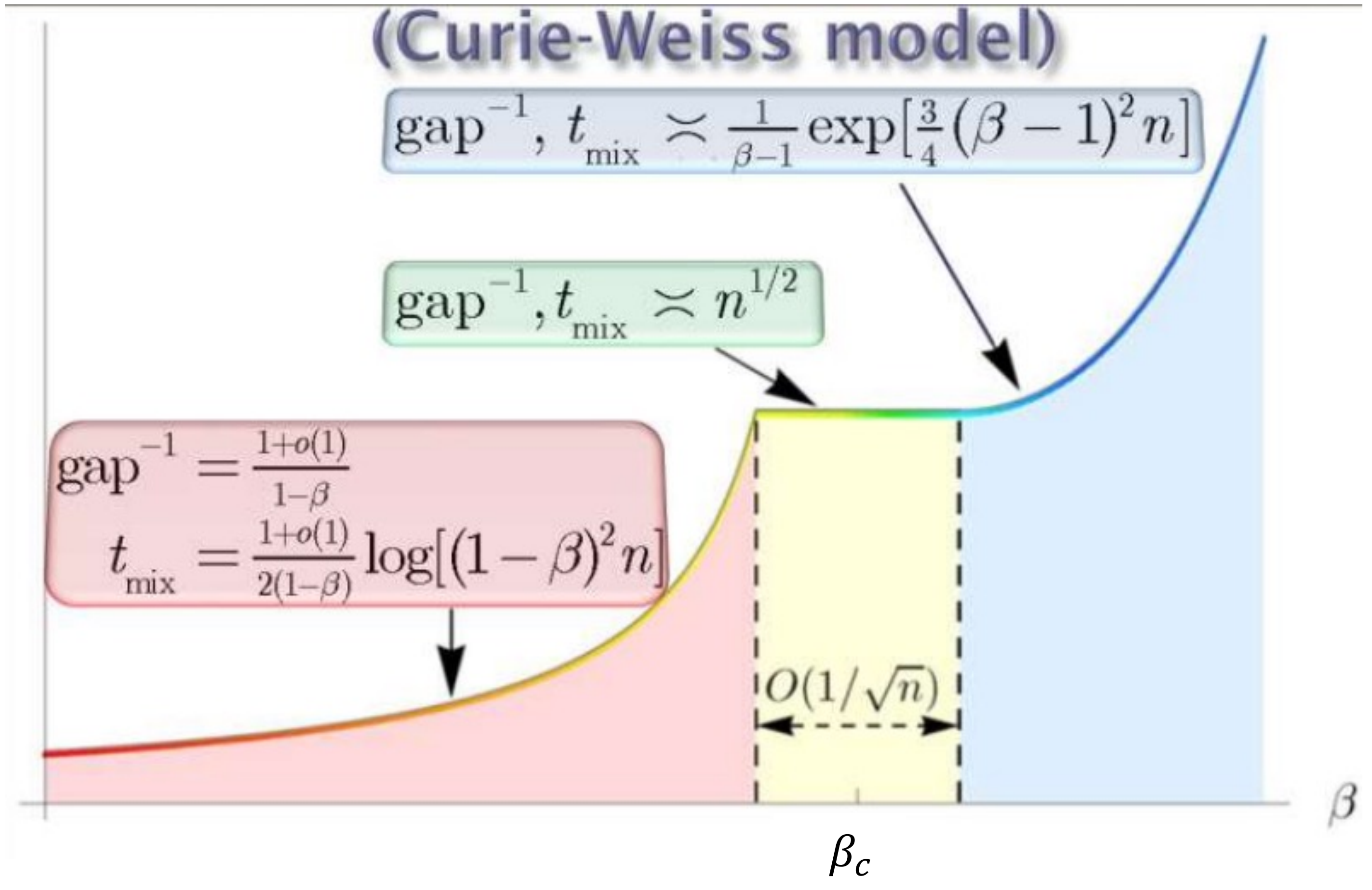
- background：Critical slowdown in Ising model
- Algorithm: Variational quantum Imaginary Evolution
- Results: On the specific heat, susceptibility and running coupling

Critical slowdown in Ising model

Curie-Weiss model:

$$\mu_n(\sigma) \propto \exp\left(\frac{\beta}{n}\sum_{x<y}\sigma(x)\sigma(y)\right).$$

- $\sigma \in \{+1, -1\}$
- n: number of vertices
- μ_n: Stationary distribution of Monte-Carlo sampling



[Ding,L., Peres 09]

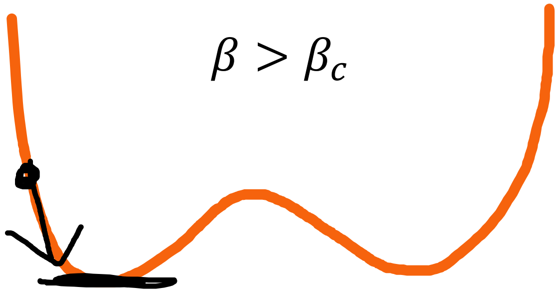
Critical slowdown in Ising model

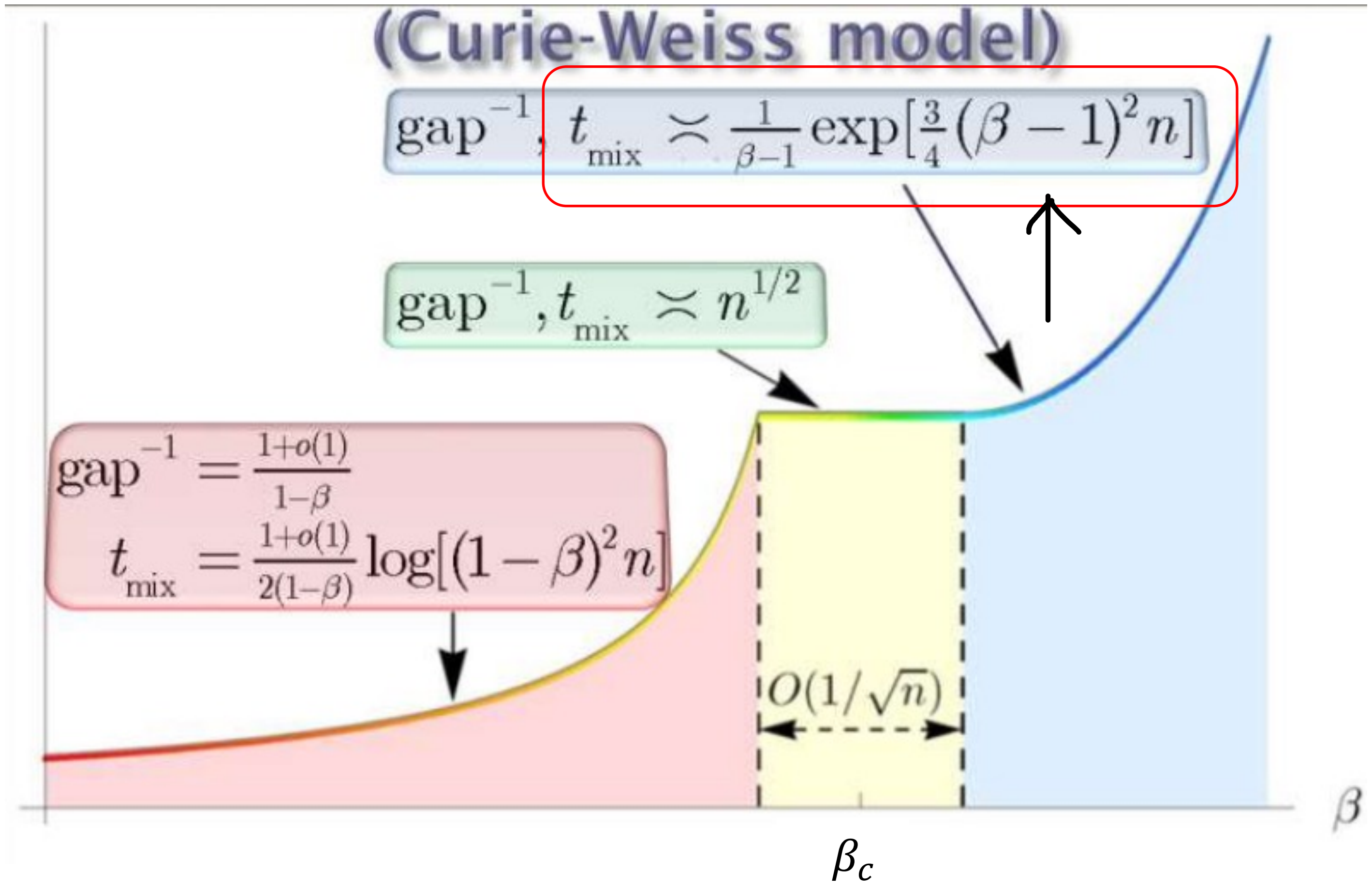
- Measuring time of convergence to equilibrium:

Mixing time

$$t_{\text{mix}} = t:\ \max_{x\in X}\|P^t(x,\cdot\,) - \mu_n\|_{TV} \le \frac{1}{4}$$

$\beta > \beta_c$

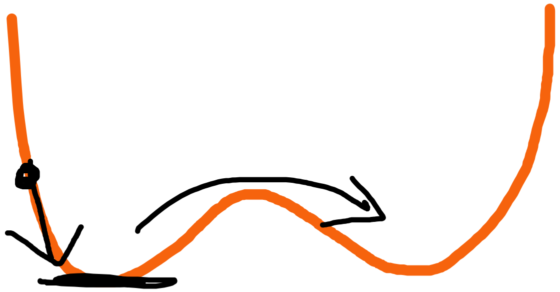


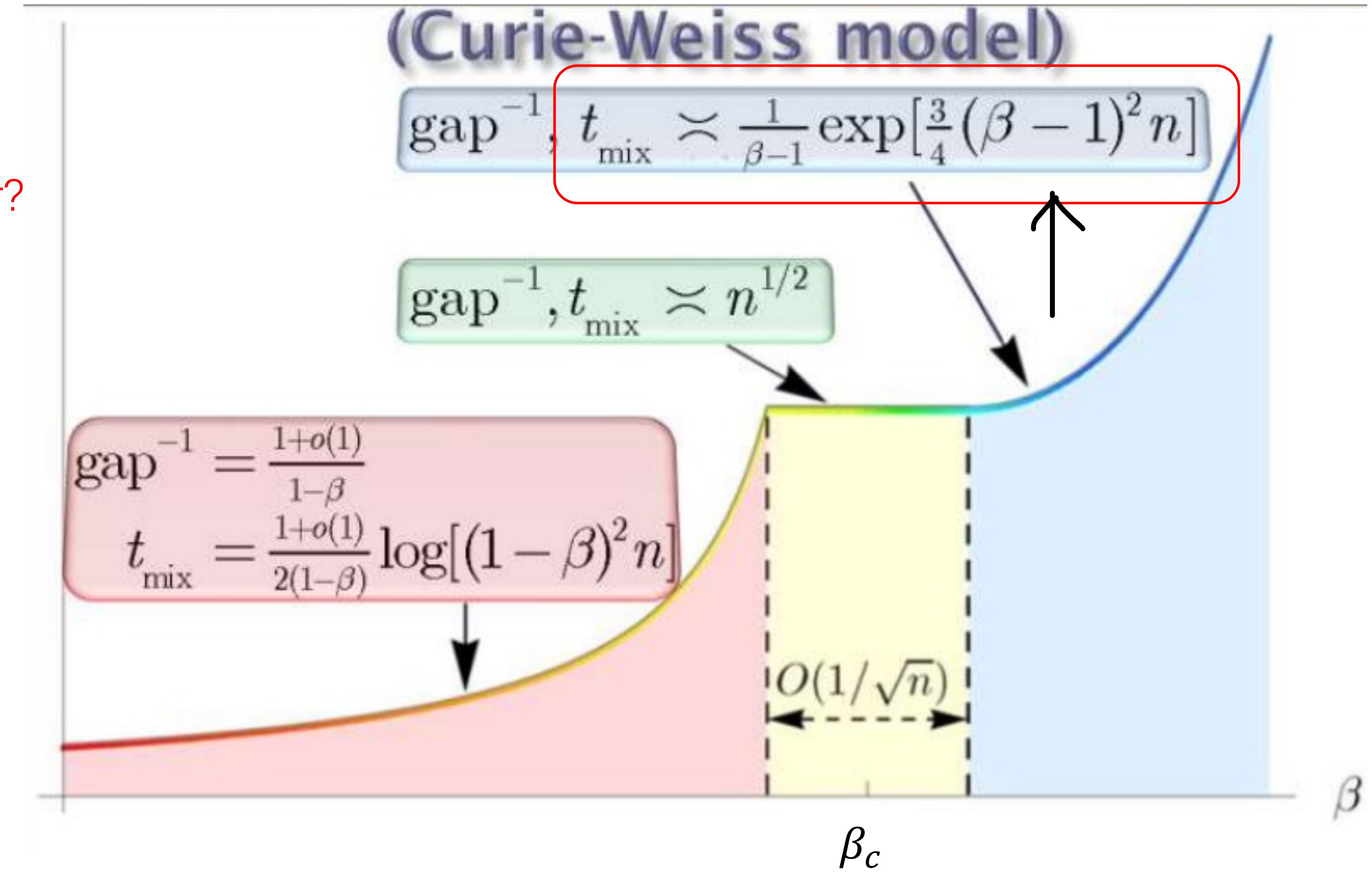


[Ding,L., Peres 09]

Critical slowdown in Ising model

How it behaves on quantum computer?

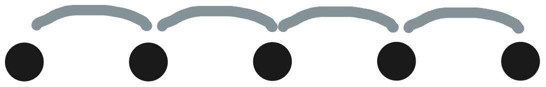




[Ding,L., Peres 09]

Long-range interacting Ising model

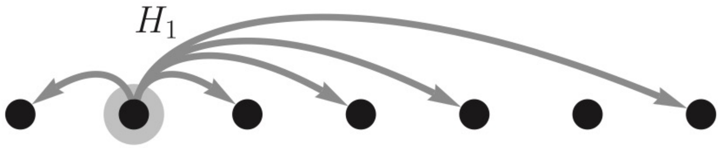
$$H = -\sum_{\substack{i,j=1 \\ i<j}}^{N} \frac{J}{|r_i - r_j|^{\alpha}} Z_i Z_j - h \sum_{i=1}^{N} X_i$$



$\alpha = \infty$

Nearest neighbor Ising model

$$H = -J \sum_{\langle i,j \rangle} Z_i Z_j - h \sum_{i=1}^{N} X_i$$



$\alpha = 0$

Curie-Weiss model

$$H = -J \sum_{i<j} Z_i Z_j - h \sum_{i=1}^{N} X_i$$

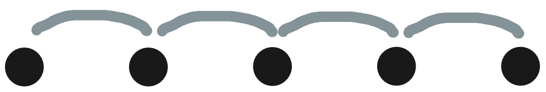
Higher dimension with periodic boundary condition(PBC):

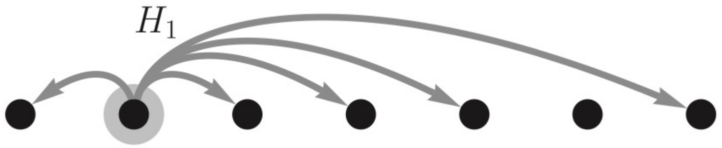
$$r_i \to \vec{r}^{\,i} = (r_1^i, \dots r_D^i)$$

$$|r_i - r_j| \to \sum_{d=1}^{D} \min(|r_d^i - r_d^j|, N_d - |r_d^i - r_d^j|)$$

Long-range interacting Ising model

$$H = -\sum_{\substack{i,j=1 \\ i<j}}^{N} \frac{J}{|r_i - r_j|^{\alpha}} Z_i Z_j - h \sum_{i=1}^{N} X_i$$





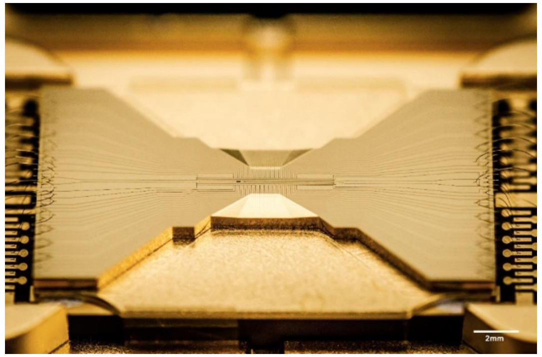
$\alpha = \infty$ → Nearest neighbor Ising model

$$H = -J \sum_{\langle i,j \rangle} Z_i Z_j - h \sum_{i=1}^{N} X_i$$

$\alpha = 0$ → Curie-Weiss model

$$H = -J \sum_{i<j} Z_i Z_j - h \sum_{i=1}^{N} X_i$$

- $0 \leq \alpha \leq 3$ in trapped ion experiments
- More physics like confinement [F. Liu et.al. (19)] and scattering [Vovrosh et.al. (22)]



Gibbs state on quantum computer

Quantum imaginary time evolution (QITE)

$$|\psi(\tau)\rangle = \frac{e^{-\tau H}}{\sqrt{\langle\psi(0)|e^{-2\tau H}|\psi(0)\rangle}}|\psi(0)\rangle$$

1. Choose Initial state $|\psi(0)\rangle$
2. Evolution

$$\rho = \frac{e^{-\beta H}}{Z}, Z = \mathrm{Tr}(e^{-\beta H})$$

Gibbs state on quantum computer

Quantum imaginary time evolution (QITE)

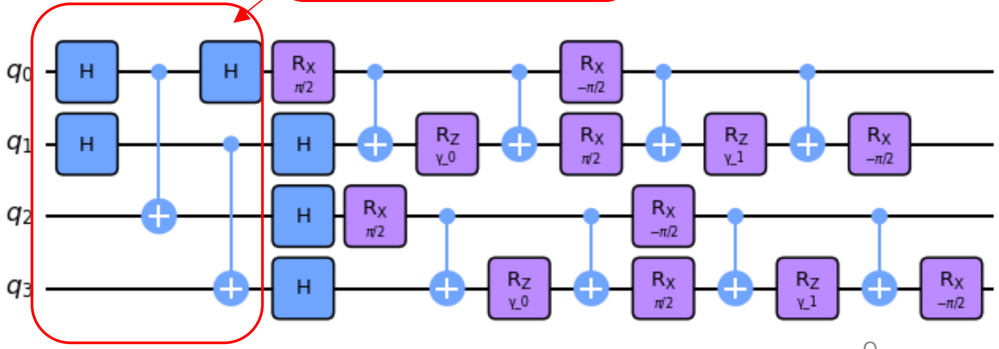
$$|\psi(\tau)\rangle = \frac{e^{-\tau H}}{\sqrt{\langle\psi(0)|e^{-2\tau H}|\psi(0)\rangle}}|\psi(0)\rangle$$

1. Choose Initial state $|\psi(0)\rangle$

- Preparing initial state as ancilla pair state:

$$|\psi_a(\tau)\rangle = \frac{e^{-\tau H\otimes \mathbf{I}_a}|\psi_a(0)\rangle}{\sqrt{\langle\psi_a(0)|\, e^{-2\tau H\otimes \mathbf{I}_a}\,|\psi_a(0)\rangle}}.$$

with $|\psi_a(0)\rangle = \frac{1}{\sqrt{d}}\sum_i |i\rangle_s |i\rangle_a$



- After imaginary time evolution for time τ, we have Gibbs state with inverse-temperature 2τ:

$$\rho = \mathrm{Tr}_a[|\psi_a(\tau)\rangle\langle\psi_a(\tau)|] = \frac{e^{-2\tau H}}{\mathrm{Tr}_s(e^{-2\tau H})}$$

Gibbs state on quantum computer

Quantum imaginary time evolution (QITE)

$$|\psi(\tau)\rangle = \frac{e^{-\tau H}}{\sqrt{\langle\psi(0)|e^{-2\tau H}|\psi(0)\rangle}}|\psi(0)\rangle$$

1. Choose Initial state $|\psi(0)\rangle$

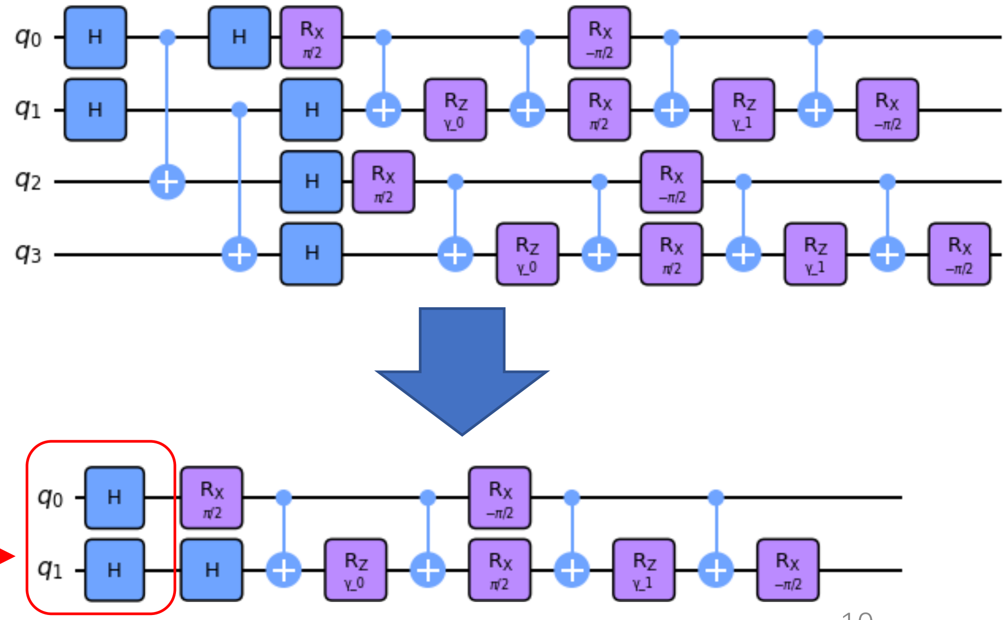
Simplification for Ising model:

- The Hamiltonian is consisted of $Z_i Z_j$
- The observable is consisted of Z:

$$H, H^2, M = \sum Z_i \cdots\cdots, O = \sum h_m \tilde{Z}$$

Then:

$$\langle O\rangle = \sum_m h_m \frac{\langle + \cdots + |e^{-\tau H}\, \tilde{Z} e^{-\tau H}| + \cdots + \rangle}{\langle + \cdots + |e^{-2\tau H}\, | + \cdots + \rangle}$$



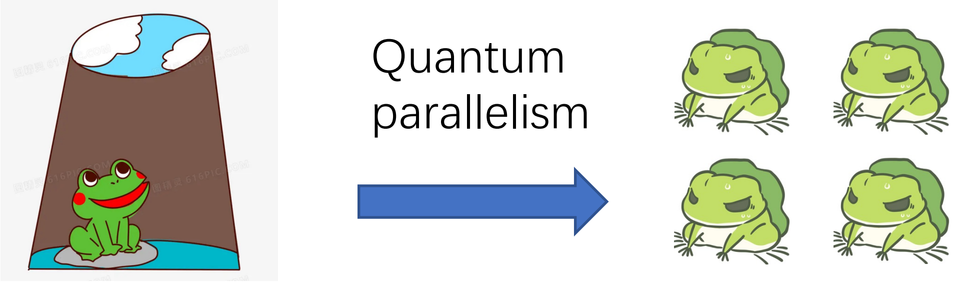
Gibbs state on quantum computer

Quantum imaginary time evolution (QITE)

$$|\psi(\tau)\rangle = \frac{e^{-\tau H}}{\sqrt{\langle\psi(0)|e^{-2\tau H}|\psi(0)\rangle}}|\psi(0)\rangle$$

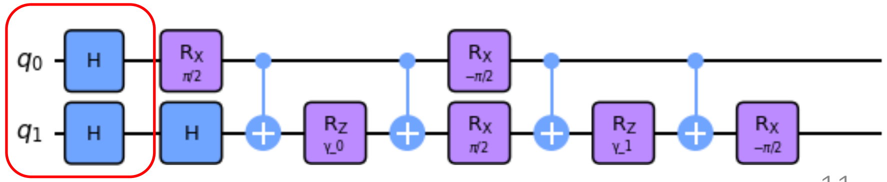
<u>1. Choose Initial state $|\psi(0)\rangle$</u>

$$|+\,+\rangle = |00\rangle + |01\rangle + |10\rangle + |11\rangle$$



2^N frogs

$$\langle O\rangle = \sum_m h_m \frac{\langle + \cdots + | e^{-\tau H}\, \tilde{Z} e^{-\tau H} | + \cdots + \rangle}{\langle + \cdots + | e^{-2\tau H} | + \cdots + \rangle}$$



Gibbs state on quantum computer

Quantum imaginary time evolution (QITE)

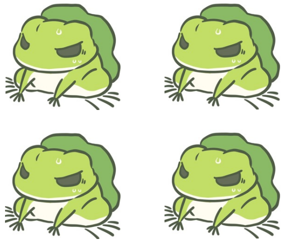
$$|\psi(\tau)\rangle = \frac{e^{-\tau H}}{\sqrt{\langle\psi(0)|e^{-2\tau H}|\psi(0)\rangle}}|\psi(0)\rangle = \left|\psi(\vec{\theta}(\tau))\right\rangle$$

Evolve the variational ansatz

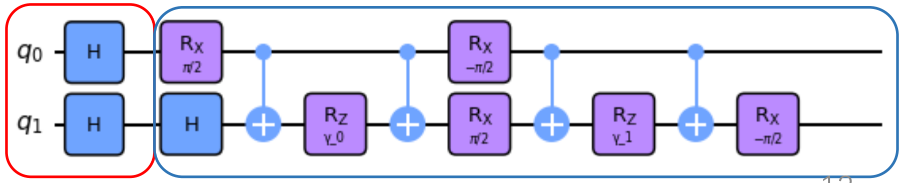
1. Choose Initial state $|\psi(0)\rangle$

$$|+\,+\rangle = |00\rangle + |01\rangle + |10\rangle + |11\rangle$$

Quantum parallelism



$$\langle O\rangle = \sum_m h_m \frac{\langle + \cdots + \left|e^{-\tau H}\,\tilde{Z} e^{-\tau H}\right| + \cdots + \rangle}{\langle + \cdots + \left|e^{-2\tau H}\right| + \cdots + \rangle}$$



Gibbs state on quantum computer

[McArdle, et.al. 19]

Quantum imaginary time evolution (QITE)

$$|\psi(\tau)\rangle = \frac{e^{-\tau H}}{\sqrt{\langle\psi(0)|e^{-2\tau H}|\psi(0)\rangle}}|\psi(0)\rangle = |\psi(\vec{\theta}(\tau))\rangle$$

2. Evolution

- Take the partial derivative on τ :

$$\frac{\partial|\psi(\tau)\rangle}{\partial\tau} = -(H - E_\tau)|\psi(\tau)\rangle, \qquad E_\tau = \langle\psi(\tau)|H|\psi(\tau)\rangle$$

- McLachlan' s variational principle

$$\delta\left\|\frac{\partial|\psi(\tau)\rangle}{\partial\tau} + (H - E_\tau)|\psi(\tau)\rangle\right\| = 0 \qquad \sum_j A_{ij}\dot{\theta}_j = C_i$$

$$A_{ij} = Re\left(\frac{\partial\langle\psi(\tau)|}{\partial\theta_i}\frac{\partial|\psi(\tau)\rangle}{\partial\theta_j}\right)$$

$$C_i = -Re\left(\frac{\partial\langle\psi(\tau)|}{\partial\theta_i}H|\psi(\tau)\rangle\right)$$

Measured on quantum computer

- The variational parameters are evolved as

$$\theta(\tau + \Delta\tau) = \theta(\tau) + \dot{\theta}(\tau)\times\Delta\tau = \theta(\tau) + A^{-1}C\times\Delta\tau$$

Ansatz design

- According to algorithm in [Motta, et.al. 20]

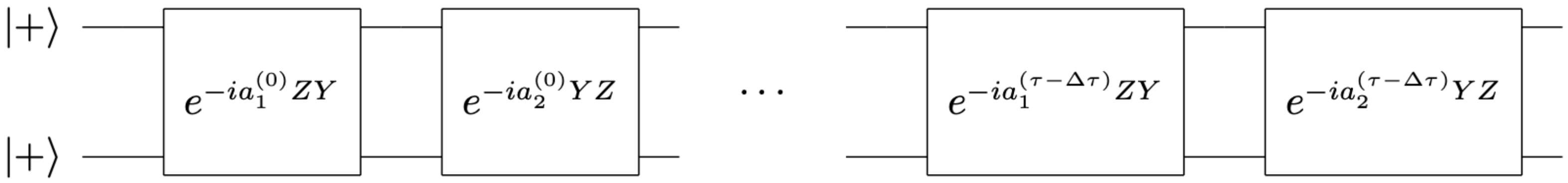
Imaginary time

$$\frac{e^{-\delta\tau Z_i Z_j}|++\rangle}{\sqrt{\langle\psi|e^{-2\delta\tau Z_i Z_j}|\psi\rangle}} = e^{-i\delta\tau_1 Z_i Y_j} e^{-i\delta\tau_2 Y_i Z_j}|++\rangle$$

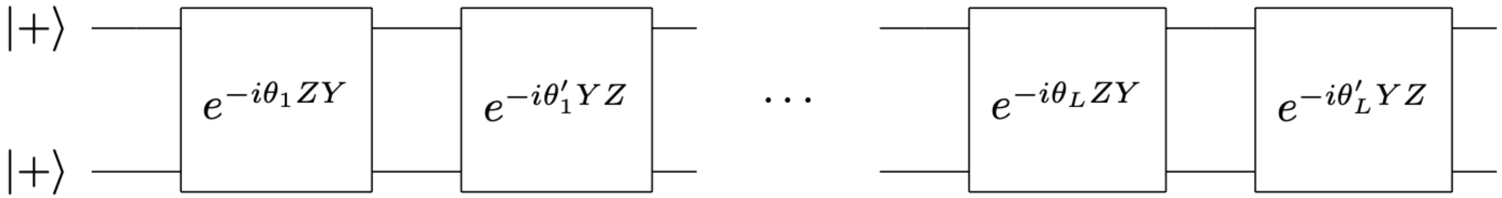
Real time

- Parametrization of the exact circuit:

Original:



Parameterized:



L: number of circuit layer

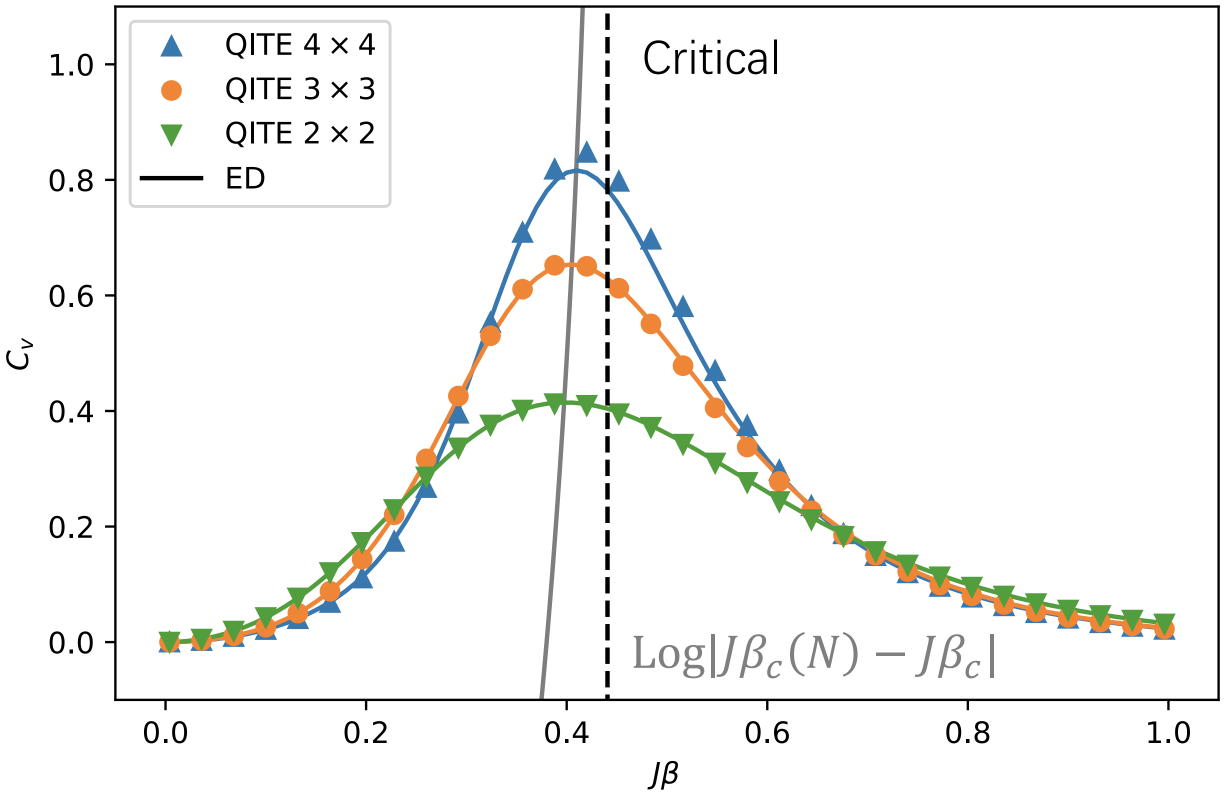
The ansatz is exact as $L \to \infty$! (similar to QAOA ansatz)

Results-Specific heat

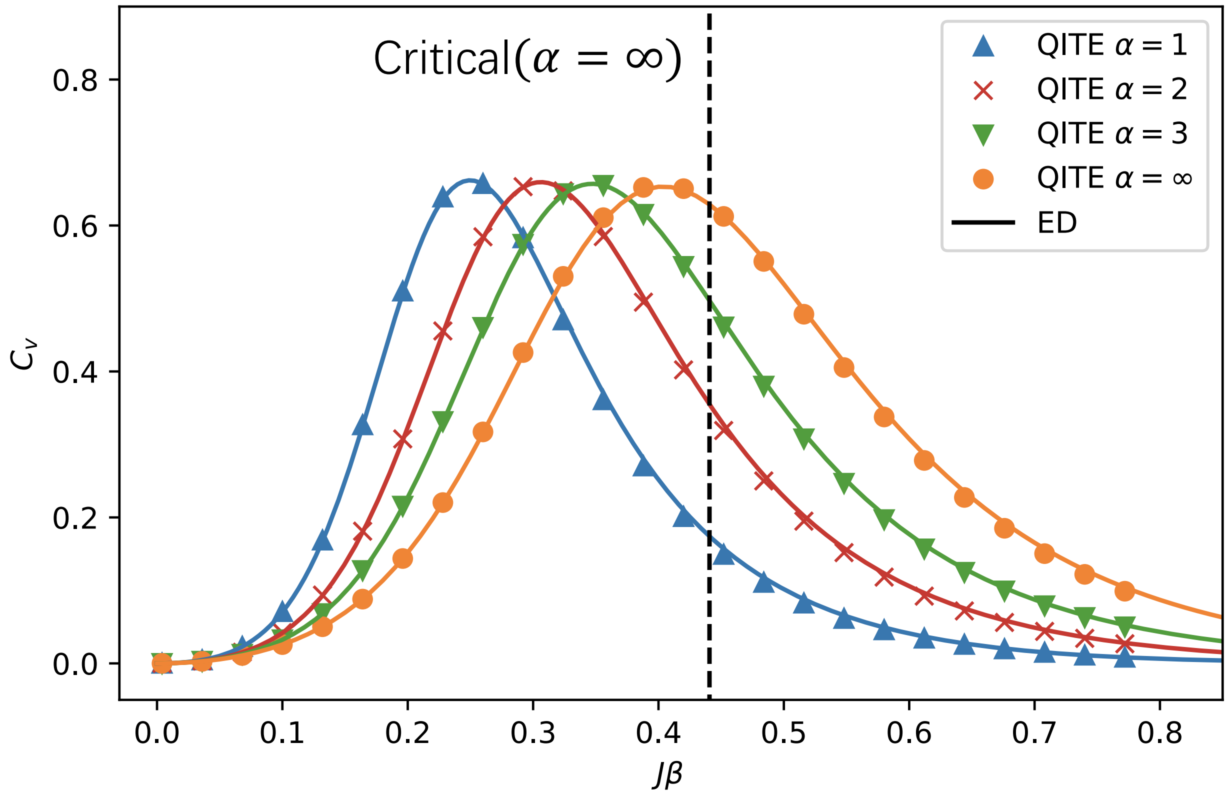
$$\langle O \rangle_{J\beta} = \frac{\mathrm{Tr}(Oe^{-\beta H(J)})}{Z}$$

$$C_v = \frac{1}{|\Lambda|T^2}(\langle H^2 \rangle - \langle H \rangle^2)$$

Dimension = 2, $\alpha = \infty$(Nearest neighbor)



Dimension = 2, $|\Lambda| = 3\times 3$



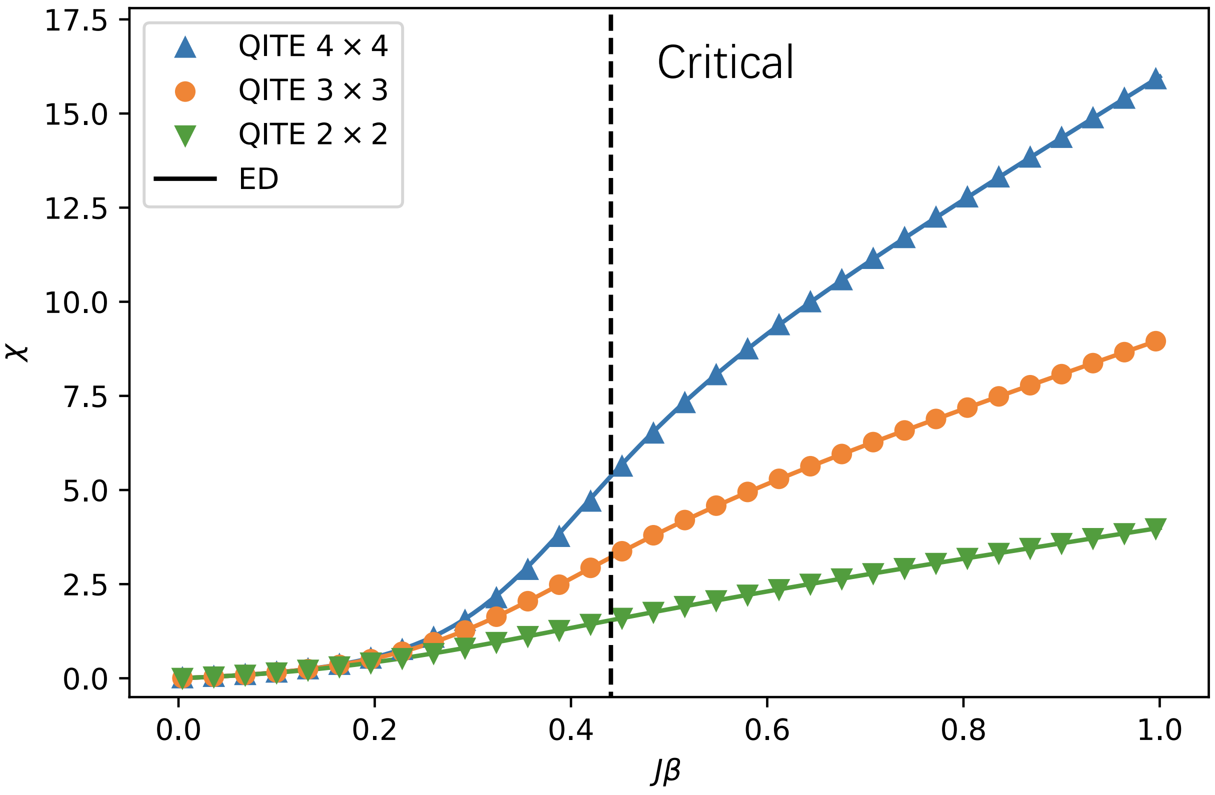
(based on quantum simulator [Qiskit])

Results-Susceptibility

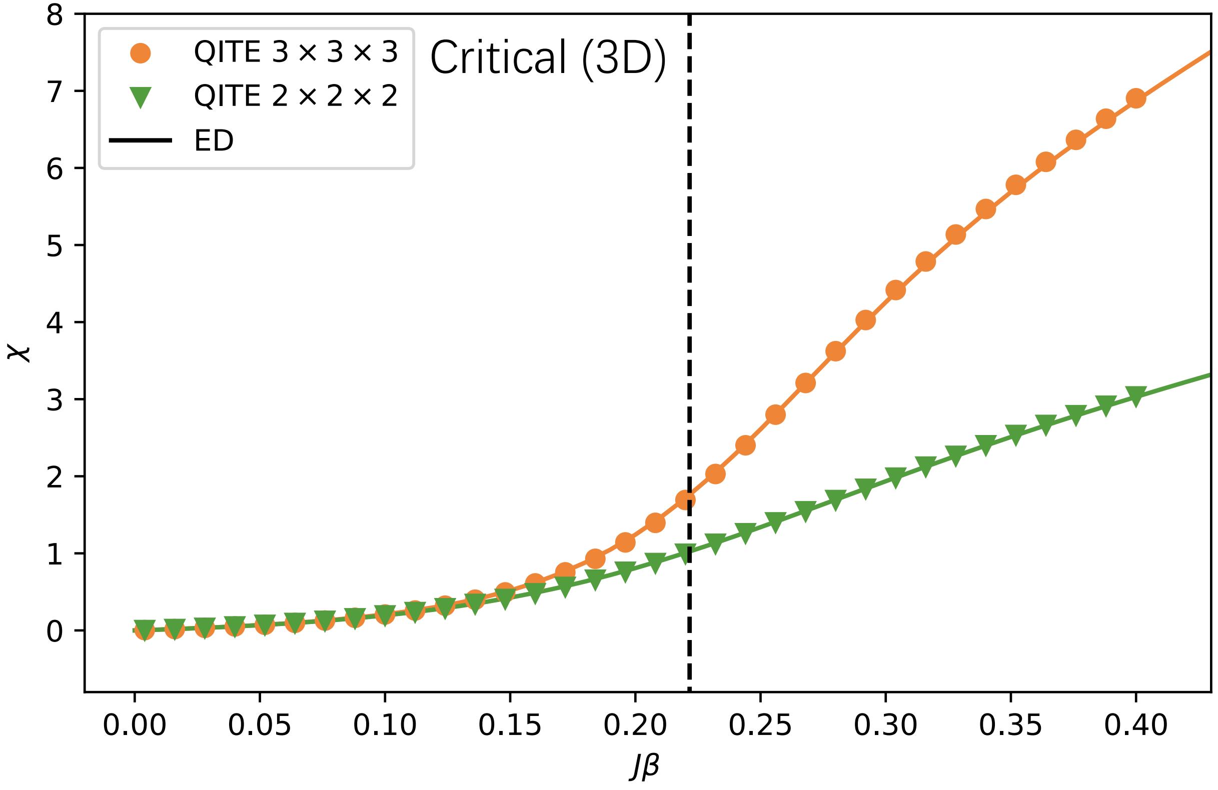
$$\langle O \rangle_{J\beta} = \frac{\mathrm{Tr}(O e^{-\beta H(J)})}{Z}$$

$$\chi = \frac{1}{|\Lambda| T}(\langle Z_{tot}^2 \rangle - \langle Z_{tot} \rangle^2), \quad Z_{tot} = \sum_{i \in \Lambda} Z_i$$

Dimension = 2, $\alpha = \infty$(Nearest neighbor)



Dimension = 3, $\alpha = \infty$(Nearest neighbor)



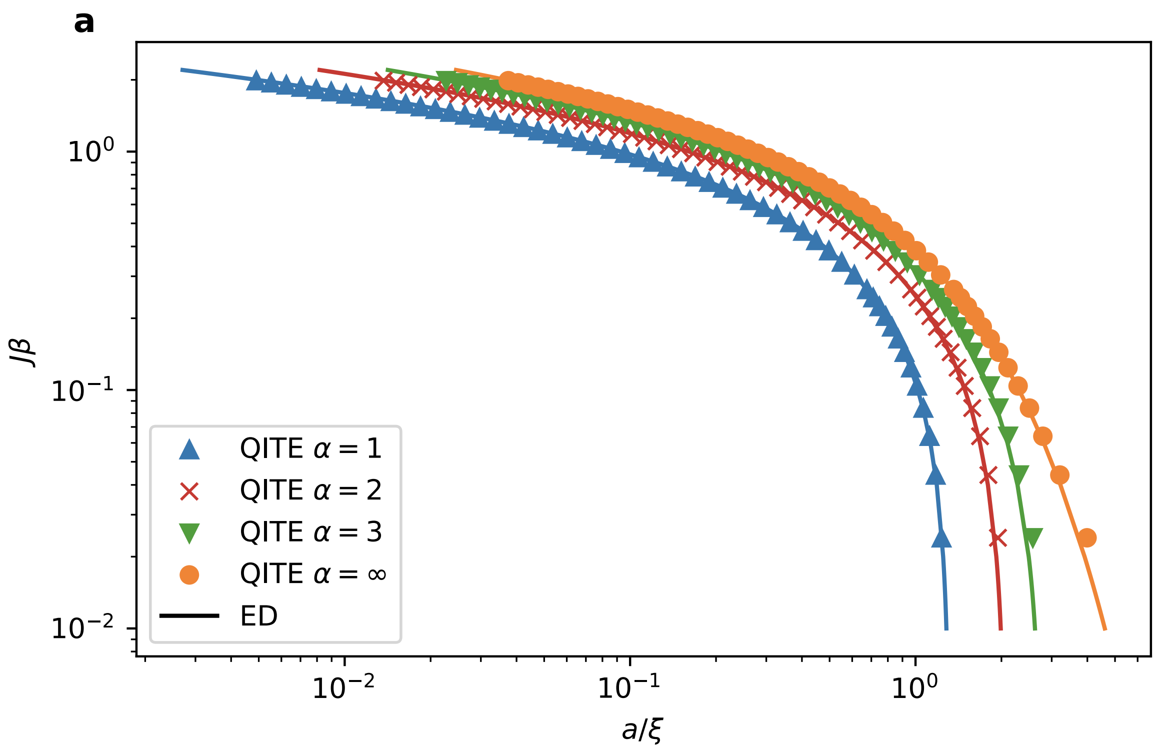
(based on quantum simulator [Qiskit])

Results-Running coupling

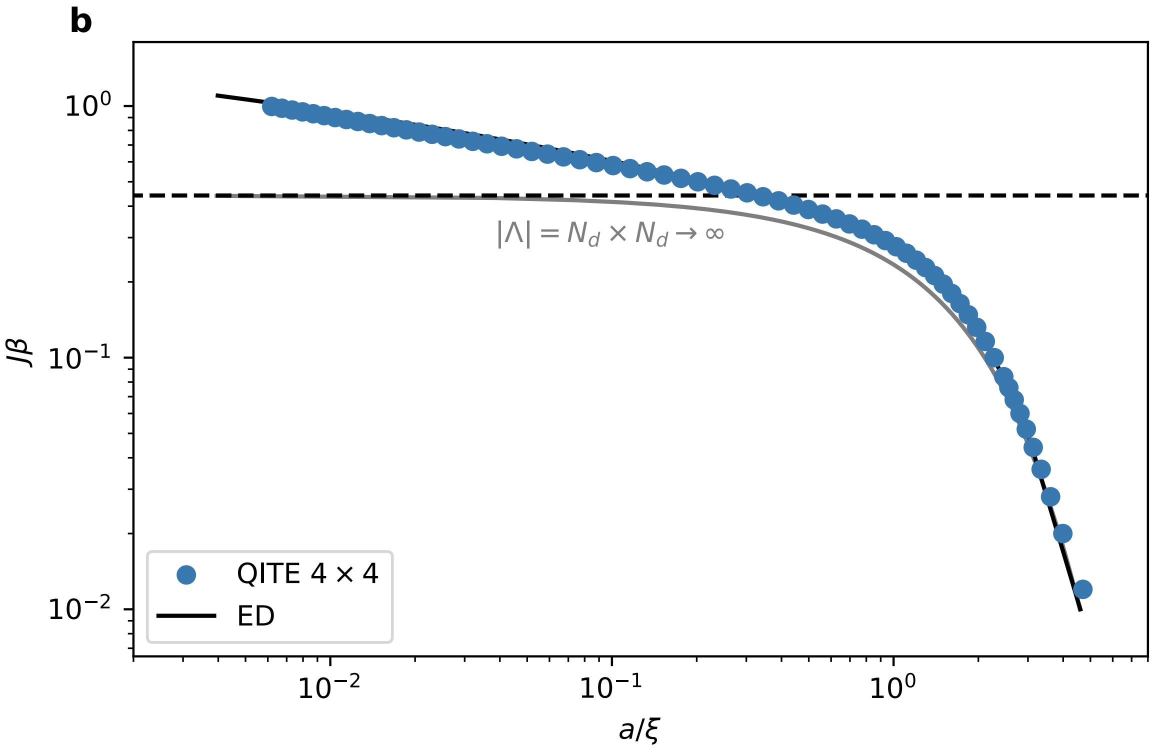
$$\langle O \rangle_{J\beta} = \frac{\mathrm{Tr}(O e^{-\beta H(J)})}{Z}$$

$$\langle Z_i Z_j \rangle_{J\beta} \sim e^{|i-j| a(J)/\xi}$$

Dimension = 1 , $|\Lambda| = 4$



Dimension = 2, $\alpha = \infty$(Nearest neighbor)



(based on quantum simulator [Qiskit])

总结

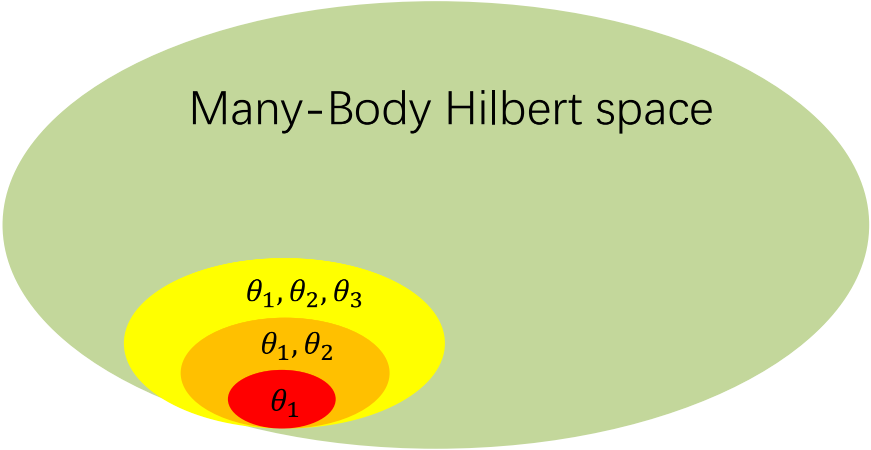
- 基于变分的量子虚时演化可以很好地生成各个温度下的Gibbs态，为Critical slowdown提供了可能的解决思路。

- 可以推广到含有横场的量子Ising模型， $\lambda\phi^4$ 模型， Q-state Potts模型等等。

$\lambda\phi^4$:

$$H = \sum_{x}\left\{-2\kappa\sum_{\mu}\phi_x\phi_{x+\mu} + \phi_x^2 + \lambda(\phi_x^2 - 1)^2\right\}, \quad \phi_x \in (-\infty, +\infty)$$

Backup: Error Analysis



systematics

- Finite expressivity of variational quantum circuit
- Numerical integration

In noiseless quantum simulator

- Coherent and incoherent noise from quantum circuit

statistics

- Finite shots noise $\sim O(\frac{1}{\sqrt{N}})$

Backup: Error Analysis

- Finite expressivity of variational quantum circuit
- Numerical integration

In noiseless quantum simulator

Solved by Runge-Kutta method

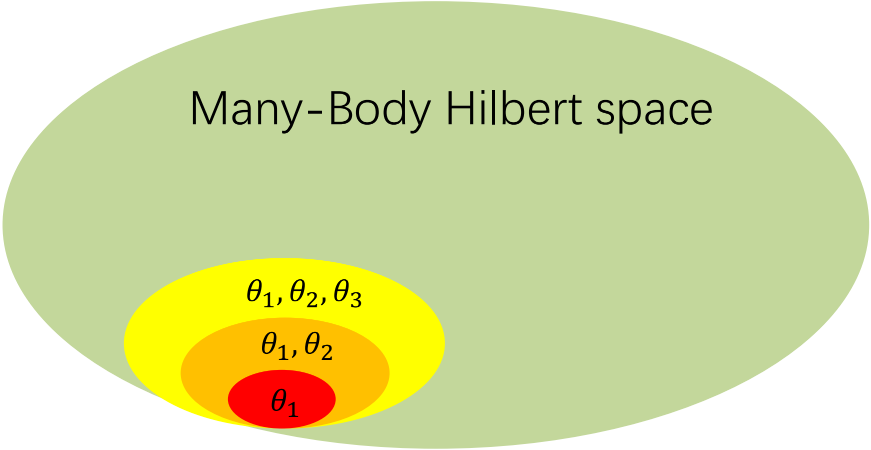
$$\theta(\tau+\Delta\tau)=\theta(\tau)+\dot{\theta}(\tau)\times\Delta\tau=\theta(\tau)+A^{-1}C\times\Delta\tau$$

Euler : $\mathrm{Error}\sim O(\Delta\tau^2)$

Runge-Kutta : $\mathrm{Error}\sim O(\Delta\tau^5)$

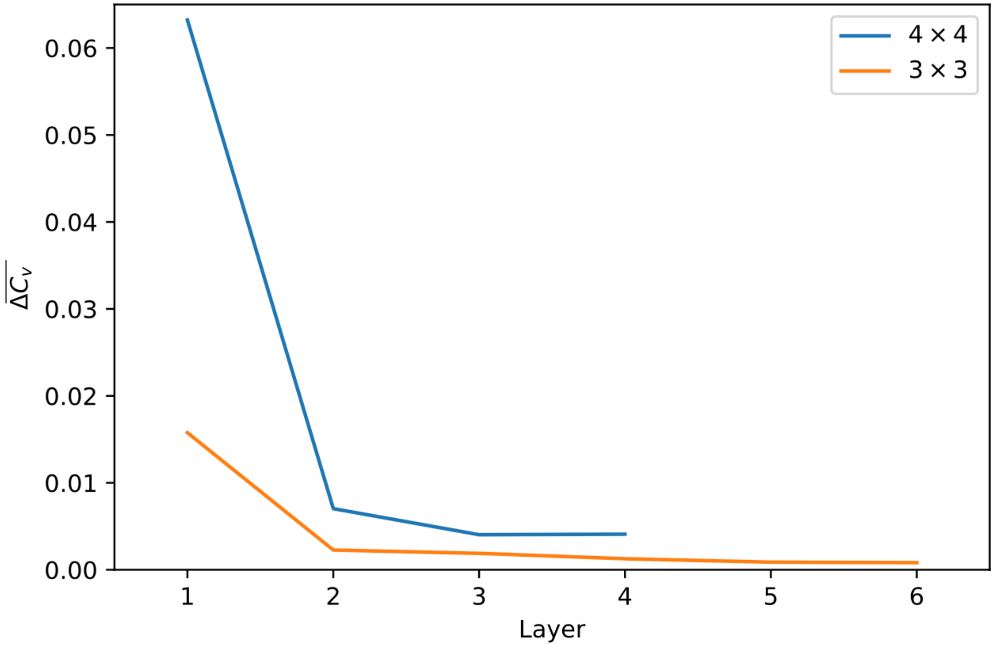
$\Delta\tau\sim10^{-3}$, $\mathrm{Error}\sim10^{-15}$

Backup: Error Analysis



- Finite expressivity of variational quantum circuit

In noiseless quantum simulator



Error reduced with deeper quantum circuit

$$\overline{\Delta C_v} = \int_0^1 |C_v - C_v^{ED}| \, \mathrm{d}\beta$$