

# Quantum Metropolis Sampling via Weak Measurement

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Arxiv:2406.16023

# Quantum Gibbs Sampling

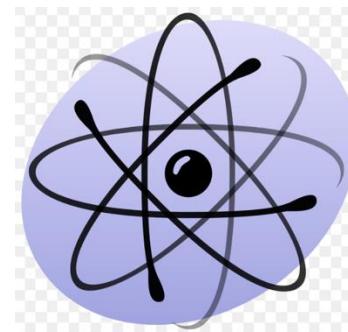
Local Hamiltonian:

$$H = H_1 + \dots + H_m \quad \text{Inverse temperature } \beta = 1/T$$

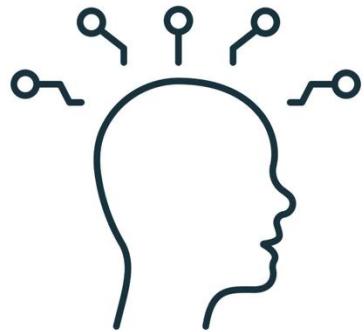


**Goal:** Given  $(H, \beta)$ , prepare Gibbs states  $e^{-\beta H} / \text{tr}(e^{-\beta H})$

❖ Distribution over eigenstates



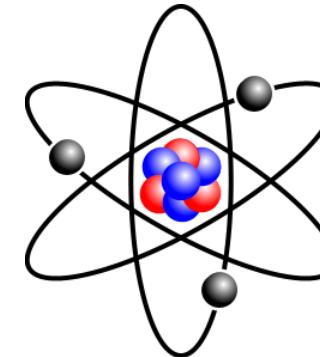
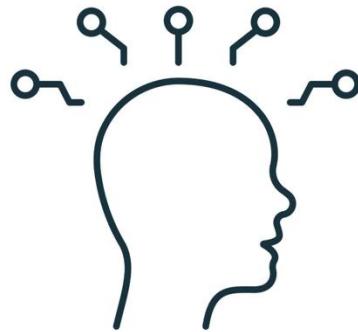
# Application of Quantum Gibbs Sampling



$$\rho_\beta := e^{-\beta H} / \text{tr}(e^{-\beta H})$$

**Quantum Boltzmann Machine**

# Application of Quantum Gibbs Sampling

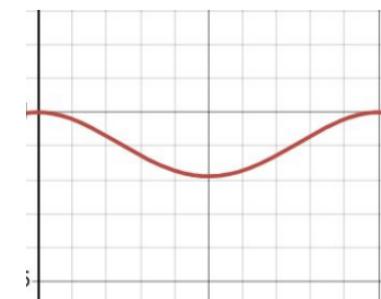


**Quantum Chemistry**  
2D Hubbard model

$$\rho_\beta := e^{-\beta H} / \text{tr}(e^{-\beta H})$$

## Quantum Boltzmann Machine

- compute the gradient  $\text{tr}(H\rho_\beta)$
- Sampling task



**Optimization**  
Simulated annealing

# Quantum Gibbs sampling

**Goal:** given  $(H, \beta)$ , prepare Gibbs states

$$\frac{\exp(-\beta H)}{\text{tr}(\exp(-\beta H))}$$

Today's focus



**Correctness**

Converge in **finite** time



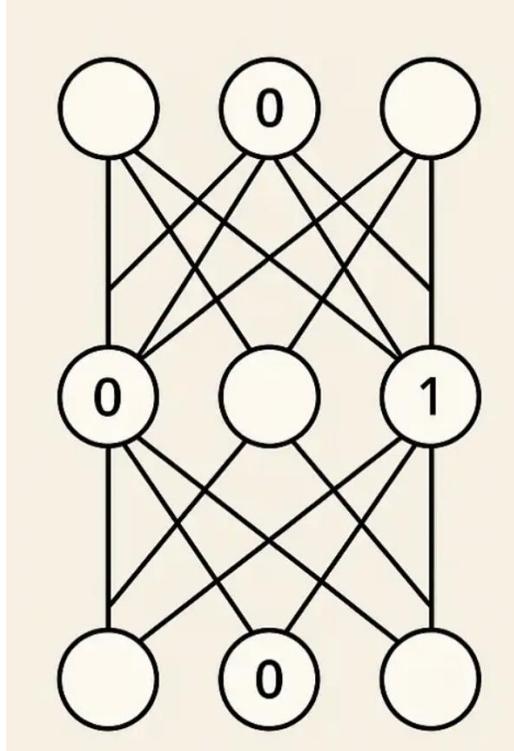
**Efficiency**

Converge in **poly(n)** time

# Outline

- Classical Metropolis Algorithm
- Quantum Metropolis Algorithm & Challenge
- Our algorithm
- Comparison Previous work

# Classical Gibbs sampling



Classical Boltzmann machine

$$H = \sum_{\langle i,j \rangle \in G} w_{ij} Z_i Z_j$$

Goal: Generate the Gibbs state (distribution)

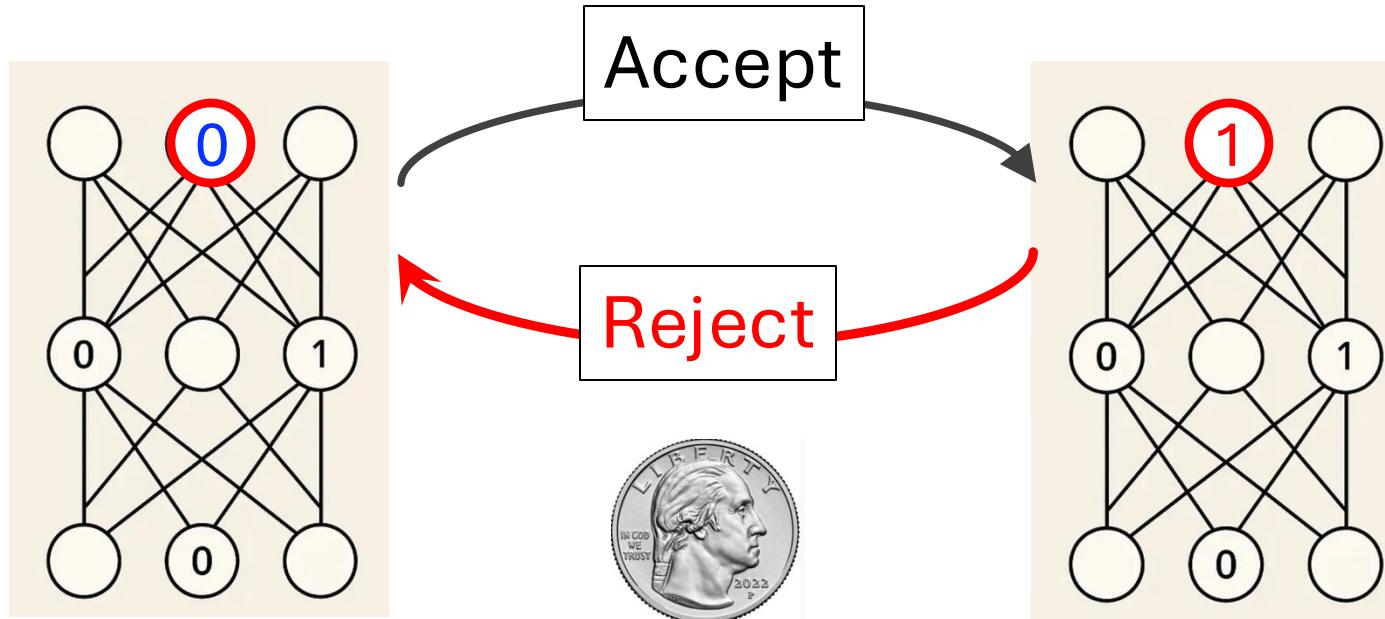
$$01011 \sim \exp(-H(01011))$$

Classical Metropolis Algorithm 1953

Markov chain → Gibbs distribution

# Classical Metropolis Algorithm 1953

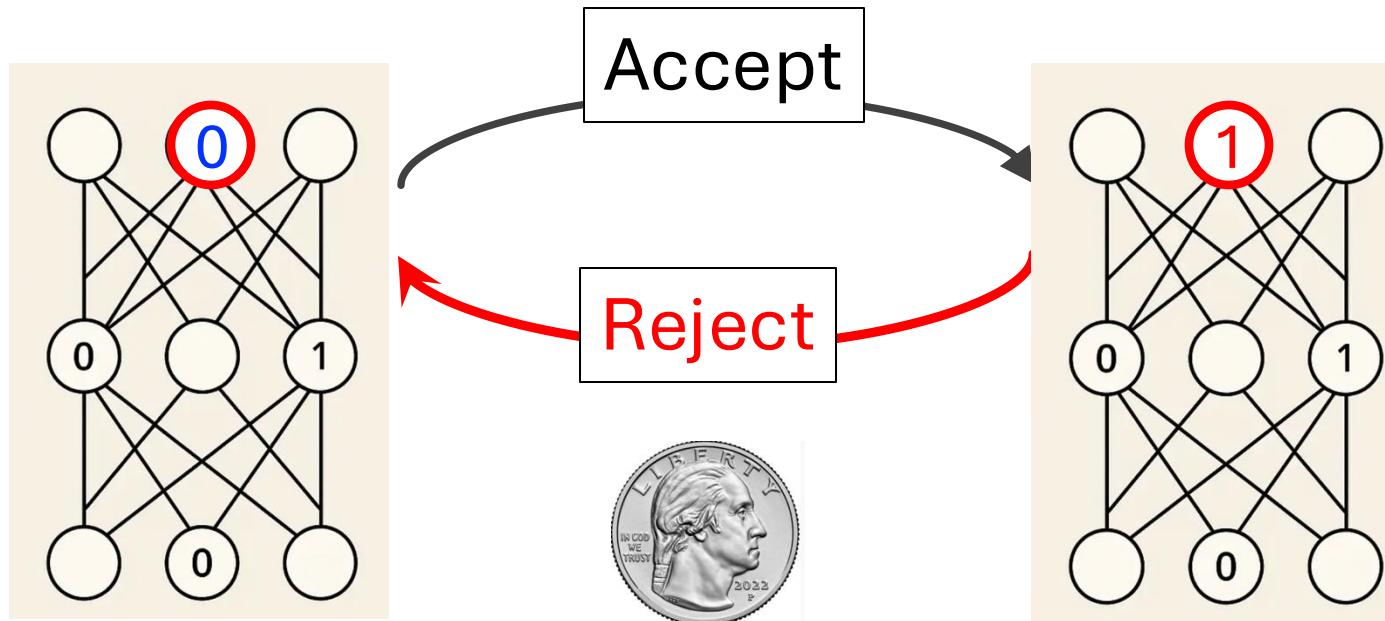
Markov chain → Gibbs distribution



- 1) Choose a random vertex and flip it
- 2) Flip a coin and choose **Accept/Reject**

# Classical Metropolis Algorithm 1953

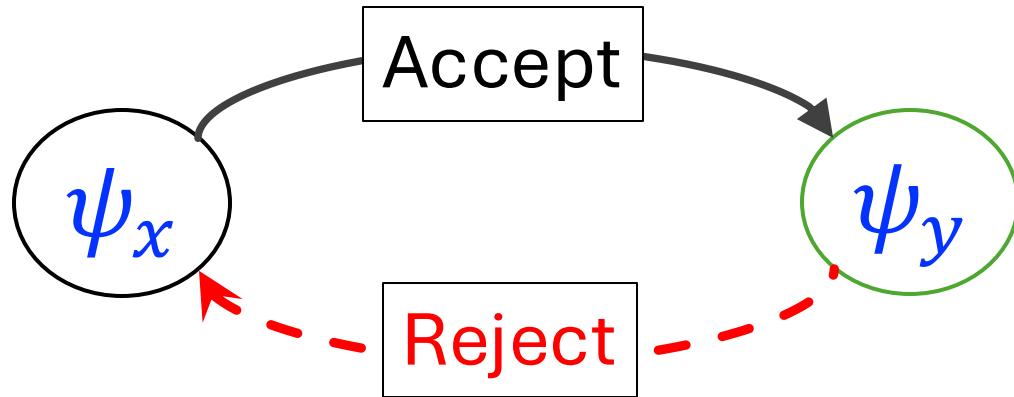
Markov chain → Gibbs distribution



- 1) Choose a random vertex and flip it
- 2) Flip a coin and choose **Accept/Reject**

$$P(\text{head}) = \min \{1, \exp(-\beta \Delta_H)\}$$

# Quantum Metropolis: challenges

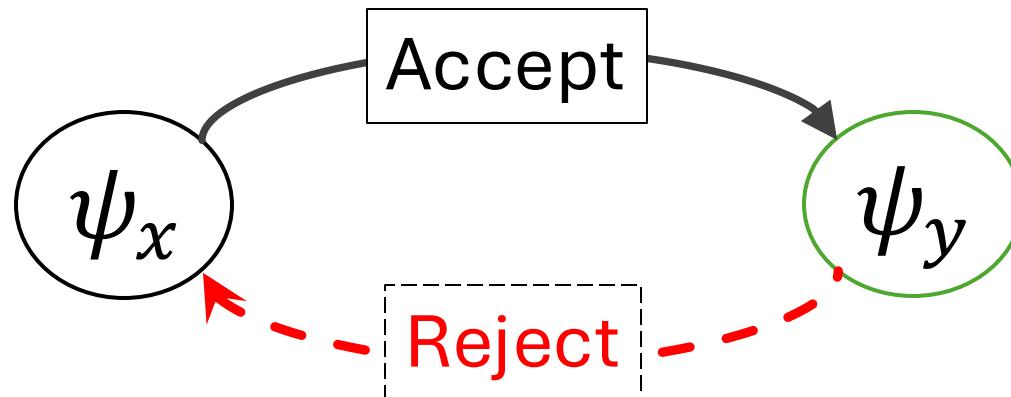


- **Challenge:** Quantum state is **unclonable**
- **Revert** quantum state **after measurement?**

**Ideas:** **Weak measurement** is easier to revert!  
**Alternate Accept**

# Our ideas to revert measurement

- 1) Weak measurement
- 2) Alternate Accept



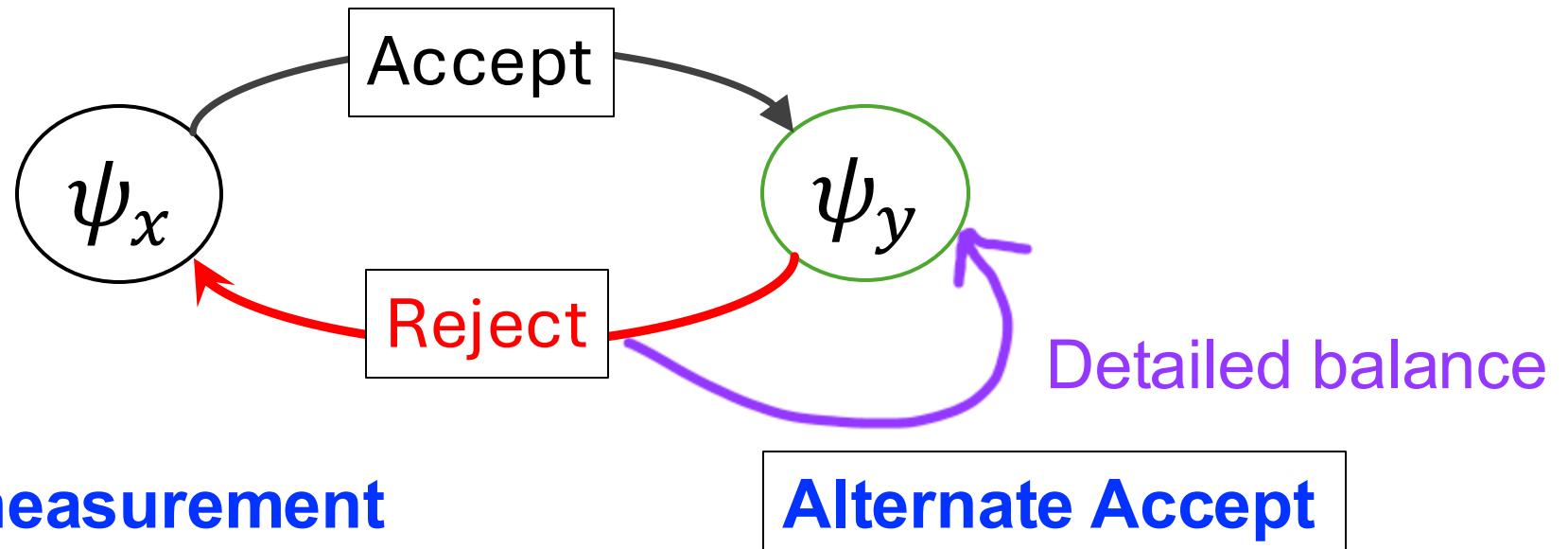
## Weak measurement



$$\tau = 1/poly$$

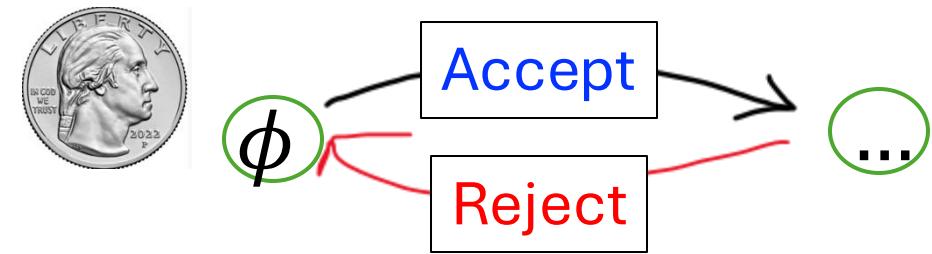
# Our ideas to revert measurement

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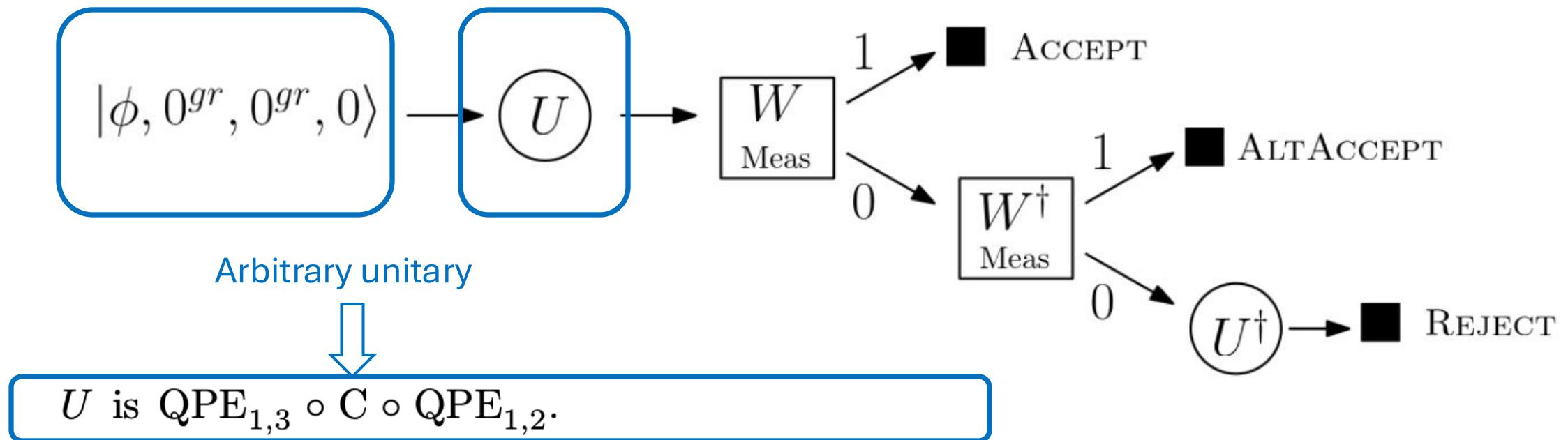


$$\tau = 1/\text{poly}$$

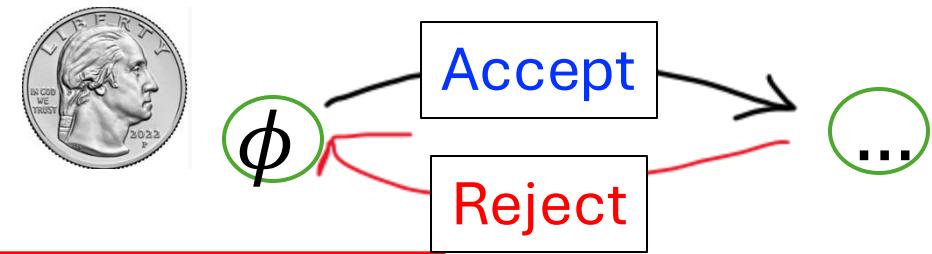
# Our algorithm in details



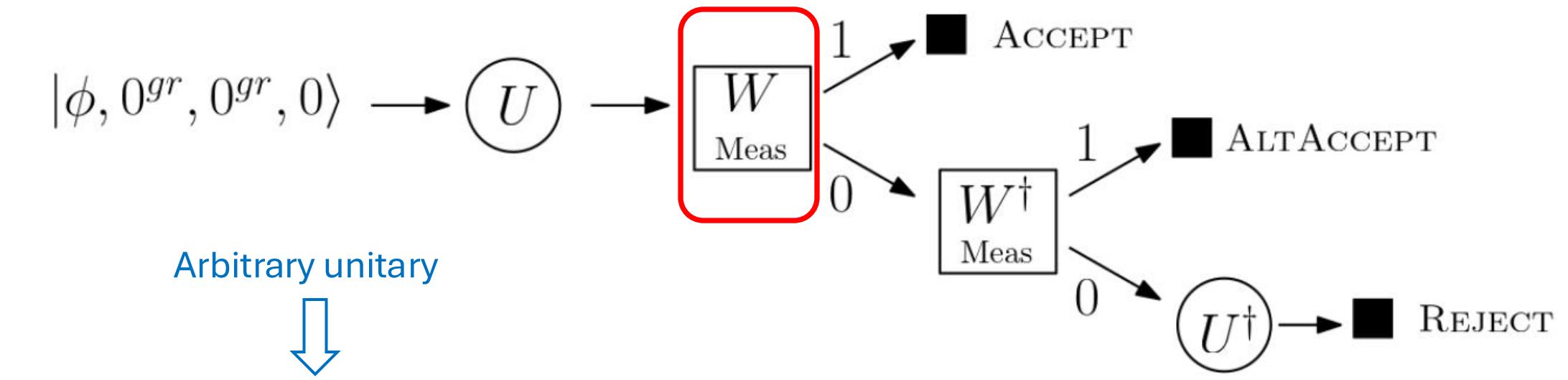
Do something random, then reject with some probability.



# Our algorithm in details



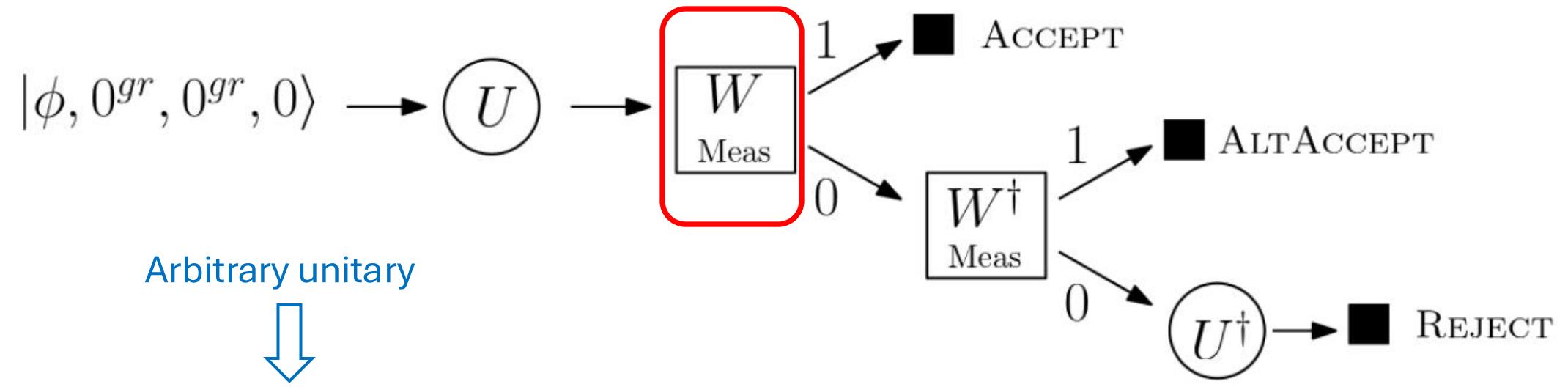
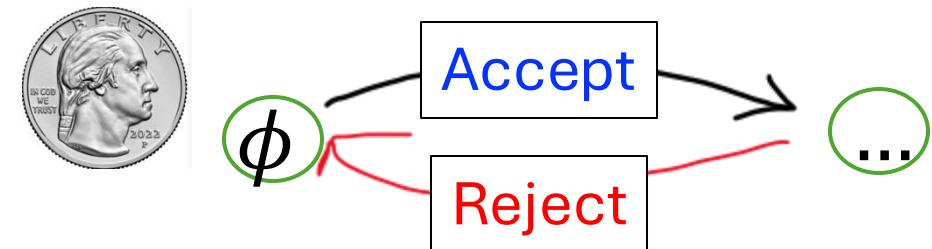
Do something random, then reject with some probability.



$$W |EE'\rangle |0\rangle = |EE'\rangle \left( \sqrt{1 - \tau^2 f_{EE'}} |0\rangle + \tau \sqrt{f_{EE'}} |1\rangle \right)$$

Weak Measurement

# Our algorithm in details

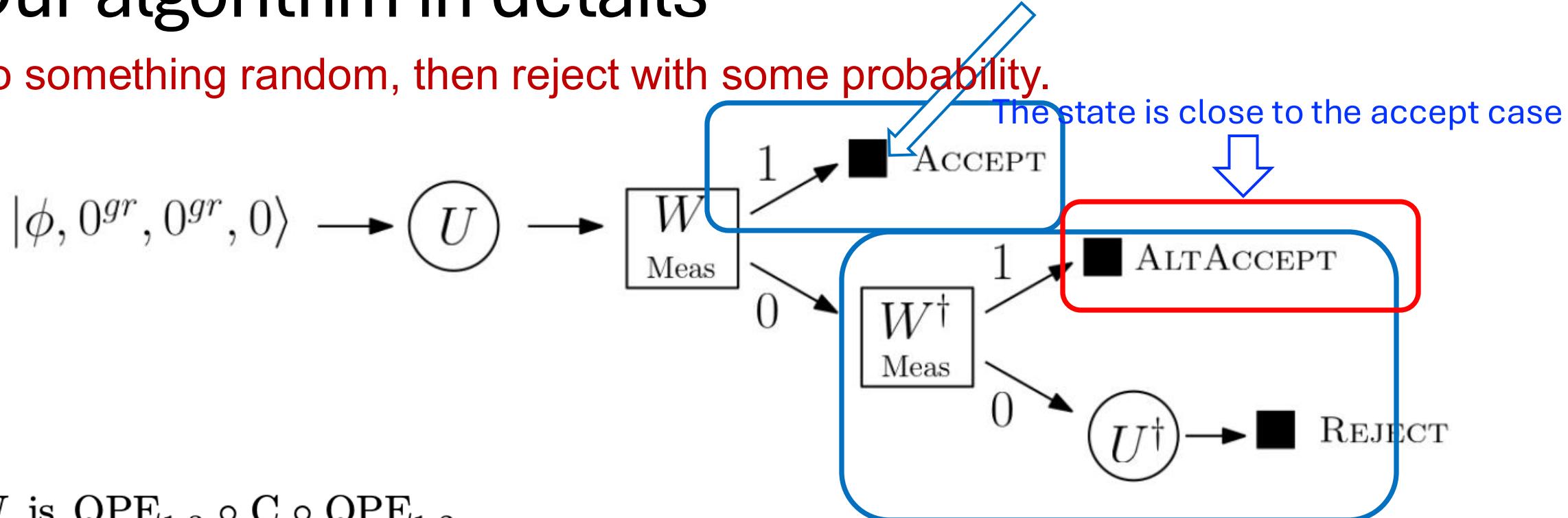


$$W |EE'\rangle |0\rangle = |EE'\rangle \left( \sqrt{1 - \tau^2 f_{EE'}} |0\rangle + \tau \sqrt{f_{EE'}} |1\rangle \right)$$

$$W := \sum_{E, E' \in S(r)^{\otimes g}} |EE'\rangle \langle EE'| \otimes \begin{bmatrix} \sqrt{1 - \tau^2 f_{EE'}} & \tau \sqrt{f_{EE'}} \\ \tau \sqrt{f_{EE'}} & -\sqrt{1 - \tau^2 f_{EE'}} \end{bmatrix}.$$

# Our algorithm in details

Do something random, then reject with some probability.



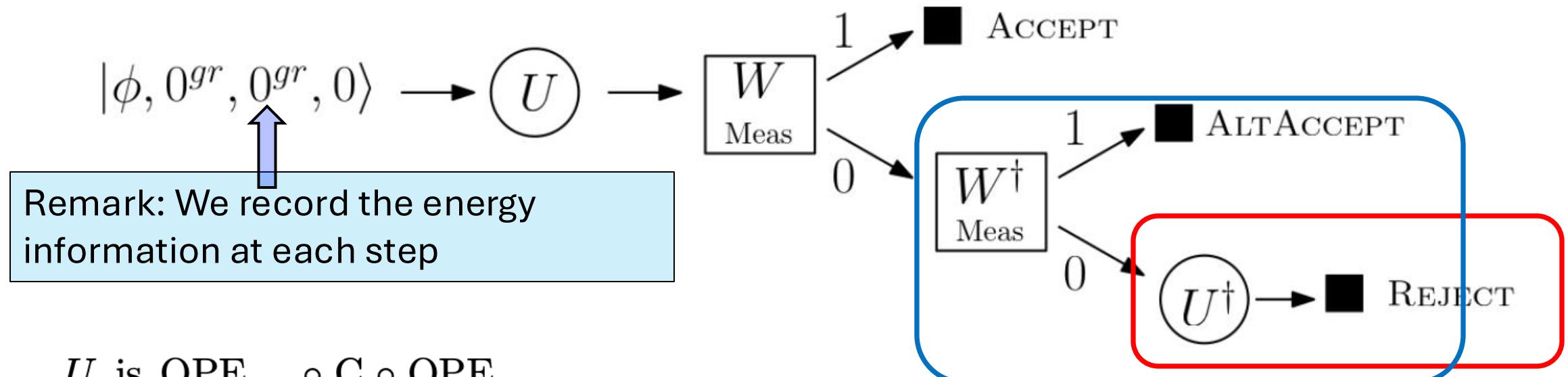
$U$  is  $\text{QPE}_{1,3} \circ \text{C} \circ \text{QPE}_{1,2}$ .

$$W |EE'\rangle |0\rangle = |EE'\rangle \left( \sqrt{1 - \tau^2 f_{EE'}} |0\rangle + \tau \sqrt{f_{EE'}} |1\rangle \right)$$

Try rewinding  
by performing inverse operations

# Our algorithm in details

Do something random, then reject with some probability.



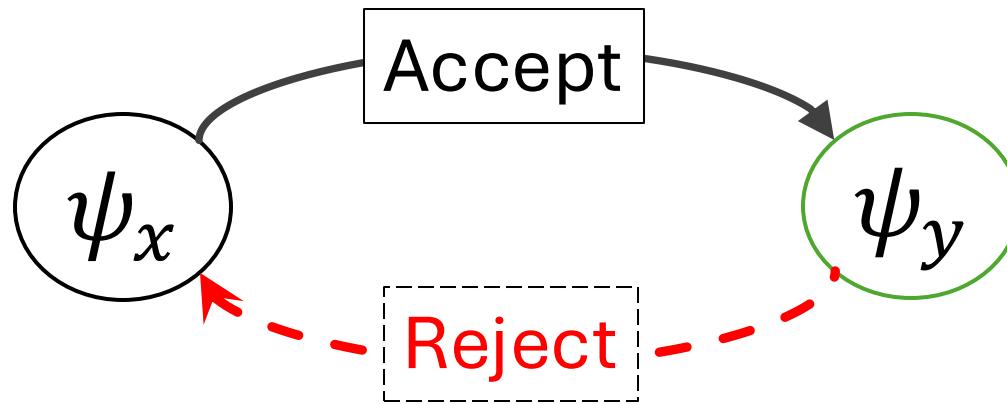
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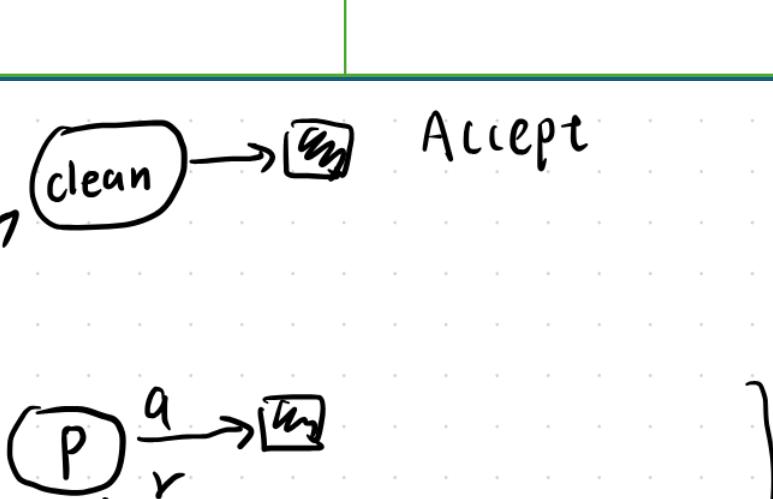
Try rewinding  
by performing inverse operations

# Comparison to existing work

- Revert quantum state **after measurement?**



# Comparison to existing work

[TOV+11]	Marriot-Watrous rewinding	Metropolis-type, errors in proof
 <p>measure 2,3,4</p> <p>user 12, trace out 34</p>	<p>Accept</p>	<p>Boosted + Shift-invariant QPE does not exist. [CKBG23]</p>

# Comparison to existing work

[TOV+11]	Marriot-Watrous rewinding	Metropolis-type, errors in proof
[CKBG23,DLL24]	Davies generator + Operator Fourier transform	provably-correct, differ from Metropolis

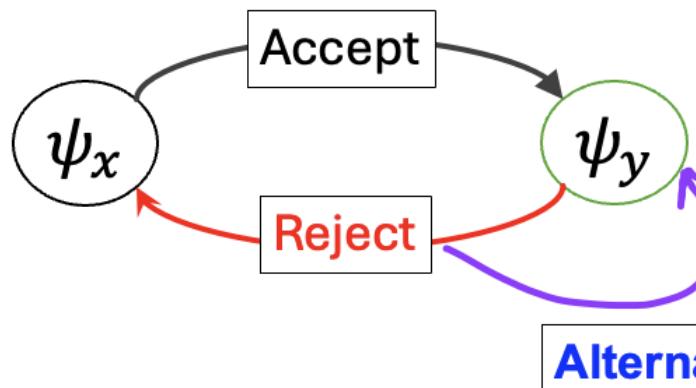
$$\mathcal{L}_\beta[\cdot] := \underbrace{-i[\mathbf{B}, \cdot]}_{\text{"coherent"}} + \sum_{a \in A} \int_{-\infty}^{\infty} \gamma(\omega) \left( \underbrace{\hat{\mathbf{A}}^a(\omega)(\cdot)\hat{\mathbf{A}}^a(\omega)^\dagger}_{\text{"transition"}} - \underbrace{\frac{1}{2}\{\hat{\mathbf{A}}^a(\omega)^\dagger \hat{\mathbf{A}}^a(\omega), \cdot\}}_{\text{"decay"}} \right) d\omega$$

$$\hat{\mathbf{A}}^a(\omega) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\mathbf{H}t} \mathbf{A}^a e^{-i\mathbf{H}t} e^{-i\omega t} f(t) dt$$

$$\gamma(\omega) = \exp\left(-\frac{(\omega + \omega_\gamma)^2}{2\sigma_\gamma^2}\right)$$

# Comparison to existing work

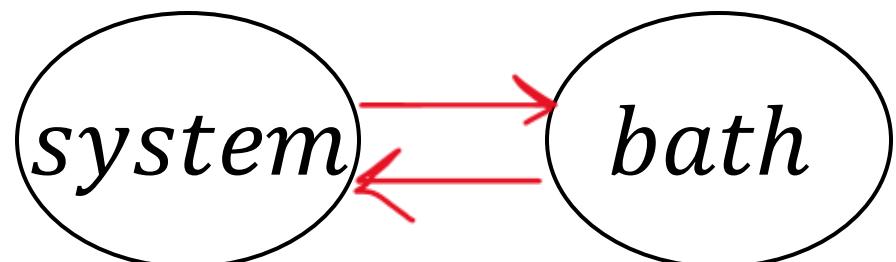
[TOV+11]	Marriot-Watrous rewinding	Metropolis-type, errors in proof
[CKBG23,DLL24]	Davies generator + Operator Fourier transform	provably-correct, differ from Metropolis
Our work [JI24]	<b>Weak measurement + Alternate accept</b>	<b>conceptually-simple</b> and provably correct



Make it easier to **generalize classical techniques to quantum** Gibbs sampling

# Comparison to existing work

[TOV+11]	Marriot-Watrous rewinding	Metropolis-type, errors in proof
[CKBG23,DLL24]	Davies generator + Operator Fourier transform	provably-correct, differ from Metropolis
Our work [JI24]	<b>Weak measurement + Alternate accept</b>	<b>conceptually-simple</b> and <b>provably correct</b>
[DZPL25,HW25,HP B25, LA25... ]	... System bath interactions...	conceptually simple and provably correct



$$H_\alpha(t) = H + H_E + \alpha f(t) \left( A_S \otimes B_E + A_S^\dagger \otimes B_E^\dagger \right).$$

# In summary....

**Most existing work**



**Correctness**

Converge in **finite** time

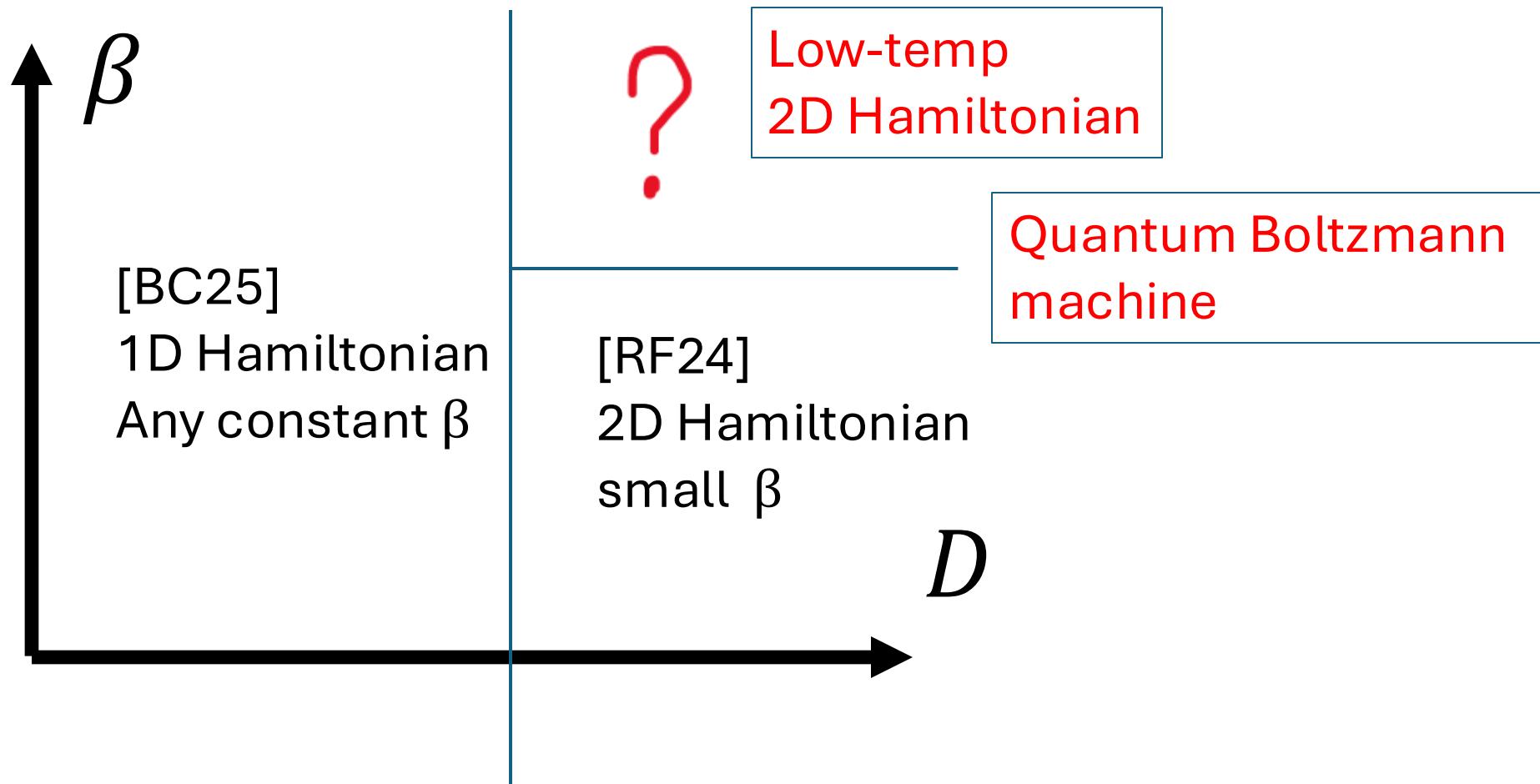
**Future direction**



**Efficiency**

Converge in **poly(n)** time

# Q1: When quantum Gibbs sampling\* is efficient?



## Q2: When estimating $\text{tr}(O\rho_\beta)$ is efficient?

- [?] Design an algorithm that requiring  $\text{tr}(O\rho_t) \rightarrow \text{tr}(O\rho_\beta)$   
might be much easier than requiring  $\rho_t \rightarrow \rho_\beta$

# Q2: When estimating $\text{tr}(O\rho_\beta)$ is efficient?

- [?] Design an algorithm that requiring  $\text{tr}(O\rho_t) \rightarrow \text{tr}(O\rho_\beta)$  might be much easier than requiring  $\rho_t \rightarrow \rho_\beta$
- Get effective independent sample of  $\rho_\beta$  with a time smaller than  $t_{mix}$  [incoming work, IPAM workshop at UCLA, 2026.1.12-202.1.16]

**New Frontiers in Quantum Algorithms for Open Quantum Systems**

[JI24] might make it easier to **generalize classical techniques to quantum** Gibbs sampling

**Thanks for listening. Questions ?**

# Appendix