Quantum Algorithms for Testing Hamiltonian Symmetry

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Joint work with Margarite LaBorde and available as arXiv:2203.10017

Mathematical Results in Quantum Theory

University of California Davis

First time visiting Davis, CA!

- View from my hotel window at Residence Inn:

- Still safe to live here? California Gold rush ended a long time ago…

Motivation

- Noether's theorem elucidates the fundamental role of symmetry in physics, in which every continuous symmetry of a physical system corresponds to a conservation law
- Goal: Use quantum computers to test symmetries of Hamiltonians
- In general, this task is computationally difficult for classical computers

Recently accepted for PRL

From: prl@aps.org <prl@aps.org>

Sent: Monday, September 12, 2022 9:45:45 AM

To: mlabo15@lsu.edu <mlabo15@lsu.edu>

Subject: Acceptance [redacted] LaBorde

Re: [redacted]

Quantum algorithms for testing Hamiltonian symmetry
by Margarite L. LaBorde and Mark M. Wilde

Dear Mrs. LaBorde,

We are pleased to inform you that your manuscript has been accepted for publication as a Letter in Physical Review Letters.

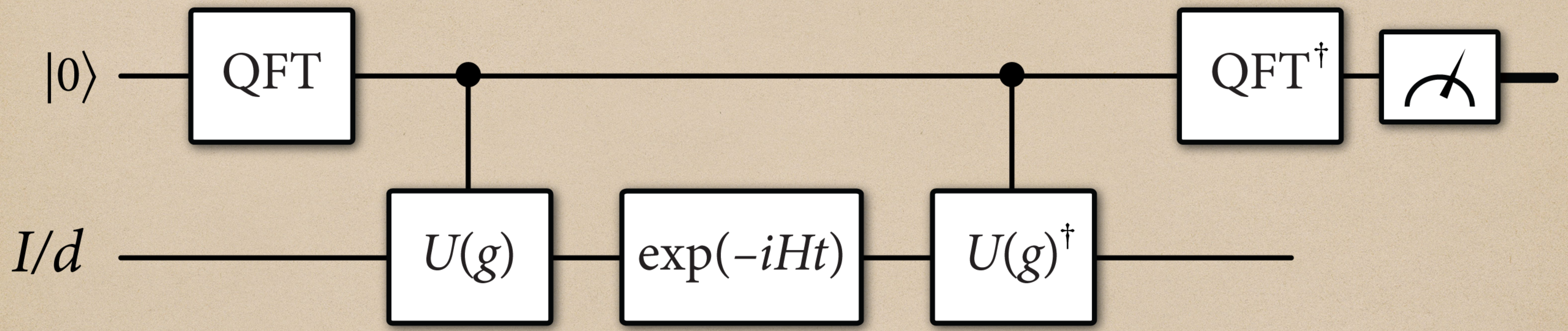
Hamiltonian Symmetry

- Let $\{U(g)\}_{g\in G}$ denote a unitary representation of a finite group G
- A Hamiltonian H is G-symmetric if $[U(g), H] = 0$ for all $g \in G$
- Can measure approximate symmetry via the commutator norm
$$\frac{1}{|G|}\sum_{g\in G} \left\| [U(g), H] \right\|_2^2, \text{ where } \|A\|_2 \equiv \sqrt{\mathrm{Tr}[A^\dagger A]}$$

Assumptions for Algorithm

- Assumption: $\exists$ efficient circuit implementing $U(g)$ for all $g \in G$
- Can take advantage of group structure in some cases to efficiently implement controlled-$U(g)$ circuit
- Hamiltonian is either k-local or described by a sparse matrix (such that efficient Hamiltonian simulation is possible)

Efficient Algorithm for Hamiltonian Symmetry Testing



- Initialize control qubits to all zeros state $|0\rangle$ and system qubits to maximally mixed state I/d
- Apply quantum Fourier transform (QFT) to control qubits
- Apply controlled unitaries and Hamiltonian simulation $\exp(-iHt)$
- Apply inverse QFT to control qubits, measure them, and accept iff the all zeros outcome occurs

Acceptance probability

- Acceptance probability $= \frac{1}{d|G|} \sum_{g \in G} \mathrm{Tr}\left[U(g)^\dagger e^{iHt} U(g) e^{-iHt}\right]$

$$= 1 - \frac{t^2}{2d|G|} \sum_{g \in G} \| [U(g), H] \|_2^2 + O(t^4)$$

- Algorithm thus accepts with certainty if and only if H is G-symmetric
- Also: It accepts approximately iff H is approximately G-symmetric

Steps of the algorithm

- Initial state: $|0\rangle_C |\psi\rangle_S$ (suppose for now system S prepared as $|\psi\rangle$)
- After first QFT: $|+\rangle_C |\psi\rangle_S$ where $|+\rangle_C \equiv |G|^{-\frac{1}{2}} \sum_{g \in G} |g\rangle_C$
- After controlled gates and Hamiltonian simulation: $|G|^{-\frac{1}{2}} \sum_{g \in G} |g\rangle_C U(g)^\dagger e^{-iHt} U(g) |\psi\rangle_S$
- Acceptance probability: $\left\| (\langle + |_C \otimes I_S) |G|^{-\frac{1}{2}} \sum_{g \in G} |g\rangle_C U(g)^\dagger e^{-iHt} U(g) |\psi\rangle_S \right\|_2^2$

Simplification of acceptance probability

$$\left\| (\langle + |_C \otimes I_S) |G|^{-\frac{1}{2}} \sum_{g \in G} |g\rangle_C U(g)^\dagger e^{-iHt} U(g) |\psi\rangle_S \right\|_2^2$$

$$= \left\| \, |G|^{-1} \sum_{g \in G} U(g)^\dagger e^{-iHt} U(g) |\psi\rangle_S \right\|_2^2$$

$$= |G|^{-2} \langle \psi | \sum_{g' \in G} U(g')^\dagger e^{iHt} U(g') \sum_{g \in G} U(g)^\dagger e^{-iHt} U(g) |\psi\rangle_S$$

$$= |G|^{-2} \sum_{g, g' \in G} \langle \psi | U(g')^\dagger e^{iHt} U(g') U(g)^\dagger e^{-iHt} U(g) |\psi\rangle_S$$

Simplification of acceptance probability (ctd.)

- When $|\psi\rangle$ is chosen uniformly at random, then previous expression becomes

$$\mathbb{E}_{\psi}\left[|G|^{-2} \sum_{g,g' \in G} \langle \psi | U(g')^{\dagger} e^{iHt} U(g') U(g)^{\dagger} e^{-iHt} U(g) | \psi \rangle_S \right]$$

$$= d^{-1} |G|^{-2} \sum_{g,g' \in G} \mathrm{Tr}\left[U(g')^{\dagger} e^{iHt} U(g') U(g)^{\dagger} e^{-iHt} U(g) \right]$$

$$= d^{-1} |G|^{-2} \sum_{g,g' \in G} \mathrm{Tr}\left[(U(g') U(g)^{\dagger})^{\dagger} e^{iHt} U(g') U(g)^{\dagger} e^{-iHt} \right]$$

$$= d^{-1} |G|^{-1} \sum_{g \in G} \mathrm{Tr}\left[U(g)^{\dagger} e^{iHt} U(g) e^{-iHt} \right]$$

Expansion of acceptance probability

Acceptance probability $\frac{1}{d|G|}\sum_{g\in G}\mathrm{Tr}\left[U(g)^\dagger e^{iHt}U(g)e^{-iHt}\right]$

is an even function of t

$\Rightarrow$ After expanding in t, odd powers in t vanish

Expansion of acceptance probability (ctd.)

- Can exploit Baker-Campbell-Hausdorff formula to find that

$$|G|^{-1}\sum_{g\in G}\mathrm{Tr}\left[U(g)^{\dagger}e^{iHt}U(g)e^{-iHt}\right] = |G|^{-1}\sum_{g\in G}\mathrm{Tr}\left[U^{\dagger}(g)\sum_{n=0}^{\infty}\frac{\left[(iHt)^{n},U(g)\right]}{n!}\right]$$

$$= |G|^{-1}\sum_{g\in G}\sum_{n=0}^{\infty}\frac{(-1)^{n}\,t^{2n}}{(2n!)}\left\|\,\left[(H)^{n},U(g)\right]\,\right\|_{2}^{2}$$

- where the nested commutator is defined as

$$[(X)^{n},Y]\equiv\underbrace{[X,\cdots[X,[X,Y]]\cdots]}_{n\text{ times}},\qquad [(X)^{0},Y]\equiv Y\,.$$

Expansion of acceptance probability (ctd.)

- Thus, it expands as

$$\frac{1}{d|G|}\sum_{g\in G}\mathrm{Tr}\left[U(g)^{\dagger}e^{iHt}U(g)e^{-iHt}\right]=\sum_{n=0}^{\infty}\frac{(-1)^{n}\,t^{2n}}{d|G|(2n!)}\sum_{g\in G}\left\|\left[(H)^{n},U(g)\right]\right\|_{2}^{2}$$

- Keeping the first two terms gives

$$\frac{1}{d|G|}\sum_{g\in G}\mathrm{Tr}\left[U(g)^{\dagger}e^{iHt}U(g)e^{-iHt}\right]=1-\frac{t^{2}}{2d|G|}\sum_{g\in G}\|\,[U(g),H]\,\|_{2}^{2}+O(t^{4})$$

- Expression for approximate symmetry appears in acceptance probability

Remark about continuous symmetries

- For finite-dimensional systems, we can also use these algorithms to test for continuous symmetries (where G is a continuous group)
- This follows because the acceptance probability can be written in terms of the twirl $\mathcal{T}_G(\cdot) \equiv |G|^{-1} \sum_{g \in G} U(g)^\dagger (\cdot) U(g)$, as

$$\frac{1}{d|G|} \sum_{g \in G} \mathrm{Tr}\left[U(g)^\dagger e^{iHt} U(g) e^{-iHt}\right] = \frac{1}{d} \mathrm{Tr}\left[\mathcal{T}_G(e^{iHt}) e^{-iHt}\right]$$

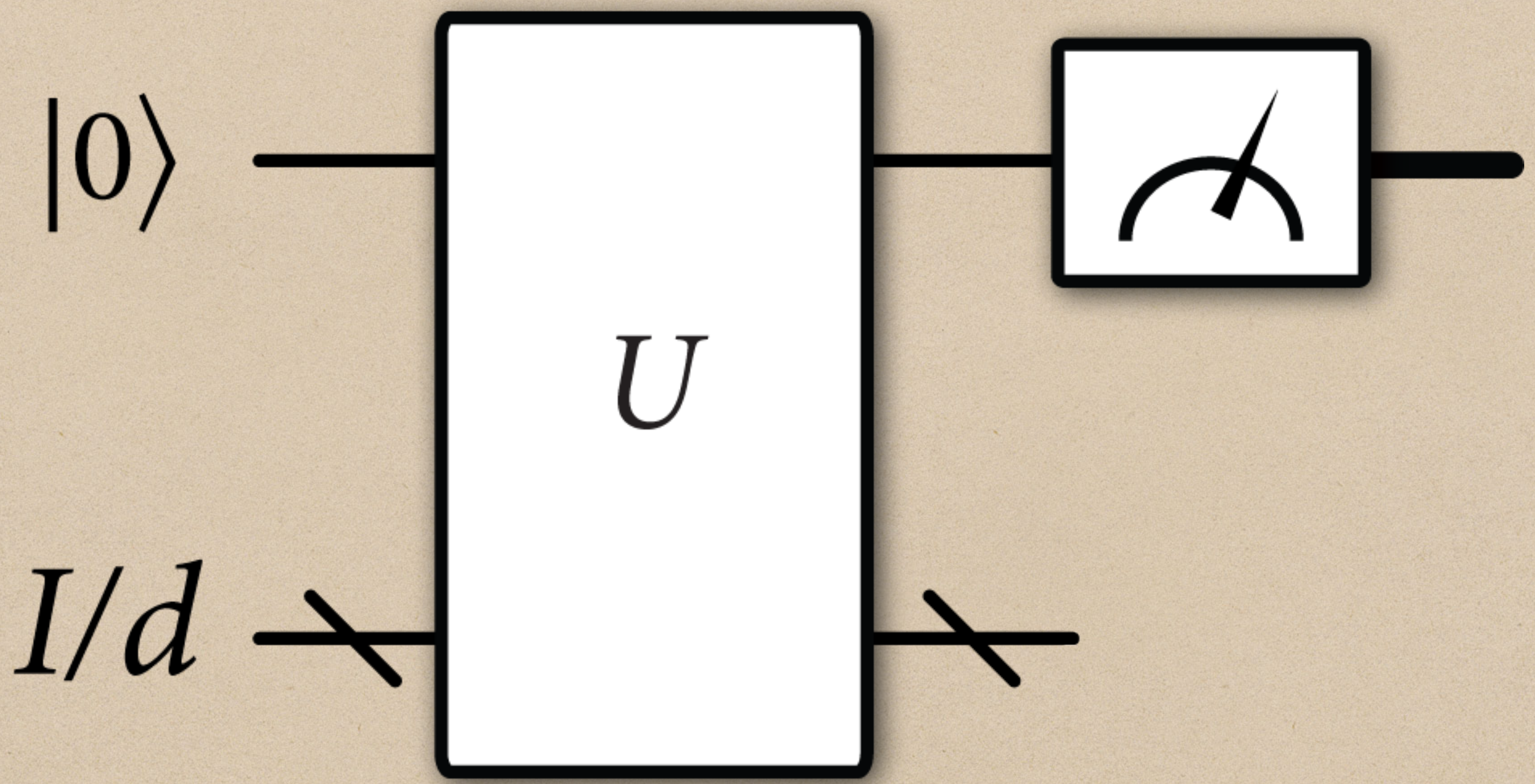
- Twirl for continuous case is $\mathcal{T}_G(\cdot) \equiv \int d\mu(g)\ U(g)^\dagger (\cdot) U(g)$
- Invoking Caratheodory's theorem, there exists a finite implementation of the twirl

Computational complexity

- We can also prove that estimating the acceptance probability is a DQC1-complete problem
- This gives evidence that the acceptance probability will be difficult to estimate using a classical computer

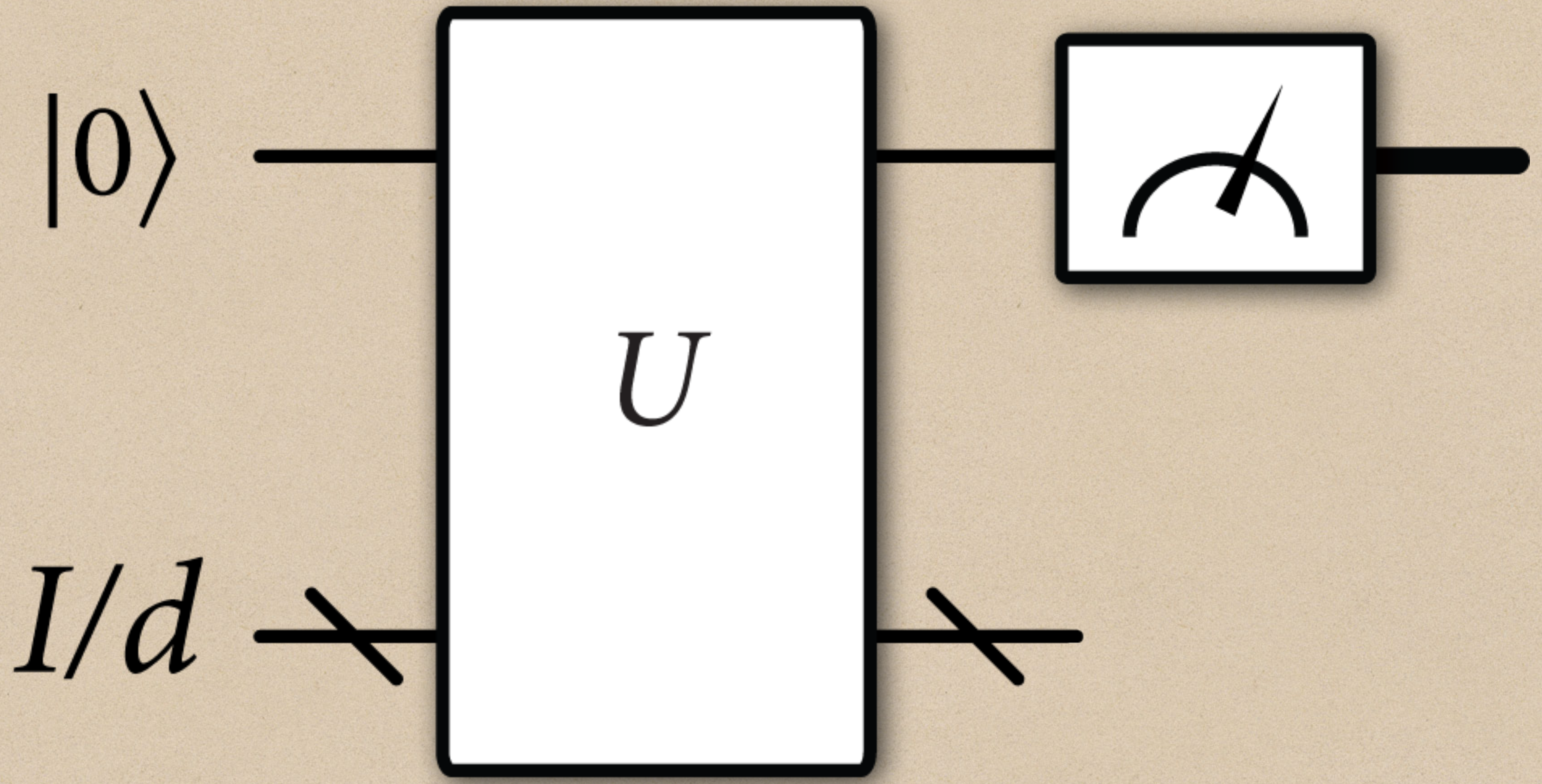
Review of DQC1

- DQC1: Only one qubit can be prepared in a pure state and all others are maximally mixed



- Thus weaker than bounded quantum polynomial time computations

Review of DQC1 (ctd.)

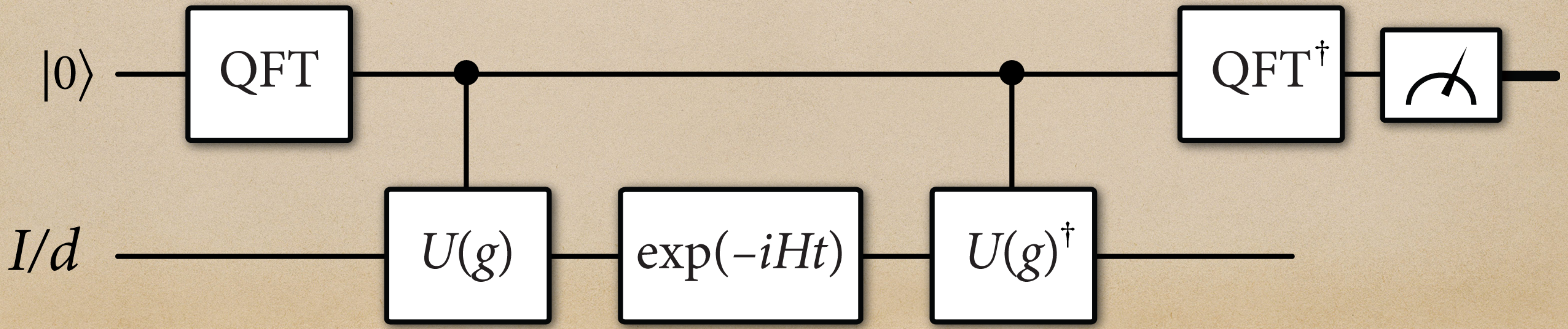


- Acceptance probability in this case given by $\mathrm{Tr}[(|1\rangle\langle 1| \otimes I)U(|0\rangle\langle 0| \otimes I/d)U^{\dagger}]$

- Goal is to estimate this quantity to within additive error

Containment in DQC1

- DQC1 complexity class does not change if there are $\log \log d$ pure qubits, because there is only a polynomial increase in number of repetitions needed to estimate acceptance probability
- By inspection, algorithm thus contained in DQC1



Hardness for DQC1

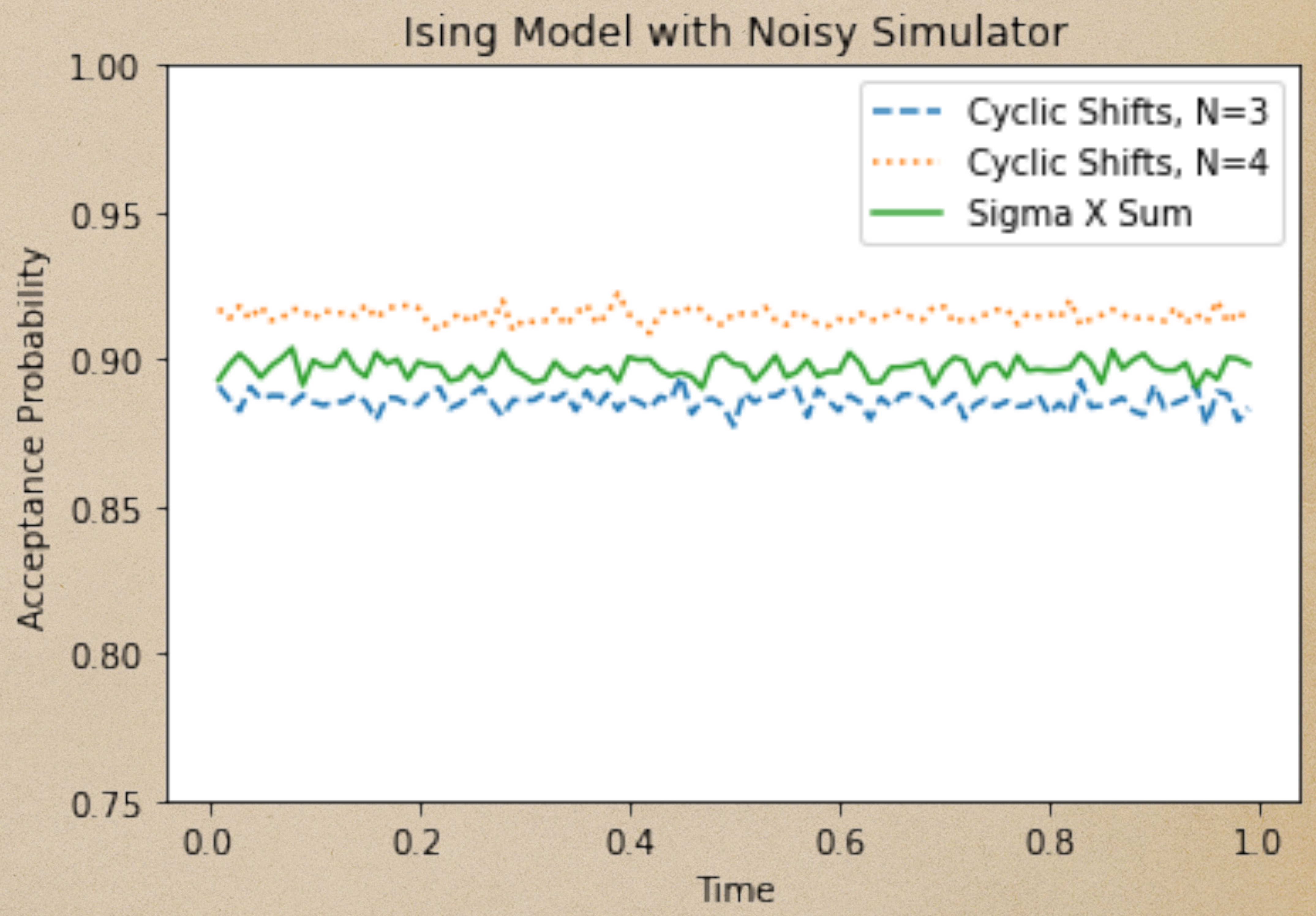
- Known: Estimating $\frac{\Re[\mathrm{Tr}[U]]}{d}$ is DQC1-complete, where U is unitary generated by quantum circuit
- We prove that estimating $\Re[\mathrm{Tr}[U^2]]/d$ is also DQC1-complete, by considering controlled unitary $\left(|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U\right)\left(\sigma_X \otimes I\right)$
- Then pick the group to be $\mathbb{Z}_2$ with representation $\{I, V\}$, where $V = |0\rangle\langle 1| \otimes U + |1\rangle\langle 0| \otimes U^\dagger$, and the Hamiltonian to be one that realizes $H_2 \otimes I$ via Hamiltonian evolution, where H_2 is a 2×2 Hadamard gate
- For the above choices, $(d|G|)^{-1} \sum_{g \in G} \mathrm{Tr}[U^\dagger(g) e^{iHt} U(g) e^{-iHt}] = \Re\left[\mathrm{Tr}\left[U^2\right]\right]/2d$

Example: Transverse-Field Ising Model

- Transverse-field Ising model w/ periodic boundary condition:

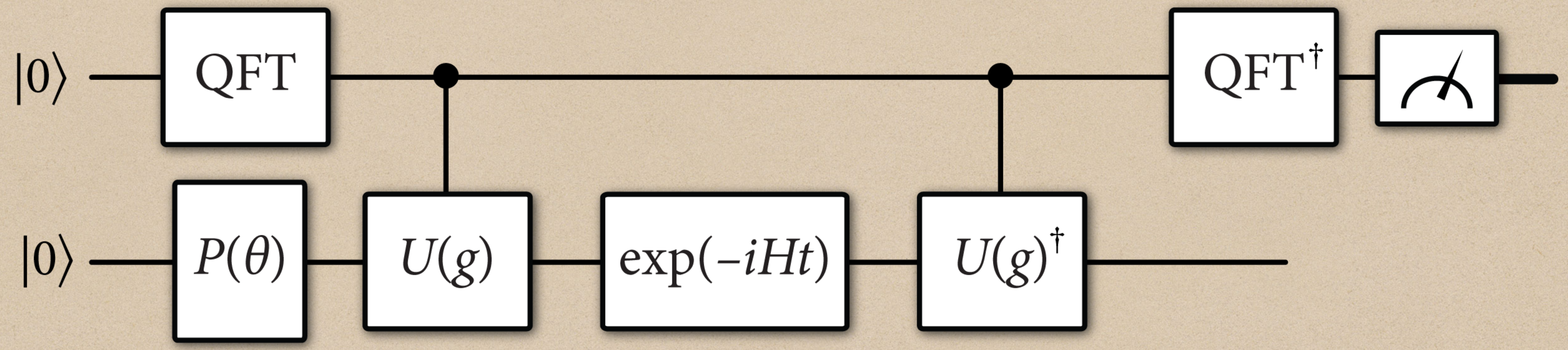
$$H_{\mathrm{TFIM}} \equiv \sigma_N^Z \otimes \sigma_1^Z + \sum_{i=1}^{N-1} \sigma_i^Z \otimes \sigma_{i+1}^Z + \sum_{i=1}^{N} \sigma_i^X$$

- Symmetries: $[H_{\mathrm{TFIM}}, (\sigma^X)^{\otimes N}] = 0$ and $[H_{\mathrm{TFIM}}, W^\pi] = 0 \quad \forall \pi \in S_N$



VQA for Hamiltonian Symmetry Testing

- By modifying the previous Hamiltonian symmetry testing algorithm to optimize over input states, we get a variational quantum algorithm:



- Acceptance probability

$$= \left\| \frac{1}{|G|} \sum_{g \in G} U(g) e^{-iHt} U(g)^\dagger \right\|_\infty^2 \geq 1 - \frac{2t}{|G|} \sum_{g \in G} \left\| [U(g), H] \right\|_\infty - O(t^2)$$

Summary

- Proposed an efficient quantum algorithm for testing Hamiltonian symmetry
- Acceptance probability contains familiar expression of Hamiltonian symmetry
- Gave evidence that acceptance probability cannot be estimated efficiently by a classical computer

Outlook

- Would like to implement larger instances of algorithm on existing quantum computers
- Would like to modify these algorithms to learn Hamiltonian symmetry
- Would like to study variational quantum algorithm further and implement it on existing quantum computers
- Can we use these algorithms to solve open problems in physics?