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INTRODUCTION TO QUANTUM PHASE ESTIMATION: EXTRACTING HIDDEN PHASES FOR SCIENTIFIC DISCOVERY

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QBI JOURNAL CLUB

OUTLINE

- Motivation
- Quantum Phase Estimation (QPE)
  - Design of QPE
  - Clarifying Questions
  - Quantum Advantage
- Practical Considerations and Recent Advances
- Closing and Discussion

MOTIVATION

The scientific problem

- Many physical and chemical properties boil down to finding eigenvalues of a Hamiltonian:

$$H|\phi_j\rangle = E_j|\phi_j\rangle$$

In chemistry: ground-state and excited-state energies.

In materials: band structures, correlation gaps.

MOTIVATION

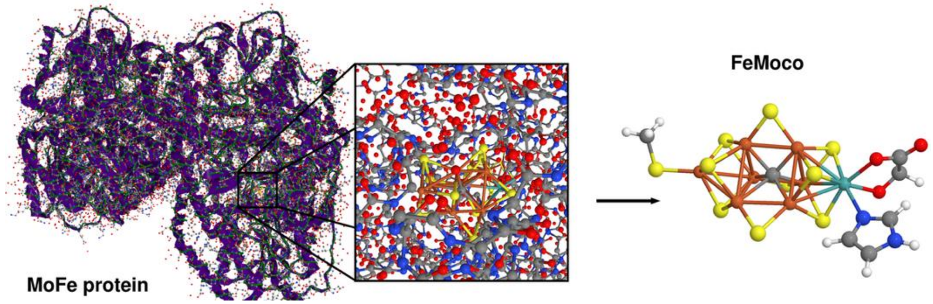
Challenge with classical methods

- The Hilbert space of an n-particle quantum system grows as 2^n
- Classical eigen solvers (Full CI, Lanczos, DMRG, etc) need to store and manipulate exponentially many amplitudes.
- Even the approximate classical methods (Hartree–Fock, CCSD) scale steeply.
- This scaling makes accurate calculations intractable for large molecules.

MOTIVATION

Quantum Phase Estimation Algorithm

- QPE is a quantum analogue of spectral decomposition — it estimates the eigenvalue of a unitary operator by measuring its phase.
- QPE was initially introduced by Alexei Kitaev in 1995
- It is a general building block behind:
  - Shor’s factoring algorithm
  - HHL linear systems of equations
  - Quantum chemistry and materials simulation



Kitaev, A. Yu. "Quantum measurements and the Abelian stabilizer problem." arXiv preprint quant-ph/9511026 (1995).

QUANTUM PHASE ESTIMATION (QPE)

EXAMPLE: GROUND STATE ENERGY

For example, given a chemistry system described by Hamiltonian H, we want to find its ground state energy:

$$H|\psi_0\rangle = E_0|\psi_0\rangle$$

Then, applying unitary $U = e^{-iHt}$ to ground state $|\psi_0\rangle$ gives:

$$U|\psi_0\rangle = e^{-iE_0 t}|\psi_0\rangle = e^{-i2\pi\phi_0}|\psi_0\rangle$$

If we can estimate the phase ϕ_0, we can recover the energy as:

$$E_0 = -\frac{2\pi\phi_0}{t}$$

PROBLEM

Input: A quantum circuit for an n-qubit operation U and an n-qubit quantum state $|\psi\rangle$

Promise: $|\psi\rangle$ is an eigenvector of U

Output: An approximation of number $\theta \in [0,1)$ satisfying:

$$U|\psi\rangle = e^{i2\pi\theta}|\psi\rangle$$

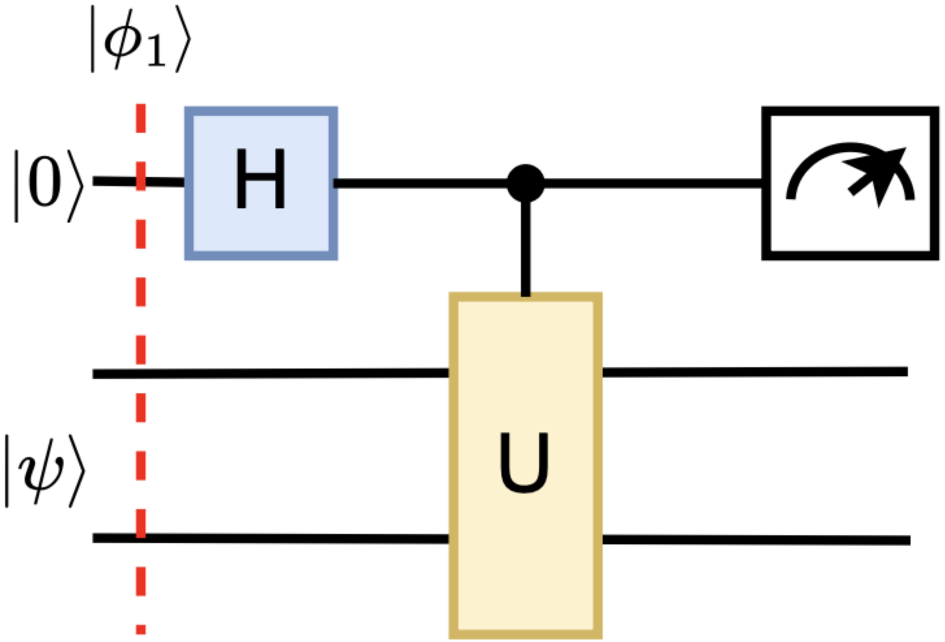
Where θ is the normalized phase of the eigenvalue. (Phase estimation)

We will store the phase in binary:

$$\theta \in [0,1)\ \theta = \frac{\theta_1}{2} + \frac{\theta_2}{4} + \cdots + \frac{\theta_m}{2^m} = 0.\theta_1\theta_2\theta_3 \ldots \theta_m$$

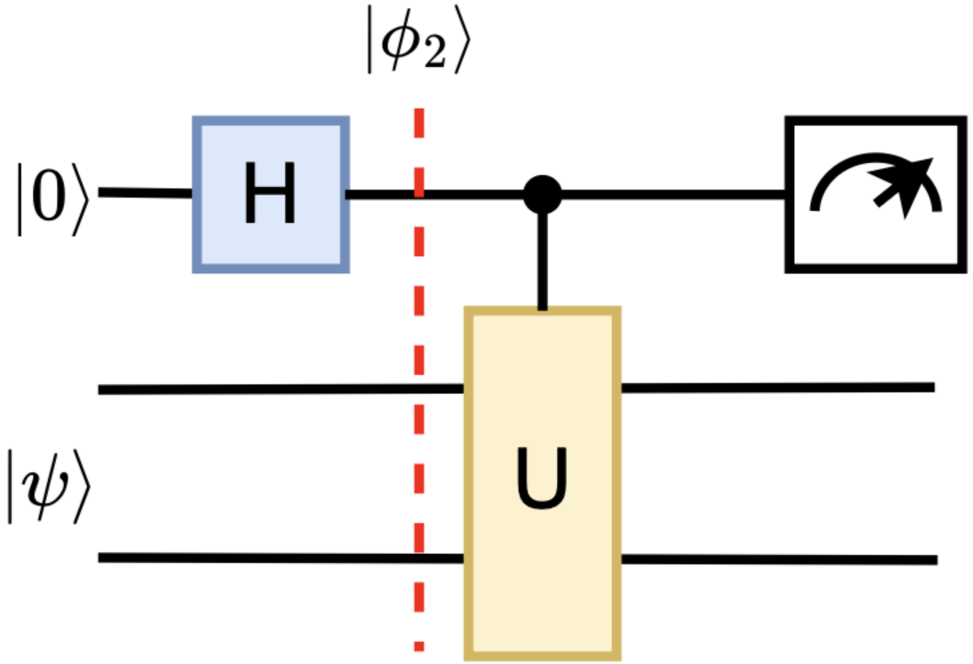
WARM UP: PHASE KICKBACK CIRCUIT

The phase kickback circuit consists of a Hadamard gate H and a controlled unitary gate.



$$|\phi_1\rangle = |\psi\rangle \otimes |0\rangle = |\psi\rangle|0\rangle$$

WARM UP: PHASE KICKBACK CIRCUIT

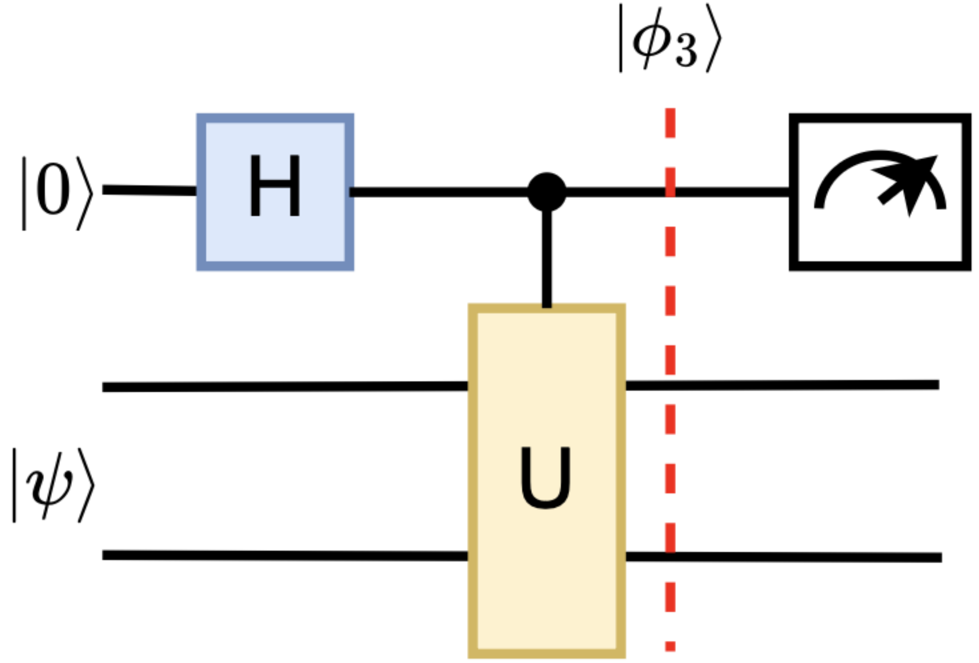


$$|\phi_2\rangle = |\psi\rangle \otimes (H|0\rangle)$$

$$= |\psi\rangle \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right)$$

$$= \frac{1}{\sqrt{2}}|\psi\rangle|0\rangle + \frac{1}{\sqrt{2}}|\psi\rangle|1\rangle$$

WARM UP: PHASE KICKBACK CIRCUIT

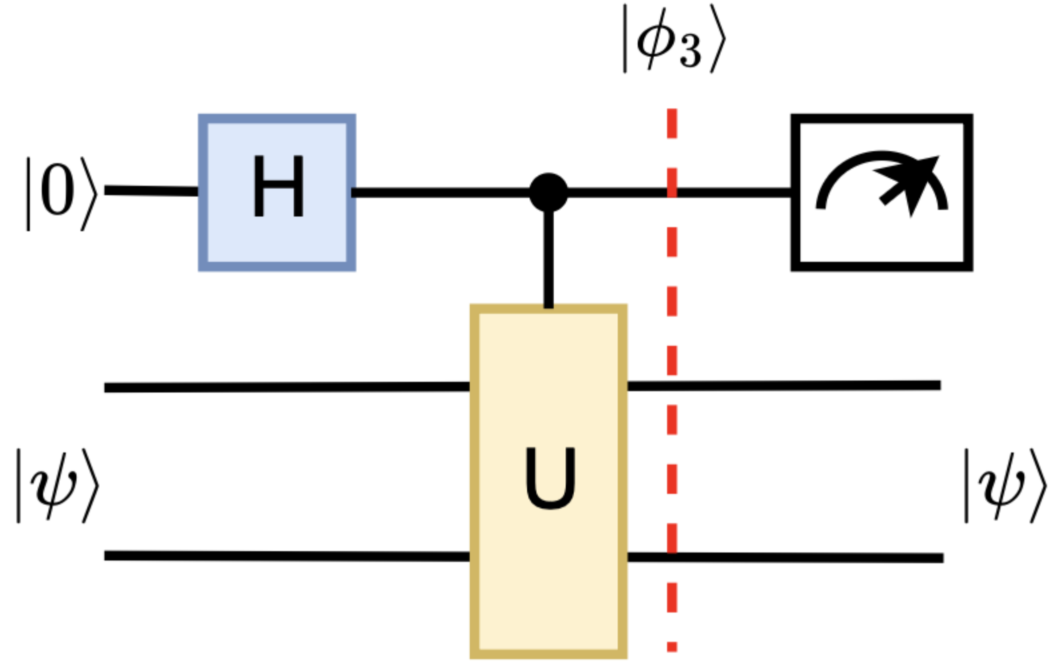


$$|\phi_3\rangle = CU|\phi_2\rangle = CU(\frac{1}{\sqrt{2}}|\psi\rangle|0\rangle + \frac{1}{\sqrt{2}}|\psi\rangle|1\rangle)$$

$$= \frac{1}{\sqrt{2}}|\psi\rangle|0\rangle + \frac{1}{\sqrt{2}}U|\psi\rangle|1\rangle = \frac{1}{\sqrt{2}}|\psi\rangle|0\rangle + \frac{1}{\sqrt{2}}e^{i2\pi\theta}|\psi\rangle|1\rangle$$

$$= |\psi\rangle \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i2\pi\theta}}{\sqrt{2}}|1\rangle\right)$$

WARM UP: PHASE KICKBACK CIRCUIT



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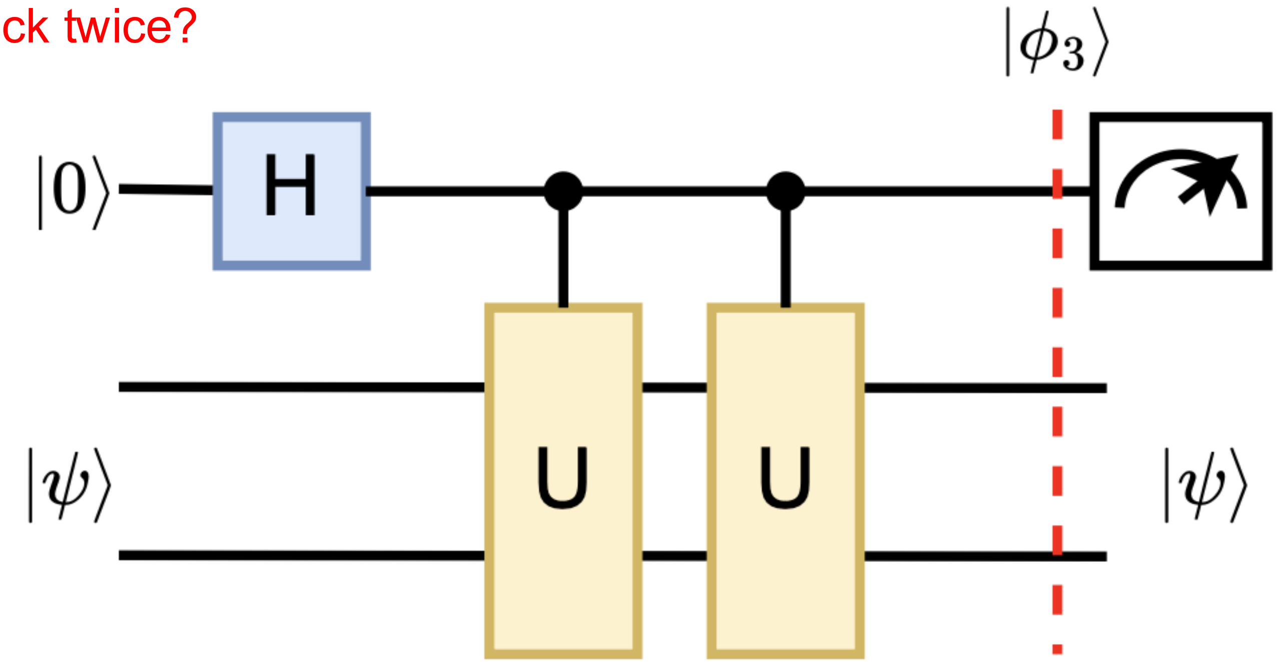
$$= \underbrace{|\psi\rangle}_{\text{qubit2,3}} \otimes \underbrace{\left(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i2\pi\theta}}{\sqrt{2}}|1\rangle\right)}_{\text{qubit1}} \longleftarrow$$

Phase kickback!
Can derive θ if measuring the phase on the first qubit.

WARM UP: PHASE KICKBACK CIRCUIT

How about Phase kickback twice?



$$|\phi_3\rangle = |\psi\rangle \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i2\pi 2\theta}}{\sqrt{2}}|1\rangle\right)$$

$$= |\psi\rangle \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i2\pi\,(2.\theta_1\theta_2\theta_3\ldots\theta_m)}}{\sqrt{2}}|1\rangle\right)$$

$$= |\psi\rangle \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i2\pi 0.\theta_2\theta_3\ldots\theta_m}}{\sqrt{2}}|1\rangle\right)$$

$$\theta = \frac{\theta_1}{2} + \frac{\theta_2}{4} + \cdots + \frac{\theta_m}{2^m} = 0.\theta_1\theta_2\theta_3\ldots\theta_m$$

WARM UP: PHASE KICKBACK CIRCUIT

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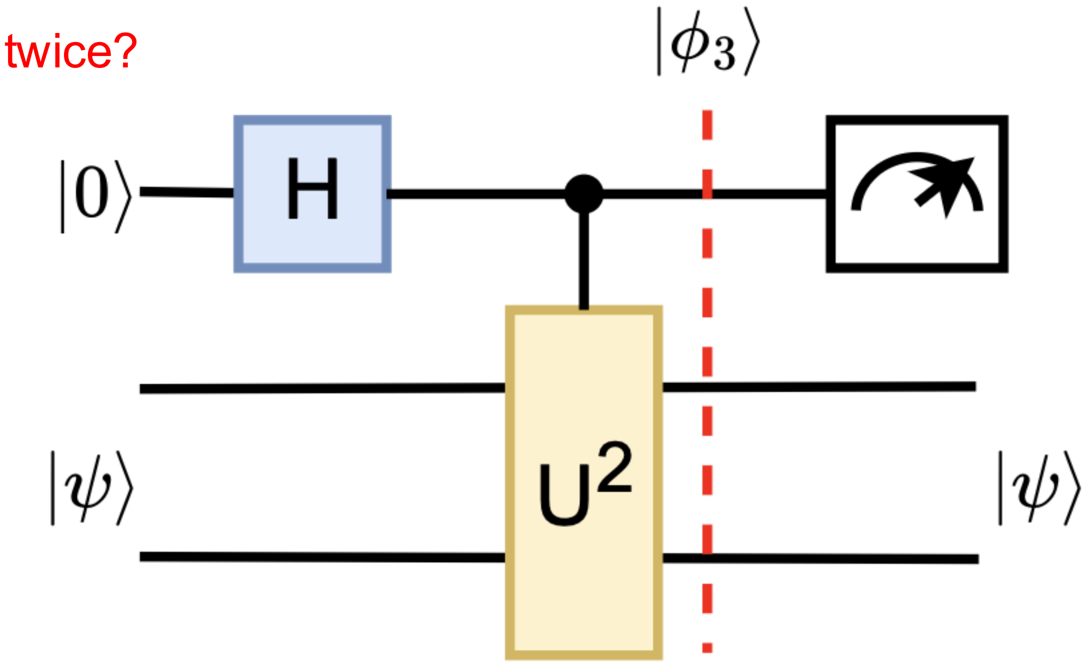

$$|\phi_3\rangle = |\psi\rangle \otimes \left(\frac{1}{\sqrt{2}} |0\rangle + \frac{e^{i2\pi 2\theta}}{\sqrt{2}} |1\rangle \right)$$

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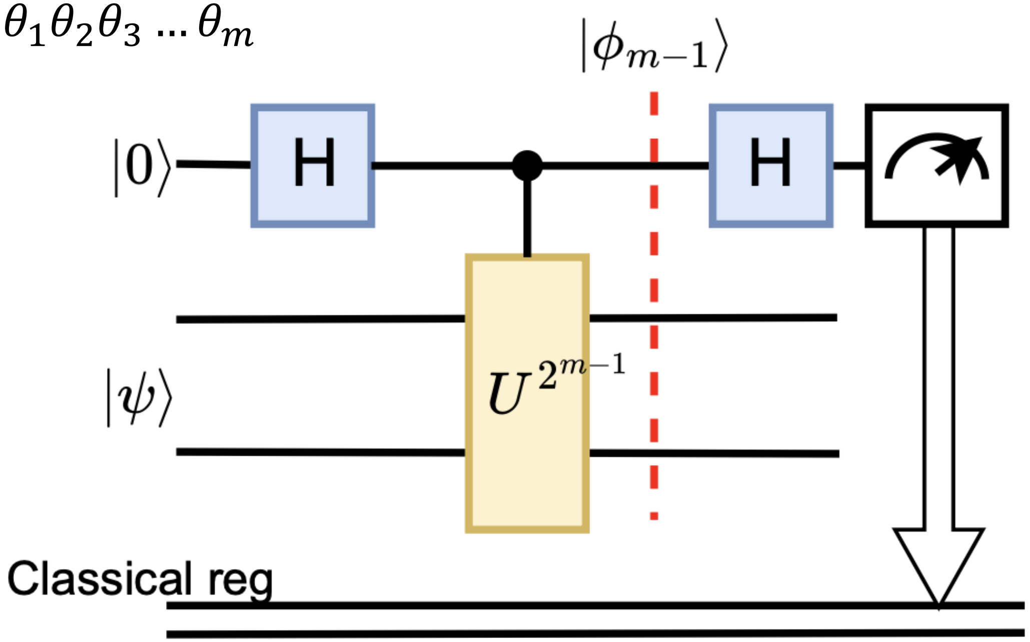
$$\theta = \frac{\theta_1}{2} + \frac{\theta_2}{4} + \cdots + \frac{\theta_m}{2^m} = 0.\theta_1\theta_2\theta_3 \ldots \theta_m$$

ITERATIVE PHASE ESTIMATION

$$\theta = \frac{\theta_1}{2} + \frac{\theta_2}{4} + \cdots + \frac{\theta_m}{2^m} = 0.\theta_1\theta_2\theta_3 \ldots \theta_m$$

Start with $U^{2^{m-1}}$



ITERATIVE PHASE ESTIMATION

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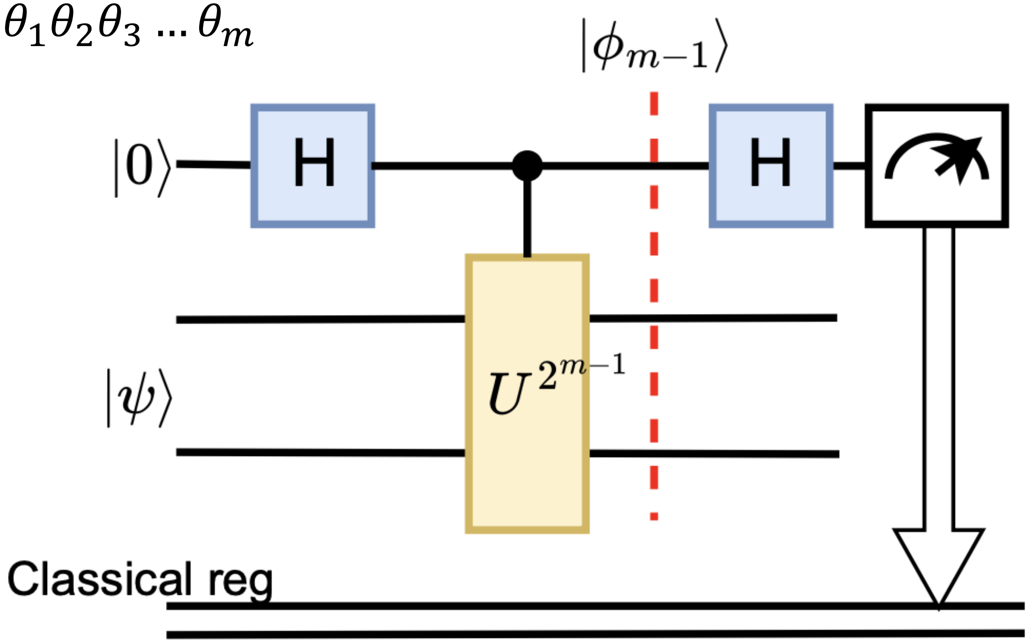


$$|\phi_{m-1}\rangle = |\psi\rangle \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i2\pi 2^{m-1}\theta}}{\sqrt{2}}|1\rangle\right)$$

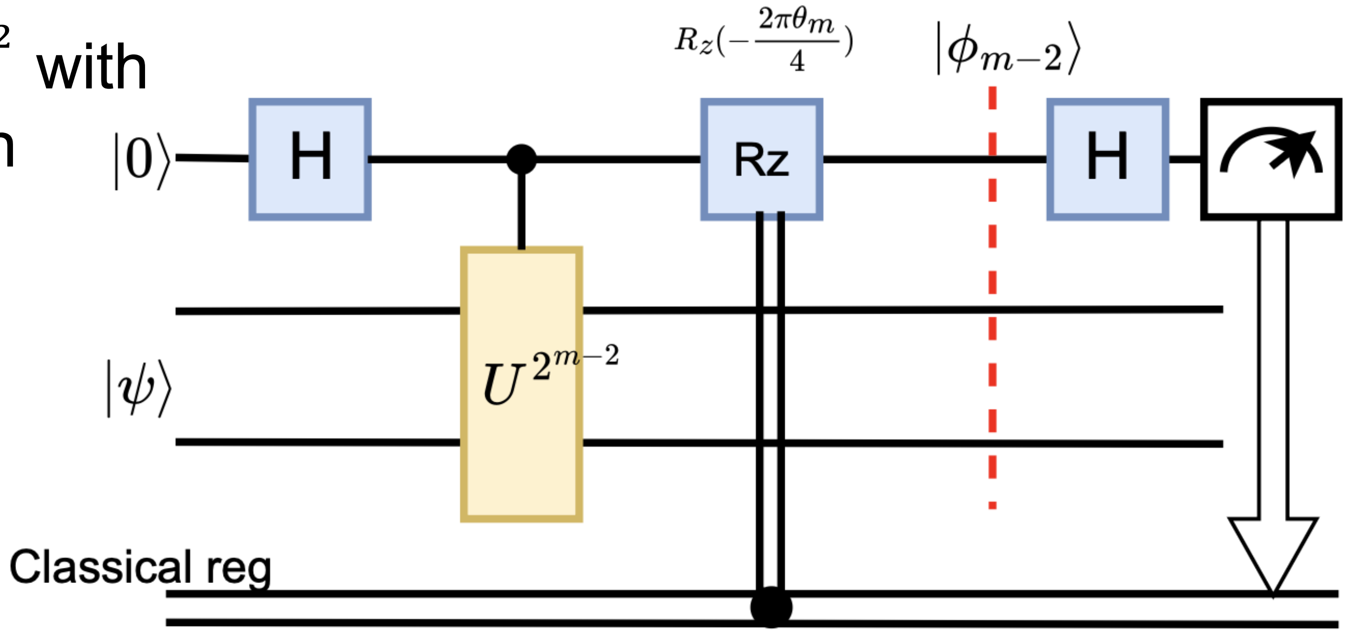
$$= |\psi\rangle \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i2\pi\,(2^{m-1}.\theta_1\theta_2\theta_3\ldots\theta_m)}}{\sqrt{2}}|1\rangle\right)$$

$$= |\psi\rangle \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i2\pi 0.\theta_m}}{\sqrt{2}}|1\rangle\right)$$

If θ_m == 0, measure result is 0,
If θ_m == 1, measure result is 1

ITERATIVE PHASE ESTIMATION

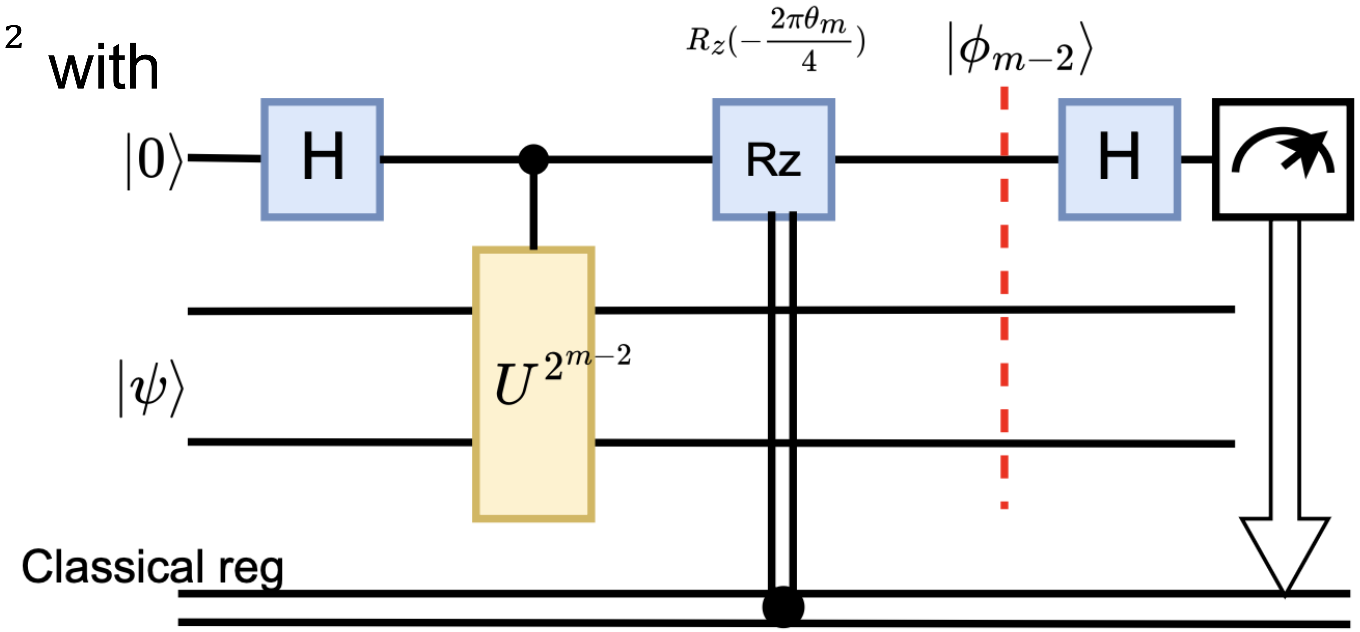
Next step: $U^{2^{m-2}}$ with phase correction based on θ_m



After controlled $U^{2^{m-2}}$: $|\psi\rangle \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i2\pi 0.\theta_{m-1}\theta_m}}{\sqrt{2}}|1\rangle\right)$

ITERATIVE PHASE ESTIMATION

Next step: $U^{2^{m-2}}$ with phase rotation based on θ_m

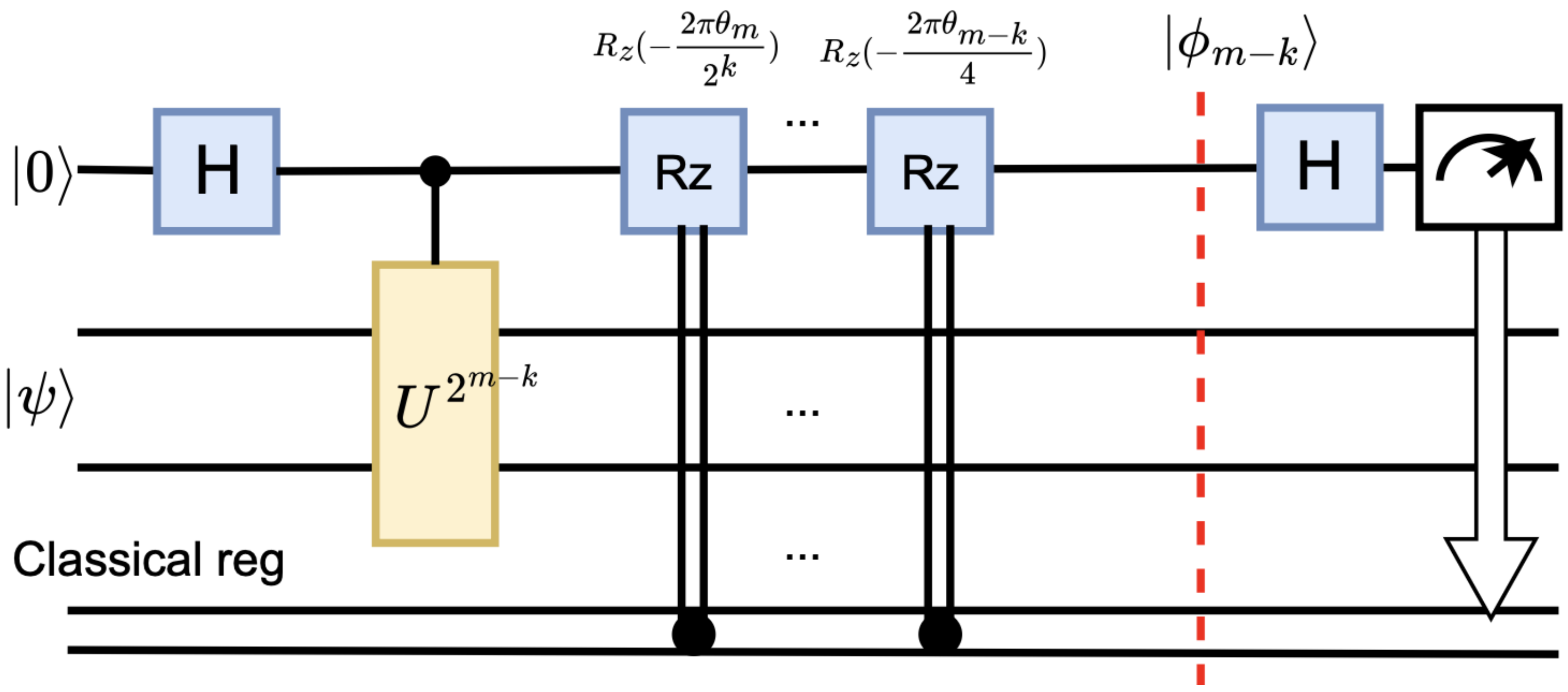


After controlled $U^{2^{m-2}}$: $|\psi\rangle\otimes\left(\frac{1}{\sqrt{2}}|0\rangle+\frac{e^{i2\pi 0.\theta_{m-1}\theta_m}}{\sqrt{2}}|1\rangle\right)$

After controlled Rz rotation: $|\phi_{m-2}\rangle=|\psi\rangle\otimes\left(\frac{1}{\sqrt{2}}|0\rangle+\frac{e^{i2\pi 0.\theta_{m-1}}}{\sqrt{2}}|1\rangle\right)$

ITERATIVE PHASE ESTIMATION

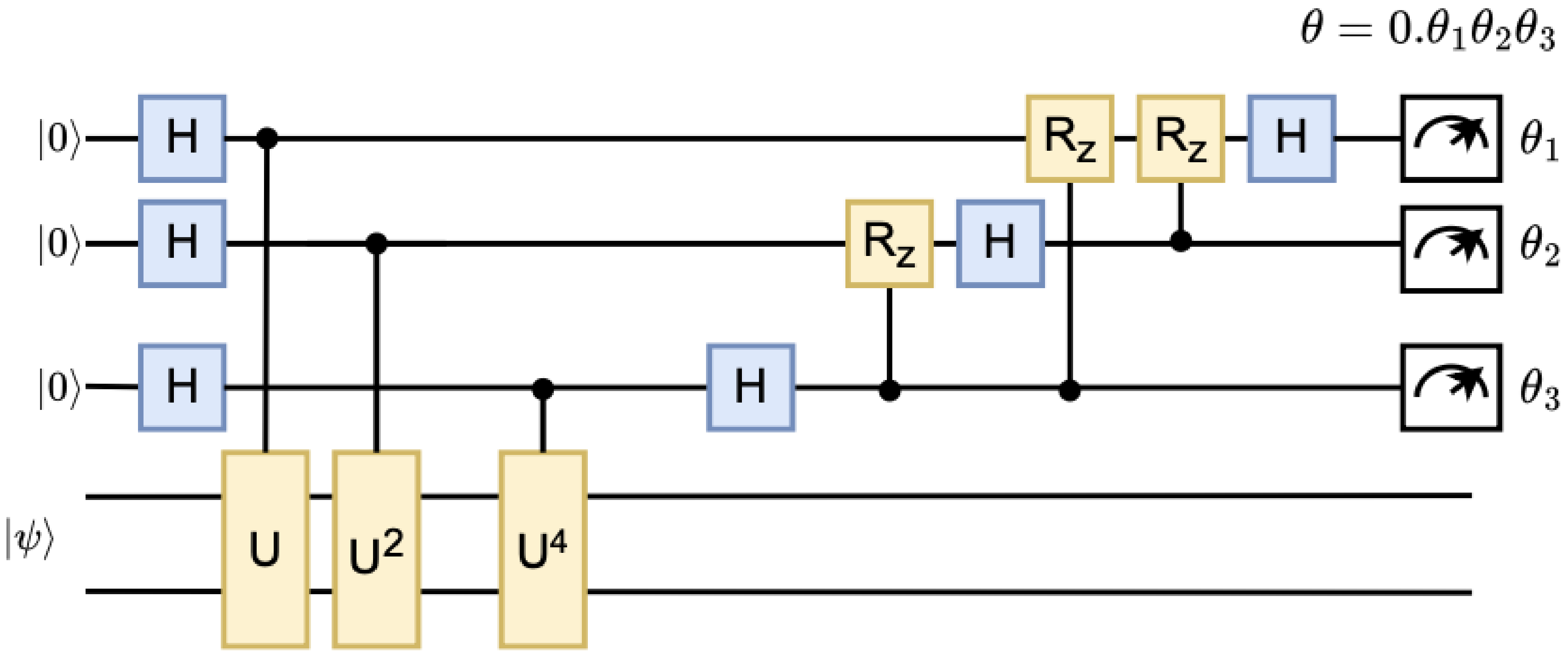
Further steps



Iterate the circuit for m times until the bitstring $\theta = 0.\theta_1\theta_2\theta_3 \ldots \theta_m$ is found!

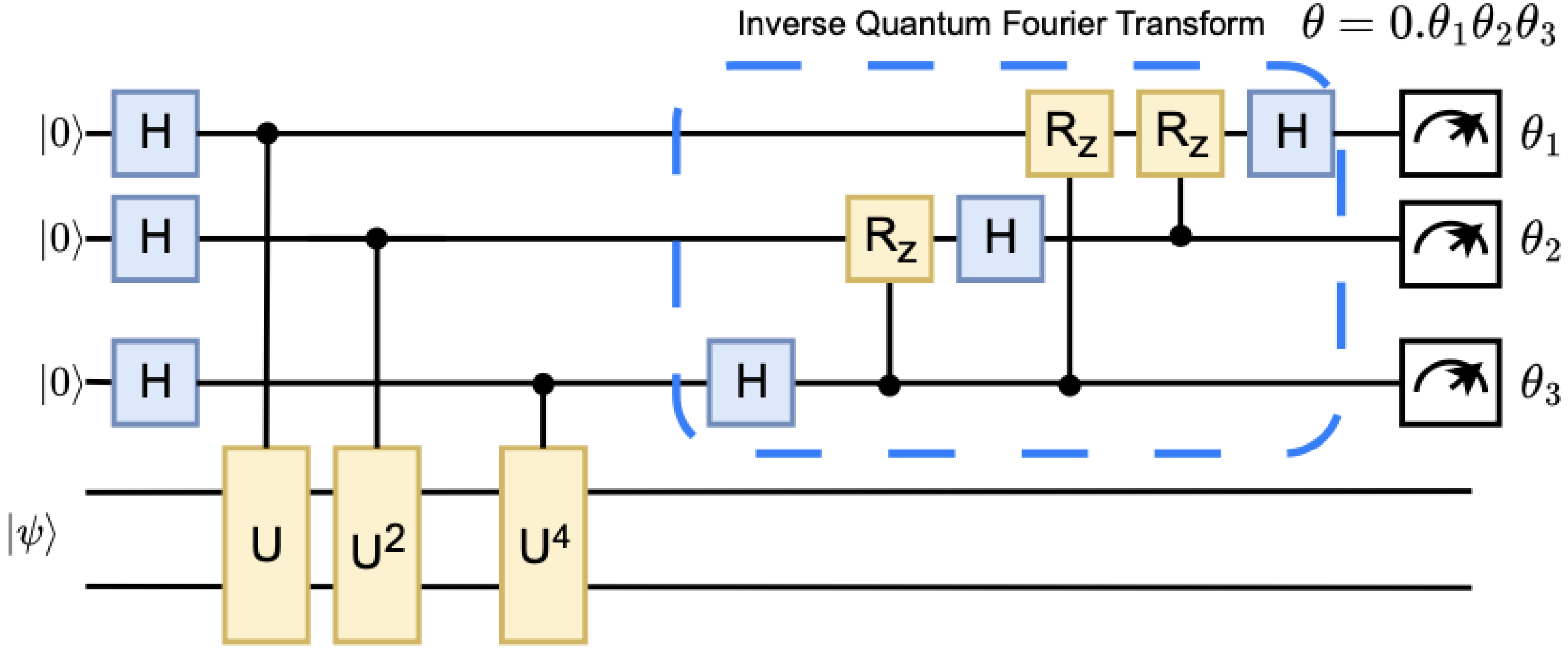
QUANTUM PHASE ESTIMATION

Put all the iterations in one circuit:



QUANTUM PHASE ESTIMATION

Quantum Phase estimation circuit:



CLARIFICATION1: PROBABILITY MEASUREMENT

Question: $\theta = 0.\theta_1\theta_2\theta_3 \dots \theta_m$ is only an approximation of the real phase

$\theta_t = 0.\theta_1\theta_2\theta_3 \dots \theta_m\theta_{m+1}\theta_{m+2} \dots$

Due to the probabilistic nature of quantum measurement, we may obtain bitstrings other than the closest one.

What is the probability of measuring the closest bitstring to the true phase?

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Due to the probabilistic nature of quantum measurement, we may obtain bitstrings other than the closest one.

What is the probability of measuring the closest bitstring to the true phase?

Answer: It can be shown that the probability of successfully measuring the closest bit string is: $P_{success} > \frac{4}{\pi^2} \approx 40\%$

Therefore, the number of required repetitions (shots) to achieve high confidence remains **a constant overhead**.

CLARIFICATION2: CIRCUIT DEPTH

Question: How does the circuit depth scale with m (accuracy) and n (problem size),

Does U^{2^m} introduce an exponential gate-count overhead?

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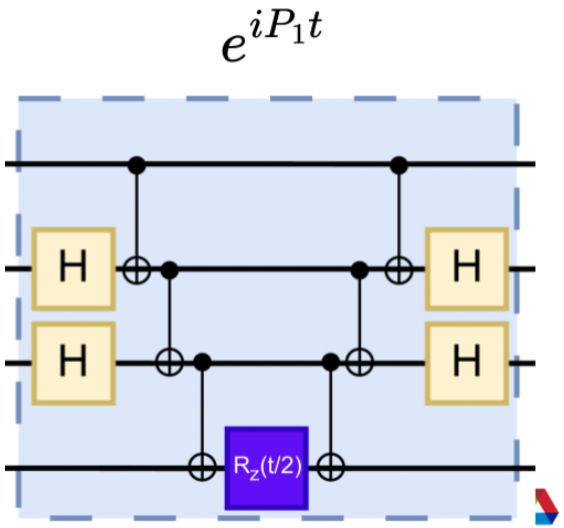
Answer: If resolution ϵ is desired, m = $log_2\left(\frac{1}{\epsilon}\right)$. One must perform $1 + 2 + \cdots + log_2\left(\frac{1}{\epsilon}\right) = O\left(\frac{1}{\epsilon}\right)$ calls to the controlled-U oracle. This dependence on ϵ is optimal, the $O\left(\frac{1}{\epsilon}\right)$ is known as **Heisenberg limit.**

However, U^{2^m} is a single unitary block, not an exponential sequence of controlled U gates.

The implementation cost varies for algorithms,

For quantum signal processing: $O\left(poly(n)\log\left(\frac{1}{\epsilon}\right)\right)$

For product formulas: $O(poly(n)\frac{1}{\epsilon^{2k}})$



CLARIFICATION3: INITIAL STATE

Question: In the derivation we assume the initial state $|\psi\rangle$ is an eigenvector of U. But what if we **do not know** the eigenstate?

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Question: In the derivation we assume the initial state $|\psi\rangle$ is an eigenvector of U. But what if we **do not know** the eigenstate?

Answer: The eigenstates of U forms a complete basis. Any initial state $|\psi_a\rangle$ can be decomposed to the superposition of the eigenstates: $|\psi_a\rangle = \sum_i \alpha_i |\psi_i\rangle$

When QPE is applied to this superposition, the measurement collapses the system to one of the eigenstates $|\psi_i\rangle$ with $|\alpha_i|^2$, and the corresponding eigenphase ϕ_i is observed.

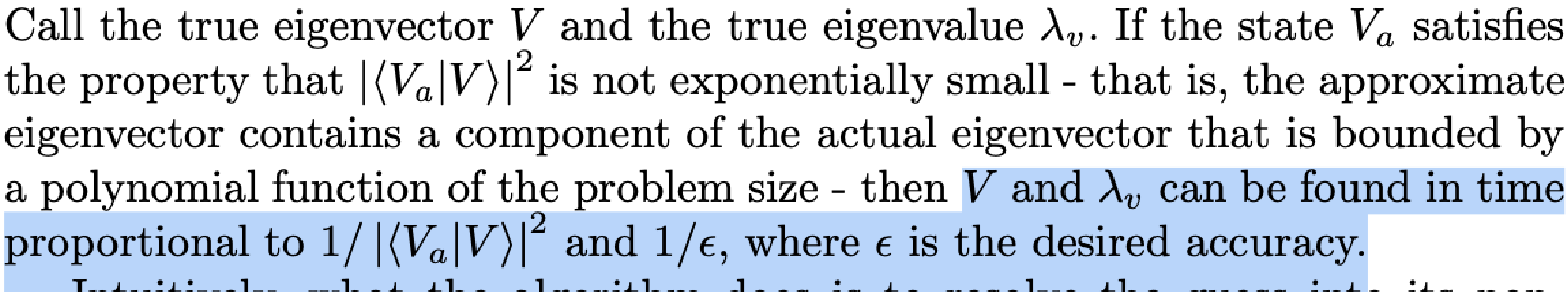
In practice, we can prepare an approximate initial state using classical methods (e.g., Hartree–Fock in quantum chemistry) to ensure non-negligible overlap with the desired eigenstate

As long as the overlap is not exponentially small, the correct eigenvalue can be obtained in polynomial time through repeated QPE runs.

CLARIFICATION3: INITIAL STATE

Daniel S. Abrams, Seth Lloyd in 1998.

“A quantum algorithm providing exponential speed increase for finding eigenvalues and eigenvectors”



Call the true eigenvector V and the true eigenvalue λ_v. If the state V_a satisfies the property that $|\langle V_a|V\rangle|^2$ is not exponentially small - that is, the approximate eigenvector contains a component of the actual eigenvector that is bounded by a polynomial function of the problem size - then V and λ_v can be found in time proportional to $1/|\langle V_a|V\rangle|^2$ and $1/\epsilon$, where ϵ is the desired accuracy.

QUANTUM VS CLASSICAL ALGORITHM

Given an n-qubit Hamiltonian and desired accuracy ϵ
Classical algorithm: Full Configuration Interaction (Full CI)

Metric	**Classical (Full CI)**	**Quantum**
Memory	$O(2^n)$	$O(n + \log(\frac{1}{\epsilon}))$
Runtime	$O(2^{3n})$	$O(poly(n)/\epsilon)$

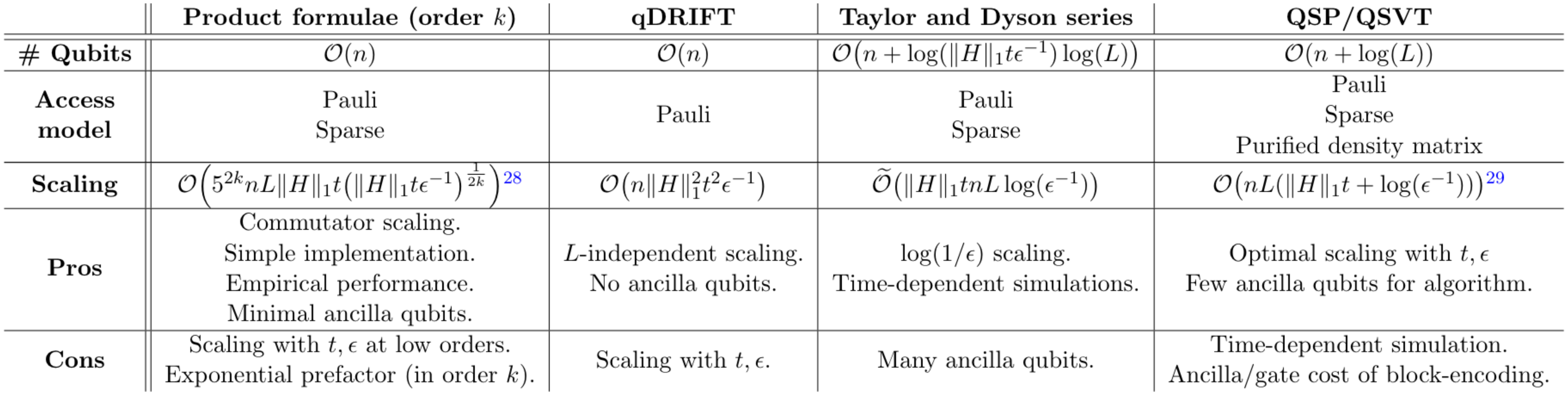
PRACTICAL CONSIDERATIONS AND RECENT ADVANCES

BUILDING UNITARY OPERATION

The controlled-U gate is the most resource-intensive operation in QPE.

Constructing $U = e^{-iHt}$ is nontrivial, this process is generally known as **Hamiltonian simulation.**

There are various approaches to realize this unitary operation and remains an active area of research.



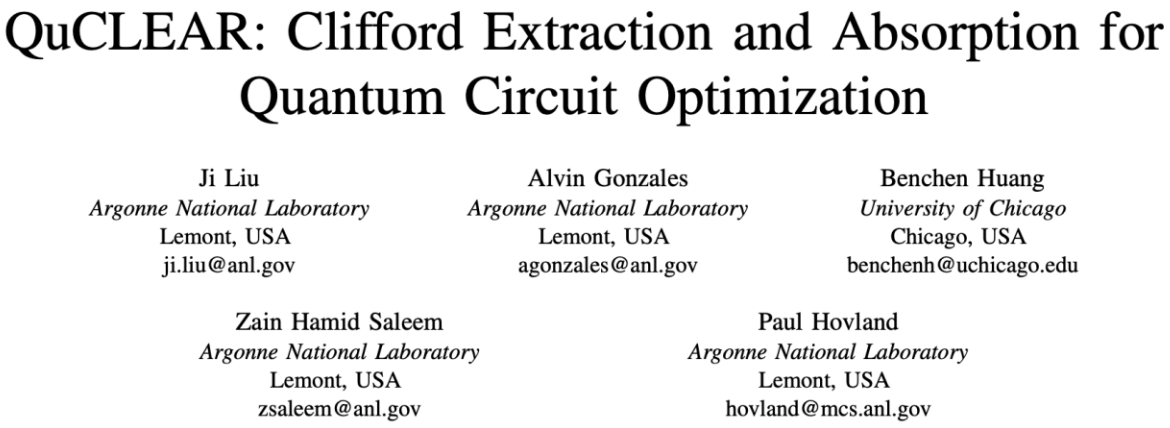
	Product formulae (order k)	**qDRIFT**	**Taylor and Dyson series**	**QSP/QSVT**
# Qubits	$\mathcal{O}(n)$	$\mathcal{O}(n)$	$\mathcal{O}\big(n + \log(\|H\|_1 t\epsilon^{-1})\log(L)\big)$	$\mathcal{O}(n + \log(L))$
Access model	Pauli Sparse	Pauli	Pauli Sparse	Pauli Sparse Purified density matrix
Scaling	$\mathcal{O}\Big(5^{2k} nL\|H\|_1 t\big(\|H\|_1 t\epsilon^{-1}\big)^{\frac{1}{2k}}\Big)$[28]	$\mathcal{O}\big(n\|H\|_1^2 t^2 \epsilon^{-1}\big)$	$\widetilde{\mathcal{O}}\big(\|H\|_1 tnL\log(\epsilon^{-1})\big)$	$\mathcal{O}\big(nL(\|H\|_1 t + \log(\epsilon^{-1}))\big)$[29]
Pros	Commutator scaling. Simple implementation. Empirical performance. Minimal ancilla qubits.	L-independent scaling. No ancilla qubits.	$\log(1/\epsilon)$ scaling. Time-dependent simulations.	Optimal scaling with t, ϵ Few ancilla qubits for algorithm.
Cons	Scaling with t, ϵ at low orders. Exponential prefactor (in order k).	Scaling with t, ϵ.	Many ancilla qubits.	Time-dependent simulation. Ancilla/gate cost of block-encoding.

Dalzell et. Al, "Quantum algorithms: A survey of applications and end-to-end complexities" arXiv:2310.03011v1, 2023

OUR WORKS AT ARGONNE

Hamiltonian Simulation

Near term: Reducing 2-qubit gates



QuCLEAR: Clifford Extraction and Absorption for Quantum Circuit Optimization

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State-of-the-art Hamiltonian Simulation synthesis work.

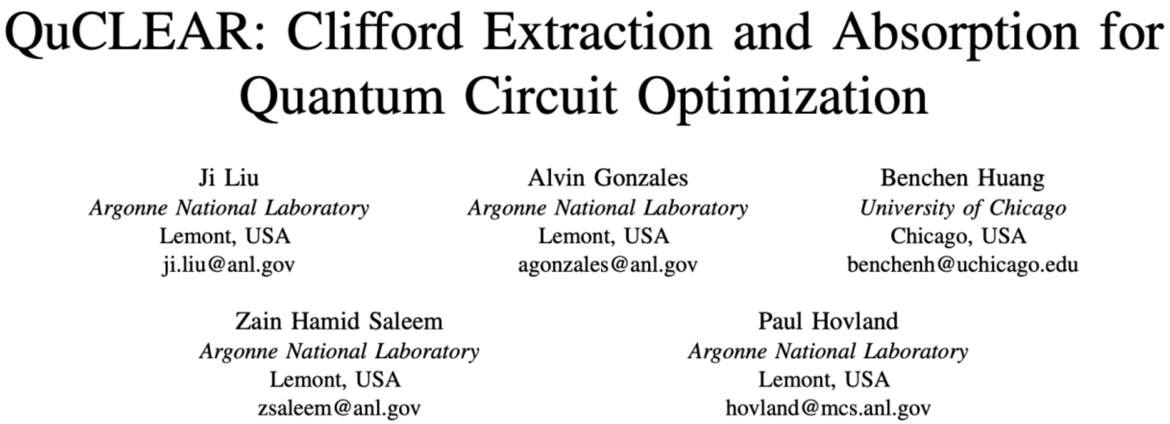
HPCA 2025,
arXiv:2408.13316v2

arXiv:2510.13573

OUR WORKS AT ARGONNE

Hamiltonian Simulation

Near term: Reducing 2-qubit gates



QuCLEAR: Clifford Extraction and Absorption for Quantum Circuit Optimization

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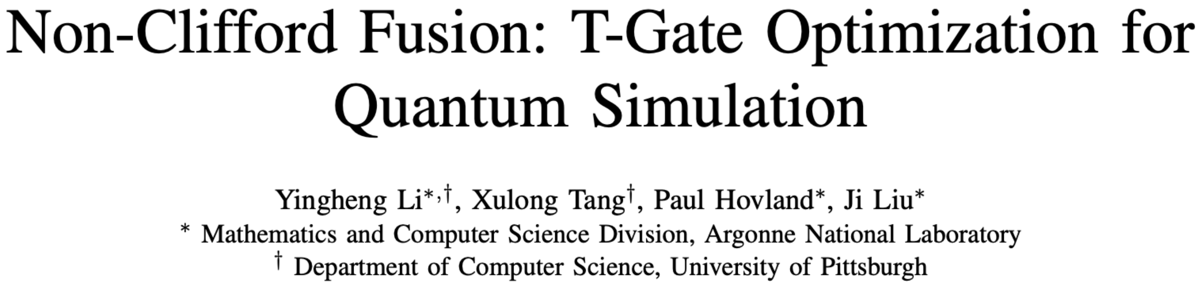
State-of-the-art Hamiltonian Simulation synthesis work.

HPCA 2025,
arXiv:2408.13316v2

Long term: Reducing T gates



Non-Clifford Fusion: T-Gate Optimization for Quantum Simulation

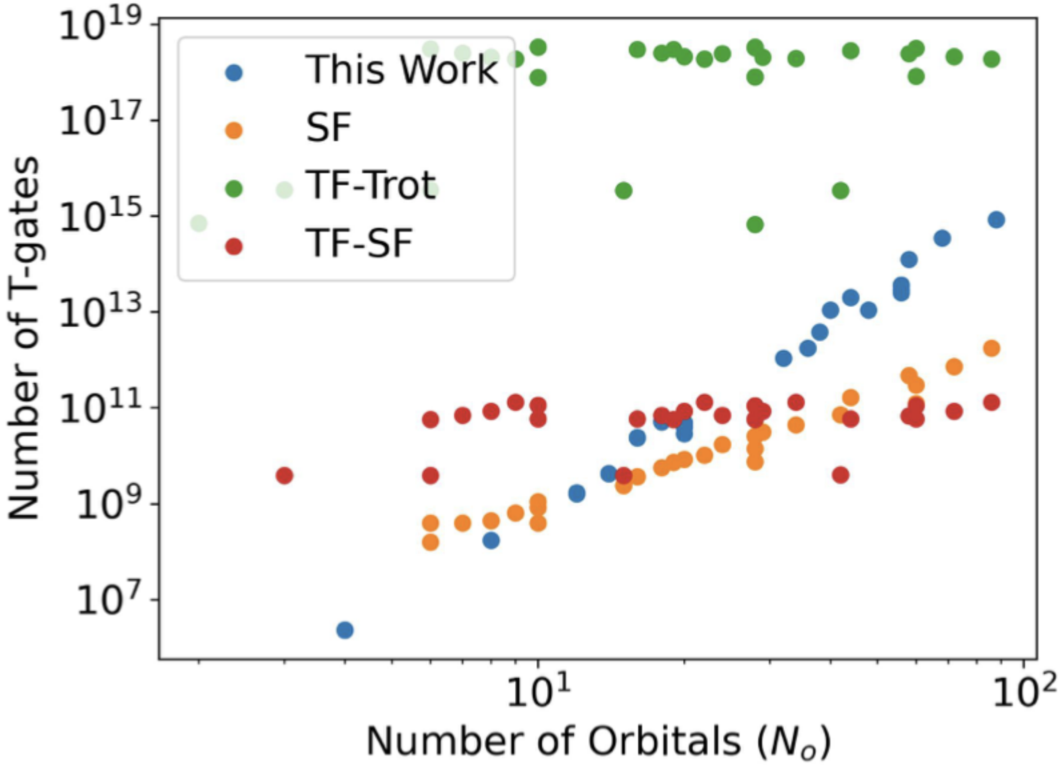
Yingheng Li[*,†], Xulong Tang[†], Paul Hovland[*], Ji Liu[*]
[*] Mathematics and Computer Science Division, Argonne National Laboratory
[†] Department of Computer Science, University of Pittsburgh

Generalized framework for optimizing T gate count and T gate depth.

arXiv:2510.13573

RESOURCE ESTIMATION

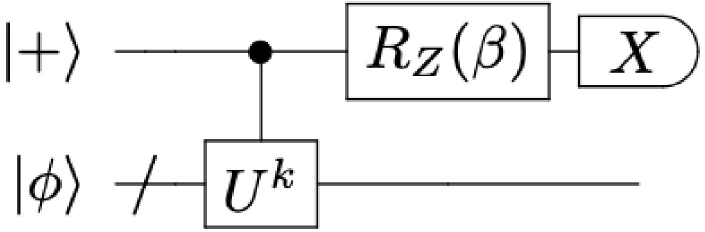
QPE is a FTQC algorithm



Otten, Matthew, Byeol Kang, Dmitry Fedorov, Joo-Hyoung Lee, Anouar Benali, Salman Habib, Stephen K. Gray, and Yuri Alexeev. "QREChem: quantum resource estimation software for chemistry applications." Frontiers in Quantum Science and Technology 2 (2023): 1232624

RECENT ADVANCES

2023: Bayesian QPE, Quantinuum



$$p(m \mid \phi, k, \beta) = \frac{1 + \cos(k\phi + \beta - m\pi)}{2}$$

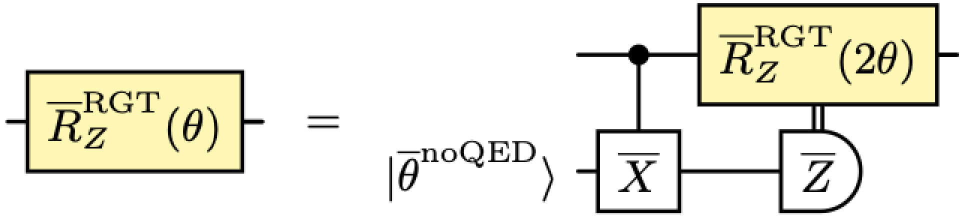
Probability of measuring $m \in \{0,1\}$ depends on k, β and unknown phase ϕ

- Use a Bayesian update process to find phase.
- Use an error detection code(iceberg code) to mitigate noise
- Hydroden, two-qubit Hamiltonian, 8-qubits, 920 two-qubit gates, 6×10^{-3} Hartree

Yamamoto, Kentaro, Samuel Duffield, Yuta Kikuchi, and David Muñoz Ramo. "Demonstrating Bayesian quantum phase estimation with quantum error detection." Physical Review Research 6, no. 1 (2024): 013221.

RECENT ADVANCES

2025: Partial Error-corrected QPE, Quantinuum

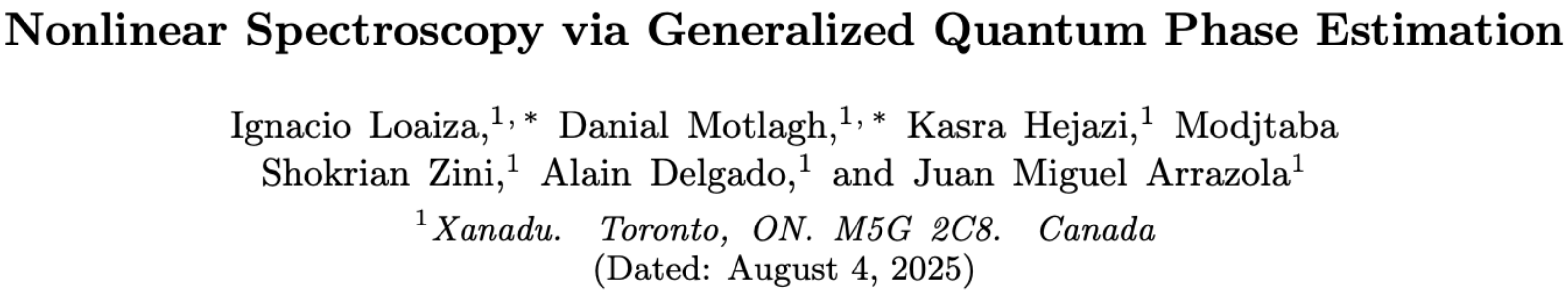


Same Bayesian QPE circuit,

- Clifford + Rz gate set, [[7,1,3]] color code
- Error correction for Clifford, Repeat until success gate for Rz.
- Hydroden, two-qubit Hamiltonian, 22 qubits, 2185 two-qubit gates, 0.018 Hartree

Yamamoto, Kentaro, Yuta Kikuchi, David Amaro, Ben Criger, Silas Dilkes, Ciarán Ryan-Anderson, Andrew Tranter et al. "Quantum Error-Corrected Computation of Molecular Energies." arXiv preprint arXiv:2505.09133 (2025).

RECENT ADVANCES

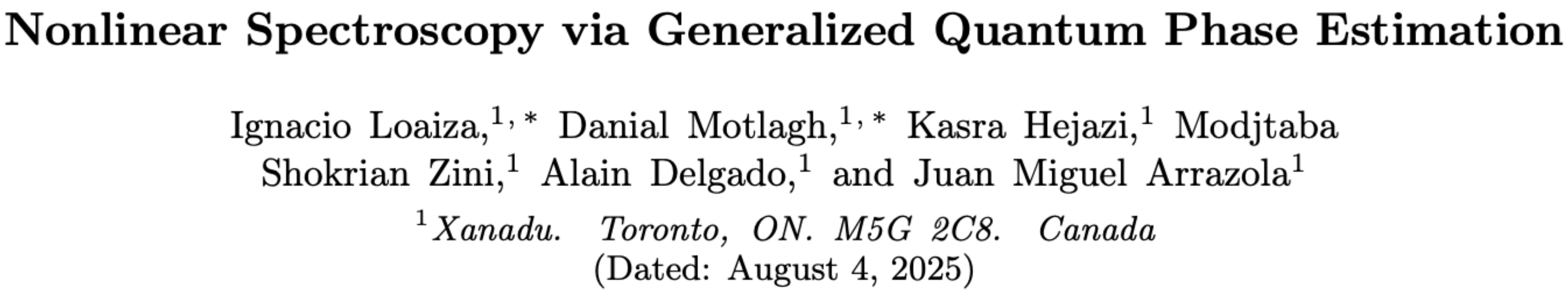


Nonlinear Spectroscopy via Generalized Quantum Phase Estimation

Ignacio Loaiza,[1,*] Danial Motlagh,[1,*] Kasra Hejazi,[1] Modjtaba
Shokrian Zini,[1] Alain Delgado,[1] and Juan Miguel Arrazola[1]
[1] *Xanadu. Toronto, ON. M5G 2C8. Canada*

(Dated: August 4, 2025)

RECENT ADVANCES



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Shokrian Zini,[1] Alain Delgado,[1] and Juan Miguel Arrazola[1]
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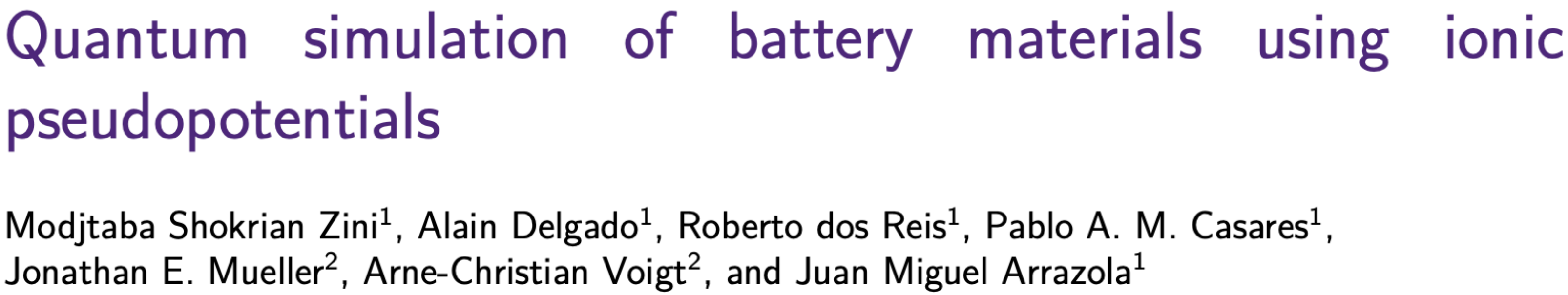
(Dated: August 4, 2025)



Quantum simulation of battery materials using ionic pseudopotentials

Modjtaba Shokrian Zini[1], Alain Delgado[1], Roberto dos Reis[1], Pablo A. M. Casares[1],
Jonathan E. Mueller[2], Arne-Christian Voigt[2], and Juan Miguel Arrazola[1]

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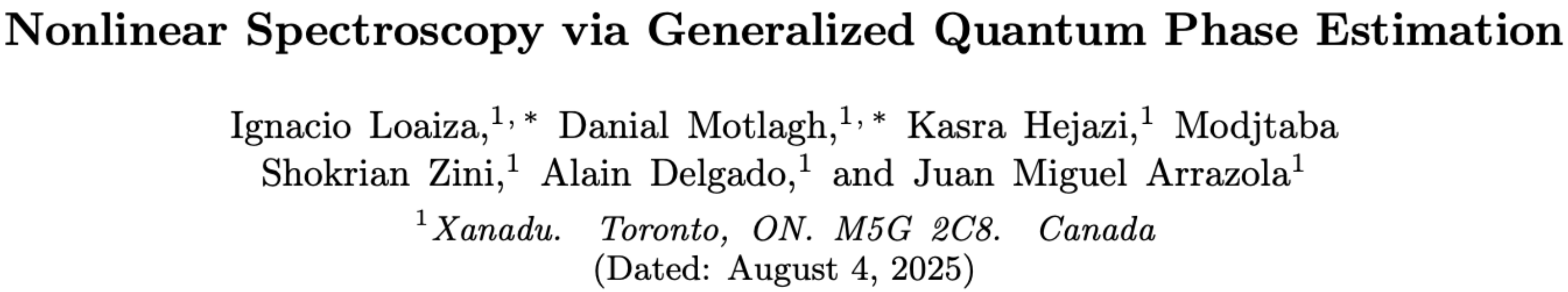

Nonlinear Spectroscopy via Generalized Quantum Phase Estimation

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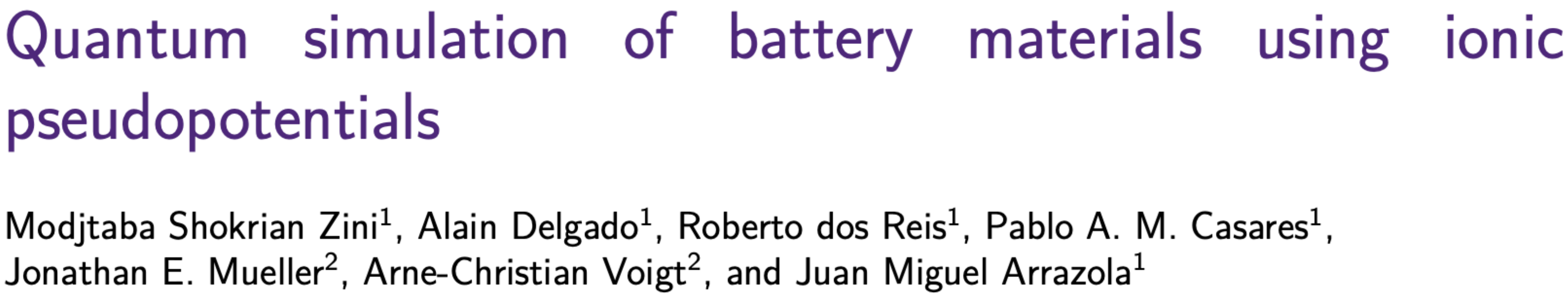

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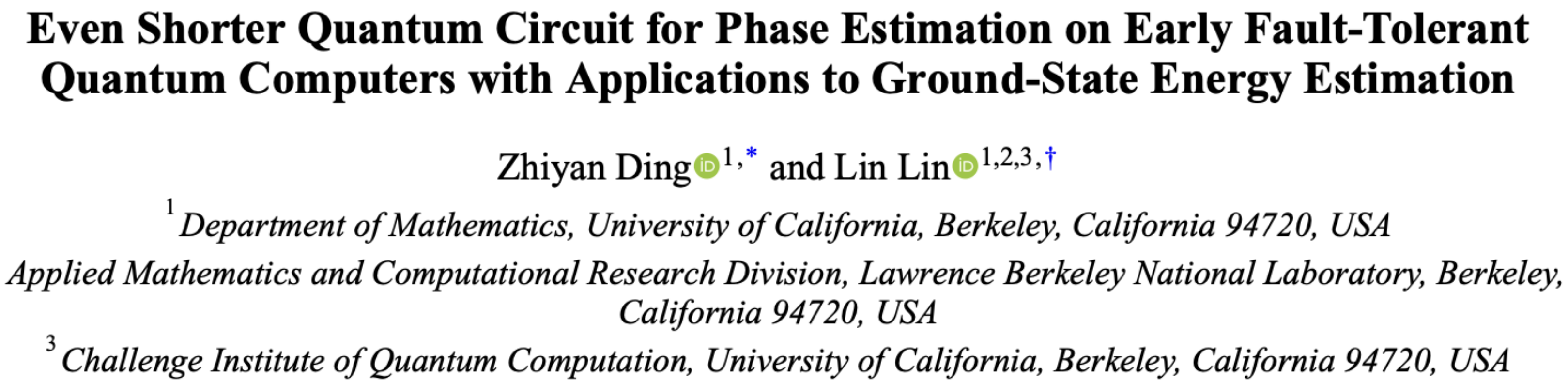

Even Shorter Quantum Circuit for Phase Estimation on Early Fault-Tolerant Quantum Computers with Applications to Ground-State Energy Estimation

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QUESTIONS?

Thank you!

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