CS 59300 – Algorithms for Data Science

Classical and Quantum approaches

Lecture 14 (10/28)

Quantum eigenvalue problems (I)

https://ruizhezhang.com/course_fall_2025.html

Slides are mostly borrowed from Yu Tong's talk at IPAM

Quick announcement

- Midterm exam
  - Time: Oct. 28 (after class) – **Oct. 30 (before class)**
  - You may either write your solutions clearly by hand or typeset them in LaTeX and print them out
  - Use of web searches or LLMs is **not allowed**
  - The midterm counts for **25%** of your final grade. The total score for the exam is **65 points**, and your final points will be calculated as:

$$\min\left\{\frac{\text{your score}}{2}, 25\right\}$$

- Course feedback

> **Office hours:** By appointment
>
> **Course information:** Here
>
> **Course feedback:** Here

Quantum algorithms

Quantum eigenvalue problems

Quantum linear algebra

Quantum Samplings

Classical Gibbs sampling

Quantum Gibbs sampling

Quantum learning theory

Variational quantum algorithms

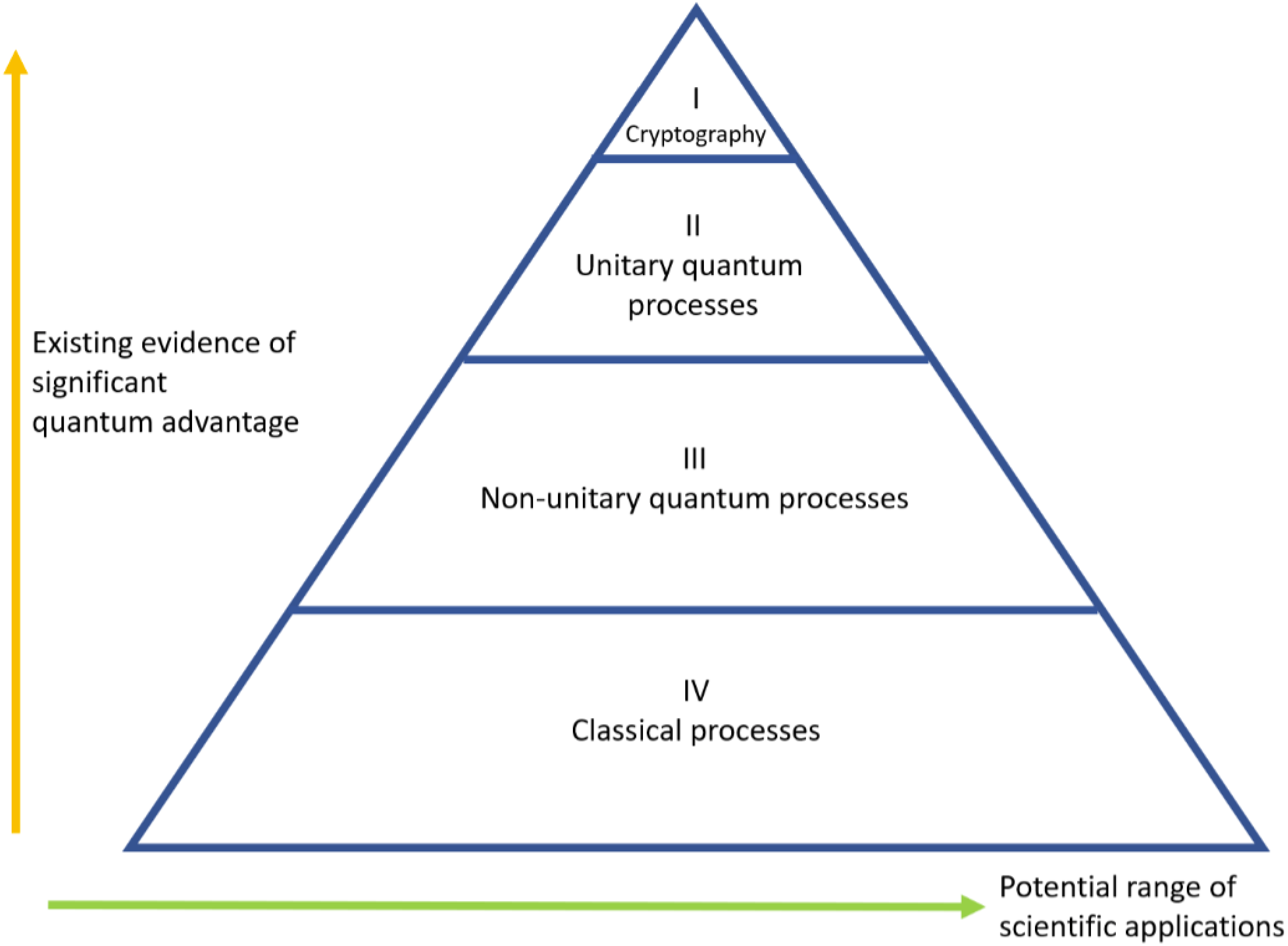
VQE, QAOA, QNN…

- Quantum SDP solvers
- Quantum gradient estimation
- Decoded Quantum Interferometry
- Adiabatic quantum computing

Quantum Hamiltonian simulation

https://quantumalgorithmzoo.org/

Quantum advantage hierarchy (as of now)



Borrowed from Lin Lin's slides

Quantum advantage hierarchy (as of now)

Level	Input Cost	Output Cost	Running Cost	Classical Cost	Examples
I	✓	✓	✓	Provably expensive	Shor's algorithm for prime number factorization
II	✓	✓	✓	Empirically expensive	Hamiltonian simulation
III	?	?	✓	Empirically expensive	Ground state energy estimation, thermal state preparation, Green's function, open quantum system dynamics
IV	?	?	?	?	Classical partial differential equations, stochastic differential equations, optimization problems, sampling problems

Basic definitions in quantum algorithms

- “Bra-Ket”: $|v\rangle$ denotes a column vector and $\langle u|$ denotes a row vector
- Single-qubit state $\cong \mathbb{C}^2 \,/\, \|\cdot\|_2$

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

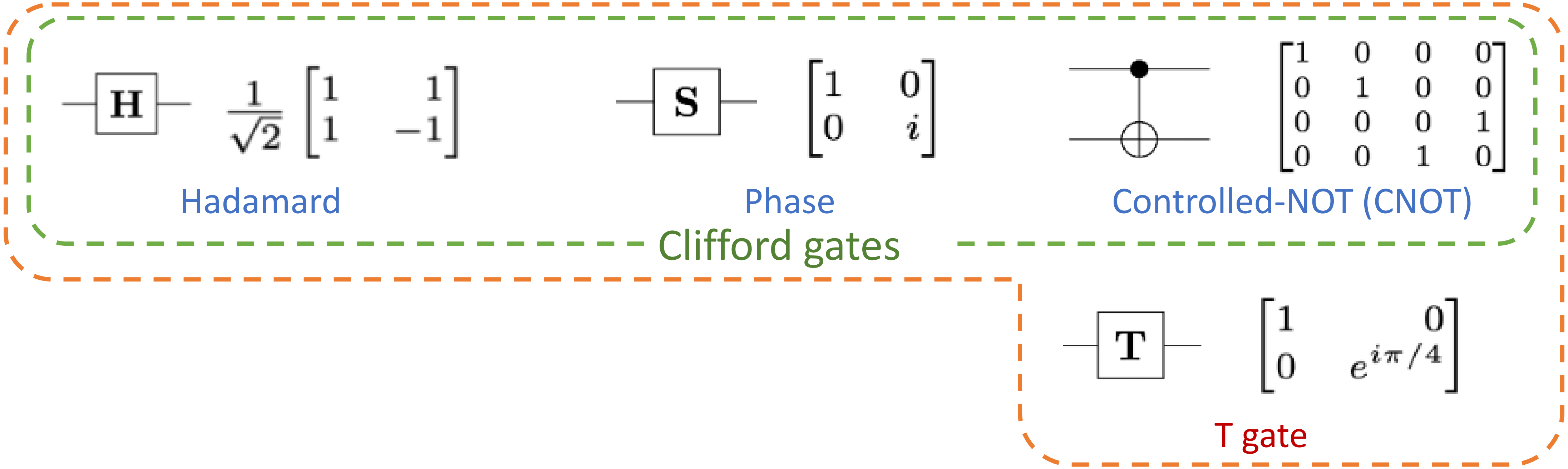
  - Measurement: we get 0 with probability $|\alpha|^2$, and get 1 with probability $|\beta|^2$
- General n qubit space: tensor product of n multiple single qubit

$$|i_1 i_2 \cdots i_n\rangle = |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \in \mathbb{C}^{2^n} / \|\cdot\|_2$$

  - We use $|j\rangle$ $(0 \le j \le 2^n - 1)$ to represent the orthonormal basis of the Hilbert space
  - $|v\rangle = \sum_{j=0}^{2^n-1} \alpha_j |j\rangle = (\alpha_0, \alpha_1, \dots, \alpha_{2^n-1})^\top$
  - Measurement: we get j with probability $|\alpha_j|^2$ (but destroy the superposition)

Quantum gates

- Each gate is a unitary operator $G \in \mathbb{C}^{2^m \times 2^m}$ applying to m qubits ($GG^\dagger = G^\dagger G = I$)
- **Solovay-Kitaev:** any large unitary operator U can be (approximately) expressed as a product of small unitary gates acting on one or two qubits (i.e., 2×2or 4×4 matrices)



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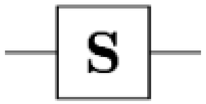
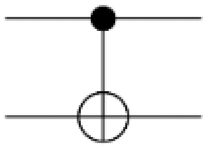
$$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Hadamard



$$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$$

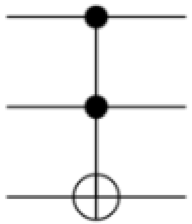
Phase



$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

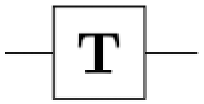
Controlled-NOT (CNOT)

Clifford gates



$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Toffoli (CCNOT)



$$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$$

T gate

Practical quantum advantages

Can we solve a practically useful problem on a quantum computer faster than on a classical computer?

- Quantum chemistry may be the right place to look
- The basic problem: the ground state energy (lowest eigenvalue of H)
- Compare with classical algorithms: need very high accuracy
  - Density functional theory can get to precision of 2-3 $\mathrm{kcal} \cdot \mathrm{mol}^{-1}$ (Bogojesk et al. ’20)
  - Chemical accuracy: 1 $\mathrm{kcal} \cdot \mathrm{mol}^{-1}$
- We should care **very much** about how the cost of the quantum algorithm scales with precision

Example: from eigenstate to eigenvalue

- The precision scaling is usually more complicated in the quantum setting
- For a Hamiltonian $H = \sum_i \alpha_i P_i$ (P_i is a multi-qubit Pauli operator), given an eigenstate $|\Psi\rangle$, how to get the eigenvalue λ?
- **Classical computer:** $\lambda = \langle\Psi|H|\Psi\rangle$ (one matrix-vector multiplication, one inner-product, machine precision)
- **Quantum computer:** measure each Pauli operator, obtain 0/1 outputs, take average to get $\langle\Psi|P_i|\Psi\rangle$, then add up all Pauli terms

Example: from eigenstate to eigenvalue

Consider measuring $X \otimes X$

- We can apply $\mathbf{H} \otimes \mathbf{H}$ to the quantum state, so that we can now measure in the computational basis ($Z \otimes Z$):

$$\langle\Psi|X \otimes X|\Psi\rangle = \langle\Psi|(\mathbf{H} \otimes \mathbf{H})Z \otimes Z(\mathbf{H} \otimes \mathbf{H})|\Psi\rangle$$

$$X = \begin{bmatrix} & 1 \\ 1 & \end{bmatrix}, \qquad H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \qquad Z = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix}$$

- We will get a random output $\hat{m} \in \{0,1\}$, such that

$$\mathbb{E}\left[(-1)^{\hat{m}}\right] = \langle\Psi|X \otimes X|\Psi\rangle$$

- Taking average over N_s samples, the variance is $\mathcal{O}(1/N_s)$ i.e. $\mathcal{O}(\epsilon^{-2})$ samples for ϵ-accuracy

Example: from eigenstate to eigenvalue

- We need to do this for all terms. Can measure some of them simultaneously (e.g. for $X \otimes X$ and $Z \otimes Z$ because they commute), but this creates correlated error
- The total number of measurements to reach ϵ precision for H is

$$\frac{(\text{some norm of } H)^2}{\epsilon^2}$$

And we require roughly this many copies of $|\Psi\rangle$ (measurement destroys the superposition)

- Quantum phase estimation can do the same by evolving with H for $\mathcal{O}(\epsilon^{-1})$ time (Heisenberg limit), with a single copy of $|\Psi\rangle$

The Heisenberg limit

- The quantum version of parameter estimation: estimate θ from parameterized quantum state $\rho(\theta)$, $\|\mathrm{d}\rho/\mathrm{d}\theta\|_1 \leq 1$ (here $\|\cdot\|_1$ is the trace norm)
- Information-theoretic lower bound: this requires $\Omega(\epsilon^{-2})$ samples (the standard quantum limit, SQL)
- Beyond-SQL example: estimate eigenvalue to precision ϵ using QPE with exact eigenstate requires runtime $\mathcal{O}(\epsilon^{-1})$
- Information theoretic lower bound: this requires $\Omega(\epsilon^{-1})$ total evolution time (how long we evolve with H). This is the Heisenberg limit

Toward Heisenberg-Limited Spectroscopy with Multiparticle Entangled States

D. LEIBFRIED, M. D. BARRETT, T. SCHAETZ, J. BRITTON, J. CHIAVERINI, W. M. ITANO, J. D. JOST, C. LANGER, AND D. J. WINELAND Authors Info & Affiliations

SCIENCE • 4 Jun 2004 • Vol 304, Issue 5676 • pp. 1476-1478 • DOI: 10.1126/science.1097576

Algorithms for different development stages of QC

NISQ

FTQC

Variational algorithms (VQE, QAOA…) (ϵ^{-2})

- Few ancillary qubits
- Short circuit depth
- Small number of repetitions
- Proper error mitigation and correction strategies

Fully fault-tolerant algorithms (ϵ^{-1})

- Total runtime dominated by non-Clifford gates)
- Parallelization
- energy consumption
- …

No universally accepted definition of EFT regime. See recent discussion (Katabarwa et al. ’24)

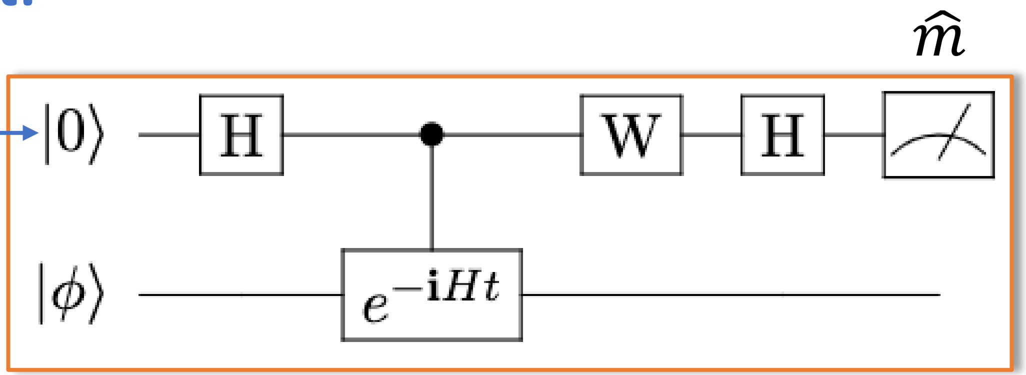
Quantum eigenvalue problem

- We have a target a Hamiltonian $H = \sum_{k=0}^{N-1} \lambda_k |E_k\rangle\langle E_k|$ (a Hermitian matrix of size $N \times N$)
- $\lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{N-1}$, λ_0 is the ground state energy, and $|E_0\rangle$ is the ground state
- $|\phi\rangle$ is an initial guess for the ground state
- We can apply control-$e^{-\mathbf{i}\tau H}$ where τ is a rescaling factor

Single-ancilla phase estimation

The Hadamard test circuit:

One ancilla qubit

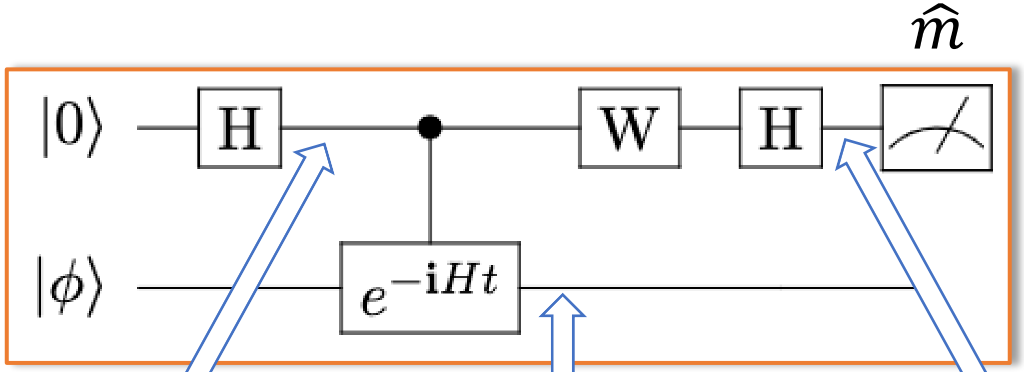


- From the measurement outcome $\hat{m}$ we can compute the expectation value $\langle\phi|e^{-\mathbf{i}tH}|\phi\rangle$
- Real and imaginary parts are computed separately (corresponding to $W = I$ and $W = S^\dagger$ respectively)

Single-ancilla phase estimation

The Hadamard test circuit:

For the real part:



$$\frac{1}{\sqrt{2}}(|0\rangle|\phi\rangle + |1\rangle|\phi\rangle)$$

$$\frac{1}{\sqrt{2}}(|0\rangle|\phi\rangle + |1\rangle e^{-\mathbf{i}Ht}|\phi\rangle)$$

$$\frac{1}{2}\Big(|0\rangle(|\phi\rangle + e^{-\mathbf{i}Ht}|\phi\rangle) + |1\rangle(|\phi\rangle - e^{-\mathbf{i}Ht}|\phi\rangle)\Big)$$

$$\mathbf{H} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

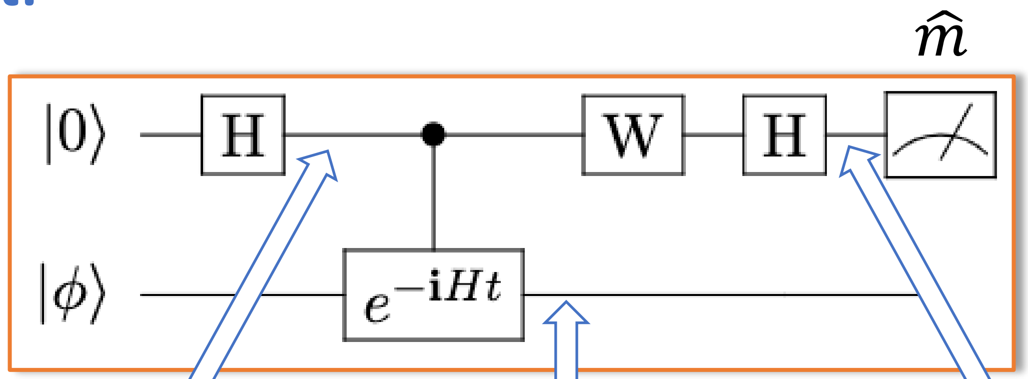
$$|0\rangle \mapsto \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$|1\rangle \mapsto \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

Single-ancilla phase estimation

The Hadamard test circuit:

For the real part:



$$\frac{1}{\sqrt{2}}(|0\rangle|\phi\rangle + |1\rangle|\phi\rangle)$$

$$\frac{1}{\sqrt{2}}(|0\rangle|\phi\rangle + |1\rangle e^{-\mathbf{i}Ht}|\phi\rangle)$$

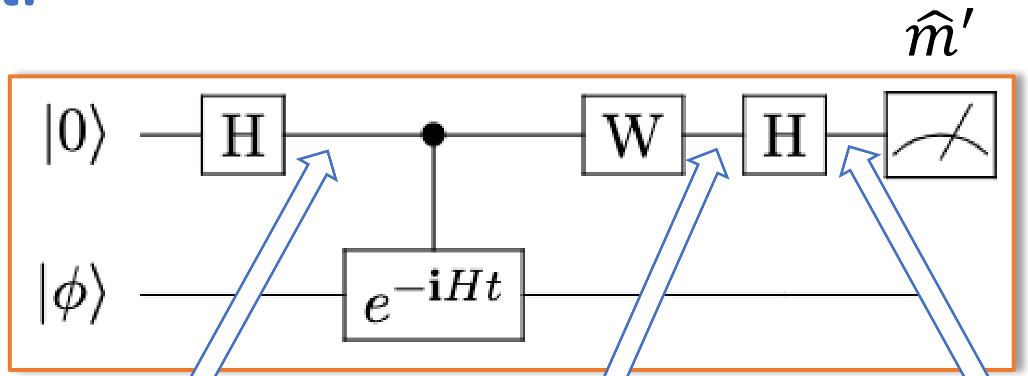
$$\frac{1}{2}\Big(|0\rangle(|\phi\rangle + e^{-\mathbf{i}Ht}|\phi\rangle) + |1\rangle(|\phi\rangle - e^{-\mathbf{i}Ht}|\phi\rangle)\Big)$$

$$\mathbb{E}[(-1)^{\hat{m}}] = \frac{1}{4}\left(\left\||\phi\rangle + e^{-\mathbf{i}Ht}|\phi\rangle\right\|^2 - \left\||\phi\rangle - e^{-\mathbf{i}Ht}|\phi\rangle\right\|^2\right) = \mathrm{Re}(\langle\phi|e^{-\mathbf{i}Ht}|\phi\rangle)$$

Single-ancilla phase estimation

The Hadamard test circuit:

For the imaginary part:



$$\frac{1}{\sqrt{2}}(|0\rangle|\phi\rangle + |1\rangle|\phi\rangle)$$

$$\frac{1}{\sqrt{2}}(|0\rangle|\phi\rangle - \mathbf{i}|1\rangle e^{-\mathbf{i}Ht}|\phi\rangle)$$

$$\frac{1}{2}\Big(|0\rangle\big(|\phi\rangle - \mathbf{i}e^{-\mathbf{i}Ht}|\phi\rangle\big) + |1\rangle\big(|\phi\rangle + \mathbf{i}e^{-\mathbf{i}Ht}|\phi\rangle\big)\Big)$$

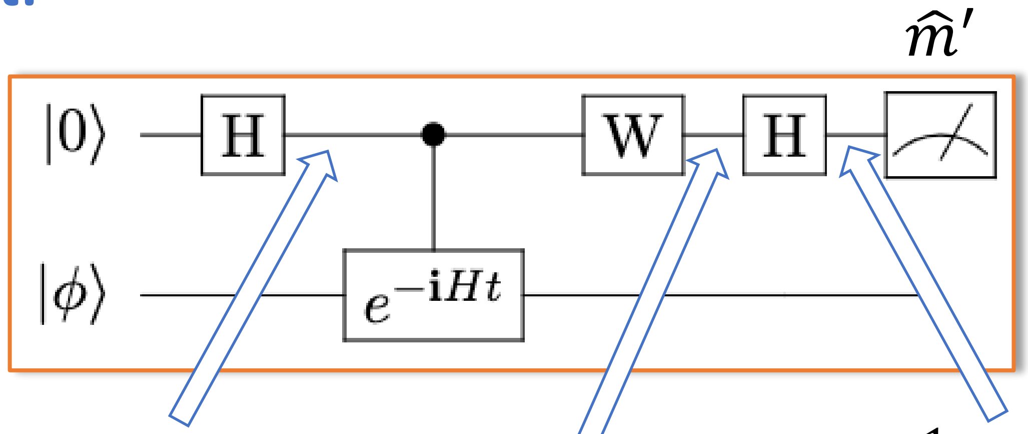
$$\mathbf{S}^\dagger = \begin{bmatrix} 1 & \\ & -\mathbf{i} \end{bmatrix}$$

$$|0\rangle \mapsto |0\rangle$$
$$|1\rangle \mapsto -\mathbf{i}|1\rangle$$

Single-ancilla phase estimation

The Hadamard test circuit:

For the imaginary part:



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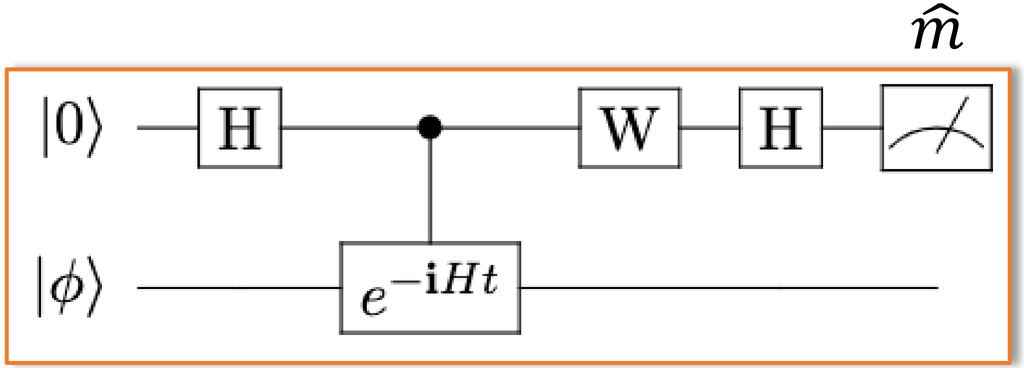
$$\frac{1}{2}\Big(|0\rangle\big(|\phi\rangle - \mathbf{i}e^{-\mathbf{i}Ht}|\phi\rangle\big) + |1\rangle\big(|\phi\rangle + \mathbf{i}e^{-\mathbf{i}Ht}|\phi\rangle\big)\Big)$$

$$\mathbb{E}\big[(-1)^{\widehat{m}'}\big] = \frac{1}{4}\left(\big\||\phi\rangle - \mathbf{i}e^{-\mathbf{i}Ht}|\phi\rangle\big\|^2 - \big\||\phi\rangle + \mathbf{i}e^{-\mathbf{i}Ht}|\phi\rangle\big\|^2\right) = \mathrm{Im}\big(\langle\phi|e^{-\mathbf{i}Ht}|\phi\rangle\big)$$

Single-ancilla phase estimation

The Hadamard test circuit:



- For any t we can estimate $\langle\phi|e^{-\mathbf{i}Ht}|\phi\rangle$ by

$$S(t) = \langle\phi|e^{-\mathbf{i}Ht}|\phi\rangle + e(t)$$

  where $e(t)$ is the statistical noise

- The signal contains eigenvalue information

$$\langle\phi|e^{-\mathbf{i}Ht}|\phi\rangle = \sum_k e^{-\mathbf{i}\lambda_k t}\, |\langle\phi|E_k\rangle|^2$$

Signal processing problem

Single frequency recovery

From the Hadamard test circuit we can generate $S(t), t \geq 0$

$$S(t) = \sum_k e^{-\mathbf{i}\lambda_k t} |\langle \phi | E_k \rangle|^2 + e(t)$$

The simplest case: $|\phi\rangle = |E_0\rangle$ and $S(t) = e^{-\mathbf{i}\lambda_0 t} + e(t)$

We want to estimate $\lambda_0 \in [-1,1)$ (rescaling the Hamiltonian properly) to precision ϵ

- We can take $t = \pi/2$, average out the noise, and estimate E_0 with $\mathcal{O}(\epsilon^{-2})$ samples
- **Caution:** if H is not rescaled (i.e. $\lambda_0 \in [-F, F]$), there could be the "aliasing effect"
  - → We need to choose different t and use binary search to locate λ_0 (https://theory.epfl.ch/kapralov/madalgo15/lec1.pdf)

Single frequency recovery

From the Hadamard test circuit we can generate $S(t), t \geq 0$

$$S(t) = \sum_k e^{-\mathbf{i}\lambda_k t} \, |\langle\phi|E_k\rangle|^2 + e(t)$$

The simplest case: $|\phi\rangle = |E_0\rangle$ and $S(t) = e^{-\mathbf{i}\lambda_0 t} + e(t)$

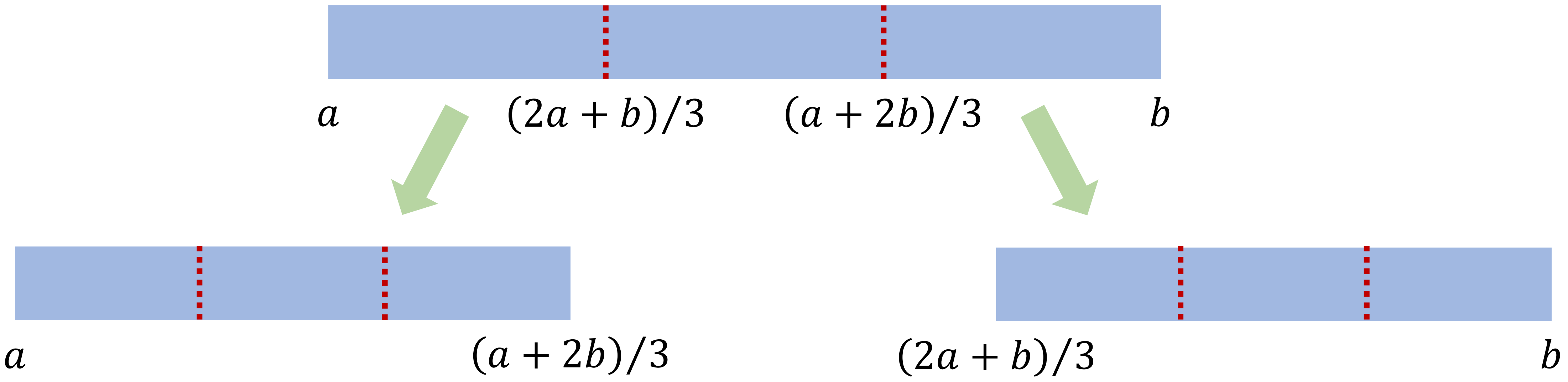
We want to estimate $\lambda_0 \in [-1,1)$ (rescaling the Hamiltonian properly) to precision ϵ

- We can take $t = \pi/2$, average out the noise, and estimate E_0 with $\mathcal{O}(\epsilon^{-2})$ samples
- I will outline a method (Kimmel-Low-Yoder '15) that uses
  - $\mathcal{O}(\log(\epsilon^{-1}))$ samples
  - $\mathcal{O}(\epsilon^{-1})$ total evolution time
- Suppose our samples are $S(t_1), \dots, S(t_{N_S})$, then the total evolution time is $t_1 + \cdots + t_{N_S}$

Robust phase estimation: algorithm

Suppose we know $a \leq -\lambda_0 \leq b$. We want to determine

1. $a \leq -\lambda_0 \leq \frac{a+2b}{3}$
2. $\frac{2a+b}{3} \leq -\lambda_0 \leq b$



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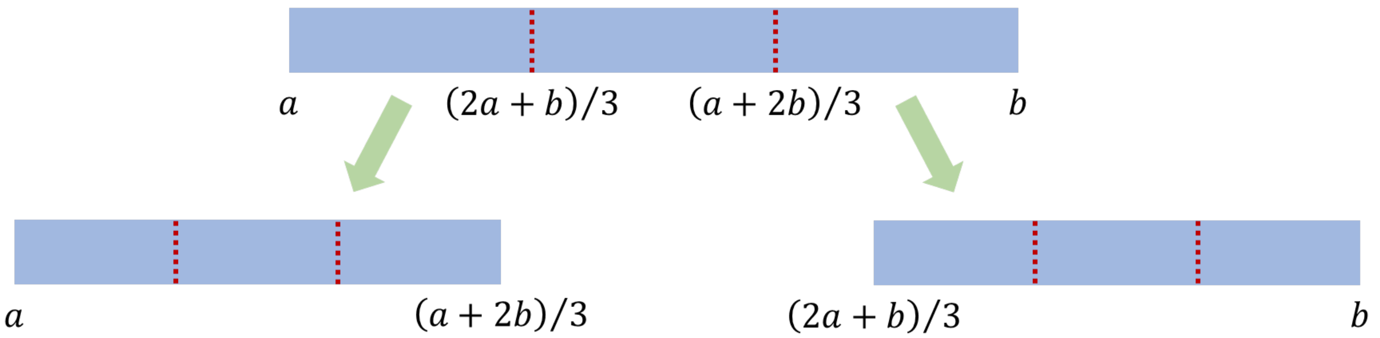


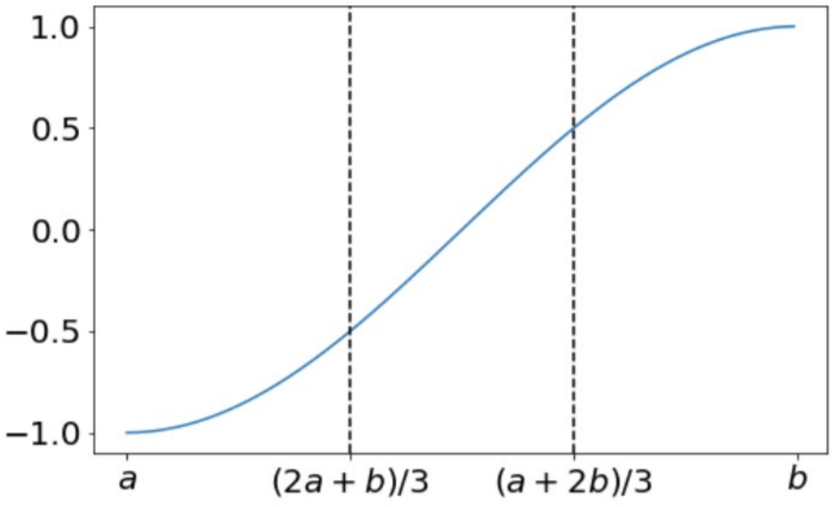
- If we can do that then we can reduce the uncertainty by $1/3$ at each step
- $\mathcal{O}(\log(\epsilon^{-1}))$ iterations are needed for ϵ precision

Robust phase estimation: algorithm

Define a function

$$f_{a,b}(-\lambda_0) := \sin\left(\frac{\pi}{b-a}\left(-\lambda_0 - \frac{a+b}{2}\right)\right) = \mathrm{Im}\left(S(t^*)e^{\mathbf{i}\phi^*}\right)$$

where $t^* = \frac{\pi}{b-a}$ and $\phi^* = -\frac{(a+b)\pi}{2(b-a)}$



- If $f_{a,b}(-\lambda_0) \leq \frac{1}{2}$, then $a \leq -\lambda_0 \leq \frac{a+2b}{3}$
- If $f_{a,b}(-\lambda_0) \geq -\frac{1}{2}$, then $\frac{2a+b}{3} \leq -\lambda_0 \leq b$
- Evaluating $f_{a,b}(-\lambda_0)$ to precision $\frac{1}{2}$ suffices
- Can get confidence level $1 - \delta'$ with $\mathcal{O}(\log(1/\delta'))$ samples

Robust phase estimation: costs

- In the last iteration, $b_K - a_K = \mathcal{O}(\epsilon)$, and thus $t_K^* = \frac{\pi}{b_K - a_K} = \mathcal{O}(\epsilon^{-1})$
- The cost of the last step is $\mathcal{O}(t^* \log(1/\delta')) = \mathcal{O}(\epsilon^{-1} \log(1/\delta'))$
- In the $(K-1)$-th iteration, $b_{K-1} - a_{K-1} = \frac{3}{2}(b_K - a_K)$, and $t_{K-1}^* = \frac{2}{3} t_K^*$
- Therefore, the total cost is

$$\mathcal{O}(\epsilon^{-1} \log(1/\delta')) \times \left(1 + \frac{2}{3} + \left(\frac{2}{3}\right)^2 + \left(\frac{2}{3}\right)^3 + \cdots\right) = \mathcal{O}(\epsilon^{-1} \log(1/\delta'))$$

- If we take $\delta' = \mathcal{O}(\delta / \log(\epsilon^{-1}))$, then by union bound, the overall success probability is $1 - \delta$
- Total evolution time is $\mathcal{O}(\epsilon^{-1} \log(1/\delta))$, and the sample complexity is $\mathcal{O}(\log(\epsilon^{-1}))$
- Robust to noise (need $|e(t)| \leq 1/2$ w.p. $2/3$)

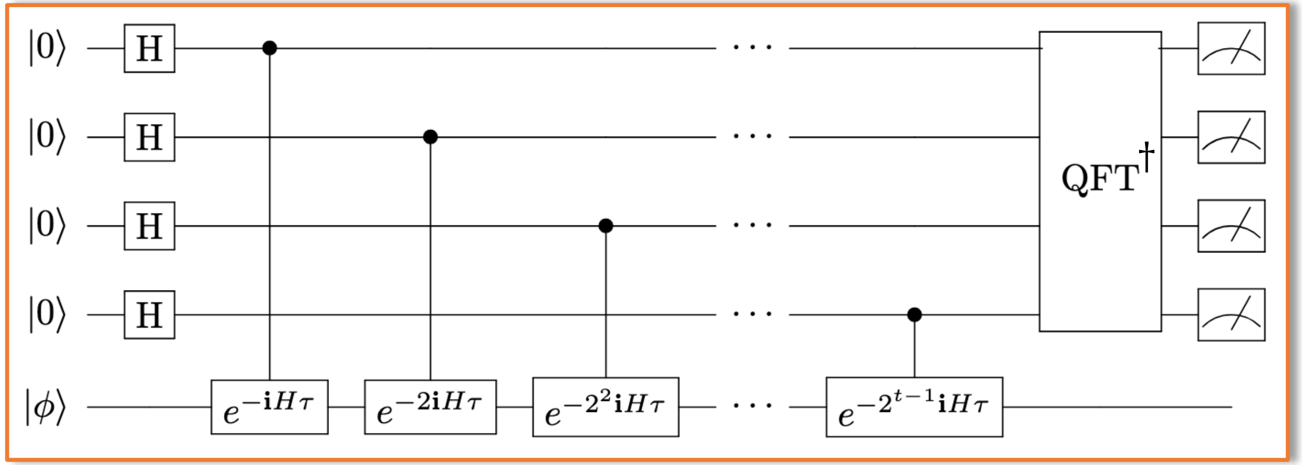
Summary: single-ancilla phase estimation

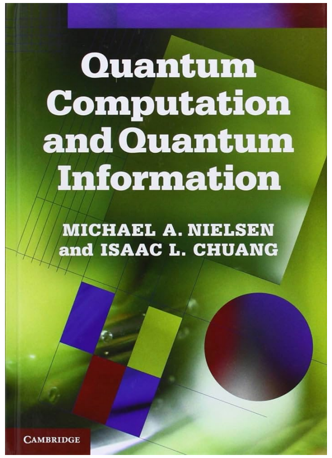
- We can use the Hadamard test circuit to estimate the eigenvalue given the corresponding eigenstate with Heisenberg-limited scaling. Itis also robust to constant amount of noise

- We can do the above with $\mathcal{O}(\epsilon^{-1}\log(1/\delta))$ total evolution time to get confidence level $1-\delta$. We will still get correct estimate when $|e(t)| \leq 1/2$ w.p. $2/3$

Quantum phase estimation

Kitaev's QPE (textbook version)





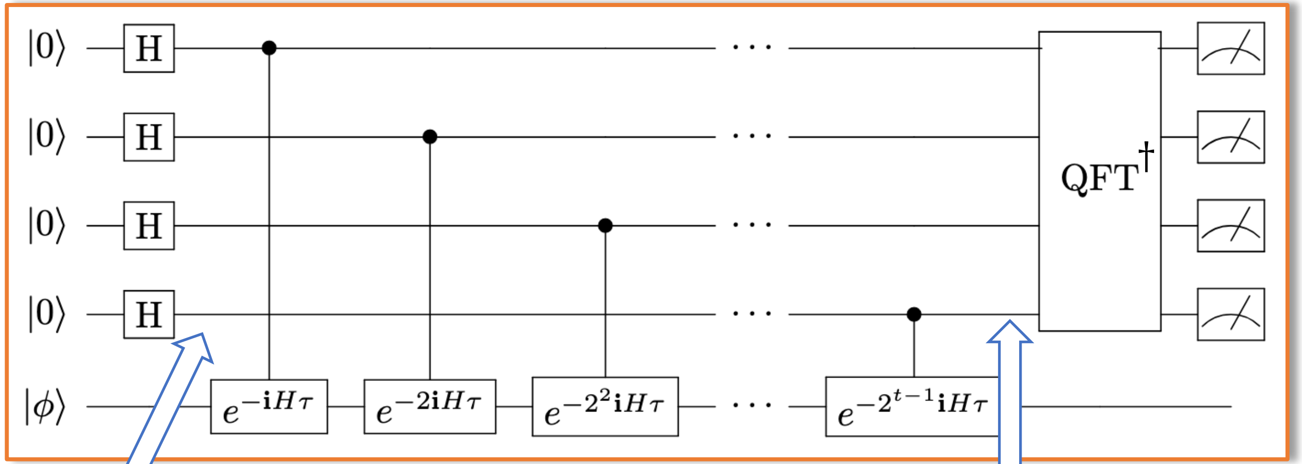
Alexei Kitaev

- Two registers: energy register (r qubits) and state register ($\log N$ qubits)
- Measuring the energy register yields a bit string $\widehat{m}$, which we convert to an energy estimate

$$\tau\hat{\lambda} = 2\pi\widehat{m}/2^r$$

Quantum phase estimation

Kitaev's QPE (textbook version)



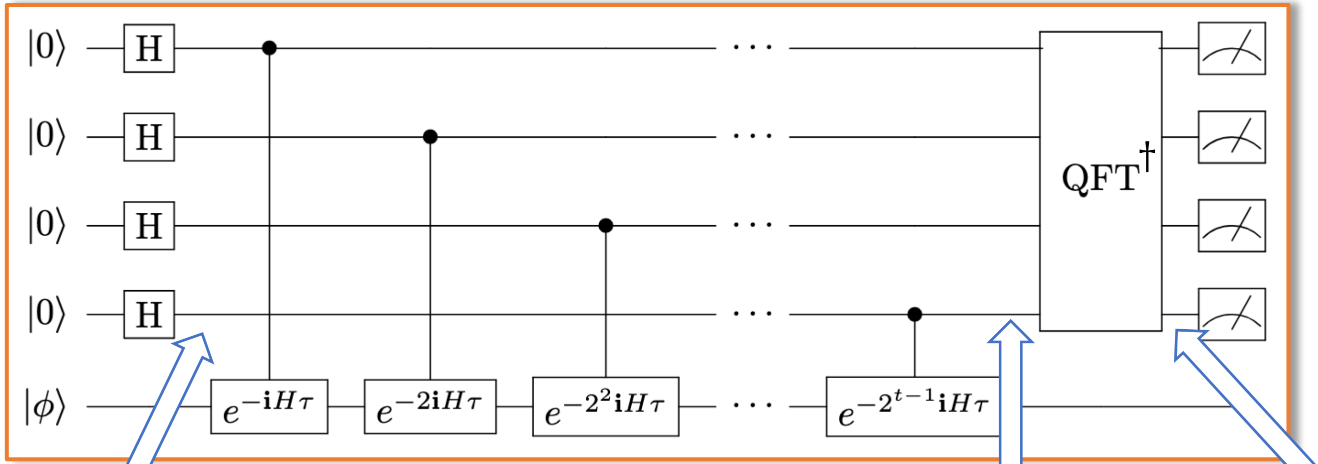
$$\frac{1}{\sqrt{2^r}}\sum_{j=0}^{2^r-1}|j\rangle\,|\phi\rangle$$

$$\frac{1}{\sqrt{2^r}}\sum_{j=0}^{2^r-1}|j\rangle e^{-\mathbf{i}j\tau H}|\phi\rangle$$

$$(\mathbf{H}\otimes\mathbf{H})|0\rangle\otimes|0\rangle = |++\rangle = \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle)$$

Quantum phase estimation

Kitaev's QPE (textbook version)



$$\frac{1}{\sqrt{2^r}}\sum_{j=0}^{2^r-1}|j\rangle\,|\phi\rangle$$

$$\frac{1}{\sqrt{2^r}}\sum_{j=0}^{2^r-1}|j\rangle e^{-\mathbf{i}j\tau H}|\phi\rangle$$

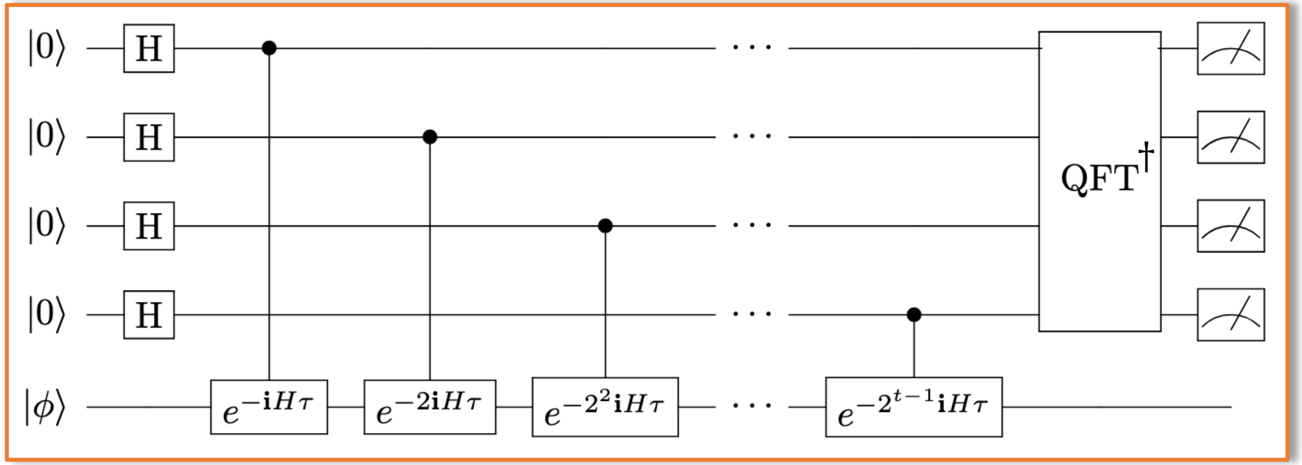
$$\frac{1}{2^r}\sum_{j=0}^{2^r-1}\sum_{m=0}^{2^r-1}e^{2\pi\mathbf{i}\frac{jm}{2^r}}|m\rangle\, e^{-\mathbf{i}j\tau H}|\phi\rangle$$

$$\mathrm{QFT}|j\rangle=\frac{1}{\sqrt{2^r}}\sum_{m=0}^{2^r-1}e^{-2\pi\mathbf{i}\frac{jm}{2^r}}|m\rangle$$

$$\mathrm{QFT}^\dagger|j\rangle=\frac{1}{\sqrt{2^r}}\sum_{m=0}^{2^r-1}e^{2\pi\mathbf{i}\frac{jm}{2^r}}|m\rangle$$

Quantum phase estimation

Kitaev's QPE (textbook version)



- Let $|\phi\rangle = \sum_k c_k |E_k\rangle$

$$\frac{1}{2^r}\sum_{j=0}^{2^r-1}\sum_{m=0}^{2^r-1} e^{2\pi \mathbf{i}\frac{jm}{2^r}}|m\rangle\, e^{-\mathbf{i}j\tau H}|\phi\rangle = \sum_k c_k \sum_{m=0}^{2^r-1}|m\rangle \frac{1}{2^r}\sum_{j=0}^{2^r-1} e^{\mathbf{i}2\pi jm/2^r - \mathbf{i}j\tau\lambda_k}|E_k\rangle$$

Quantum phase estimation

$$\sum_k c_k \sum_{m=0}^{2^r-1} |m\rangle \underbrace{\frac{1}{2^r} \sum_{j=0}^{2^r-1} e^{\mathbf{i}2\pi jm/2^r - \mathbf{i}j\tau\lambda_k}}_{\Gamma(2\pi m/2^r - \tau\lambda_k)} |E_k\rangle$$

- $\Gamma(\theta) \coloneqq 2^{-r} \sum_{j=0}^{2^r-1} e^{\mathbf{i}j\theta} \approx \delta(\theta)$ i.e. the Dirac delta function
- Thus, the quantum state before measurement is roughly equal to:

Energy register

$$\approx \sum_k c_k \sum_{m=0}^{2^r-1} |m\rangle \delta(2\pi m/2^r - \tau\lambda_k) |E_k\rangle = \sum_k c_k \left| \frac{2^r \tau\lambda_k}{2\pi} \right\rangle |E_k\rangle$$

- This is the idealized version of QPE

Quantum phase estimation

- The kernel function $\Gamma(\theta)$ is

$$\Gamma(\theta) := \frac{1}{2^r}\sum_{j=0}^{2^r-1} e^{\mathbf{i}j\theta} = \frac{1}{2^r}\frac{1-e^{\mathbf{i}2^r\theta}}{1-e^{\mathbf{i}\theta}}$$

- The quantum state before measurement is precisely equal to

$$\sum_k c_k \sum_{m=0}^{2^r-1} |m\rangle\Gamma(2\pi m/2^r - \tau\lambda_k)|E_k\rangle$$

- Measuring the energy register $|m\rangle$ yields m with probability

$$\Pr[\widehat{m} = m] = \sum_k |c_k|^2 |\Gamma(2\pi m/2^r - \tau\lambda_k)|^2$$

Quantum phase estimation

$$\Pr[\hat{m} = m] = \sum_k |c_k|^2 |\Gamma(2\pi m/2^r - \tau\lambda_k)|^2$$

- Imagine there is a random variable $\hat{k}$ such that $\Pr\left[\hat{k} = k\right] = |c_k|^2$
- Then,

$$\Pr[\hat{m} = m] = \sum_k \Pr\left[\hat{m} = m \mid \hat{k} = k\right] \cdot \Pr\left[\hat{k} = k\right]$$

where

$$\Pr\left[\hat{m} = m \mid \hat{k} = k\right] = |\Gamma(2\pi m/2^r - \tau\lambda_k)|^2$$

the probability of getting energy measurement $\hat{m}$ given an eigenstate $|E_k\rangle$

- We will show that $\Pr\left[\hat{m} = m \mid \hat{k} = k\right]$ is concentrated around $\frac{2^r \tau \lambda_k}{2\pi}$

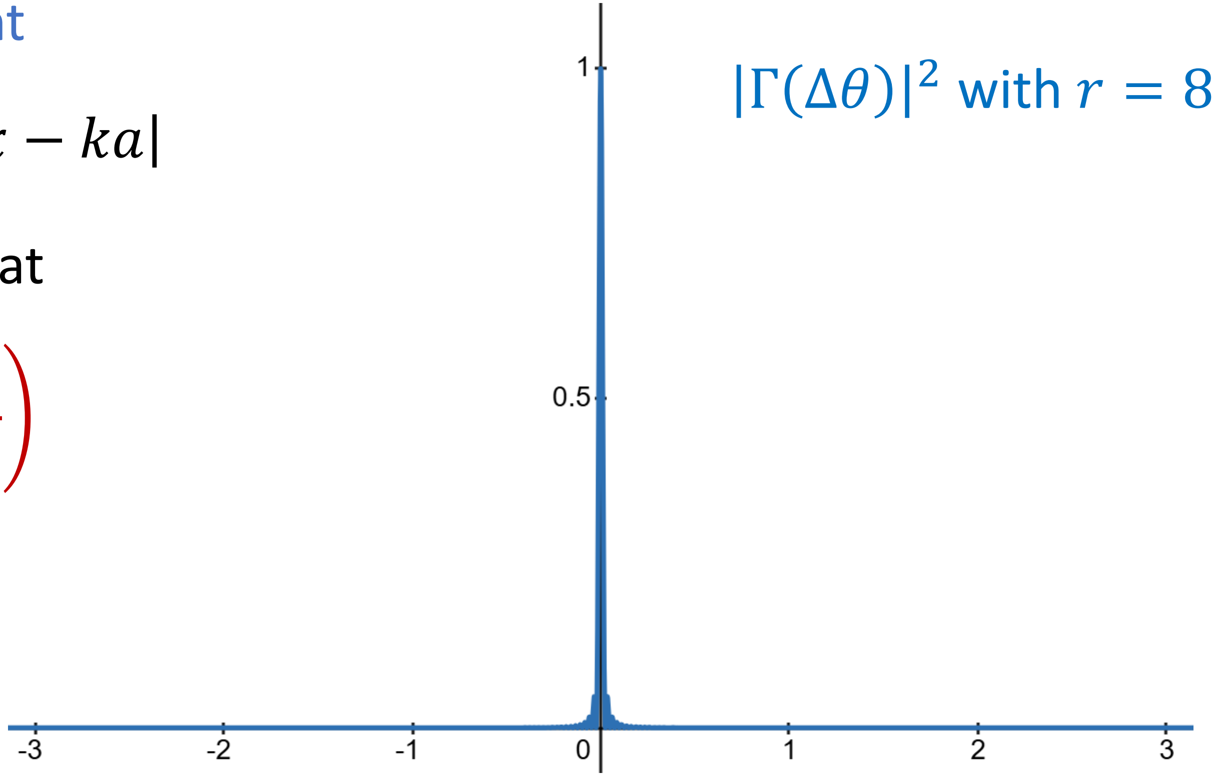
Quantum phase estimation

- Let $\Delta\theta \coloneqq 2\pi m/2^r - \tau\lambda_k$

$$\Pr\left[\hat{m} = m \mid \hat{k} = k\right] = |\Gamma(\Delta\theta)|^2 = \frac{1}{2^{2r}} \frac{\left|1 - e^{\mathrm{i}2^r\Delta\theta}\right|^2}{|1 - e^{\mathrm{i}\Delta\theta}|^2} = \frac{1}{4^r} \frac{\sin^2(2^{r-1}\Delta\theta)}{\sin^2(\Delta\theta/2)}$$

- Let $\tau\hat{\lambda} = 2\pi\hat{m}/2^r$ be the energy measurement
- Recall the wrap-around distance $|x|_a = \min_{k\in\mathbb{Z}} |x - ka|$
- The concentration of the $\Gamma(\Delta\theta)$ guarantees that

$$\Pr\left[\left|\tau\hat{\lambda} - \tau\lambda_k\right|_{2\pi} > \epsilon \,\middle|\, \hat{k} = k\right] = \mathcal{O}\left(\frac{1}{2^r\epsilon}\right)$$



Quantum phase estimation: Thought experiment

- For an initial state $|\phi\rangle = \sum_k c_k |E_k\rangle$, we first sample $\hat{k} = k$ w.p. $|c_k|^2$
- An energy estimate $\tau\hat{\lambda}$ is generated by QPE that is ϵ-close to $\tau\lambda_k$ with probability at least

$$1 - \mathcal{O}\left(\frac{1}{2^r \epsilon}\right)$$

- In this sense we are sampling from the spectrum of τH, and each sample is close to an (rescaled) eigenvalue with large probability (exact in the limit of $r \to \infty$)

Proof of the concentration of the kernel

$$\Pr\left[\left|\tau\hat{\lambda} - \tau\lambda_k\right|_{2\pi} > \epsilon \,\middle|\, \hat{k} = k\right] = \mathcal{O}\left(\frac{1}{2^r \epsilon}\right)$$

- Let $\epsilon := 2\pi\ell/2^r$

$$\Pr\left[\left|\frac{2\pi\widehat{m}}{2^r} - \tau\lambda_k\right|_{2\pi} > \frac{2\pi\ell}{2^r} \,\middle|\, \hat{k} = k\right] = \Pr\left[\left|\widehat{m} - \frac{2^r\tau\lambda_k}{2\pi}\right|_{2^r} > \ell \,\middle|\, \hat{k} = k\right]$$

$$= \sum_{\substack{0 \le m < 2^r - 1: \\ \left|m - \frac{2^r\tau\lambda_k}{2\pi}\right|_{2^r} > \ell}} \frac{1}{4^r} \frac{\sin^2\left(2^{r-1}(2\pi m/2^r - \tau\lambda_k)\right)}{\sin^2((2\pi m/2^r - \tau\lambda_k)/2)}$$

$$\le \sum_{\substack{0 \le m < 2^r - 1: \\ \left|m - \frac{2^r\tau\lambda_k}{2\pi}\right|_{2^r} > \ell}} \frac{1}{4^r} \frac{1}{\sin^2((2\pi m/2^r - \tau\lambda_k)/2)}$$

Proof of the concentration of the kernel

- Since $\left|\sin\left(\frac{x}{2}\right)\right| \geq \frac{|x|_{2\pi}}{\pi}$, we have

$$\begin{aligned}
\sum_{\substack{0\leq m<2^r-1:\\ \left|m-\frac{2^r\tau\lambda_k}{2\pi}\right|_{2^r}>\ell}} \frac{1}{4^r}\frac{1}{\sin^2((2\pi m/2^r-\tau\lambda_k)/2)} &\leq \sum_{\substack{0\leq m<2^r-1:\\ \left|m-\frac{2^r\tau\lambda_k}{2\pi}\right|_{2^r}>\ell}} \frac{1}{4^r}\frac{\pi^2}{|2\pi m/2^r-\tau\lambda_k|_{2\pi}^2} \\
&= \sum_{\substack{0\leq m<2^r-1:\\ \left|m-\frac{2^r\tau\lambda_k}{2\pi}\right|_{2^r}>\ell}} \frac{1}{4|m-2^{r-1}\tau\lambda_k/\pi|_{2^r}^2} \\
&\leq 2\cdot\frac{1}{4}\sum_{n=\ell}^{\infty}\frac{1}{n^2} \\
&\leq \frac{1}{2(\ell-1)} = \mathcal{O}\left(\frac{1}{2^r\epsilon}\right)
\end{aligned}$$

■

Summary: quantum phase estimation

- QPE returns an energy estimate that is close to a random eigenvalue of τH with large probability

- QPE returns an energy estimate $\hat{\lambda}$ that is ϵ-close to a random $\tau\lambda_{\hat{k}}$ with probability at least $1 - \mathcal{O}(2^{-r}\epsilon^{-1})$, where $\hat{k} = k$ with probability $|c_k|^2$
- QPE applies the controlled-$e^{-\mathbf{i}\tau H}$ 2^r times in total, where $2^r = \mathcal{O}(\epsilon^{-1})$ for a constant success probability

Use QPE for ground state energy estimation

- **Goal:** estimate λ_0 with ϵ precision, given that the initial state satisfies $|c_0|^2 \geq \eta$
- To ensure that the energy we get correspond to the ground state rather than excited states (i.e. $\hat{k} = 0$):
  - Generate $\mathcal{O}(1/|c_0|^2) = \mathcal{O}(\eta^{-1})$ samples $\hat{\lambda}$
  - Take the minimum
- The probability of all the samples the energy estimate being close to some eigenvalue is

$$\left(1 - \mathcal{O}\left(\frac{1}{2^r \epsilon}\right)\right)^{\mathcal{O}(1/|c_0|^2)} = \Omega(1)$$

if we take $2^r \epsilon = \Omega(1/|c_0|^2) = \Omega(\eta^{-1})$, i.e. $r = \Omega(\log(\eta^{-1}\epsilon^{-1}))$

Use QPE for ground state energy estimation

- **Goal:** estimate λ_0 with ϵ precision, given that the initial state satisfies $|c_0|^2 \geq \eta$

- **Total cost:**

$$\mathcal{O}\left(\frac{1}{|c_0|^2}\right) \times \Theta\left(\frac{1}{\epsilon |c_0|^2}\right) = \mathcal{O}(\eta^{-2}\epsilon^{-1})$$

Heisenberg-limited scaling

- **Circuit depth:**

$$2^r = \Theta(\eta^{-1}\epsilon^{-1}) \geq \frac{\pi}{\epsilon}$$

- **Number of ancilla qubits:**

$$r = \Theta(\log(\eta^{-1}\epsilon^{-1}))$$

Two different approaches

	Heisenberg limit	Allow $p_0 < 1$	#ancilla	Circuit depth
Hadamard test	✗	✗	1	Short
Kitaev's QPE	✓	✓	Many	Long

Can we design an algorithm with all these good properties?

Early fault-tolerant (EFT) phase estimation

- Post-Kitaev type: (Lin-Tong '22; Dong et al. '22; **Z.** et al. '22; Ding-Lin '23; Wang et al. '23; Ni et al. '23; Ding et al. '24; Yi et al. '24; Castaldo-Corni '25…)
- Quantum Krylov subspace type: (Parrish-McMahon '19; Stair et al. '20; Epperly et al. '22; Klymko et al. '22; Shen et al. '23; Li et al. '23; Ding et al. '24...)
- Experimental relevance: (Blunt et al. '23; Kiss et al. '24…)