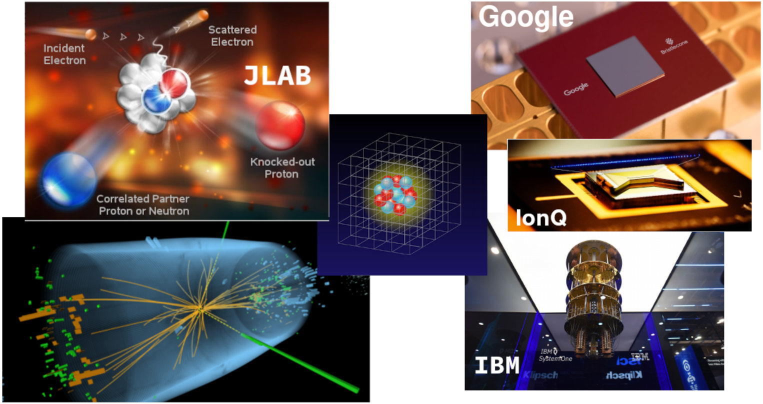
Quantum Simulations - I

Alessandro Roggero

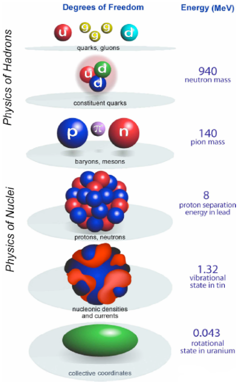


Trento Institute for
Fundamental Physics
and Applications

NNP Summer School

MIT – 18 July, 2022

Introduction: the nuclear many-body problem



Bertsch, Dean, Nazarewicz (2007)

$$\mathcal{L}_{QCD} = \sum_f \overline{\Psi}_f \left(i\gamma^\mu D_\mu - m_f\right)\Psi_f - \frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a$$

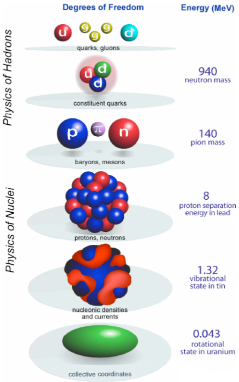
- in **principle** can derive everything from here

Effective theory for nuclear systems

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i,j} V_{ij} + \frac{1}{6}\sum_{i,j,k} W_{ijk} + \cdots$$

- easier to deal with than the QCD lagragian
- describes correctly low energy physics
- non-perturbative $\rightarrow$ still very challenging

Introduction: the nuclear many-body problem



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Two main goals:

- energy spectrum (eigenvalues)
- scattering cross sections/response to external probes (eigenvectors)

Why is this difficult?

GOAL: compute the ground state energy with error at most ϵ

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PROBLEM: large dimension of the Hilbert space $N = dim(\mathcal{H}) > 4^A$

Classical computational cost

- Full diagonalization: $O(N^3)$
- sparse Lanczos*: $O\left(dN\frac{\log(N)}{\sqrt{\epsilon}}\right)$
- MC no sign prob.: $O\left(\frac{\log(N)^\alpha}{\epsilon^2}\right)$
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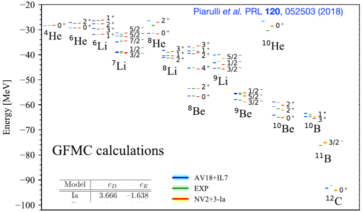
*see eg. Kuczynski & Wozniakowski (1989)



What is a Quantum Computer?

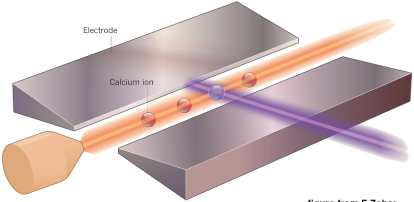


figure from E.Zohar

A Quantum Computer is a controllable quantum many-body system that allows to enact unitary transformations on an initial state ρ_0

$$\rho_0 \rightarrow U\rho_0 U^\dagger$$

n degrees of freedom so $\rho \in \mathcal{H}^{\otimes n}$

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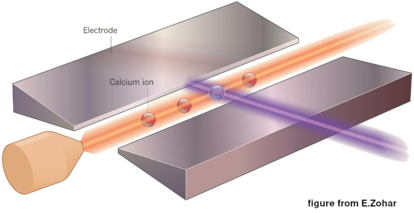

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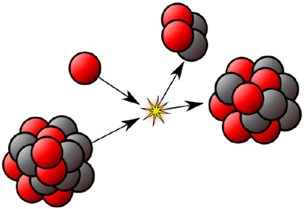
In a Quantum Simulation we want to use this freedom to describe the time-evolution of a closed system

$$\rho(t) \rightarrow U(t) \rho_0 U(t)^\dagger$$

described by some Hamiltonian

$$U(t) = \exp\left(itH\right) \ .$$



Black box model for a quantum computer

Blume-Kohout et al. (2013)

Box contains n qubits (2-level sys.) together with a set of buttons

- initial state preparation ρ
- projective measurement $\mathcal{M}$
- quantum operations G_k

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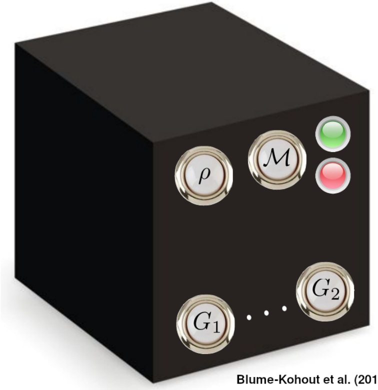

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Solovay–Kitaev Theorem

We can build a **universal** black box with only a **finite number** of buttons

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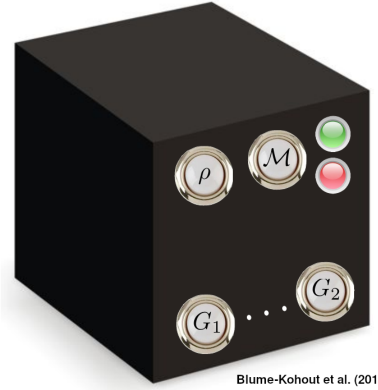

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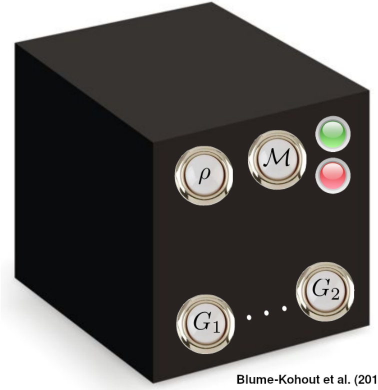

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1. discretize the physical problem

$$|\Psi(0)\rangle \rightarrow |\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle$$

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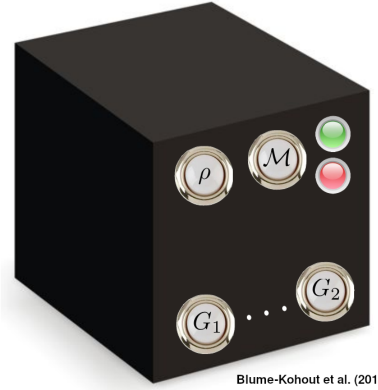

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2. map physical states to bb states

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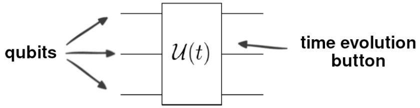

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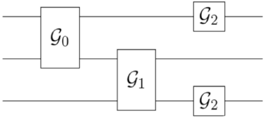
Lloyd (1996) We can simulate time evolution of local Hamiltonians

1. discretize the physical problem
2. map physical states to bb states
3. push correct button sequence

$$|\Psi(0)\rangle \rightarrow |\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle$$

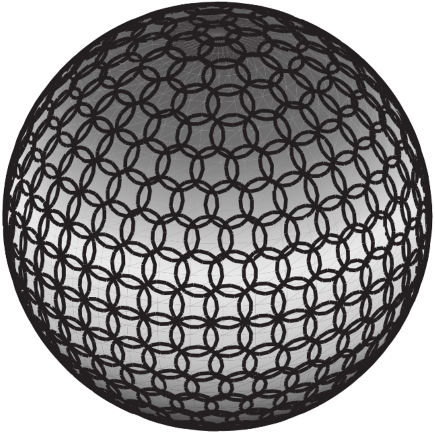


Can we always do this?

image from Nielsen&Chuang

Any unitary operation can be thought as the time evolution operator for some (Hermitian) Hamiltonian

$$U \quad \leftrightarrow \quad e^{iH}$$



A simple counting argument shows that for a fixed choice of universal buttons (quantum gates) there are unitary operations on n qubits which will require $O(2^n)$ operations

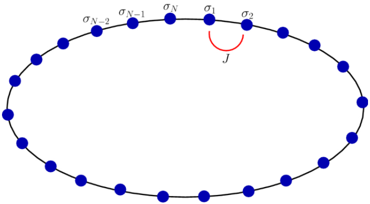
We can find Hamiltonians whose time evolution cannot be simulated **efficiently**

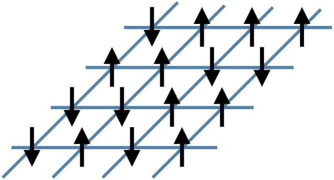
Efficient Hamiltonian Simulation

Hamiltonians encountered in physics have usually structure, like locality

$$H^{1D}_{Ising} = J\sum_{i=1}^{N} Z_i Z_{i+1} + h\sum_{i=1}^{N} X_i$$

$$H^{1D}_{Heis} = J\sum_{i=1}^{N} \vec{\sigma}_i \cdot \vec{\sigma}_{i+1}$$





$$H^{2D}_{Ising} = J\sum_{\langle i,j\rangle} Z_i Z_j + h\sum_{i} X_i$$

$$H^{2D}_{Heis} = J\sum_{\langle i,j\rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j$$

All these situations are examples of 2-local spin Hamiltonians

Quantum Simulation of k-local Hamiltonians

- locality constraints number of terms appearing in the Hamiltonian
- one can approximate full evolution with products of evolutions

$$e^{it(A+B)} = e^{itA}e^{itB} + \mathcal{O}\left(t^2\|[A,B]\|\right)$$

- locality constrains how expensive any individual term can be

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S. LLOYD (1996): k-local hamiltonians can be simulated efficiently

Consider a system of n qubits and a k-local Hamiltonian $H = \sum_j^{N_j} h_j$ where each term h_j acts on at most $k = \mathcal{O}(1)$ qubits at a time for $N_j = \mathcal{O}(\text{poly}(n))$, then using the Trotter-Suzuki decomposition

$$\left\| U(\tau) - \prod_j^{N_j} \exp\left(i\tau h_j\right) \right\| \leq C\tau^2$$

we can implement $U(\tau)$ with error ϵ using $\mathcal{O}\left(\text{poly}(\tau, 1/\epsilon, n)4^k\right)$ gates.

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PROBLEM: large dimension of the Hilbert space $N = dim(\mathcal{H}) > 4^A$

Classical computational cost

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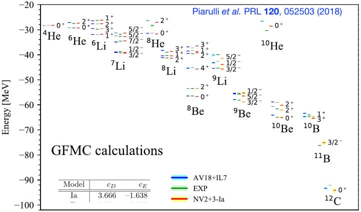

*see eg. Kuczynski & Wozniakowski (1989)

Why quantum computing for nuclear physics?

GOAL: compute the ground state energy with error at most ϵ

$$H = \sum_i \frac{p^2}{2m} + \frac{1}{2}\sum_{i,j} V_{ij} + \frac{1}{6}\sum_{i,j,k} W_{ijk} + \cdots$$

Quantum Phase Estimation (QPE)

Time evolution can be cheap

- many Hamiltonians such that

  $$|\Psi(t+\tau)\rangle = \exp(i\tau H)\,|\Psi(t)\rangle$$

  costs only $O\left(\tau \log(N)^\alpha\right)$
- QPE uses this to solve our goal in $O\left(\frac{\log(N)^\gamma}{\epsilon^\kappa}\right)$ for $1 \leq \kappa \leq 3$

IMPORTANT REMARKS:

1. many repetitions required, need stable quantum processor for only $O\left(\frac{\log(N)^\gamma}{\epsilon}\right)$ operations
2. this is not always possible
3. if it is, dynamics is as easy/complicated as static

General scheme for many-body quantum simulations

- Discretize physical problem on finite Hilbert space
- Encode discrete problem into spin problem
- Prepare an encoded low energy state
- Manipulate state, e.g. evolve under unitary time evolution
- Measure properties of final state

General scheme for many-body quantum simulations

- Discretize physical problem on finite Hilbert space
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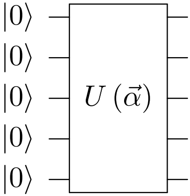
- many options for preparing low energy states with a given encoding

Variational State Preparation

Exploit variational principle for the energy to find some reasonable parametrization for the ground-state

$$E(\vec{\alpha}) = \langle \Psi(\vec{\alpha}) | H | \Psi(\vec{\alpha}) \rangle \geq E_0$$



see e.g. J.McClean, J. Romero, et.al. (2016), M. Cerezo, A. Arrasmith, R. Babbush, et al. (2021)

Quick introduction to quantum gates

single-qubit gates

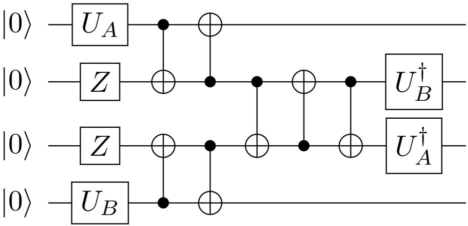
$$-\boxed{R_{\hat{n}}(\theta)}- = \exp\left(i\theta\frac{\hat{n}\cdot\vec{\sigma}}{2}\right)$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -\boxed{X}-$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -\boxed{Y}-$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -\boxed{Z}-$$

$$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = -\boxed{S}-$$



two-qubit entangling gate

$$\text{CNOT} = (\text{control } \bullet, \text{ target } \oplus) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$|\Phi_0\rangle = a\,|00\rangle + b\,|01\rangle + c\,|10\rangle + d\,|11\rangle$$

$$|\Phi_1\rangle = a\,|00\rangle + b\,|01\rangle + c\,|11\rangle + d\,|10\rangle$$

EXERCISE: show that $\forall U_A, U_B$ the output of the circuit above is $|0000\rangle$

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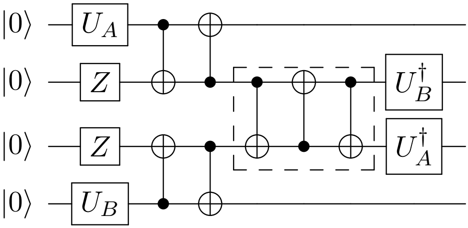
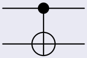


two-qubit entangling gate

CNOT =  $= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

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Quick introduction to quantum gates II

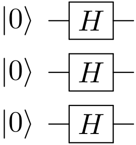
Hadamard Gate

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

- rotates between Z and X basis

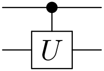
$$\left.\begin{aligned} H|0\rangle &= |+\rangle \\ H|1\rangle &= |-\rangle \end{aligned}\right\} \qquad X|\pm\rangle = \pm|\pm\rangle$$

- generates uniform superposition



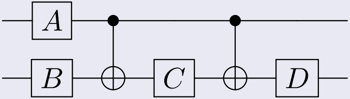
$$H^{\otimes 3}|0\rangle = \frac{1}{\sqrt{2^3}}\sum_{k=0}^{2^3-1}|k\rangle$$

Generic controlled unitary

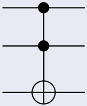


$$= \begin{pmatrix}\mathbb{1} & 0\\ 0 & U\end{pmatrix}$$

Single qubit U Barenco et al. (1995)



Controlled CNOT: Toffoli



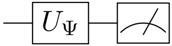
= [6 CNOT + 9 single qubit]∗

* see eg. Nielsen & Chuang

Measuring an observable: single qubit case

Computational basis is eigenbasis of Z so that, if $|\Psi\rangle = U_\Psi |0\rangle$, we have

$$\langle\Psi|Z|\Psi\rangle = |\langle 0|\Psi\rangle|^2 - |\langle 1|\Psi\rangle|^2 \equiv \; |0\rangle$$



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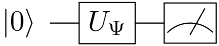

We now need to repeat calculation M times to estimate the probabilities

$$P(0) = |\langle 0|\Psi\rangle|^2 \sim \frac{\sum_k \delta_{s_k,0}}{M} \qquad Var\left[P(0)\right] \sim \frac{v_0}{M} \longrightarrow 0 \; .$$

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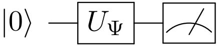

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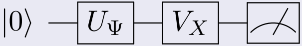
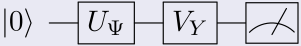
Other expectation values accessible by basis transformation

$X = V_X Z V_X^\dagger$



$Y = V_Y Z V_Y^\dagger$



- for X we can use $X = V_X Z V_X^\dagger$ where V_X is the Hadamard

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

- for Y we can use $Y = SXS^\dagger$ so that $V_Y = SV_X = SH$

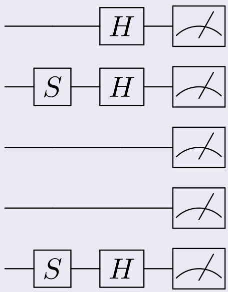
Measuring an observable: the Pauli group

Given a state $|\Psi\rangle$ defined over n qubits and an encoded operator

$$O = \sum_{k=1}^{N_K} c_k P_k \quad P_k \in \{(\mathbb{1}, X, Y, Z)^{\otimes n}\}$$

we want to measure the expectation value $\langle\Psi|O|\Psi\rangle$ [McClean et al. (2014)].

Example: $X_0 Y_1 Z_2 Z_3 Y_4$



- $\forall k$ perform M experiments to get $\langle P_k \rangle$ with

$$Var[P_k] \sim \frac{\langle P_k^2 \rangle - \langle P_k \rangle^2}{M} = \frac{1 - \langle P_k \rangle^2}{M}$$

- we can now evaluate $\langle O \rangle$ with variance

$$Var[O] = \sum_{k=1}^{N_K} |c_k|^2 Var[P_k]$$

$\Rightarrow$ total error $\propto \sqrt{N_K/M}$.

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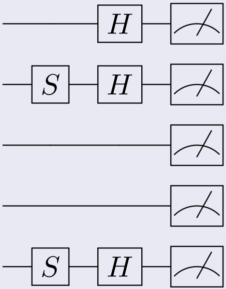
Given a state $|\Psi\rangle$ defined over n qubits and an encoded operator

$$O = \sum_{k=1}^{N_K} c_k P_k \quad P_k \in \{(\mathbb{1}, X, Y, Z)^{\otimes n}\}$$

we want to measure the expectation value $\langle\Psi|O|\Psi\rangle$ [McClean et al. (2014)].

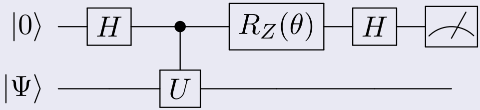
Example: $X_0 Y_1 Z_2 Z_3 Y_4$



- naive estimator has total error $\propto \sqrt{N_K/M}$
- we can measure multiple terms together!

$$X_0 Y_1 Z_2 Z_3 Y_4 \begin{cases} X_0 Y_1 \mathbb{1}_2 Z_3 Y_4 \\ X_0 Y_1 \mathbb{1}_2 \mathbb{1}_3 Y_4 \\ \dots \\ \mathbb{1}_0 Y_1 \mathbb{1}_2 \mathbb{1}_3 \mathbb{1}_4 \\ X_0 X_1 Z_2 Z_3 X_4 \\ \dots \end{cases} \Rightarrow \epsilon_{tot} \propto \sqrt{\frac{N_G}{M}}$$

Measuring an observable: Hadamard test



Kitaev (1995)

When $\theta = 0$ we have:

1. $|\Phi_0\rangle = |0\rangle \otimes |\Psi\rangle$
2. $|\Phi_1\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |\Psi\rangle$
3. $|\Phi_2\rangle = \frac{|0\rangle \otimes |\Psi\rangle}{\sqrt{2}} + \frac{|1\rangle \otimes U|\Psi\rangle}{\sqrt{2}}$
4. $|\Phi_3\rangle = \frac{|0\rangle \otimes (\mathbb{1} + U)|\Psi\rangle}{2} + \frac{|1\rangle \otimes (\mathbb{1} - U)|\Psi\rangle}{2}$

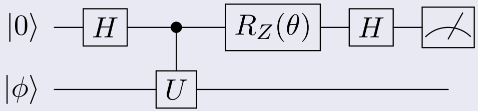
Result of ancilla measurement

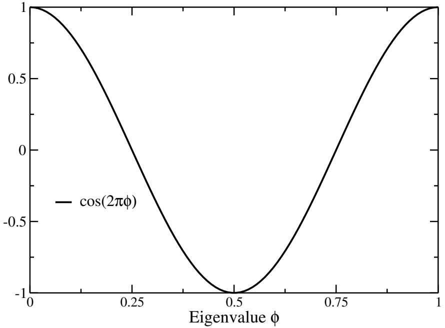
$$\langle Z \rangle_a = \frac{\langle \Psi | \left(U + U^\dagger \right) | \Psi \rangle}{2} = \mathcal{R} \langle \Psi | U | \Psi \rangle$$

EXERCISE: find the proper angle θ needed to measure the imaginary part

EXAMPLE: eigenvalue estimation

Take a unitary U and an eigenvector $|\phi\rangle$ so that: $U|\phi\rangle = e^{i2\pi\phi}|\phi\rangle$





- for $\theta = 0$: $\langle Z\rangle_a = cos(2\pi\phi)$

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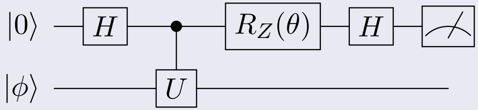

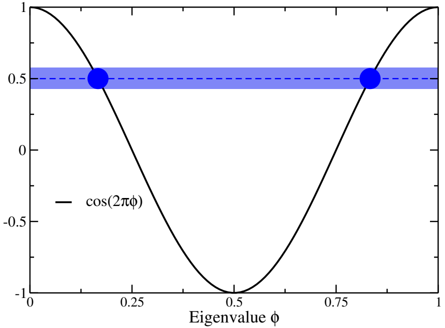

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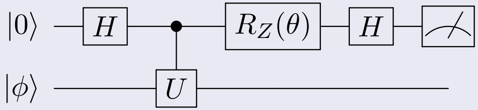

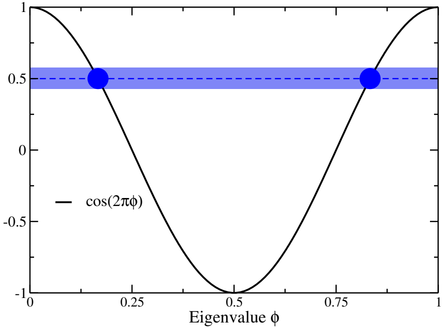

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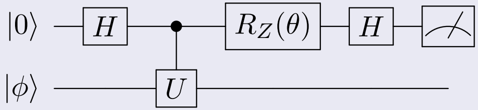

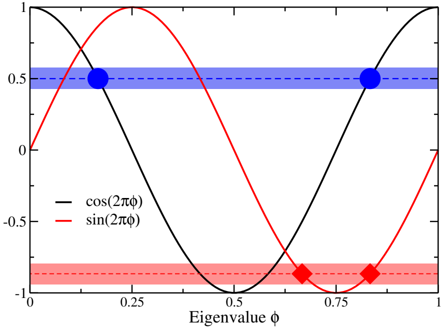

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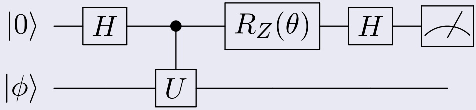

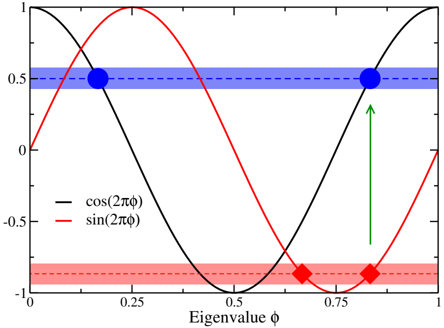

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Quantum phase estimation in one slide

GOAL: compute eigenvalue ϕ with error δ using exact eigenvector $|\phi\rangle$

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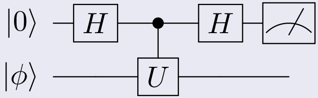

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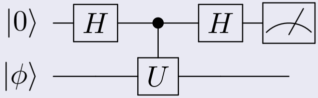
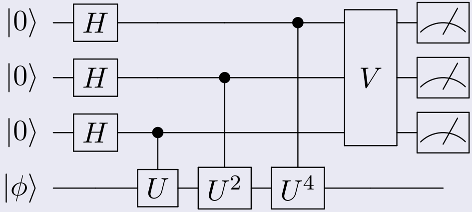


- Quantum Phase Estimation (QPE) uses $O(1/\delta)$ controlled-U operations, $O(\log(1/\delta))$ ancilla qubits and only $O(1)$ experiments



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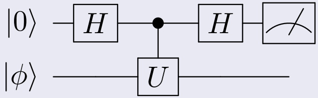

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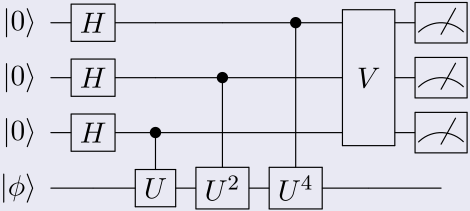
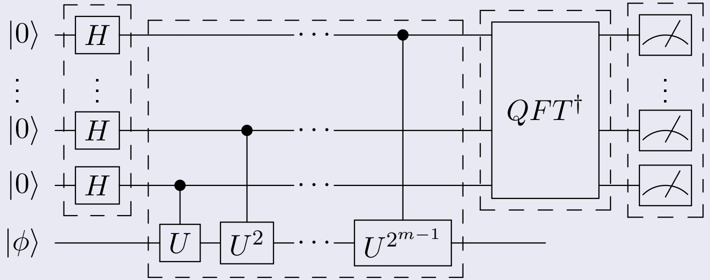


BONUS: works even if $|\phi\rangle \to \alpha|\phi\rangle + \beta|\xi\rangle$ with $O(1/\alpha^2)$ experiments

Filling in the details

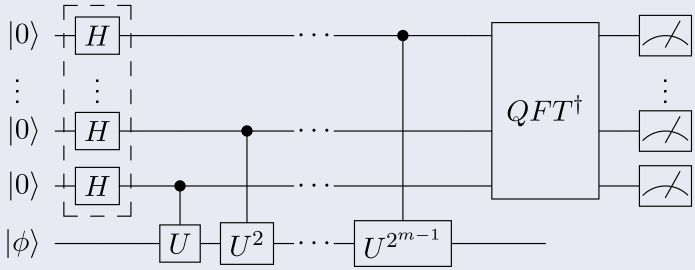
Abrams & Lloyd (1999)



The QPE algorithm has 4 main stages

1. prepare m ancilla in uniform superposition of basis states
2. apply controlled phases using U^k with $k = 2^0, 2^1, \ldots, 2^{m-1}$
3. perform (inverse) Fourier transorm on ancilla register
4. measure the ancilla register

Filling in the details: state preparation

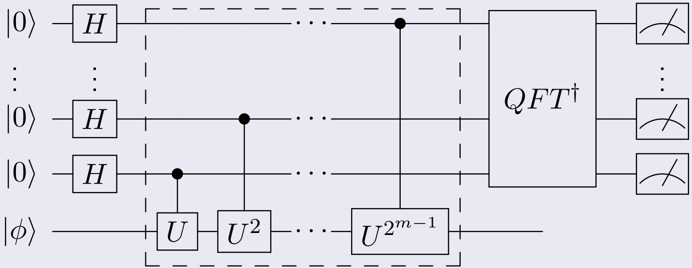


1. prepare m ancilla in uniform superposition of basis states

$$|\Phi_1\rangle = H^{\otimes m}|0\rangle_m = \left(\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right)\otimes\left(\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right)\otimes\cdots\otimes\left(\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right)$$
$$= \frac{1}{\sqrt{2^m}}\sum_{k=0}^{2^m-1}|k\rangle$$

BINARY REPRESENTATION: use $|3\rangle$ to indicate $|00011\rangle$

Filling in the details: phase kickback



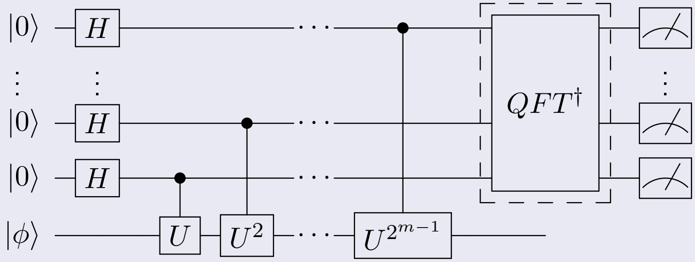
The state $|\phi\rangle$ is an eigenstate of U with $U|\phi\rangle = \exp(i2\pi\phi)|\phi\rangle$

2. each c-U^k applies a phase $\exp(i2\pi k\phi)$ to the $|1\rangle$ state of the ancilla

$$|\Phi_2\rangle = \left(\frac{|0\rangle + e^{i2\pi\phi}|1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle + e^{i4\pi\phi}|1\rangle}{\sqrt{2}} \otimes \cdots \otimes \frac{|0\rangle + e^{i2^{m-1}\pi\phi}|1\rangle}{\sqrt{2}}\right) \otimes |\phi\rangle$$

$$= \frac{1}{\sqrt{2^m}} \sum_{k=0}^{2^m-1} \exp\left(i2\pi\phi k\right)|k\rangle \otimes |\phi\rangle$$

Filling in the details: inverse QFT

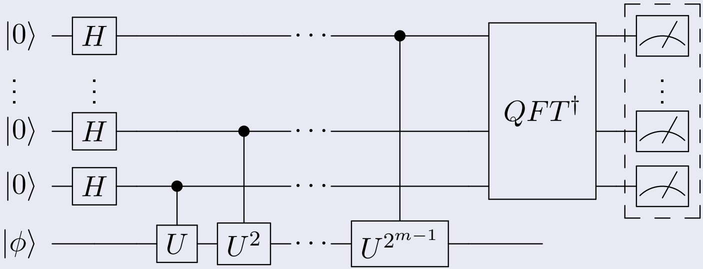


Recall that: $QFT^\dagger |k\rangle = \frac{1}{\sqrt{2^m}} \sum_{q=0}^{2^m-1} \exp\left(-i\frac{2\pi}{2^m}qk\right)|q\rangle$

3. after an inverse QFT the final state is

$$|\Phi_3\rangle = QFT^\dagger |\Phi_2\rangle = \frac{1}{2^m}\sum_{k=0}^{2^m-1}\sum_{q=0}^{2^m-1} \exp\left(i2\pi k\left(\phi - \frac{q}{2^m}\right)\right)|q\rangle \otimes |\phi\rangle$$

Filling in the details: final measurement



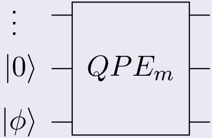
$$|\Phi_3\rangle = \sum_{q=0}^{2^m-1} \left(\frac{1}{2^m} \sum_{k=0}^{2^m-1} \exp\left(i \frac{2\pi k}{2^m} (2^m \phi - q) \right) \right) |q\rangle \otimes |\phi\rangle$$

4. if phase ϕ is a m-bit number we can find $0 \leq p < 2^m$ s.t. $2^m \phi = p$

$$|\Phi_3\rangle = \sum_{q=0}^{2^m-1} \delta_{q,p} |q\rangle \otimes |\phi\rangle = |p\rangle \otimes |\phi\rangle$$

$\Rightarrow$ exact solution with only 1 measurement!

Final measurement: generic phase



$$| \Phi_3\rangle = \sum_{q=0}^{2^m-1} \left(\frac{1}{2^m} \sum_{k=0}^{2^m-1} e^{i \frac{2\pi k}{2^m}(2^m \phi - q)} \right) |q\rangle \otimes |\phi\rangle$$

- when $2^m\phi$ is not an integer we can sum the term in parenthesis as

$$\sum_{k=0}^{2^m-1} e^{ixk} = \frac{1-e^{i2^m x}}{1-e^{ix}} = \exp\left(i\frac{x}{2}(2^m-1)\right)\frac{\sin\left(2^m x/2\right)}{\sin\left(x/2\right)}$$

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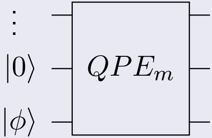

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- we will measure the ancilla register in $|q\rangle$ with probability

$$P(q) = \frac{1}{M^2}\frac{\sin^2\left(M\pi(\phi - q/M)\right)}{\sin^2\left(\pi(\phi - q/M)\right)}$$

where we have defined $M = 2^m$

Final measurement: generic phase example

example taken from A. Childs lecture notes (2011)

$$P(q) = \frac{1}{M^2} \frac{\sin^2\left(M\pi(\phi - q/M)\right)}{\sin^2\left(\pi(\phi - q/M)\right)}$$

EXERCISE: show that if $r = \lceil M\phi \rfloor$ then $P(r) \geq 4/\pi^2 \approx 0.4$

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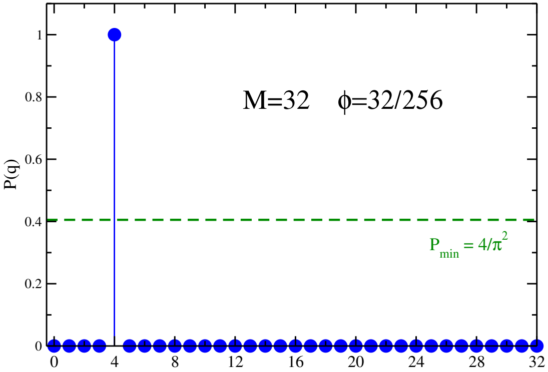

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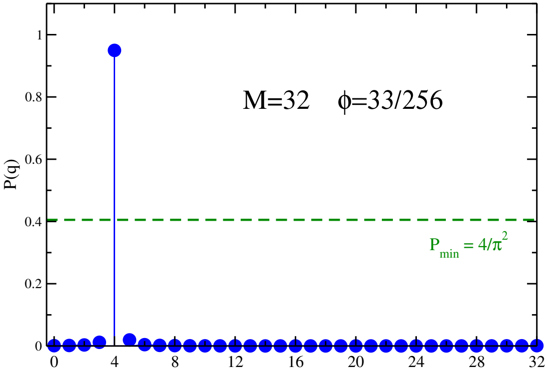

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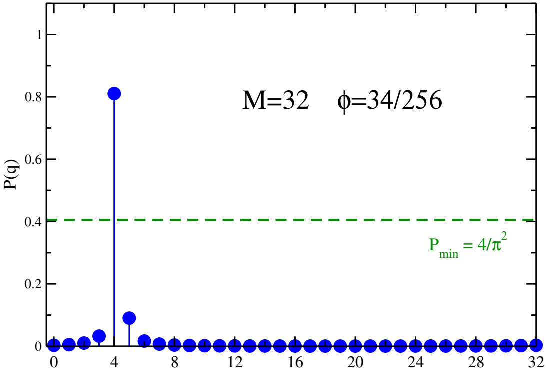

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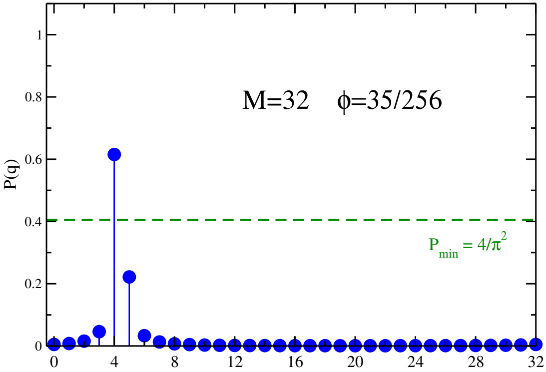

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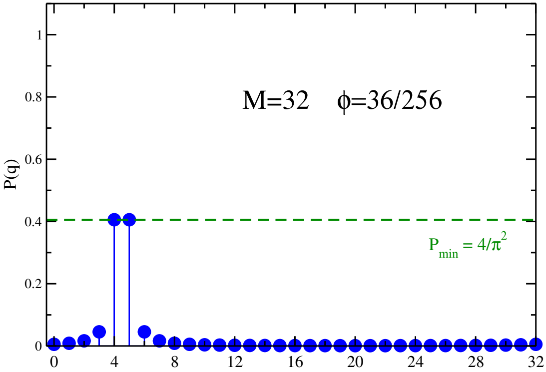

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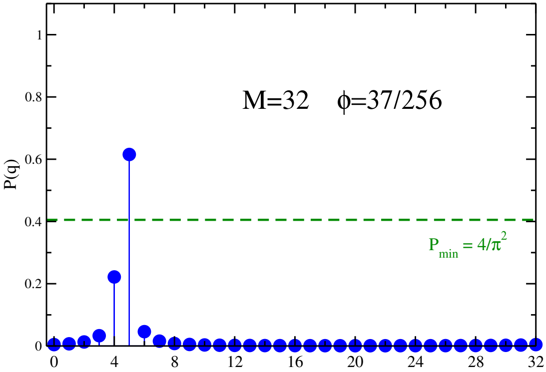

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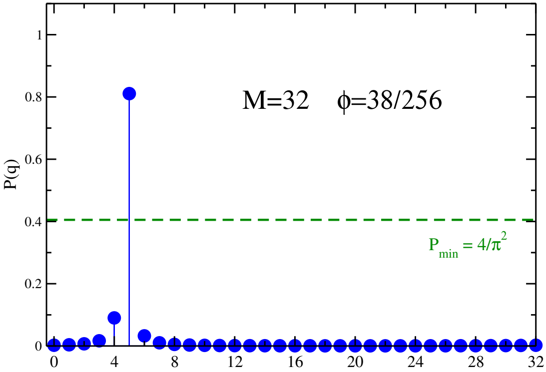

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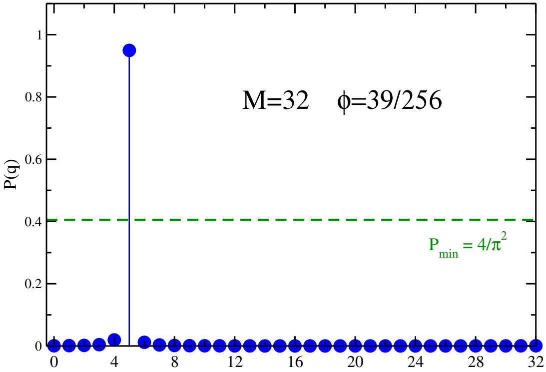

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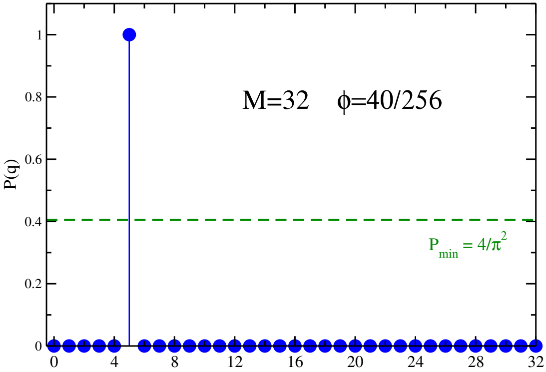

Final measurement: generic phase II

$$P(q) = \frac{1}{M^2}\frac{\sin^2\left(M\pi(\phi - q/M)\right)}{\sin^2\left(\pi(\phi - q/M)\right)}$$

- the best m-bit approximation to ϕ is p/M with $p = \lceil M\phi \rfloor$
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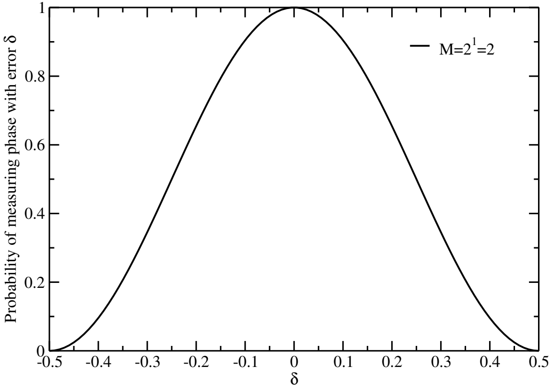

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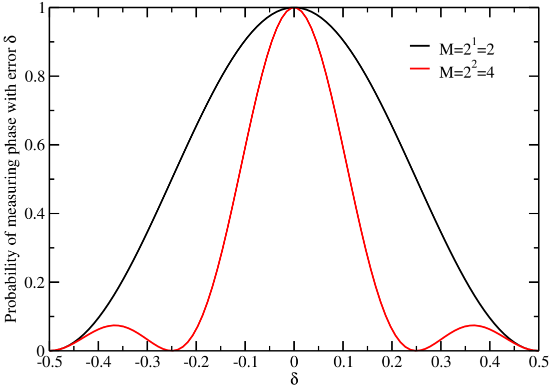

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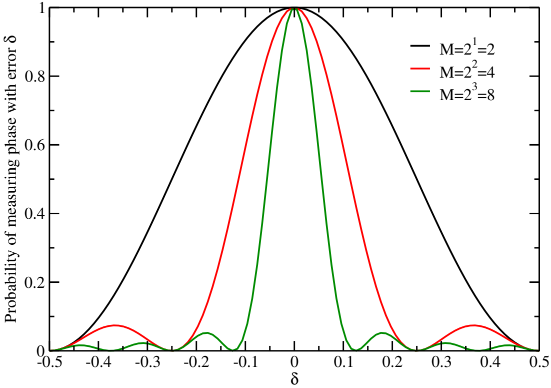

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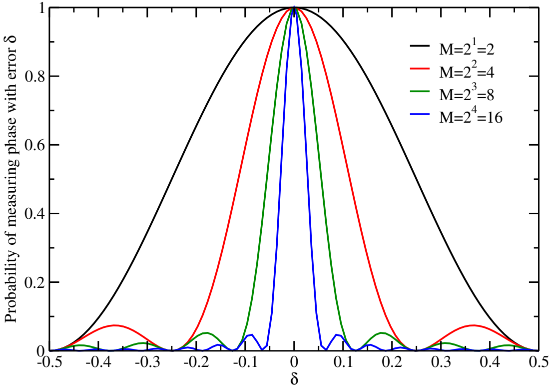

Final measurement: generic phase II

$$P(q) = \frac{1}{M^2} \frac{\sin^2\left(M\pi(\phi - q/M)\right)}{\sin^2\left(\pi(\phi - q/M)\right)}$$

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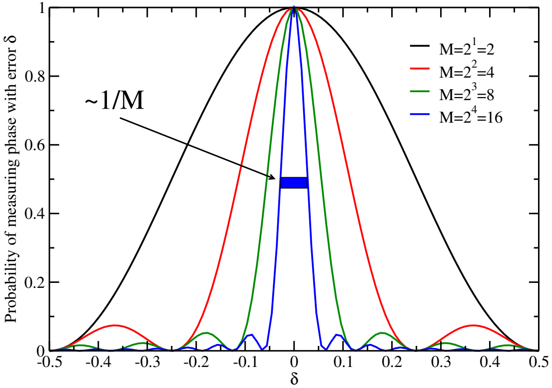
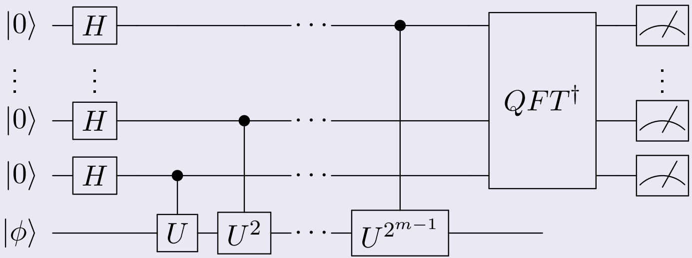


Quick recap of QPE for eigenstates



- given an eigenstate $|\phi\rangle$ QPE can provide an estimate for the phase ϕ with precision δ using $M \sim 1/\delta$ with probability $P > 4/\pi^2$

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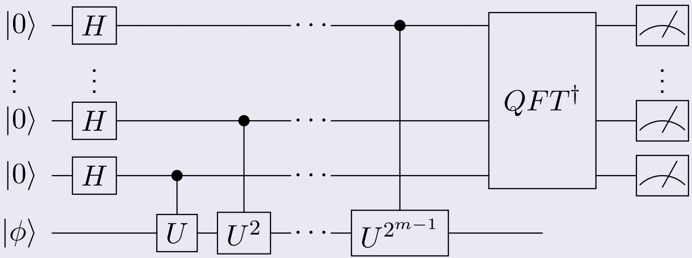

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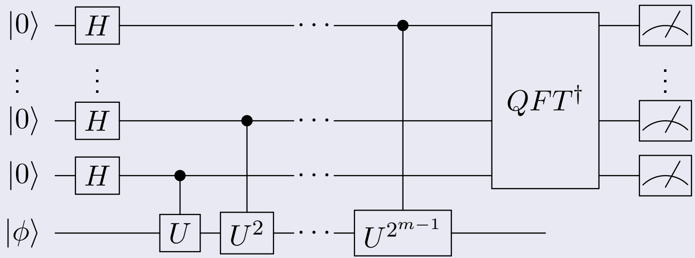
- this probability can be amplified to $1-\epsilon$ using more ancilla qubits*

$$m' = m + \left\lceil \log\left(\frac{1}{2\epsilon}+2\right)\right\rceil \quad \Rightarrow \quad M' \sim \frac{1}{\delta\epsilon}$$

*see eg. Nielsen & Chuang

Quick recap of QPE for eigenstates



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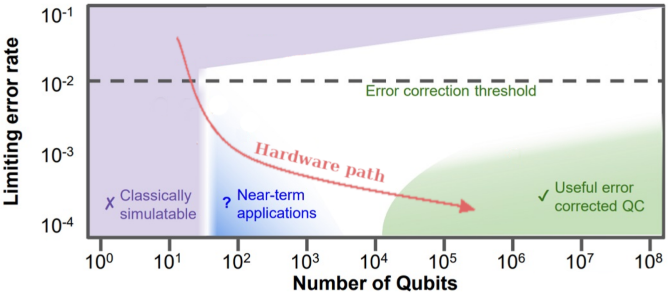
- we can also repeat this $O(\log(1/\eta))$ times and take a majority vote to increase the probability to $1-\eta$ (see Chernoff bound)

Final recap of first day

1. quantum computers can simulate efficiently the time-evolution operator $U(\tau) = \exp(i\tau H)$ for k-local Hamiltonians
   - for target error ϵ this requires $\mathcal{O}(\text{poly}(n, \tau, 1/\epsilon)4^k)$ gates
2. if we can prepare an energy eigenstate $|\phi\rangle$ we can use this to measure it's phase with accuracy Δ using a total propagation time $\tau \sim 1/\Delta$
3. this might be preferable to directly estimating the energy as an expectation value as this would cost $\mathcal{O}(1/\Delta^2)$ measurements

from Google AI



EXAMPLE 2: the SWAP test

- State Tomography: reconstruction of state $|\Psi\rangle$ costs $O(N)$ samples
- State Overlap: we can compute $|\langle\Psi|\Phi\rangle|^2$ using only $O(\log(N))$ gates

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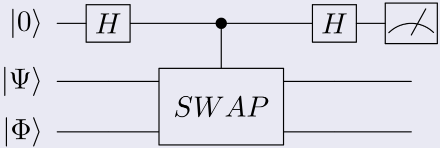
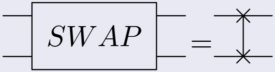


Buhrman, Cleve, Watrous & de Wolf (2001)

$$\Rightarrow \langle Z\rangle_a = |\langle\Psi|\Phi\rangle|^2$$

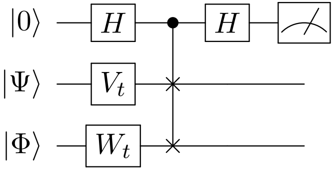
The SWAP gate

$$\text{SWAP}\,|\Psi\rangle\otimes|\Phi\rangle = |\Phi\rangle\otimes|\Psi\rangle$$



$$2 \text{ qubits} \Rightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Why should we care?



$$\Rightarrow M(\Psi\leftrightarrow\Phi) = \left|\langle\Psi|V_t^\dagger W_t|\Phi\rangle\right|^2$$

Efficient transition matrix element!