Nuclear structure (and reactions) with Quantum Computers - II

Alessandro Roggero

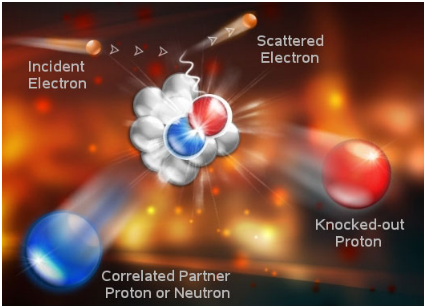

figure credit: JLAB collab.

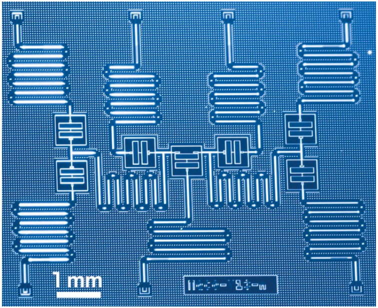

figure credit: IBM

QC and QIS for NP

JLAB – 17 March, 2020

Quantum phase estimation in one slide

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

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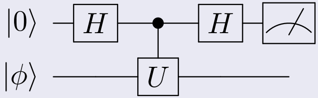
- Hadamard test: one controlled-U operation and $O(1/\delta^2)$ experiments



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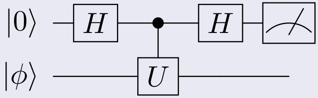
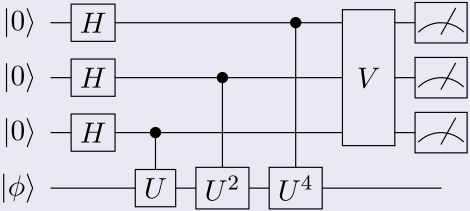


- Quantum Phase Estimation (QPE) uses $O(1/\delta)^*$ controlled-U operations, $O(\log(1/\delta))^*$ ancilla qubits and only $O(1)^*$ experiments



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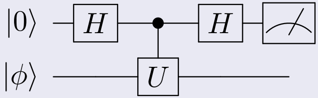

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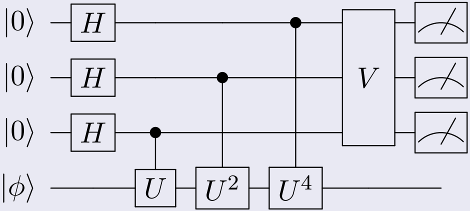
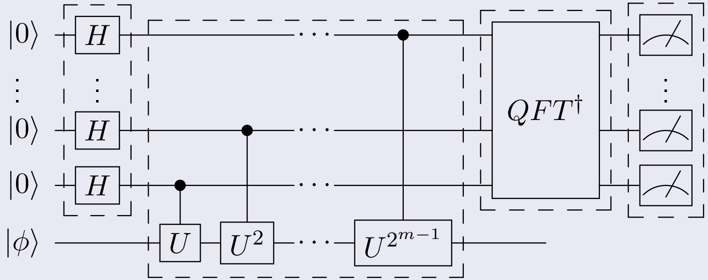


BONUS: works even if $|\phi\rangle \to \alpha\,|\phi\rangle + \beta\,|\xi\rangle$ with $O(1/\alpha^2)^*$ experiments

Filling in the details

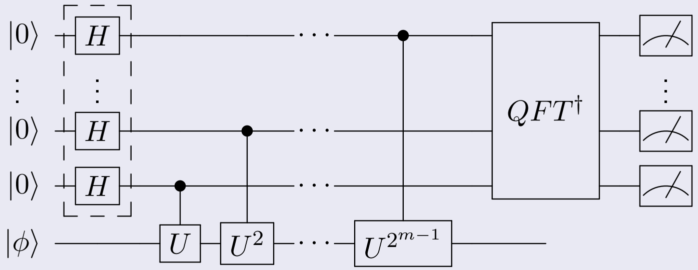
Abrams & Lloyd (1999)



The QPE algortihm 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



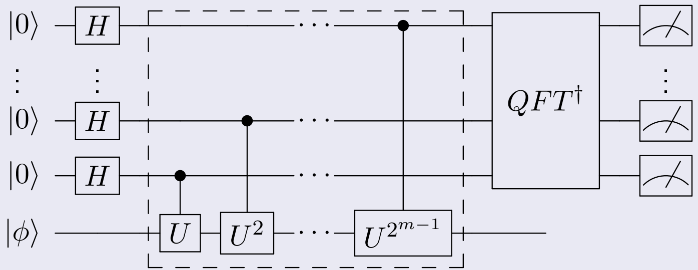
1. prepare m ancilla in uniform superposition of basis states

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

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

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

Filling in the details: phase kickback



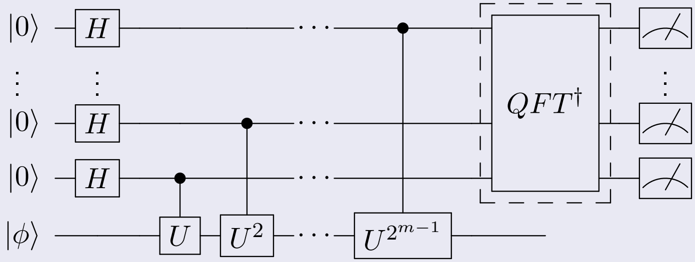
The state $|\phi\rangle$ is an eigenstate of U with $U|\phi\rangle = \exp(i2\pi\phi)|\phi\rangle$

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

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

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

Filling in the details: inverse QFT

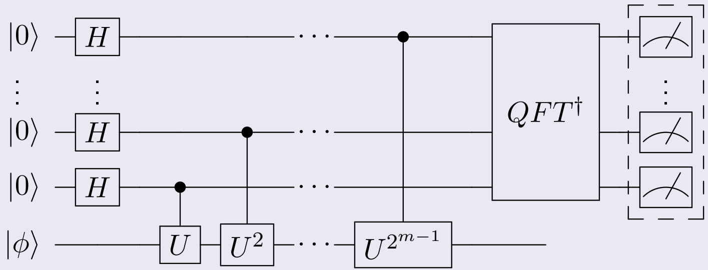


Recall that: $QFT^\dagger |k\rangle = \frac{1}{\sqrt{2^m}} \sum_{q=0}^{2^m-1} \exp\left(-i2\pi \frac{qk}{2^m}\right) |q\rangle$ see DL lectures

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



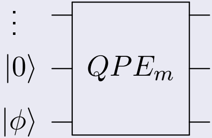
$$|\Phi_3\rangle = \sum_{q=0}^{2^m-1} \left(\frac{1}{2^m} \sum_{k=0}^{2^m-1} \exp\left(i \frac{2\pi k}{2^m} (2^m \phi - q) \right) \right) |q\rangle \otimes |\phi\rangle$$

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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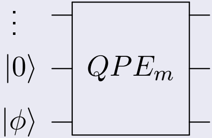

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- we will measure the ancilla register in $|q\rangle$ with probability

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

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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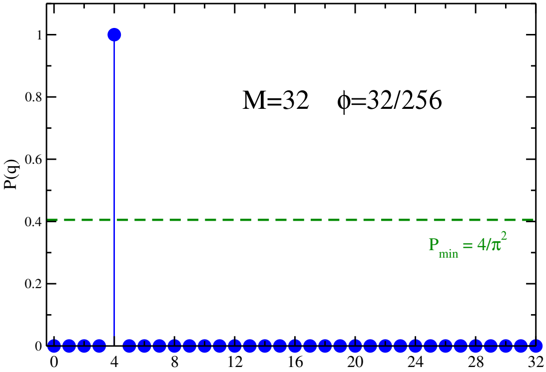

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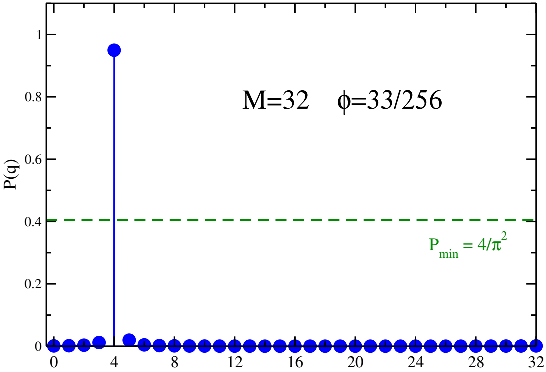

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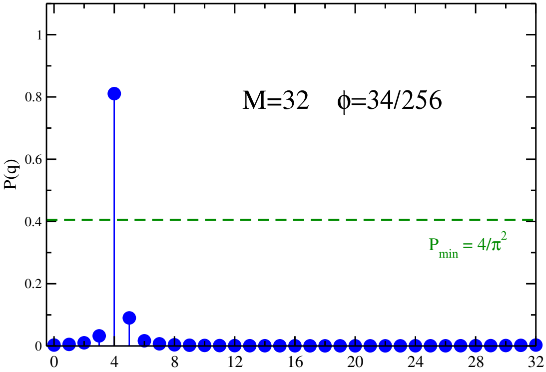

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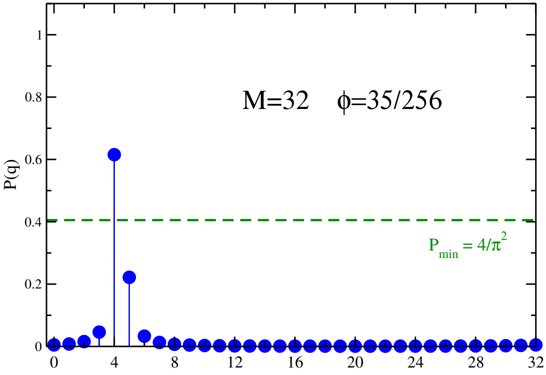

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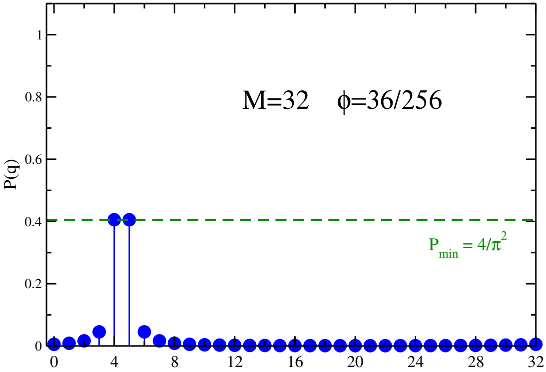

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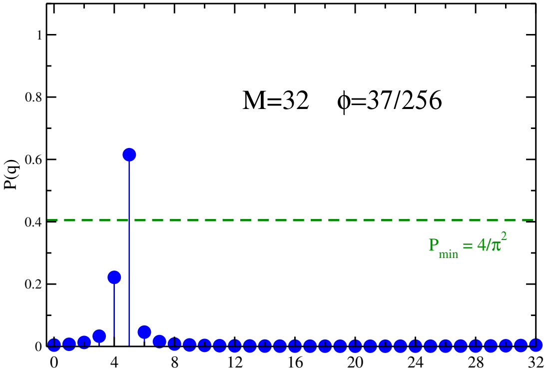

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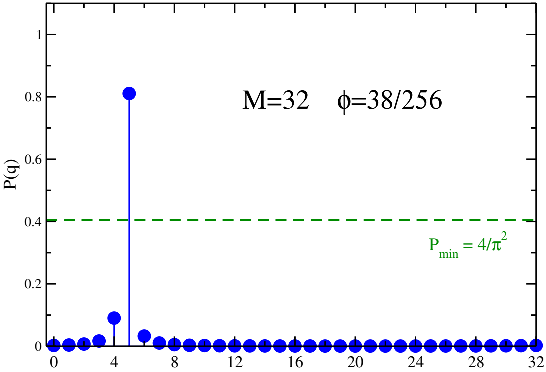

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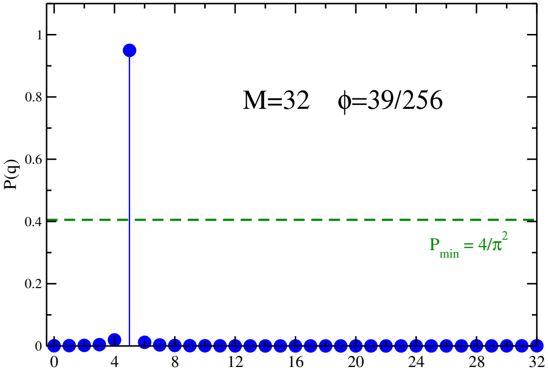

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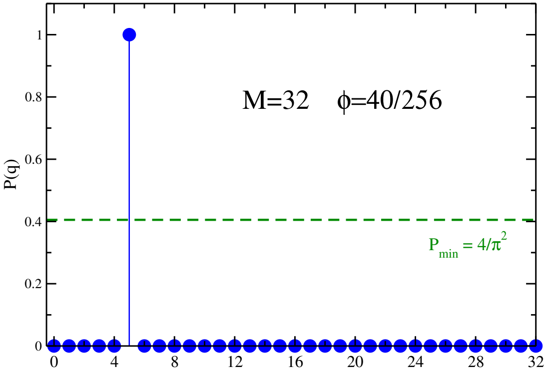
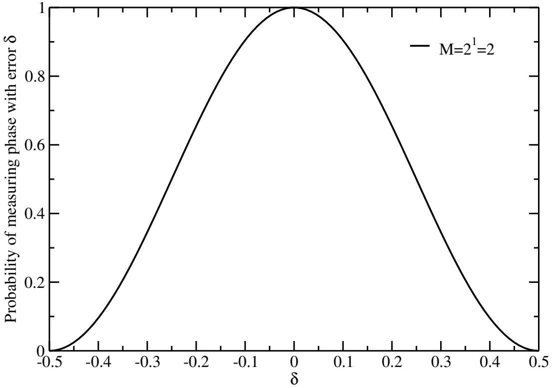


Final measurement: generic phase II

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

- the best m-bit approximation to ϕ is p/M with $p = \lceil M\phi \rfloor$
- the probabilty of making an error $\delta = (q-p)/M$ is



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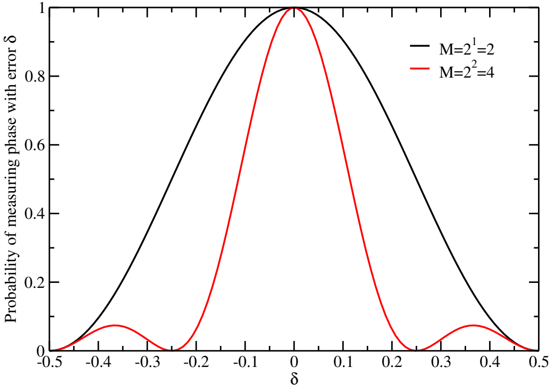

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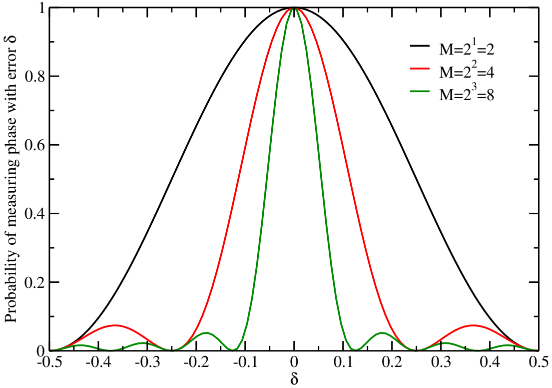

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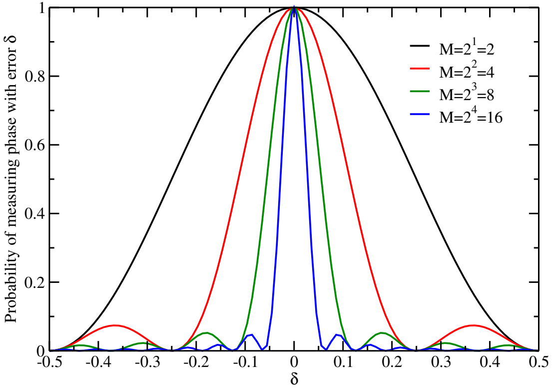

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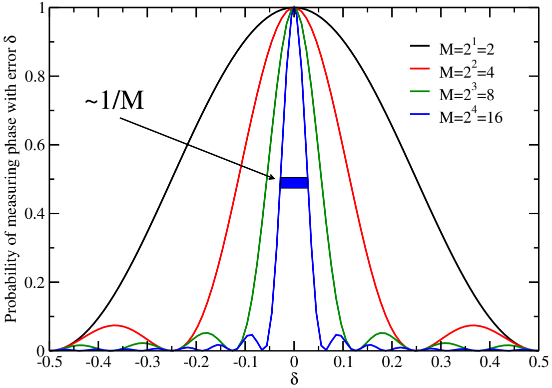
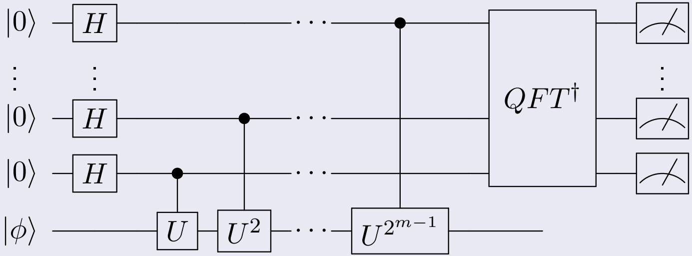


Quick recap of QPE for eigenstates



- 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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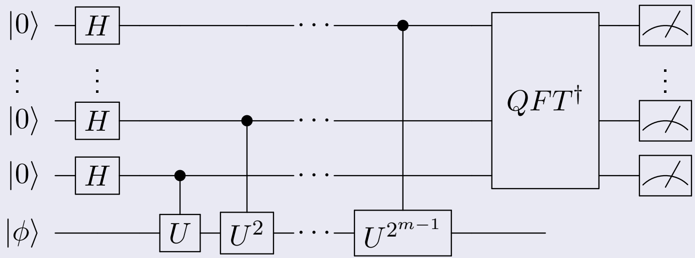
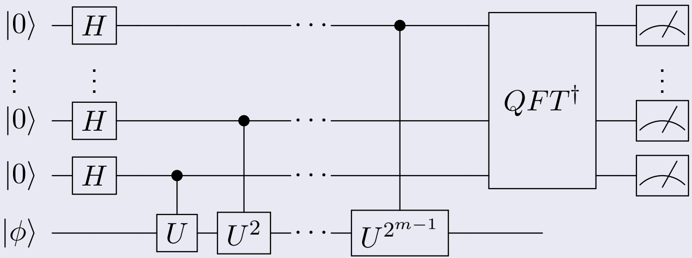


- given an eigenstate $|\phi\rangle$ QPE can provide an estimate for the phase ϕ with precision δ using $M \sim 1/\delta$ with probability $P > 4/\pi^2$
- this probability can be amplified to $1-\epsilon$ using more ancilla qubits*

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

*see eg. Nielsen & Chuang

Quick recap of QPE for eigenstates



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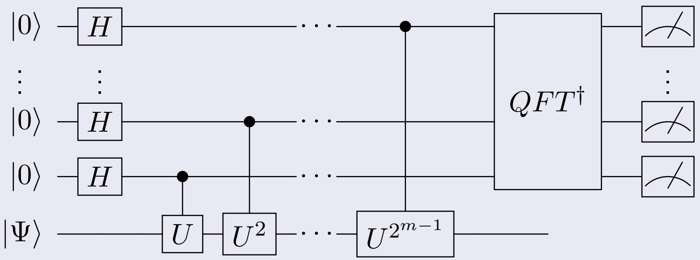
*see eg. Nielsen & Chuang

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

QPE on general states



If we start with a generic state $|\Psi\rangle = \sum_j c_j |\phi_j\rangle$ we find

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

The new probability becomes

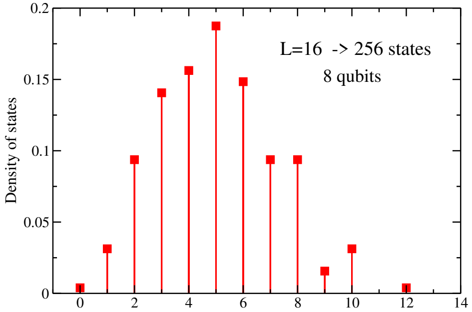
$$P(q) = \frac{1}{M^2} \sum_j |c_j|^2 \frac{\sin^2\left(M\pi(\phi_j - q/M)\right)}{\sin^2\left(\pi(\phi_j - q/M)\right)}$$

EXAMPLE: Spectrum of 1D Hubbard model

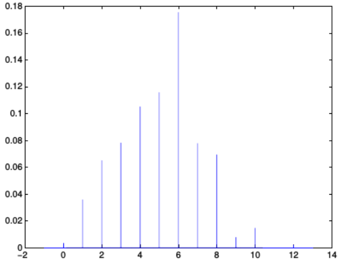
example taken from Ovrum & Horth-Jensen (2007)

$$H_H = \sum_{i}^{L} \sum_{\sigma=\uparrow,\downarrow} \left[\epsilon a^\dagger_{i,\sigma} a_{i,\sigma} - t \left(a^\dagger_{i+1,\sigma} a_{i,\sigma} + a^\dagger_{i,\sigma} a_{i+1,\sigma} \right) \right] + U \sum_{i}^{L} n_{i,\uparrow} n_{i,\downarrow}$$

- we can estimate the spectrum using QPE with random initial states
- consider simple case with $t = 0$, $\epsilon = U = 1$ Ovrum&Horth-Jensen (2007)



$m = 16$ ancilla qubits



Fermion to spin mapping: Jordan Wigner transformation

The fermionic Fock space with M modes can be mapped into the Hilbert space of M spins using the following identification see DL lectures

$$\left.\begin{aligned} a_k &= \left(\prod_{j=0}^{k-1} -Z_j\right) \frac{X_k + iY_k}{2} \\ a_k^\dagger &= \left(\prod_{j=0}^{k-1} -Z_j\right) \frac{X_k - iY_k}{2} \end{aligned}\right\} \quad \Rightarrow \quad \{a_j, a_k^\dagger\} = \delta_{j,k}$$

- occupation encoded into value of spin projection, $\sigma^\pm = \frac{X_k \pm iY_k}{2}$

$$|vac\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle \quad a_2^\dagger |vac\rangle = |\uparrow\uparrow\downarrow\uparrow\rangle \quad a_2^\dagger |\uparrow\uparrow\downarrow\uparrow\rangle = 0$$

- fermionic phase encoded into the string of Pauli Z operators

$$a_2^\dagger a_1^\dagger |vac\rangle = -a_1^\dagger a_2^\dagger |vac\rangle \quad a_2^\dagger a_0^\dagger a_1^\dagger |vac\rangle = a_0^\dagger a_1^\dagger a_2^\dagger |vac\rangle$$

Many other mappings available

- Bravy-Kitaev, BK-Superfast
- auxiliary fermions
- error-correcting codes
- LDPC codes

Bravyi & Kitaev (2000) , Verstraete & Cirac (2005), Havlicek et al. (2017), Steudtner & Wehner (2017)

Time evolution for Hubbard model

$$H'_H = \sum_i^L \sum_{\sigma=\uparrow,\downarrow} n_{i,\sigma} + \sum_i^L n_{i,\uparrow} n_{i,\downarrow} \qquad n_{i,\sigma} = a^\dagger_{i,\sigma} a_{i,\sigma}$$

- using Jordan-Wigner transformation we can map this into $2L$ qubits

$1\uparrow$ $1\downarrow$ $2\uparrow$ $2\downarrow$ $3\uparrow$ $3\downarrow$ $4\uparrow$ $4\downarrow$

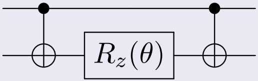
$$n_{i,\uparrow} = \frac{\mathbb{1} + Z_{2i-1}}{2} \qquad n_{i,\downarrow} = \frac{\mathbb{1} + Z_{2i}}{2}$$

$$H_{JW} = h_0 + h_1 \sum_{j=1}^{2L} Z_j + h_2 \sum_{j<k=1}^{2L} Z_j Z_k$$

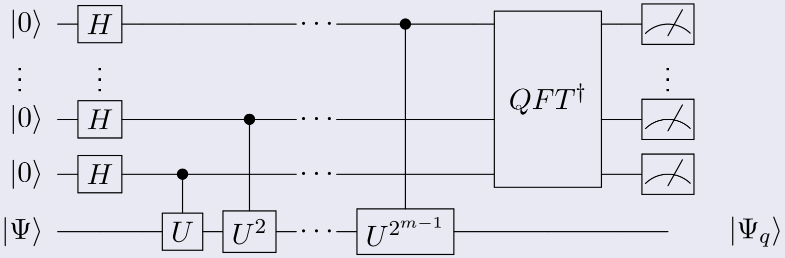
- propagator $U(\tau)$ can be obtained using one and two-qubit Z rotatations

EXERCISE

Show that $U_2 = e^{-i\frac{\theta}{2}Z_1 Z_2}$ is



QPE as state preparation



- before the ancilla measurement we have

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

- after measuring the integer value q the system qubits are left in

$$|\Psi_q\rangle = \frac{1}{M\sqrt{P(q)}} \sum_j c_j \frac{\sin\left(M\pi(\phi_j - q/M)\right)}{\sin\left(\pi(\phi_j - q/M)\right)} |\phi_j\rangle \approx \sum_{|\phi_j - \frac{q}{M}| \lesssim \frac{1}{M}} c_j |\phi_j\rangle$$

Recap of first day (so far)

- given a state $|\Psi\rangle$ prepared on a register with n qubits we can

- compute expectation value $\langle\Psi|O|\Psi\rangle = \sum_k^{N_k} o_k \langle\Psi|P_k|\Psi\rangle$ with error ϵ using $\mathcal{O}(N_K^3/\epsilon^2)$ repetitions and no additional quantum gate
- compute overlap $|\langle\Psi|\Phi\rangle|^2$ with another state saved in an ancillary register using $\mathcal{O}(n)$ gates and $\mathcal{O}(1/\epsilon^2)$ repetitions

- let $|\Psi\rangle = \sum_k c_k |\phi_k\rangle$ be the decomposition in the eigenbasis of U
  - we can obtain the eigenvalue spectrum with resolution δ and error ϵ using $m = \mathcal{O}(\log(1/\delta))$ controlled-U^k operations with exponent $k = 2^0, 2^1, \ldots, 2^{m-1}$, an additional register of m ancilla qubits and $\mathcal{O}(1/\epsilon^2)$ repetitions
  - project to final state $|\Psi_q\rangle \approx |\phi_q\rangle$ with resolution δ using the same setup
  - if $|\Psi\rangle$ is an eigenstate we only need $\mathcal{O}(1)$ repetitions

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Was this worth it?

Can we implement efficiently a controlled-U^M operation for $M \gg 1$?

- remember that $U(\tau)^k = U(k\tau) = \exp(ik\tau H)$ for some Hamiltonian

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

Consider a system of n qubits and a r-local Hamiltonian $H = \sum_j^{N_j} h_j$ where each term h_j acts on at most $r = \mathcal{O}(1)$ 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 $\mathcal{O}\left(\text{poly}(\tau, 1/\epsilon, n) 4^r\right)$ gates.

PROBLEM: the Jordan-Wigner transformation leads to n-local terms

Final recap of first day

1. quantum computers can simulate efficiently the time-evolution operator $U(\tau) = \exp(i\tau H)$ for r-local Hamiltonians
   - for target error ϵ this requires $\mathcal{O}(\text{poly}(n, \tau, 1/\epsilon)4^r)$ gates
   - Jordan Wigner on n qubits leads to n-local terms!
     - SPOILER: this might not be a problem in practice
   - tomorrow we'll generalize this and find better scaling
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. if $|\Psi\rangle$ has overlap $\alpha = |\langle\phi|\Psi\rangle|^2$, we just add $\mathcal{O}(1/\alpha)$ repetitions

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