



# Introduction to Quantum Simulation

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## The Problem

- **How do you simulate the evolution of a quantum system, and extract useful predictions, *efficiently*?**
  - Problem appears to be impossible classically for all but the simplest systems
- **All phases of the quantum simulation must be efficient**
  - Preparing the initial state
  - Evolving the state
  - Extracting an answer
- **In 1982 Feynman speculated quantum computers might simulate quantum systems efficiently**
  - Bosons (yes) / fermions (???)
  - Lloyd showed this is true for bosons and fermions
  - ... and we now know its true for anyons too
  - Lloyd/Abrams then constructed an explicit quantum algorithm for computing properties of a quantum system

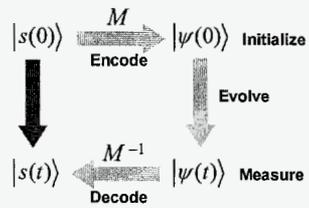
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## The Solution

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- Idea: use the evolution of one quantum system to emulate the evolution of another



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*Quantum Simulation*



## Quantum Simulation in Small Increments



- Schrödinger equation with time independent, local, Hamiltonian

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = H|\psi\rangle$$

- i.e.,  $H = \sum_{\ell=1}^L H_{\ell}$  and only involves few-body interactions
- Solution  $|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle = U|\psi(0)\rangle$

- If you can find an efficient quantum circuit for  $U$ , then you're done

- But, in general, this is hard and/or costly to do exactly
- Moreover, if  $\exists \ell, \ell' : [H_{\ell}, H_{\ell'}] \neq 0$  then  $\exp(-iHt/\hbar) = \exp(-i \sum_{\ell=1}^L H_{\ell} t/\hbar) \neq \prod_{\ell=1}^L \exp(-iH_{\ell} t/\hbar)$

- How then do you build a circuit for  $U$  ?

- Break evolution up into small increments

$$|\psi(t)\rangle = \underbrace{e^{-iH\Delta t/\hbar} e^{-iH\Delta t/\hbar} \dots e^{-iH\Delta t/\hbar}}_{M \text{ factors}} |\psi(0)\rangle$$

$$= \left( \prod_{j=1}^M U(\Delta t) \right) |\psi(0)\rangle \quad \text{where} \quad U(\Delta t) = e^{-iH\Delta t/\hbar} \approx \prod_{\ell=1}^L e^{-iH_{\ell}\Delta t/\hbar} + O((\Delta t)^2)$$

- If each  $H_{\ell}$  is local, there is an efficient quantum circuit for  $\exp(-iH_{\ell}\Delta t/\hbar)$

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## Higher-Order Approximations



- Trotter formula (e.g.,  $H = H_1 + H_2$ )

-Basis of approximation rests on a limit

$$\lim_{n \rightarrow \infty} (e^{-iH_1 t/n} e^{-iH_2 t/n})^n = e^{-i(H_1 + H_2)t}$$

- Simplest Trotter approximation

$$e^{-iH\Delta t} = e^{-iH_1\Delta t} e^{-iH_2\Delta t} + O((\Delta t)^2)$$

- Higher-order Trotter approximations

$$\begin{aligned} e^{-iH\Delta t} &= e^{-iH_1 \frac{\Delta t}{2}} e^{-iH_2 \Delta t} e^{-iH_1 \frac{\Delta t}{2}} + O((\Delta t)^3) \\ &= e^{-iH_2 \frac{\Delta t}{2}} e^{-iH_1 \Delta t} e^{-iH_2 \frac{\Delta t}{2}} + O((\Delta t)^3) \end{aligned}$$

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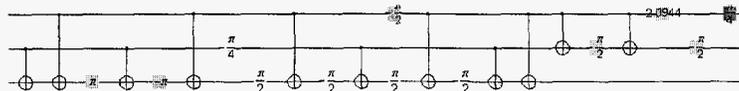
## Decompose Unitary Increments into Quantum Circuits



- Quantum circuit is a decomposition of desired unitary matrix into sequence of single and pairwise quantum logic gates
- Only requires
  - y-rotations, z-rotations, phase-shifts, and controlled-NOT gates (CNOT)

$$R_y(\theta) = \begin{pmatrix} \cos \theta/2 & \sin \theta/2 \\ -\sin \theta/2 & \cos \theta/2 \end{pmatrix}, \quad R_z(\xi) = \begin{pmatrix} e^{i\xi/2} & 0 \\ 0 & e^{-i\xi/2} \end{pmatrix}, \quad P_h(\theta) = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix}$$

$$CNOT \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \equiv \text{CNOT gate symbol}$$



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## Walsh-Hadamard Gates



- Some gates are especially useful, e.g., Walsh-Hadamard gates

$$W = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \equiv \text{Walsh-Hadamard gate symbol}$$

- $W$  gates create a superposition of exponentially many (i.e.,  $2^n$ ) terms in polynomially many (i.e.,  $n$ ) operations

$$\underbrace{(W|0\rangle) \otimes (W|0\rangle) \otimes (W|0\rangle)}_{n \text{ operations}} = \frac{1}{2\sqrt{2}} \underbrace{(|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle)}_{2^n \text{ components}}$$

$$\left. \begin{array}{l} |0\rangle \xrightarrow{W} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |0\rangle \xrightarrow{W} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |0\rangle \xrightarrow{W} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \end{array} \right\} = \frac{1}{2\sqrt{2}} (|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle)$$

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# Extracting Answers from Quantum Simulations



## Extracting Answers from Quantum Simulations



- **You cannot “read” the answer, i.e., the full solution  $|\psi(t)\rangle$** 
  - It is stored in a quantum state
  - If you try to read it, you collapse the state
- **What can you do with it?**
  - You can sample from it
  - You can repeat the simulation and perform state tomography to estimate  $|\psi(t)\rangle$
  - ... but this is likely to be inefficient
  - You can use it as an input to another quantum algorithm (the key!!)
- **If we feed  $|\psi(t)\rangle$  into another quantum algorithm, we can ...**
  - Obtain mean values of operators efficiently
  - Calculate correlation functions
  - Measure (some) spectral properties
  - Estimate a ground state eigenvalue / eigenvector

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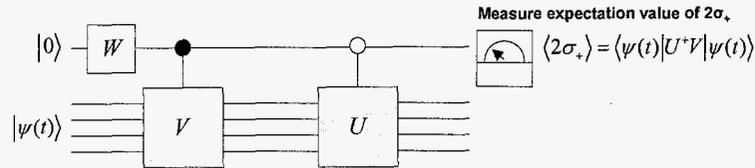
## Ancilla-Assisted Measurements



- Suppose we computed  $|\psi(t)\rangle$  because we would like to estimate  $\langle \psi(t) | U^\dagger V | \psi(t) \rangle = \langle U^\dagger V \rangle$

–Where  $U, V$  are unitary

- With  $2\sigma_+ = \sigma_x + i\sigma_y$  the following circuit is found to measure  $\langle U^\dagger V \rangle$



- Only a single output qubit is monitored
  - Estimating the state of a single qubit can be done efficiently
  - Then, if the Controlled-0- $U$  and Controlled-1- $V$  can be implemented efficiently ...
  - ... the (polynomial cost) quantum simulation (needed to create the input to this circuit) need only be repeated polynomially many times

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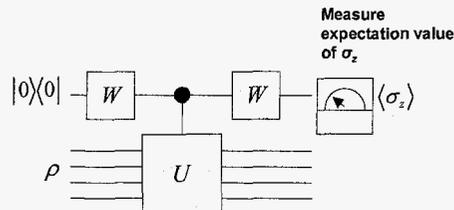


## Tomography c.f. Spectroscopy



- Circuits for measuring  $\text{Re}[\text{Tr}(\rho U)]$  and  $\text{Im}[\text{Tr}(\rho U)]$  for any unitary operator  $U$

–Find  $\langle \sigma_z \rangle = \text{Re}[\text{Tr}(\rho U)]$  and  $\langle \sigma_x \rangle = -\text{Im}[\text{Tr}(\rho U)]$



- N.B. polarization measurement reveals a property that depends on both  $\rho$  and  $U$ 
  - Hence can use this circuit to extract information about  $\rho$  if  $U$  is known (tomography)
  - Or to extract information about  $U$  if  $\rho$  is known (spectroscopy)

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# Quantum Fourier Transform



## From DFT to QFT



- **Discrete Fourier Transform (DFT)**

$$(x_0, x_1, \dots, x_{N-1}) \xrightarrow{\text{DFT}} (y_0, y_1, \dots, y_{N-1}): y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j e^{2\pi i j k / N}$$

- **Quantum Fourier Transform (QFT)**

- Same except "vector" is now stored in amplitudes of a superposition state

$$\sum_{j=0}^{N-1} x_j |j\rangle \xrightarrow{\text{QFT}} \sum_{k=0}^{N-1} y_k |k\rangle: |j\rangle \rightarrow \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i j k / N} |k\rangle$$

- Defining  $|j\rangle \equiv |j_1, j_2, \dots, j_n\rangle: j = j_1 2^{n-1} + j_2 2^{n-2} + \dots + j_n 2^0$

- Defining  $0.j_\ell j_{\ell+1} \dots j_m \equiv j_\ell / 2 + j_{\ell+1} / 4 + \dots + j_m / 2^{m-\ell+1}$

- Can factor mapping of basis state into following product state

$$|j\rangle \equiv |j_1 j_2 \dots j_n\rangle \rightarrow \frac{1}{2^{n/2}} \left[ (|0\rangle + e^{2\pi i 0.j_n} |1\rangle) (|0\rangle + e^{2\pi i 0.j_{n-1} j_n} |1\rangle) \dots (|0\rangle + e^{2\pi i 0.j_1 j_2 \dots j_n} |1\rangle) \right]$$

- Hence QFT maps basis states into product states and therefore has an efficient quantum circuit factorization



# Quantum Circuit for QFT

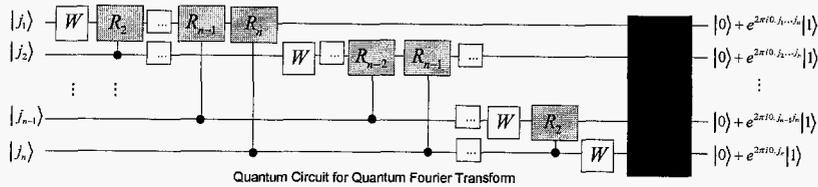


- Need Walsh-Hadamard and controlled 1-qubit gates

$$W = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad R_k = \begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi i / 2^k} \end{pmatrix}$$

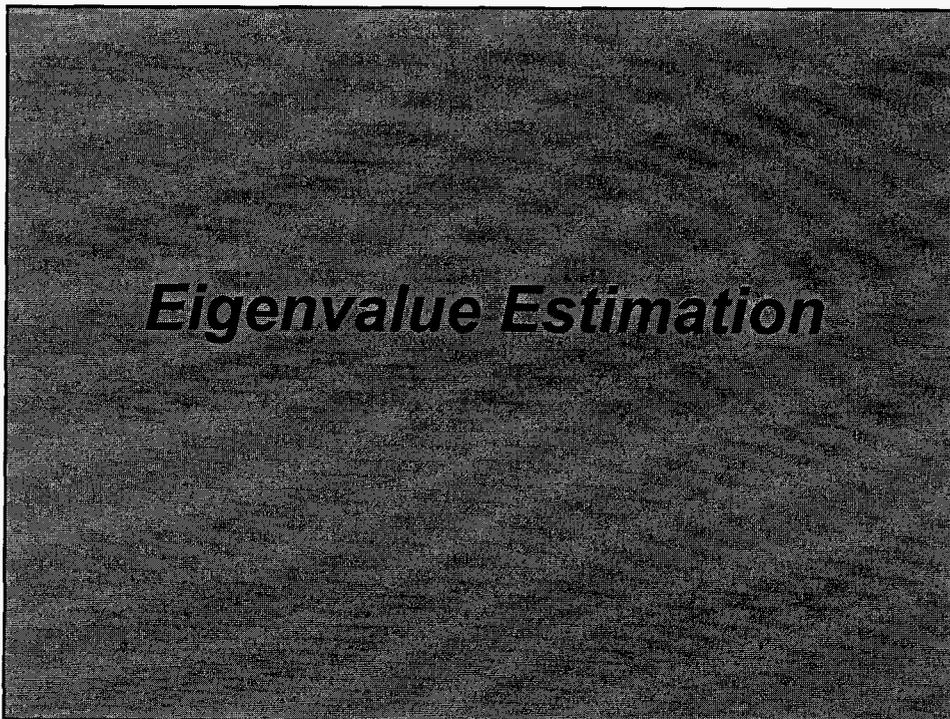


$$\equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{2\pi i / 2^k} \end{pmatrix}$$



- DFT (actually FFT) of length  $N$  vector takes  $O(N \log N)$  steps
  - QFT of length  $N$  vector takes  $O((\log N)^2)$  steps
    - Exponential speedup
    - But cannot see the result, can only compute with it or sample from it
- QFT maps eigenstates into phase factors
    - QFT<sup>-1</sup> maps phase factors into eigenstates

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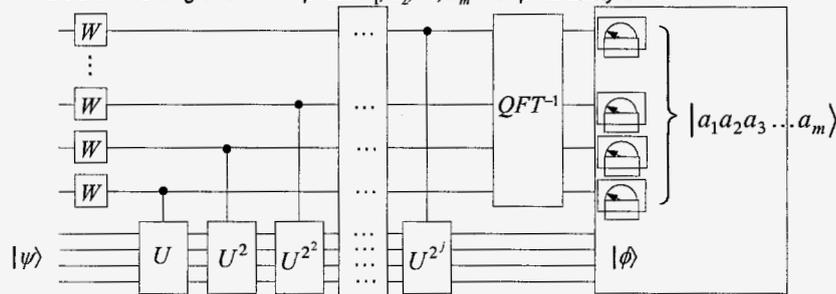




# Eigenvalue Estimation



- **Problem:** Given a Hamiltonian,  $H$ , and a state,  $|\psi\rangle$ , which approximates a true eigenstate,  $|\phi\rangle$
- **Goal:** Determine the corresponding eigenvalue,  $e^{2\pi i\phi} : 0 \leq \phi \leq 1$
- **Some observations:**
  - First notice an eigenvector of  $H$  is also an eigenvector of  $U = e^{-iHt/\hbar}$
  - If  $H$  is "local",  $U$  (and powers of  $U$ ) can be implemented efficiently
- **Let  $a/2^m = 0.a_1a_2\dots a_m$  (in binary) is the best  $m$ -bit estimate of  $\phi$** 
  - Then the following circuit computes  $a_1, a_2, \dots, a_m$  with probability 0.405



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# How Does Eigenvalue Estimation Work?



- **Hamiltonian,  $H$ , and a state,  $|\psi\rangle$ , which approximates a true eigenstate,  $|\phi_u\rangle$**
- **Goal: Determine the corresponding eigenvalue,  $a_u$**

### Algorithm AbramsLloydEigenvalue:

Step 1: Initialize state to  $|0\rangle|\psi\rangle = |0\rangle\sum_u d_u|\phi_u\rangle$  where  $|\phi_u\rangle$  are eigenvectors of  $U$

Step 2: Apply Walsh-Hadamard's to the  $b$  ancillae to create  $\frac{1}{\sqrt{2^b}}\sum_{j=0}^{2^b-1}|j\rangle\sum_u d_u|\phi_u\rangle$

Step 3: Apply powers of  $U$ , conditioned on ancillae  $\frac{1}{\sqrt{2^b}}\sum_{j=0}^{2^b-1}|j\rangle U^j \sum_u d_u|\phi_u\rangle$

Step 4: Since  $U$  unitary its eigenvalues can be written as  $e^{2\pi i a_u}$  where  $a_u \in \mathbb{R}$

Step 5: Re-write last state using eigenvalues and change order of summation

$$\frac{1}{\sqrt{2^b}} \sum_u d_u e^{2\pi i j a_u} |j\rangle |\phi_u\rangle$$

Step 6: Perform an inverse QFT in the ancillae  $\sum_u d_u \left( \sum_{j=0}^{2^b-1} g(a_u, j) |j\rangle \right) |\phi_u\rangle$

$$\text{where } g(a_u, j) = \begin{cases} \frac{\sin(\pi(2^b a_u - j)) e^{2\pi i(a_u - j/2^b)2^{b-1}}}{2^b \sin(\pi(a_u - j/2^b))} & 2^b a_u \neq j \\ 1 & 2^b a_u = j \end{cases}$$

Step 7: Measure the ancillae qubits to obtain outcome  $j$  with probability

$$p_j = \sum_u |d_u|^2 |g(a_u, j)|^2 \text{ and project second register into state } \sum_u \frac{d_u g(a_u, j)}{\sqrt{p_j}} |\phi_u\rangle$$

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# Fermionic Simulations



## Fermionic Simulations



- (In 1<sup>st</sup> quantization) fermionic simulations pose a special challenge in terms of creating the antisymmetric initial state

– Input state needs to be a superposition of Slater determinants

– i.e.,  $|\psi\rangle = \sum_{\alpha=1}^L g_{\alpha} |\phi_{\alpha}\rangle$  where  $|\phi_{\alpha}\rangle = \prod_{j=1}^{N_{\alpha}} c_j^{\dagger} |vac\rangle$

- In 2<sup>nd</sup> quantization must convert creation/annihilation operator algebra to that of spin-1/2 systems

– E.g., in a Hamiltonian  $H = \sum_{i=1}^M V_{ij} n_{i\uparrow} n_{j\downarrow} + \sum_{\langle i,j \rangle > \sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma}$

– Map creation/annihilation operators to spin operations using Jordan-Wigner transformation, i.e., with  $\sigma_{\pm}^j = \frac{\sigma_x^j \pm i\sigma_y^j}{2}$

$$c_j \rightarrow \left( \prod_{\ell=1}^{j-1} -\sigma_z^{\ell} \right) \sigma_-^j$$

$$c_j^{\dagger} \rightarrow \left( \prod_{\ell=1}^{j-1} -\sigma_z^{\ell} \right) \sigma_+^j$$

# Conclusions



## Conclusions

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- **Quantum computers *can* simulate quantum systems exponentially faster than classical computers**
- **But this does not imply you can obtain information about *all* properties of the system exponentially faster**
  - E.g., if you want the complete eigenspectrum there is no advantage
- **Obtaining certain properties exponentially faster is possible**
  - Often using some ancilla-assisted readout scheme
  - Expectation values of operators
  - Correlation functions
  - Gross spectral features (e.g., spectral regularity, density of states)
  - Ground state eigenvalues /eigenvectors
- **Aside: Quantum simulation of a fault tolerant quantum computer confers fault tolerance to the simulation**
  - Is this exploitable to make an error free computation?

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