Seminar 3 Quantum Computations

#### Schedule

- 1. Introduction to Quantum Computing
- 2. Formalisms in QM & Computing
- 3. Quantum Circuits Today
- 4. Fourier Analysis & Search Algorithms
- 5. Realisations of Quantum Computers
- More to come...
- I rescheduled the overall syllabus as now we require more time to explain concepts.

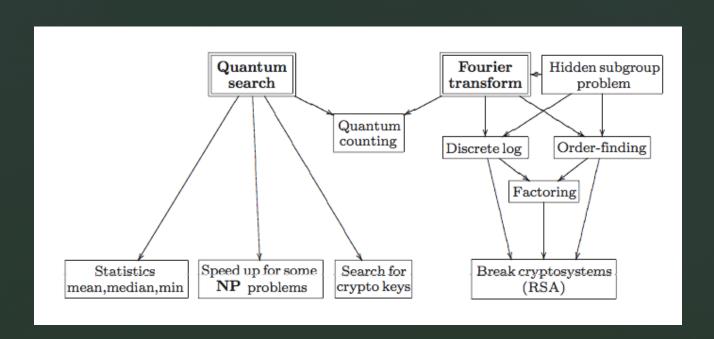
## Before going in...

- From now, we are entering the 'real' Quantum Computing.
- Recall our first seminar? We shall prove many theorems and elaborate further on the topics I introduced at then.
- It shall be little more technical and hard than before, but I think it will be transmittable.

# Before going in...

- Today, our content is based on chapters 4 on Nielsen & Chuang.
- First, we go through algorithms and little more on Quantum Circuits.
- I tried to incorporate some exercises. Harder exercises are explained, you must solve the easier ones.

#### An Overview



#### Some Extra Gates

• 
$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
,  $Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ ,  $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ 

Think of the Pauli Spin Matrices.

• Hadamard Gate 
$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

• Phase Gate 
$$S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$$

• 
$$\pi/8$$
 Gate  $T = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix} = e^{i\pi/8} \begin{bmatrix} e^{-i\pi/8} & 0 \\ 0 & e^{i\pi/8} \end{bmatrix}$ 

#### Rotations of Quantum Gates

$$R_{x}(\theta) \equiv e^{-\frac{i\theta X}{2}} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}X = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

$$R_{y}(\theta) \equiv e^{-\frac{i\theta Y}{2}} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}Y = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

$$R_{z}(\theta) \equiv e^{-\frac{i\theta Z}{2}} = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}Z = \begin{bmatrix} e^{-\frac{i\theta}{2}} & 0\\ 0 & e^{\frac{i\theta}{2}} \end{bmatrix}$$

The Rotation operators rotate the state ket on the Bloch sphere. Check it!

## Z-Y Decomposition for a Single Qubit

- Theorem. Suppose U is a unitary operation on a single qubit. Then there exist real numbers  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\delta$  such that U =  $\exp(i\alpha)Rz(\beta)Ry(\gamma)Rz(\delta)$ .
- Proof. The right hand side can be expressed as

$$U = \begin{bmatrix} e^{i(\alpha - \frac{\beta}{2} - \frac{\delta}{2})} \cos \frac{\gamma}{2} & -e^{i(\alpha - \frac{\beta}{2} + \frac{\delta}{2})} \sin \frac{\gamma}{2} \\ e^{i(\alpha + \frac{\beta}{2} - \frac{\delta}{2})} \sin \frac{\gamma}{2} & e^{i(\alpha + \frac{\beta}{2} + \frac{\delta}{2})} \cos \frac{\gamma}{2} \end{bmatrix}$$

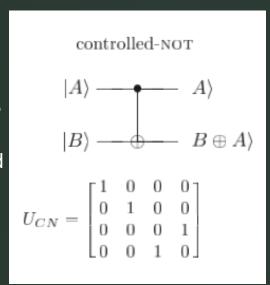
- Since U is unitary and therefore the rows and columns are orthonormal, we can decide the four variables.
- Should it be just Z & Y?

#### A Little Generalisation

- We can generalise the axes and state that:
- Suppose m and n are non-parallel real unit vectors in three dimensions.
- $U = \exp(i\alpha)Rn(\beta)Rm(\gamma)Rn(\delta)$ .
- Corollary: Suppose U is a unitary gate on a single qubit. Then
  there exist unitary operators A, B, C on a single qubit such that
  ABC = I and U = exp(iα)AXBXC, where α is some overall phase
  factor.

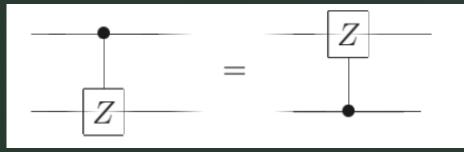
# **Controlled Operations**

- Matrix Representations: Remember this?
- If the control qubit is set then U is applied to the target qubit, otherwise the target qubit is left alone; that is,  $|c\rangle|t\rangle \rightarrow |c\rangle U^c|t\rangle$   $U_{CN} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
- (Generalisation)



#### Exercises

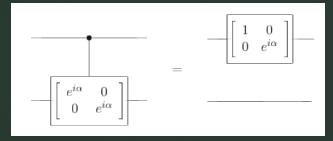
- 1. Construct a gate from one controlled-Z gate, that is, the gate whose action in the computational basis is specified by the unitary matrix and two Hadamard gates.
- 2. Show



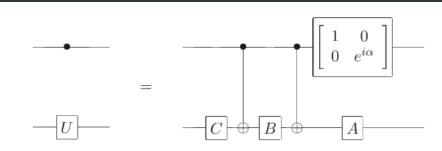
3. Flip of CNOT basis:

# Construction of the Controlled-U Opeartions

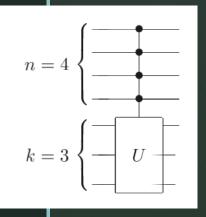
- Recall ABC = I and U = exp(iα)AXBXC
- Also, we have to give the phase, which is not very hard as



From this,



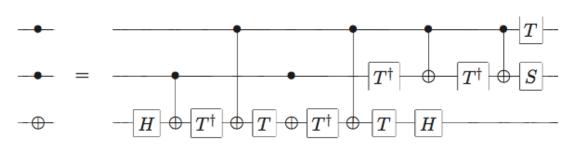
# Conditioning of Multiple Qubits



- $\overline{C^n(U)|x_1x_2}x_3\dots x_n\rangle|\psi\rangle = |x_1x_2x_3\dots x_n\rangle U^{x_1x_2x_3\dots x_n}|\psi\rangle$
- (More generally, suppose we have n + k qubits, and U is a k qubit unitary operator.)
- For U to operate in the k target qubits, all slots in  $x_1x_2x_3 ... x_n$  should be 1!

#### Construction of the Toffoli Gate

Doesn't the content in the last slide REALLY imply that we can make Toffoli gates?

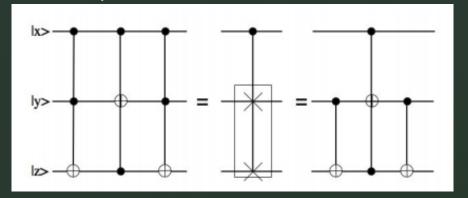


- Actually, we can create all CCU Gates with just CNOT and single Qubit operations.
- (You know what to do from here.)

#### Fredkin Gates

- Known as the CSWAP gate
- 1. Construct the Fredkin Gate using THREE Toffoli gates.
- 2. Actually, the first and third Toffoli can be replaced with CNOT.

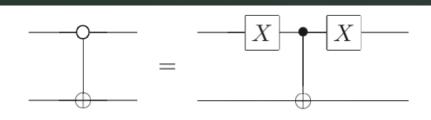
3. More simply, we can just make this with 5 two-qubit operations.



Ш	INPUT		OUTPUT		
C	<i>I</i> <sub>1</sub>	<i>l</i> <sub>2</sub>	C	<i>O</i> <sub>1</sub>	02
0	0	0	0	0	0
0	0	1	0	0	1
0	1	0	0	1	0
0	1	1	0	1	1
1	0	0	1	0	0
1	0	1	1	1	0
1	1	0	1	0	1
1	1	1	1	1	1

# Conditional Dynamics when control qubit is 0

- Until now, all the controlled operations were made only if the controlled qubits are 1.
- Constructing the gates which operates if the conrolled qubits are0 is quite useful!
- Construction is easy:



#### Two Useful Theorems for Measurement

- Principle of deferred measurement: Measurements can always be moved from an intermediate stage of a quantum circuit to the end of the circuit; if the measurement results are used at any stage of the circuit then the classically controlled operations can be replaced by conditional quantum operations.
- Principle of implicit measurement: Without loss of generality, any unterminated quantum wires (qubits which are not measured) at the end of a quantum circuit may be assumed to be measured.

# Universality

- Recall seminar 1 and 2?
- Some set of gates can create all algorithms by combination of their elements.
- Our goal: CNOT gates and single qubit gates can create all quantum computer algorithms.

## **Two-Level Unitary Gates**

- Consider a unitary matrix U which acts on a d-dimensional Hilbert space.
- U may be decomposed into a product of two-level unitary matrices; that is, unitary matrices which act non-trivially only on two-or-fewer vector components.
- Considering for d=3 shall suffice the overall logic.

# Two-Level Unitary Gates are Universal

• Claim. We can construct  $U_1$ ,  $U_2$ ,  $U_3$  such that  $I = U_3 U_2 U_1 U$ .

Proof. Set 
$$U = \begin{bmatrix} a & d & g \\ b & e & h \\ c & f & i \end{bmatrix}$$

$$\text{If b=0, U1=I, else, } U_1 = \begin{bmatrix} \frac{a^*}{\sqrt{|a|^2 + |b|^2}} & \frac{b^*}{\sqrt{|a|^2 + |b|^2}} & 0 \\ \frac{b}{\sqrt{|a|^2 + |b|^2}} & \frac{-a}{\sqrt{|a|^2 + |b|^2}} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

# Two-Level Unitary Gates are Universal

• If c'=0, 
$$U_2 = \begin{bmatrix} a'^* & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
, else,  $U_2 = \begin{bmatrix} \frac{a'}{\sqrt{|a'|^2 + |c'|^2}} & 0 & \frac{c'}{\sqrt{|a'|^2 + |c'|^2}} \\ 0 & 1 & 0 \\ \frac{c'}{\sqrt{|a'|^2 + |c'|^2}} & 0 & \frac{-a'}{\sqrt{|a'|^2 + |c'|^2}} \end{bmatrix}$ 

$$\quad \bullet \quad U_2 U_1 U = \begin{bmatrix} 1 & 0 & 0 \\ 0 & e^{\prime\prime} & h^{\prime\prime} \\ 0 & f^{\prime\prime} & i^{\prime\prime} \end{bmatrix}$$

• I think it is now quite straightforward how to construct  $U_3$ .

#### **Gray Codes**

- A Gray code connecting s and t is a sequence of binary numbers, starting with s and concluding with t, such that adjacent members of the list differ in exactly one bit.
- For instance, with s = 101001 and t = 110011 we have the Gray code 101001 101011 100011 110011.

# Shortening the Unitary operator to Two-Level Unitary Gates

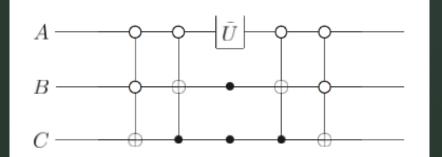
- Implementing each step of the Gray code is easy: Use the controlled bit flip.
- Stop just before the final step: By now, the remaining operation is a controlled one-qubit gate. We know that this can be implemented using CNOT and single qubit operations.
- Then, just do the inverse process, and we are done.

# Example

Implement U.

$$\widetilde{U} = \begin{bmatrix} a & c \\ b & d \end{bmatrix}$$

 Note that only 000 and 111 gives nontrivial terms.



## **Approximation of Unitary Operators**

- A discrete set of gates can't be used to implement an arbitrary unitary operation exactly, since the set of unitary operations is continuous.
- A discrete set CAN be used to approximate any unitary operation.
- Definition of  $\overline{Error}$ :  $E(U,V) = \max_{|\psi\rangle} ||(U-V)|\psi\rangle||$ , where U is the real operator and V is the approximated one.

#### Approximation of Unitary Operators

Suppose a quantum system starts in the state  $|\psi\rangle$ , and we perform either the unitary operation U, or the unitary operation V. Following this, we perform a measurement. Let M be a POVM element associated with the measurement, and let  $P_U$  (or  $P_V$ ) be the probability of obtaining the corresponding measurement outcome if the operation U (or V) was performed. Then

$$|P_U - P_V| = |\langle \psi | U^{\dagger} M U | \psi \rangle - \langle \psi | V^{\dagger} M V | \psi \rangle|. \tag{4.64}$$

Let  $|\Delta\rangle\equiv (U-V)|\psi\rangle$ . Simple algebra and the Cauchy–Schwarz inequality show that

$$|P_U - P_V| = |\langle \psi | U^{\dagger} M | \Delta \rangle + \langle \Delta | M V | \psi \rangle|. \tag{4.65}$$

$$\leq |\langle \psi | U^{\dagger} M | \Delta \rangle| + |\langle \Delta | M V | \psi \rangle| \tag{4.66}$$

$$\leq \||\Delta\rangle\| + \||\Delta\rangle\| \tag{4.67}$$

$$\leq 2E(U,V). \tag{4.68}$$

What does this inequality mean?

Ans: If the error is small, the difference of probabilities in measurement outcomes are also small.

- We CAN generalise this to n operators, and the result is:
- $E(U_m U_{m-1} \dots U_1, V_m V_{m-1} \dots V_1) \le \sum_{j=1}^m E(U_j, V_j)$

#### Some Additional Theorems

- 1. The standard set of gates, comprised of Hadamard, Phase, CNOT, and  $\frac{\pi}{8}$  gates are universal.
- Proof is made by picturing those gates at the Bloch sphere, which turns the gates into a rotation operators. We then use some  $\epsilon \delta$  technique to prove the theorem.

#### Some Additional Theorems

- Solovay-Kitaev Theorem: An arbitrary single qubit gate can be approximated to an accuracy  $\epsilon$  requires  $O(\log^c(1/\epsilon))$  gates from our discrete set, where c is a constant approximately equal to 2.
- This is a polylogarithmic increase over the size of the original circuit, which is likely to be acceptable for virtually all applications.

# Simulation of Quantum Systems

- Of course, this is possible in classical computers, albeit very inefficiently.
- Schrodinger's Equation:  $i \frac{\partial}{\partial t} \psi(x) = (-\frac{1}{2m} \frac{\partial^2}{\partial x^2} + V(x)) \psi(x)$
- This means we have to solve exponential amounts of equations for many-particle systems...

#### Quantum Simulation Algorithm

- $i\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle \rightarrow |\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$
- Yeah..of course we can just approximate to the first order. But srsly, do you really think this will be accurate?
- What we should do?: Let's class Hamiltonians to many local interactions.  $H = \sum_{k=1}^{L} H_k$
- Each  $H_k$  shall work on finite numbers (actually, usually two) of particles and therefore be quite easy to evaluate using Quantum Circuits. (i.e.  $e^{-iH_kt}$  is much easier to evaluate than  $e^{-iHt}$ .)

#### Quantum Simulation Algorithm

- Okay, but we do have some problems.
- If  $[H_i, H_k]$  is NOT zero (which is the default),  $e^{-iHt} \neq \prod_{k=1}^L e^{-iH_kt}$
- Trotter's Formula: Let A and B be Hermitian operators. Then for any real t,  $\lim_{n\to\infty}(e^{iAt/n}e^{iBt/n})^n=e^{i(A+B)t}$
- I will not state the proof since it is little complicated, but one important consequence is  $e^{i(A+B)\Delta t}=e^{iA\Delta t}e^{iB\Delta t}+O(\Delta t^2)$

## **Quantum Simulation Algorithm**

loop

#### Algorithm: Quantum simulation

Inputs: (1) A Hamiltonian  $H = \sum_k H_k$  acting on an N-dimensional system, where each  $H_k$  acts on a small subsystem of size independent of N, (2) an initial state  $|\psi_0\rangle$ , of the system at t=0, (3) a positive, non-zero accuracy  $\delta$ , and (3) a time  $t_f$  at which the evolved state is desired.

**Outputs:** A state  $|\tilde{\psi}(t_f)\rangle$  such that  $|\langle \tilde{\psi}(t_f)|e^{-iHt_f}|\psi_0\rangle|^2 \geq 1 - \delta$ .

Runtime:  $O(\text{poly}(1/\delta))$  operations.

**Procedure:** Choose a representation such that the state  $|\tilde{\psi}\rangle$  of  $n=\text{poly}(\log N)$  qubits approximates the system and the operators  $e^{-iH_k\Delta t}$  have efficient quantum circuit approximations. Select an approximation method (see for example Equations (4.103)–(4.105)) and  $\Delta t$  such that the expected error is acceptable (and  $j\Delta t=t_f$  for an integer j), construct the corresponding quantum circuit  $U_{\Delta t}$  for the iterative step, and do:

1. 
$$|\tilde{\psi}_0\rangle \leftarrow |\psi_0\rangle$$
 ;  $j=0$  initialize state

2. 
$$\rightarrow |\tilde{\psi}_{i+1}\rangle = U_{\Delta t}|\tilde{\psi}_{i}\rangle$$
 iterative update

3. 
$$\rightarrow j = j + 1$$
; goto 2 until  $j\Delta t \ge t_f$ 

$$ightarrow | ilde{\psi}(t_f)
angle = | ilde{\psi}_j
angle$$
 final result