LibKet: A Software Framework for Quantum-Accelerated Scientific Computing

Hands-on Introduction to Quantum Computing with LibKet

2021 SIAM Conference on Computational Science and Engineering

March 1st, 2021

Matthias Möller¹ and Carmen G. Almudever²

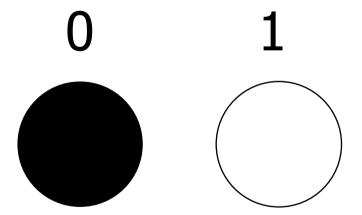
¹Delft University of Technology (m.moller@tudeflt.nl) ²Technical University of Valencia (cargara2@disca.upv.es)



Basic unit of information

Bit

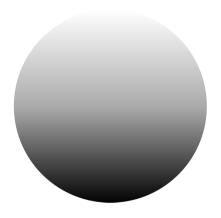
Exclusive state



Quantum bit (Qubit)

$$|0\rangle$$
 and $|1\rangle$

Superposition

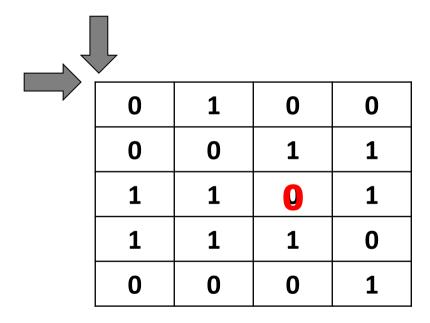


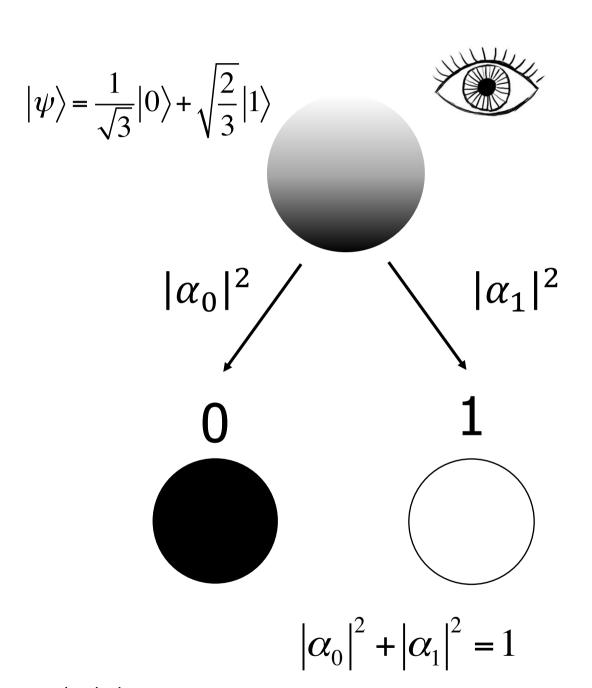
$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$$



Reading out information

Memory





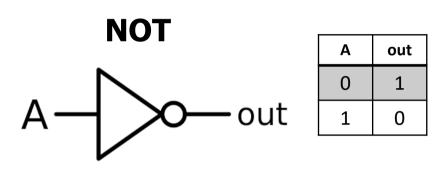
Probabilistic process



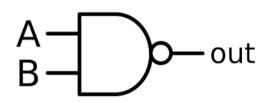
Operations

Classical gates

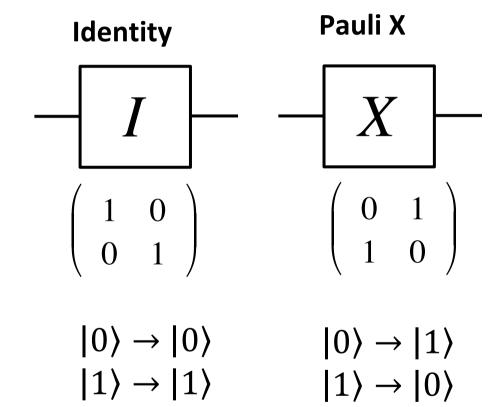
Quantum gates



NAND



Α	В	out	
0	0	1	
0	1	1	
1	0	1	
1	1	0	

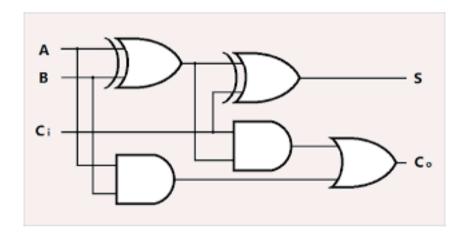


- Logical operation
- Truth tables
- Most of them only run forward
- Unitary operation
- Unitary matrix
- All quantum gates are reversible



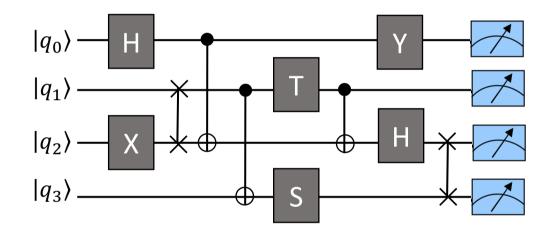
Computation

Classical circuits



Quantum circuits

Circuit model of computation



- Single-qubit gates: H, X, T, S, Y
- Two-qubit gates: CNOT and SWAP



3 bits

000 or 001 or 010 or 011 or 100 or 101 or 110

n bits hold 1 value: from 0 to 2ⁿ-1

3 qubits



$$\alpha_{000} |000\rangle + \alpha_{001} |001\rangle + \alpha_{010} |010\rangle + \alpha_{011} |011\rangle + \alpha_{100} |100\rangle + \alpha_{101} |101\rangle + \alpha_{110} |110\rangle + \alpha_{111} |111\rangle$$

000 and 001 and 010 and 011 and 100 and 101 and 110 and 111

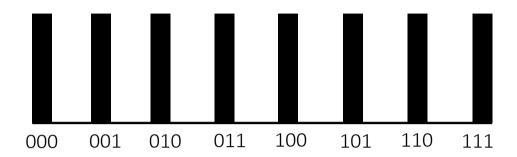
- n qubits can hold 2ⁿ values (50 qubits, 2⁵⁰ complex amplitudes)
- All states (amplitudes) can be manipulated at the same time



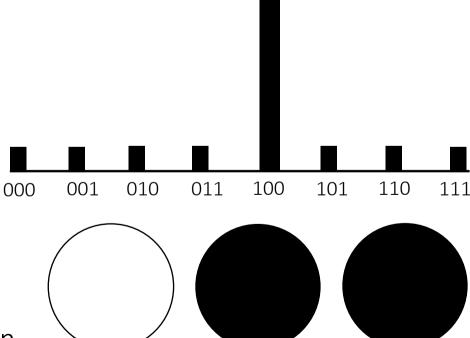
Superposition and entanglement



$$\alpha_{000} |000\rangle + \alpha_{001} |001\rangle + \alpha_{010} |010\rangle + \alpha_{011} |011\rangle + \alpha_{100} |100\rangle + \alpha_{101} |101\rangle + \alpha_{110} |110\rangle + \alpha_{111} |111\rangle$$



Interference

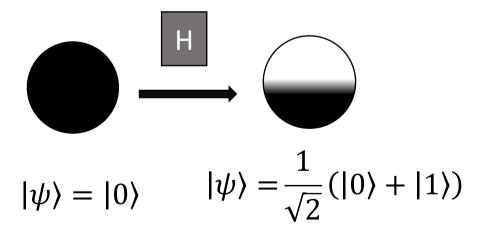


- Probabilistic computation
- Result is a binary value



In-memory computing

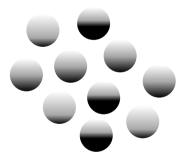
• The qubits hold the information in a form of a quantum state which is modified by applying an operation on them.



Qubits and gates are error prone

- Qubits have short coherence time
- Imperfect operations
 - Gate error rates: 10^{-2} - 10^{-3}

Quantum information needs to be protected

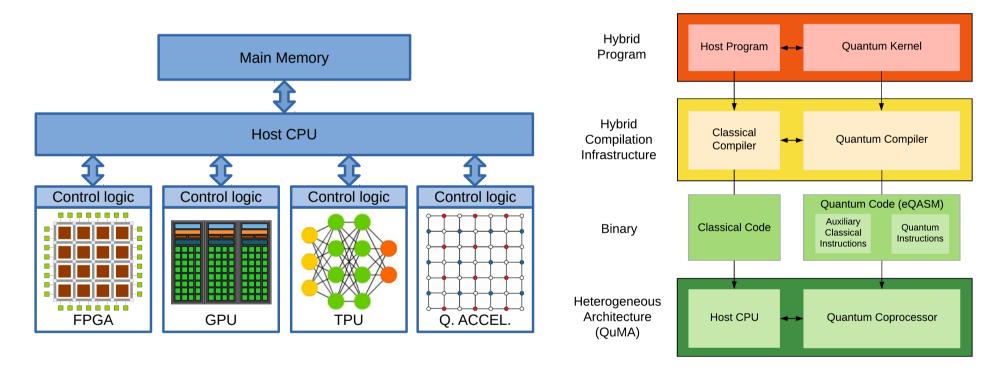


Quantum error correction



A quantum computer is not (is)

- It is not a replacement for classical computers
- It is an in-memory-computing device
- It is a co-processor in a (heterogeneous) multi-core architecture



X. Fu et. al, "eQASM: An Executable Quantum Instruction Set Architecture", IEEE International Symposium on High Performance Computer Architecture (HPCA), 2019.

Riesebos, L., et al. "Quantum Accelerated Computer Architectures." 2019 IEEE International Symposium on Circuits and Systems (ISCAS). IEEE, 2019.



Quantum Computation is based on Linear Algebra



Reading out quantum information

Measuring a qubit (quantum state)

$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$$

$$|\alpha_0|^2 \qquad |\alpha_1|^2$$

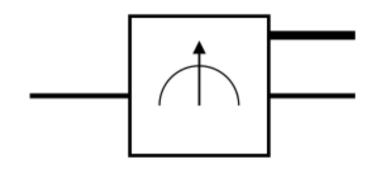
$$0 \qquad 1$$

$$|\alpha_0|^2 + |\alpha_1|^2 = 1$$

$$\alpha_0, \alpha_1 \in \mathbb{C}$$

$$\left| \boldsymbol{\alpha}_i \right|^2$$

is the probability of finding the qubit in state $|i\rangle$ when we measure it (in the computational basis)



Probabilistic process
Binary value
Projective measurement



Measuring a qubit

$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$$

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

$$\frac{1}{2} |0\rangle + \frac{\sqrt{3}}{2} |1\rangle$$

$$\frac{1}{2} |0\rangle + \frac{i\sqrt{3}}{2} |1\rangle$$

$$\frac{1}{2} |0\rangle + \frac{1}{2} |1\rangle$$

 $|\alpha_0|^2$ Prob. result 0 Prob. result 1

$$\left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$$

$$\left|\frac{1}{2}\right|^2 = \frac{1}{4}$$

$$\left|\frac{1}{2}\right|^2 = \frac{1}{4}$$

$$\left|\frac{1}{2}\right|^2 = \frac{1}{4}$$

$$|lpha_1|^2$$

$$\left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$$

$$\left|\frac{\sqrt{3}}{2}\right|^2 = \frac{3}{4}$$

$$\left|\frac{i\sqrt{3}}{2}\right|^2 = \frac{3}{4}$$

$$\left|\frac{1}{2}\right|^2 = \frac{1}{4}$$

This is not a quantum state

$$\left|\alpha_0\right|^2 + \left|\alpha_1\right|^2 = 1$$



A quantum state is a vector

$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$$

$$\begin{vmatrix} 0 \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \qquad \begin{vmatrix} 1 \rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\left| \psi \rangle = \alpha_0 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \alpha_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} \right|$$

Representation on the Bloch Sphere

$$|\psi\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} \quad \alpha_0, \alpha_1 \in \mathbb{C}$$

$$\alpha_0, \alpha_1 \in \mathbb{C}$$

•
$$|\psi\rangle = \alpha_0 |0\rangle + e^{i\varphi}\alpha_1 |1\rangle$$

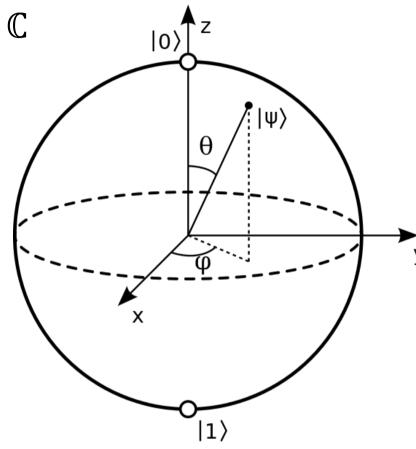
 $\alpha_0, \alpha_1 \in \mathbb{R}$

•
$$\sqrt{\alpha_0^2 + \alpha_1^2} = 1$$
 $(\sqrt{\sin^2 x + \cos^2 x} = 1)$

$$\alpha_0 = \cos\frac{\theta}{2} \qquad \qquad \alpha_1 = \sin\frac{\theta}{2}$$

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$

$$\theta, \varphi \in \mathbb{R}$$

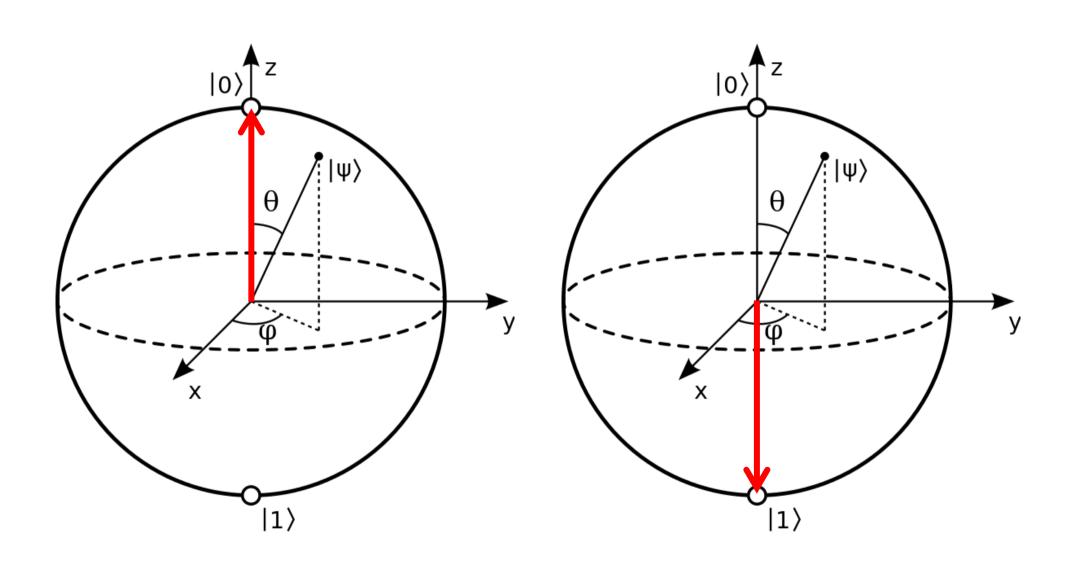


 θ : polar angle $\in [0,\pi]$

 φ : azimutal angle $\in [0,2\pi]$



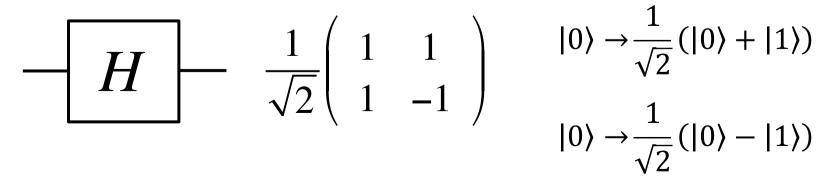
Representation on the Bloch Sphere





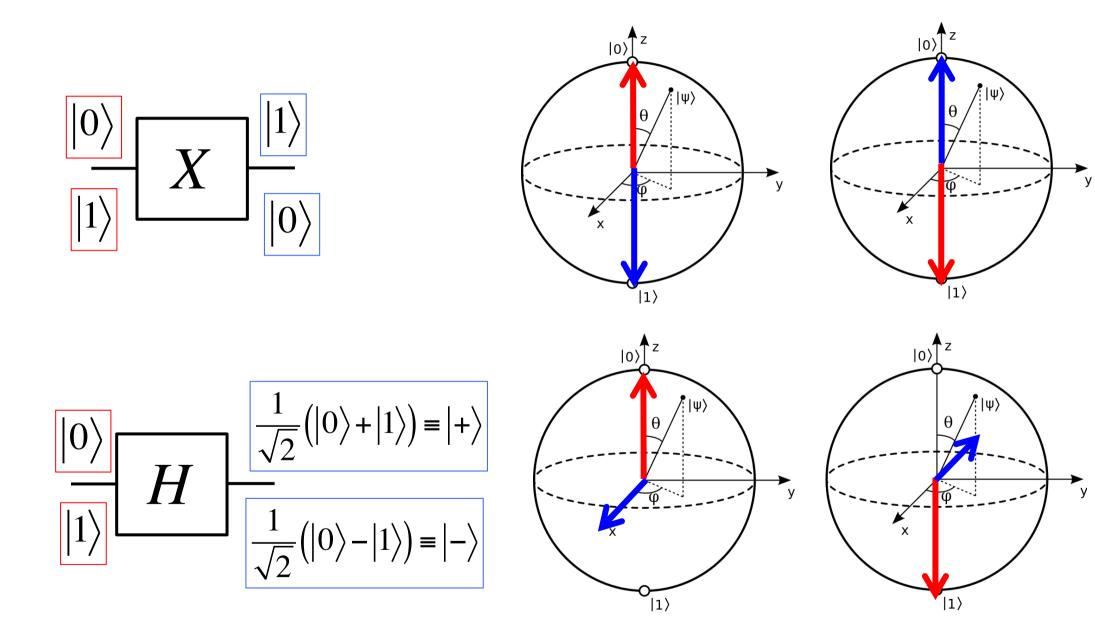
Single-qubit gates

Hadamard



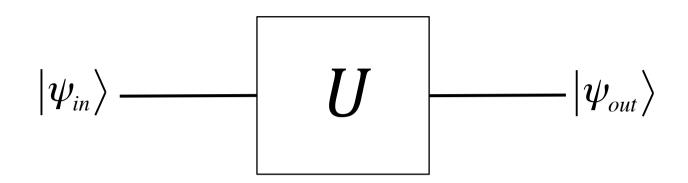


Single-qubit gates





Single-qubit gates



$$|\psi_{out}\rangle = U|\psi_{in}\rangle$$

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

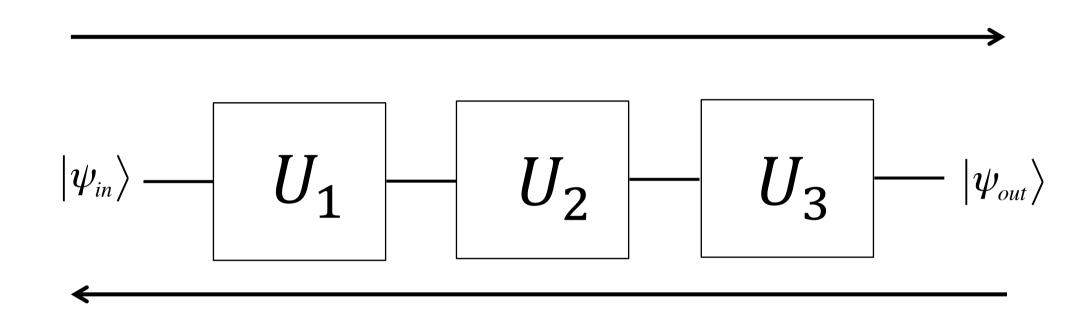
$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|0\rangle \boxed{X} ? \qquad |\psi_{out}\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$





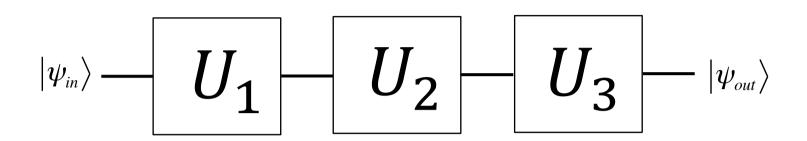
Quantum circuit (single qubit)



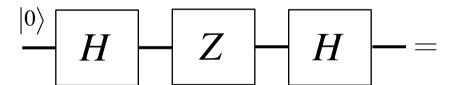
$$|\psi_{out}\rangle = U_3 U_2 U_1 |\psi_{in}\rangle$$



Quantum circuit (single qubit)



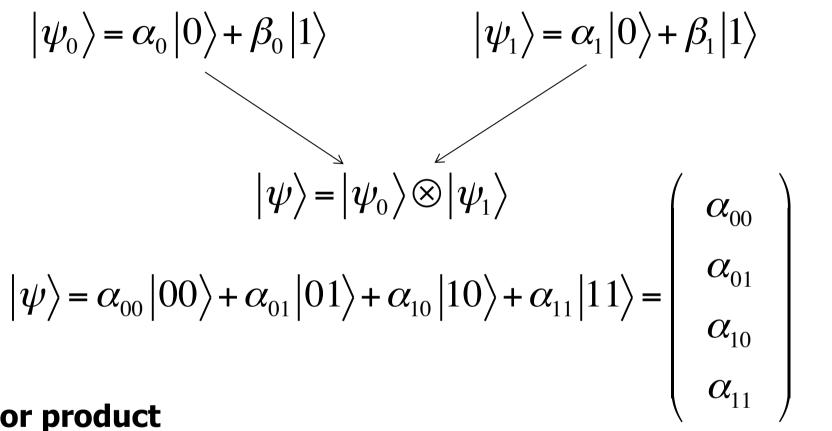
$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



$$\stackrel{|0\rangle}{-} H - X - H - =$$







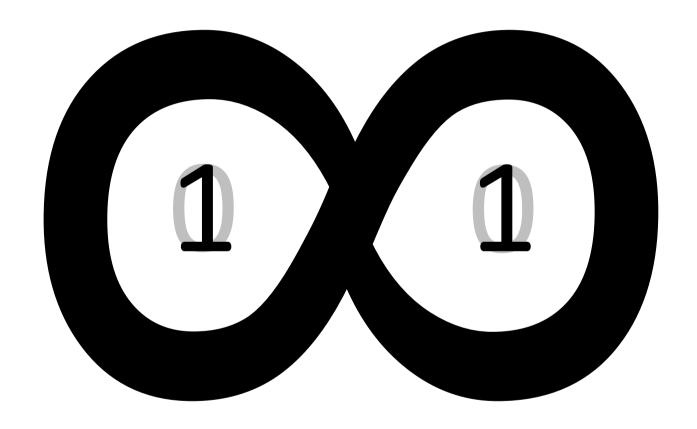
Tensor product

$$|A\rangle \otimes |B\rangle = \begin{bmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{bmatrix}$$

$$\left|\alpha_{00}\right|^{2} + \left|\alpha_{01}\right|^{2} + \left|\alpha_{10}\right|^{2} + \left|\alpha_{11}\right|^{2} = 1$$



Entanglement



Two qubits in a superposition are correlated with one another



Entanglement

Quantum entanglement means that multiple particles are linked together in a way such that the measurement of one particle's quantum state determines the possible quantum states of the other particles.

This connection isn't depending on the location of the particles in space. Even if you separate entangled particles by billions of kms, changing one particle will induce a change in the other.

$$\frac{1}{\sqrt{2}}(|00\rangle+|11\rangle)$$

https://www.youtube.com/watch?v=CC_XES4xQD4



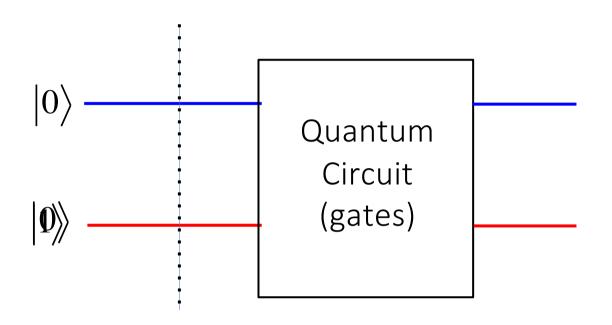
Two qubits are *entangled* when their joint states cannot possibly be separated into a product of individual qubit states

$$|\Psi\rangle = \left|\varphi\rangle \, \otimes \left|\psi\rangle \right| \quad \text{vs.} \quad \left|\Psi\rangle = \left|\varphi\rangle \, \otimes \left|\psi\rangle + \left|\varphi'\rangle \, \otimes \left|\psi'\rangle \right| \right|$$

$$\frac{1}{\sqrt{2}} \left(\left| 10 \right\rangle + \left| 11 \right\rangle \right) = \left| 1 \right\rangle \otimes \frac{1}{\sqrt{2}} \left(\left| 0 \right\rangle + \left| 1 \right\rangle \right) \quad \text{(not entangled)}$$

$$\frac{1}{\sqrt{2}} \left(\left| 00 \right\rangle + \left| 11 \right\rangle \right) = \frac{1}{\sqrt{2}} \left| 0 \right\rangle \otimes \left| 0 \right\rangle + \frac{1}{\sqrt{2}} \left(\left| 1 \right\rangle \otimes \left| 1 \right\rangle \right) \text{ (entangled)}$$





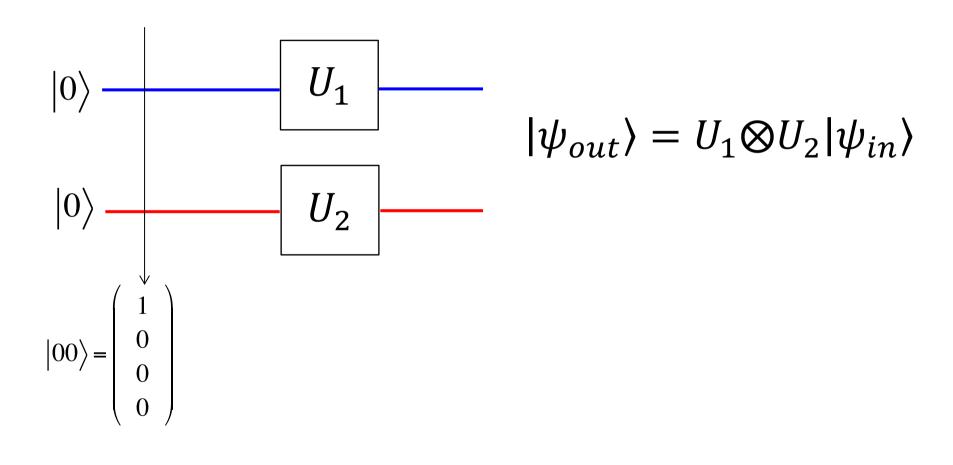
$$|0\rangle \otimes |0\rangle = |0\rangle |0\rangle = |00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{vmatrix} 01 \rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

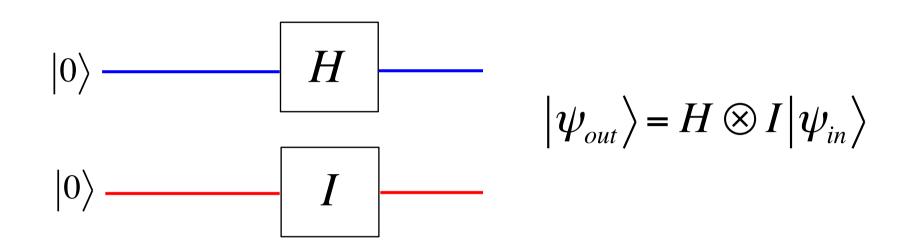
$$|10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\begin{vmatrix} 11 \rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$





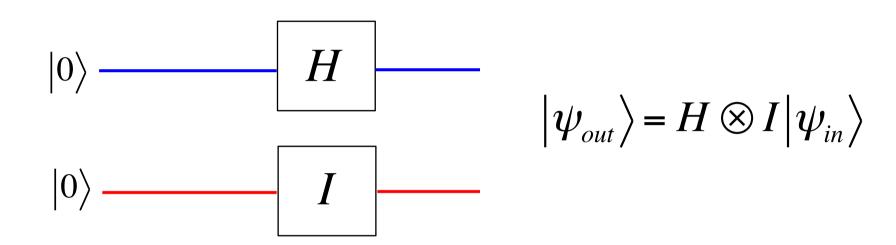




$$\hat{U}_1 \otimes \hat{U}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} =$$

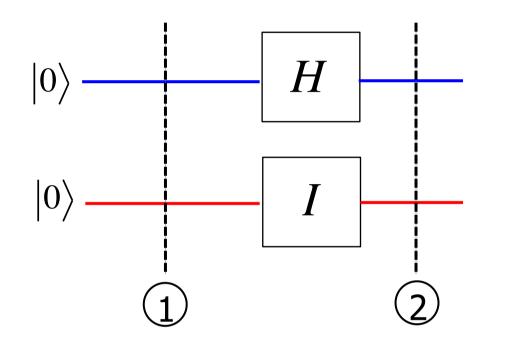
$$|A\rangle \otimes |B\rangle = \begin{bmatrix} A_{11}B & A_{12}B \\ A_{21}B & A_{22}B \end{bmatrix}$$





$$|\psi_{out}\rangle$$
 =





$$|\psi_{out}\rangle = H \otimes I |\psi_{in}\rangle$$

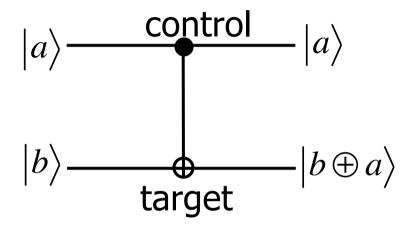
$$\bigcirc$$
 $|00\rangle$

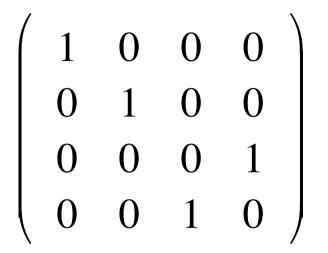


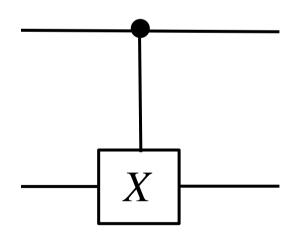


Multi-qubit gates

CNOT gate







XOR gate

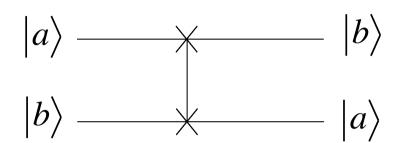
a	b out	
0	0	0
0	1	1
1	0	1
1	1	0

$$a \cdot \overline{b} + \overline{a} \cdot b$$

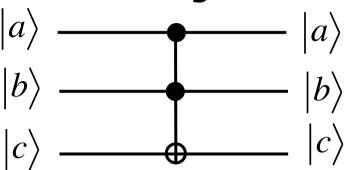


Multi-qubit gates

SWAP gate



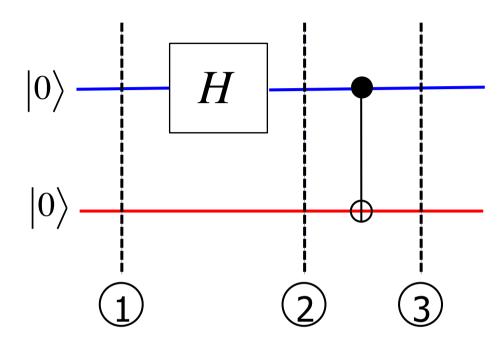




$$\left(\begin{array}{ccccc}
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1
\end{array}\right)$$

Input		Output			
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	0	1
1	1	0	1	1	1
1	1	1	1	1	0





- \bigcirc $|00\rangle$

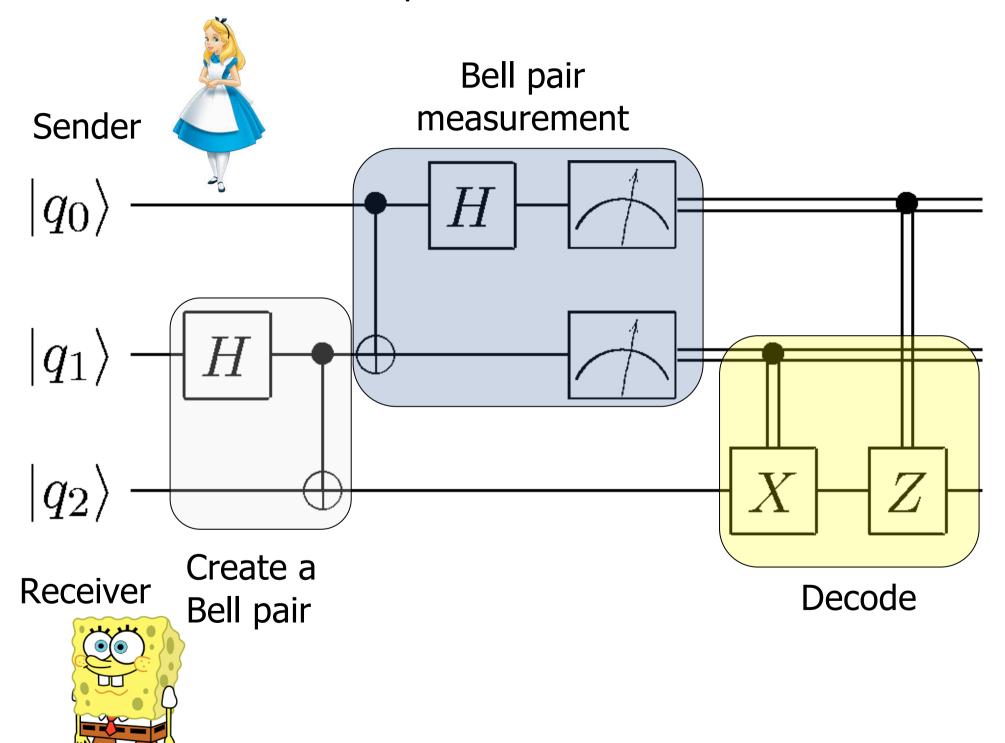


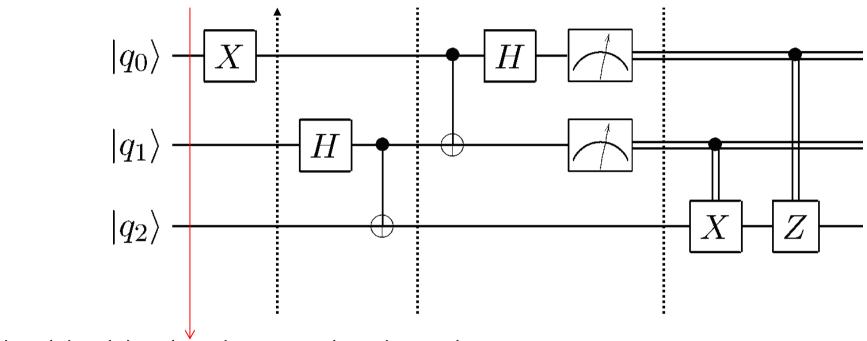
Bell states

$$|\beta_{00}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$
$$|\beta_{01}\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$
$$|\beta_{10}\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$
$$|\beta_{11}\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$









 $|q_0\rangle|q_1\rangle|q_2\rangle = |q_0q_1q_2\rangle = |000\rangle$

QASM-like code

X q0 H q1 CNOT q1,q2 CNOT q0,q1 H q0



$$|q_0\rangle|q_1\rangle|q_2\rangle = |q_0q_1q_2\rangle = |000\rangle$$

$$X q_0 \rightarrow |100\rangle$$

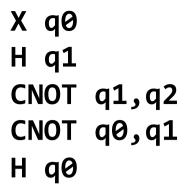
$$\mathbf{H} \mathbf{q_1} \rightarrow |1\rangle \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) |0\rangle = \frac{1}{\sqrt{2}} (|100\rangle + |110\rangle)$$

CNOT
$$q_1, q_2 \rightarrow \frac{1}{\sqrt{2}} (|100\rangle + |111\rangle)$$

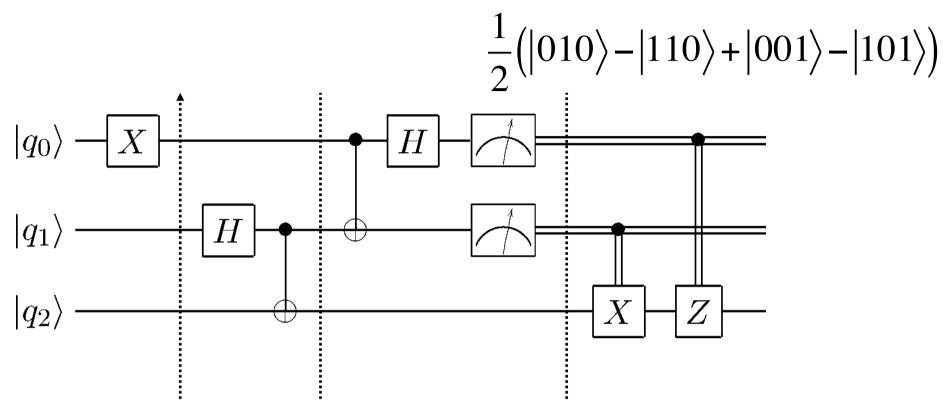
CNOT
$$q_0, q_1 \rightarrow \frac{1}{\sqrt{2}} (|110\rangle + |101\rangle)$$

$$\mathbf{H} \mathbf{q_0} \rightarrow \frac{1}{\sqrt{2}} \left[\frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) |10\rangle + \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) |01\rangle \right] =$$

$$=\frac{1}{2}(|010\rangle-|110\rangle+|001\rangle-|101\rangle)$$







- Measure 00 \rightarrow $|q_2\rangle = |1\rangle \rightarrow$ no correction
- Measure 01 \rightarrow $|q_2\rangle = |0\rangle \rightarrow$ bit-flip q2 \rightarrow $|q_2\rangle = |1\rangle$
- Measure 10 \rightarrow $|q_2\rangle = -|1\rangle$ \rightarrow phase-flip q2 \rightarrow $|q_2\rangle = |1\rangle$
- Measure 11 \rightarrow $|q_2\rangle$ = $-|0\rangle$ \rightarrow bit-flip and phase-flip \rightarrow $|q_2\rangle$ = $|1\rangle$





Qubits are very fragile!

- Extremely short coherence time: ~ us − s
- Gate error rates: $^{\sim}10^{-1}$ -10⁻³ vs. CMOS 10⁻²⁰-10⁻¹⁵

1. Bit flip error

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \rightarrow \alpha|1\rangle + \beta|0\rangle$$

$$\sigma_{x} = \left[\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right]$$

2. Phase flip error

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \rightarrow \alpha|0\rangle - \beta|1\rangle$$

$$\sigma_z = \left| \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right|$$

3. Bit and Phase flip error

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \rightarrow \alpha|1\rangle - \beta|0\rangle$$

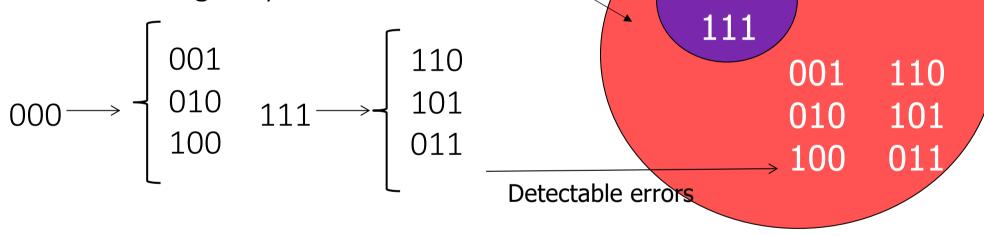
$$\sigma_{y} = \left[\begin{array}{cc} 0 & -i \\ i & 0 \end{array} \right]$$



Classical error correction encoding: 3 bit repetition code

- 0 is encoded as 000
- 1 is encoded as 111

Valid codewords Assuming only 1 bit error



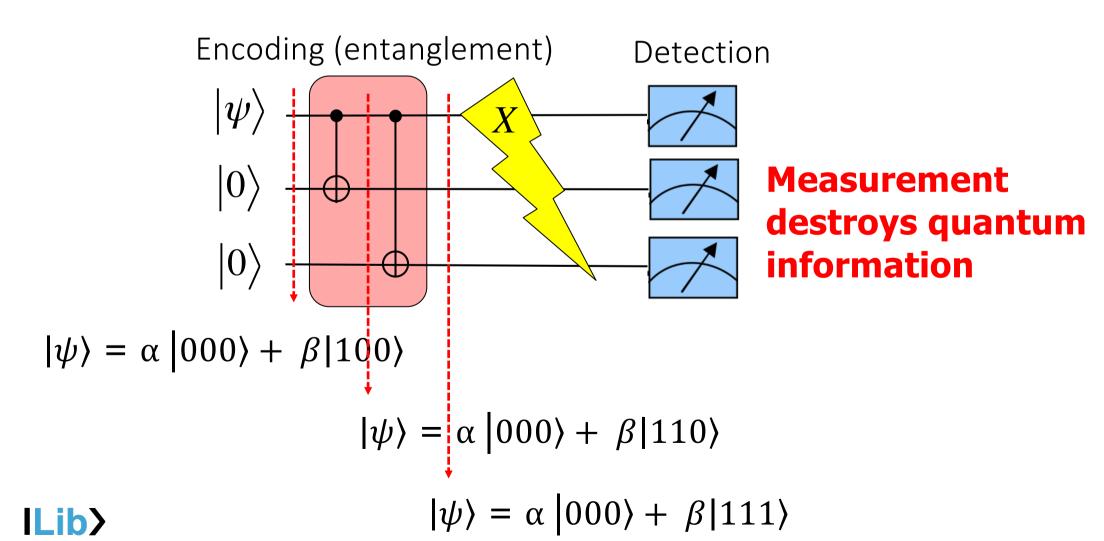
000

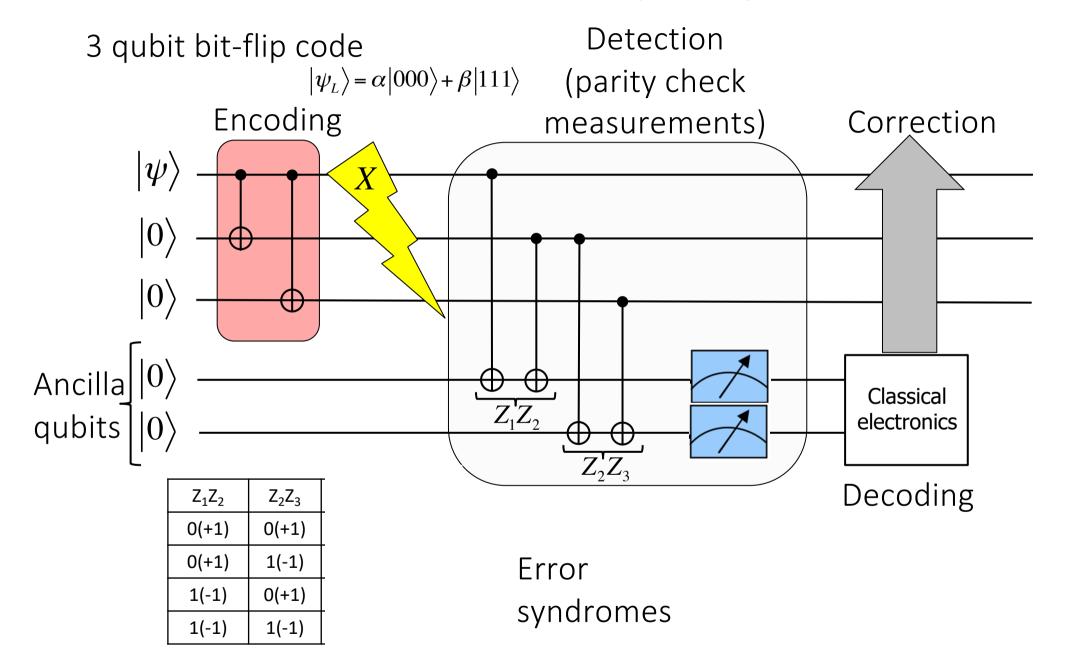
- Decoding: Majority voting
 - E.g. $000 \rightarrow 001$ \longrightarrow bit-flip bit 3



3 qubit bit-flip code: single bit-flip errors

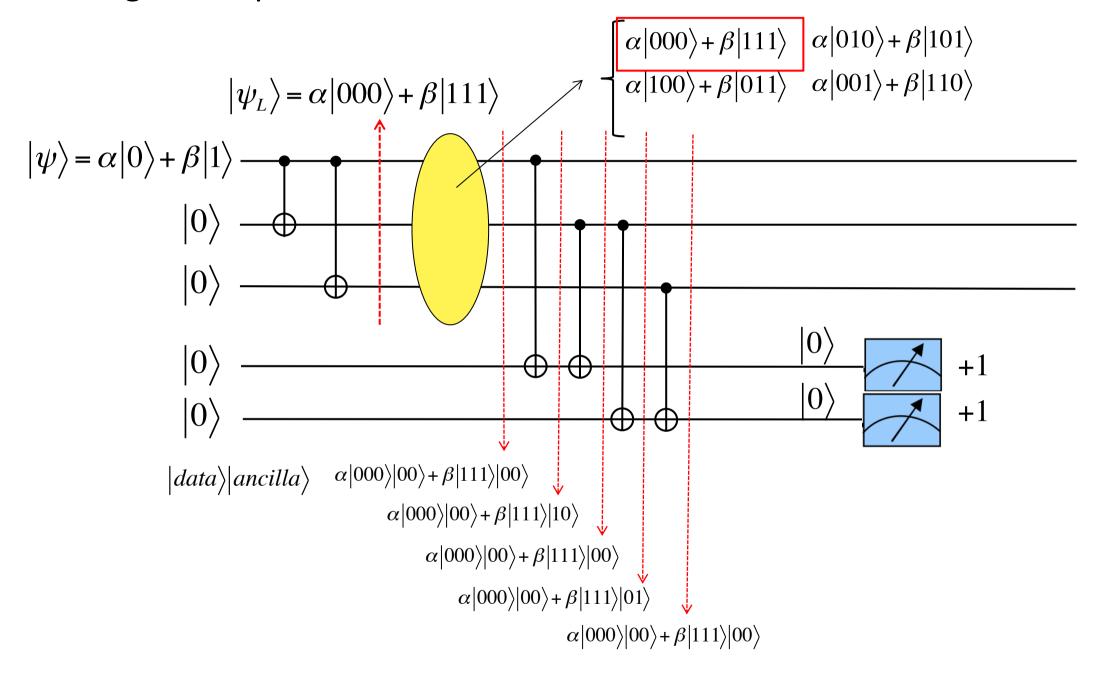
Physical qubit Logical qubit
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \rightarrow \alpha|000\rangle + \beta|111\rangle$$





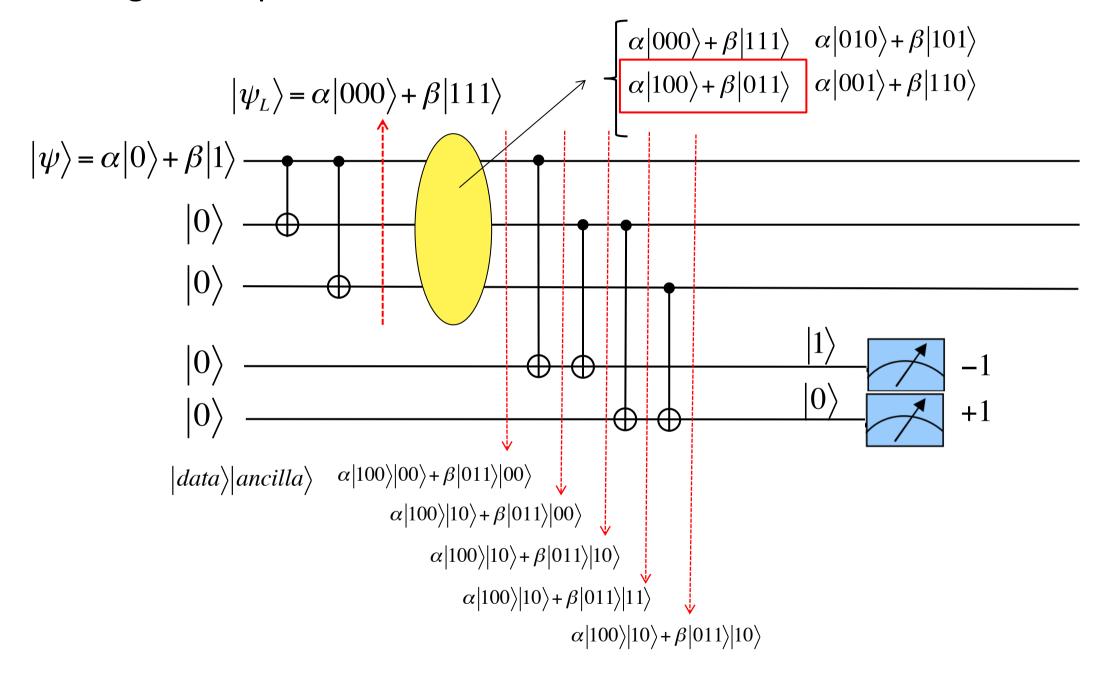


Single bit-flip error occurs...



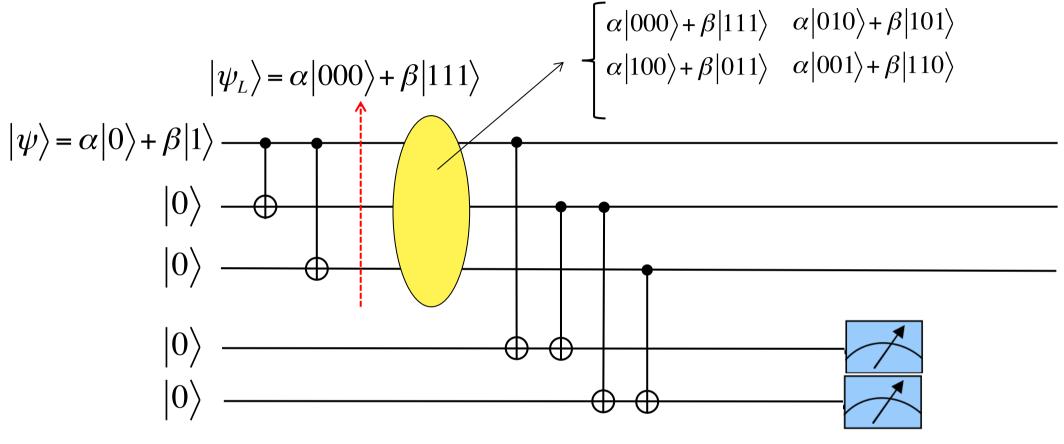


Single bit-flip error occurs...





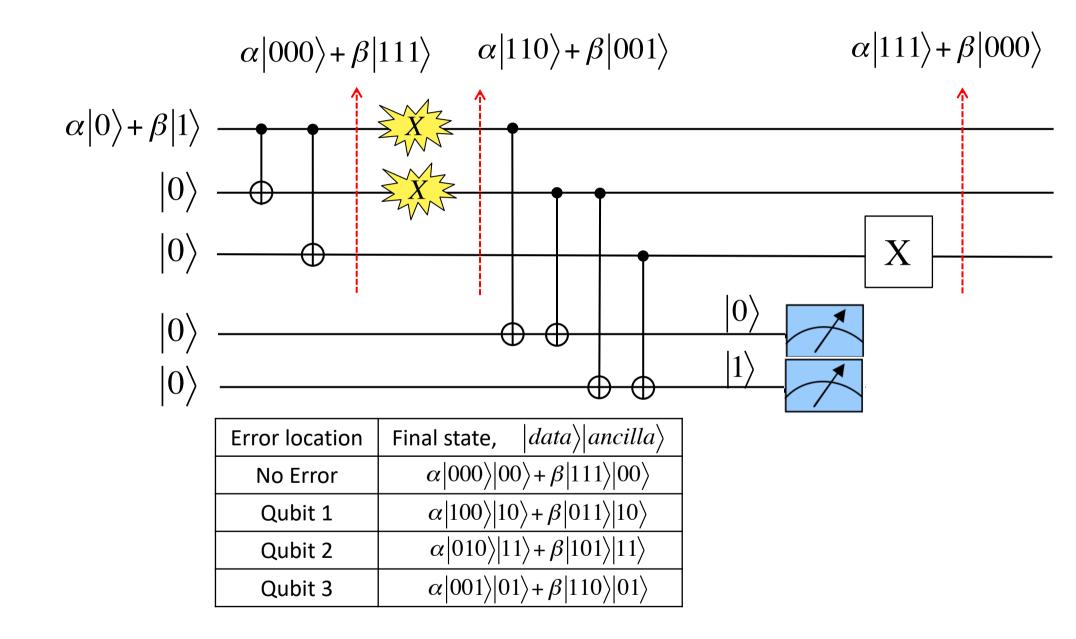
Single bit-flip error occurs...



Error location	Final state, $ data angle ancilla angle$
No Error	$\alpha 000\rangle 00\rangle$ + $\beta 111\rangle 00\rangle$
Qubit 1	$\alpha 100\rangle 10\rangle + \beta 011\rangle 10\rangle$
Qubit 2	$\alpha 010\rangle 11\rangle + \beta 101\rangle 11\rangle$
Qubit 3	$\alpha 001\rangle 01\rangle + \beta 110\rangle 01\rangle$

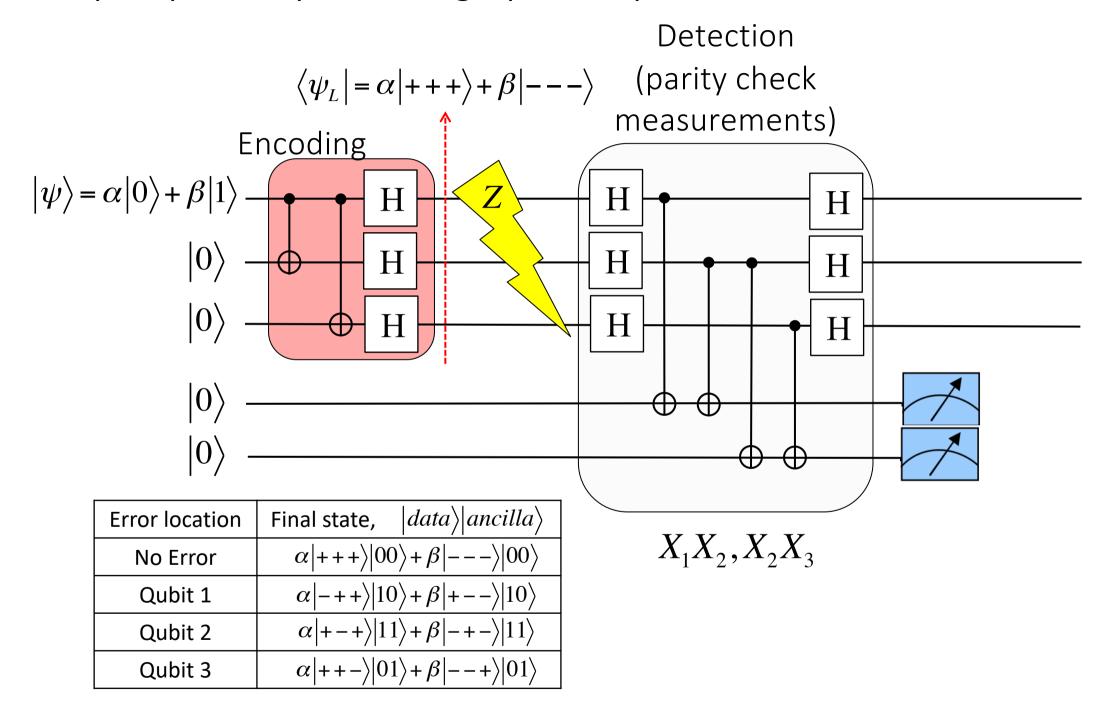


When two bit-flip errors occur...





3-qubit phase-flip code: single phase-flip errors





Quantum error correction (QEC) - Exercise

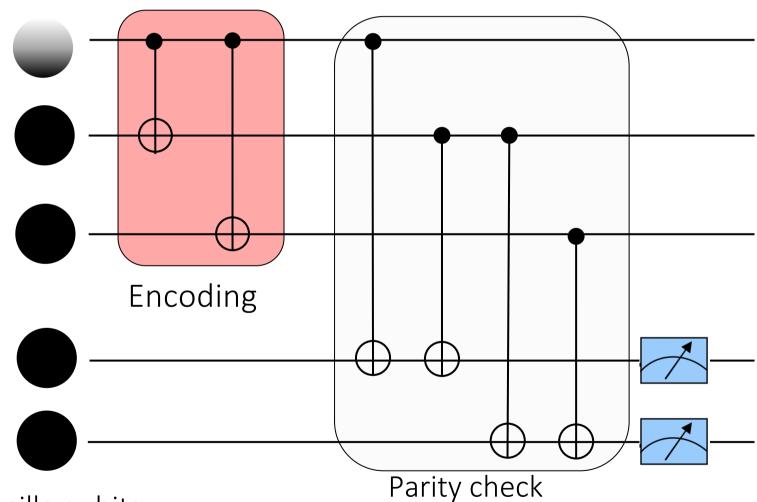
Encoding

Physical qubit

Logical qubit qubit

$$|\psi\rangle = |0\rangle$$

$$|\psi_L\rangle = |000\rangle$$



Ancilla qubits

measurements

Detection



