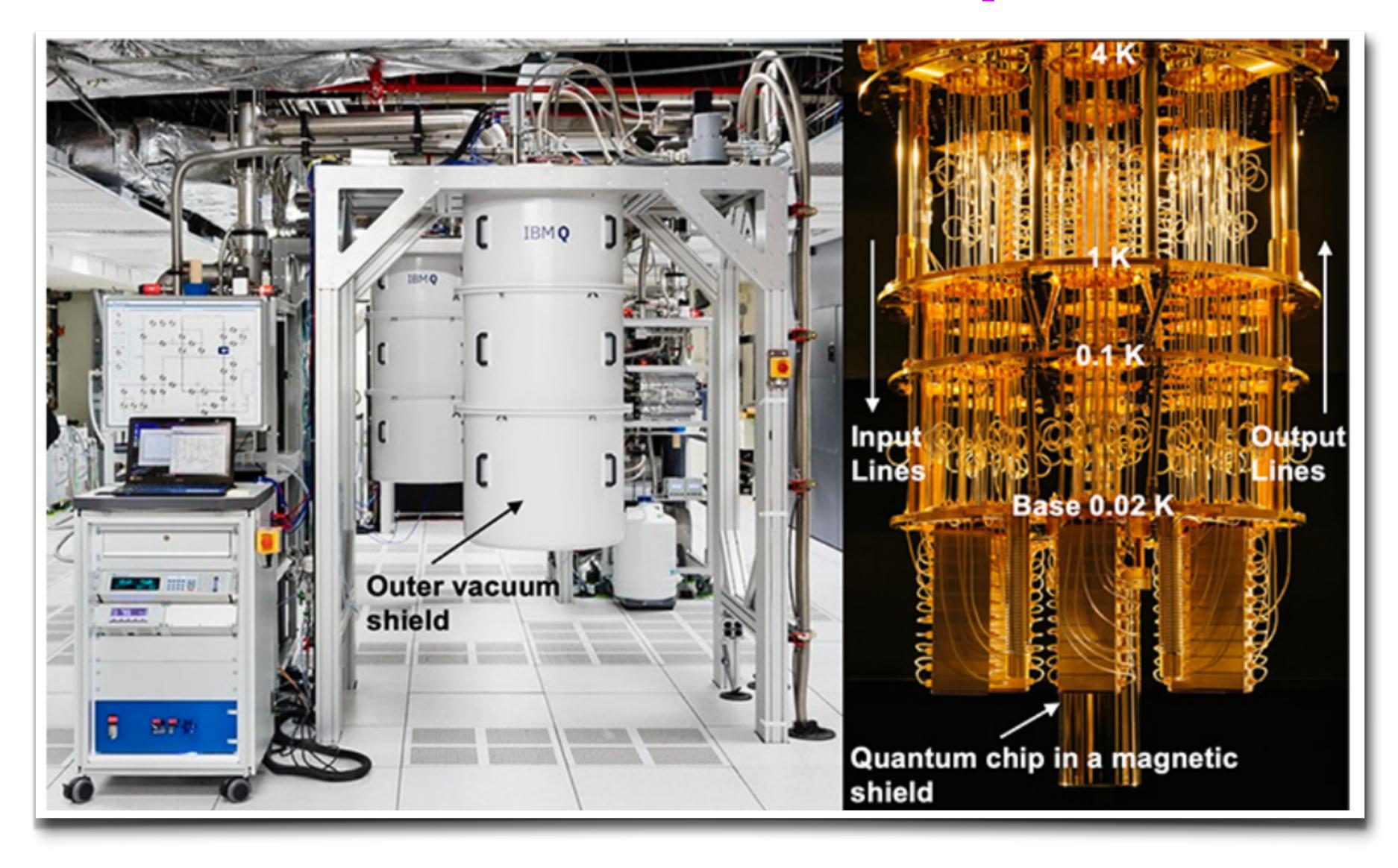
Developing Quantum Computing Circuits

Optics and Spectroscopy
Sofia University

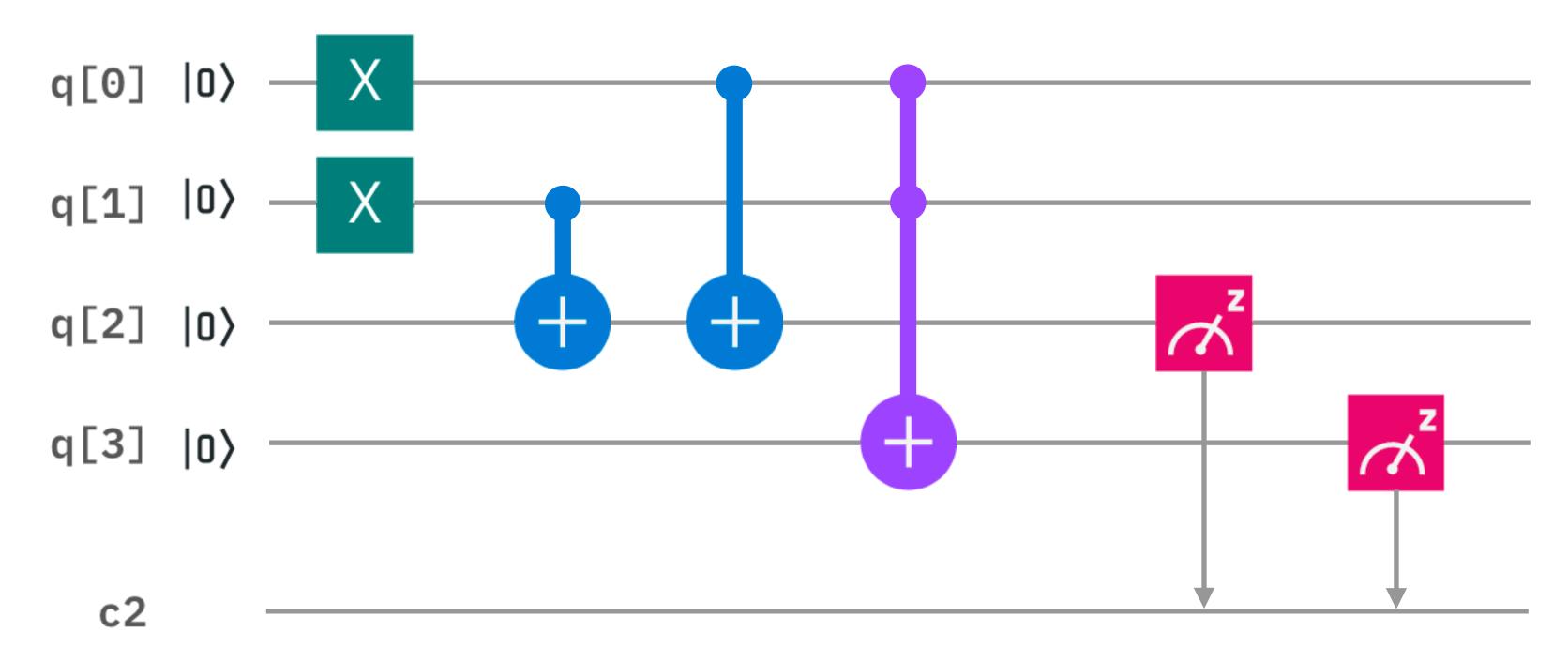
IBM's Quantum Computer



DiVincenzo's criteria

Constructing a quantum computer requires that the experimental setup meet he following conditions

- 1. A scalable physical system with well characterised qubit
- 2. The ability to initialise the state of the qubits to a simple fiducial state, such as |000...>
- 3. Long relevant decoherence times, much longer than the gate operation time
- 4. A "universal" set of quantum gates
- 5. A qubit-specific measurement capability



Qiskit

- Qiskit is an open-source SDK for working with quantum computers at the level of pulses, circuits and application modules
- Designed to work with IBM's quantum processors
- Qiskit webpage https://qiskit.org

Setup Qiskit

- 1. Install Anaconda Python https://www.anaconda.com/products/ individual
- 2. Start Anaconda Prompt
- 3. Install qiskit by typing "pip install qiskit"
- 4. Start Jupyter notebook by typing "jupyter notebook"



Get Access to Quantum Computers

1. Get access token from IBM Quantum Experience -

https://quantum-computing.ibm.com

2. Setup Access token in Qiskit



Single Qubit Quantum state

Can be written as:
$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \quad \alpha, \beta \in \mathbb{C}$$

Probability of the bit being in $|0\rangle$ is $|\alpha|^2$ and $|1\rangle$ is $|\beta|^2 \Rightarrow |\alpha|^2 + |\beta|^2 = 1$

Vector notation of
$$|\psi\rangle = {\alpha \choose \beta} \Rightarrow |0\rangle = {1 \choose 0}, \quad |1\rangle = {0 \choose 1}$$

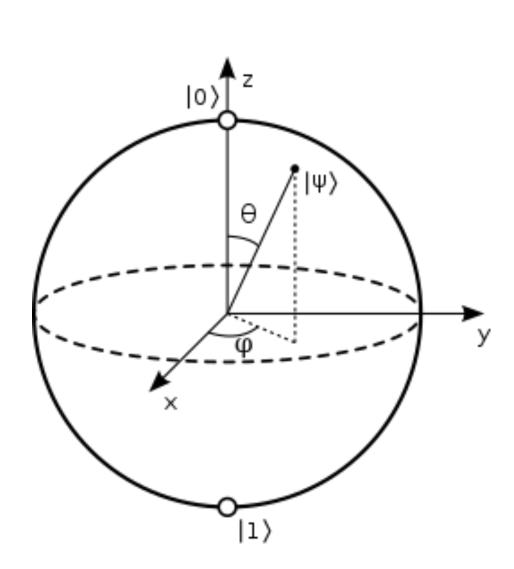
From $|\alpha|^2+|\beta|^2=1$ and since global phase is undetectable $|\psi\rangle:=e^{i\delta}\,|\psi\rangle$

$$|\psi\rangle = e^{i\delta} \left(\cos(\theta/2)|0\rangle + \sin(\theta/2)e^{i(\phi-\delta)}|1\rangle\right)$$

$$\Rightarrow |\psi\rangle = \cos(\theta/2) |0\rangle + \sin(\theta/2)e^{i\phi} |1\rangle$$

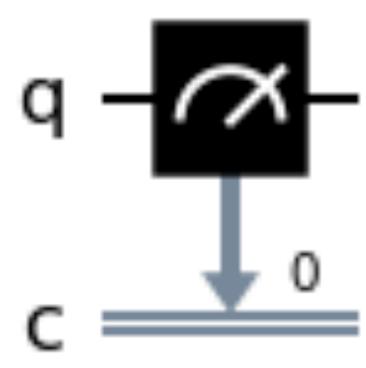
$$0 \le \phi < 2\pi$$
, $0 \le \theta \le \pi$

Bloch sphere representation of qubit state



Measurement operator

- Make once time measurement on a qubit
- Records the result in classical bit



Running Hello World

- 1. Writing 'Hello World' program
- 2. Visualising the program
- 3. Running 'Hello World' program on Simulator
- 4. Running 'Hello World' program on Quantum Computer



Initialise qubit state

- In Qiskit we can specify the initial state of a qubit
- Let's remind the Bloch representation of a qubit that will be used in the examples

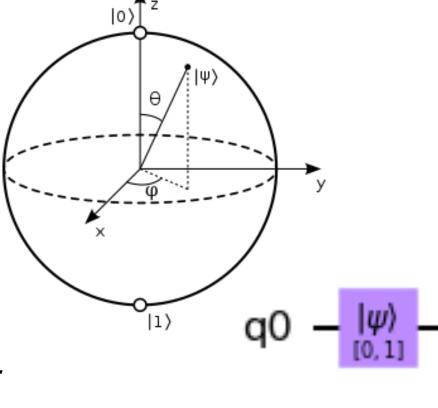
$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle = \cos(\theta/2) |0\rangle + \sin(\theta/2)e^{i\phi} |1\rangle$$



Initialise qubit in state
$$|1\rangle = 0 |0\rangle + 1 |1\rangle \Rightarrow \alpha = 0, \quad \beta = 1 \Rightarrow \quad \theta = \pi, \quad 0 \le \phi < 2\pi$$



Initialise qubit in state
$$|\psi\rangle = \left(\frac{1}{2} + \frac{1}{2}i\right) |0\rangle + \frac{\sqrt{2}}{2} |1\rangle = e^{i\frac{\pi}{4}} \left(\frac{\sqrt{2}}{2} |0\rangle + \frac{\sqrt{2}}{2}e^{-i\frac{\pi}{4}} |1\rangle\right) \Rightarrow \theta = \frac{\pi}{2}, \quad \phi = -\frac{\pi}{4}$$



$$q0 - \frac{|\psi\rangle}{[0.5 + 0.5j, 0.707]}$$

Demo Source

Quantum gates/operations

- A gate which acts on a qubit is represented by a 2×2 unitary matrix U: $\left| \psi' \right\rangle = U \left| \psi \right\rangle$
- A general unitary must be able to take the $|0\rangle$ to the state $\left|\psi\right\rangle = \cos(\theta/2) \left|0\right\rangle + \sin(\theta/2) e^{i\phi} \left|1\right\rangle = U \left|0\right\rangle$ $\Rightarrow U = \begin{pmatrix} \cos(\theta/2) & a \\ e^{i\phi} \sin(\theta/2) & b \end{pmatrix} \text{, where } a \text{ and } b \text{ are complex numbers such that } U^\dagger U = I$
- The general expression of 2×2 unitary matrix, which depends on 4 real parameters, is:

$$U = \begin{pmatrix} \alpha & -e^{-i\varphi}\beta^* \\ \beta & e^{-i\varphi}\alpha^* \end{pmatrix}, \qquad |\alpha|^2 + |\beta|^2 = 1$$

• This is the most general form of single quit unitary, if we substitute above $\phi = -\lambda - \phi$

$$U = \begin{pmatrix} \cos(\theta/2) & -e^{i\lambda}\sin(\theta/2) \\ e^{i\phi}\sin(\theta/2) & e^{i\lambda+i\phi}\cos(\theta/2) \end{pmatrix}, \quad 0 \le \phi < 2\pi, \quad 0 \le \theta \le \pi, \quad 0 \le \lambda < 2\pi$$

Why quantum operations are represented as unitary matrix?

Schrödinger equation

$$\frac{d}{dt} \left| \psi(t) \right\rangle = -\frac{i}{\hbar} \hat{H}(t) \left| \psi(t) \right\rangle,$$

where Hamiltonian $\hat{H}(t)$ is Hermitian operator $\hat{H}(t) = \hat{H}^{\dagger}(t)$

• Suppose $|\psi(t)\rangle=\hat{U}(t)\,|\psi(0)\rangle$ for some matrix $\hat{U}(t)$ which is not unitary yet

$$\frac{d\hat{U}(t)}{dt} = -\frac{i}{\hbar}\hat{H}(t)\hat{U}(t), \quad \frac{d\hat{U}^{\dagger}(t)}{dt} = -\frac{i}{\hbar}\hat{H}(t)\hat{U}(t)$$

At
$$t=0$$
, $\hat{U}(0)=\hat{I}$, so $\hat{U}^{\dagger}(0)\hat{U}(0)=\hat{I}$

$$\frac{d}{dt} \left(\hat{U}^{\dagger}(t) \hat{U}(t) \right) = \frac{1}{\hbar} \hat{U}^{\dagger}(t) \left(i\hat{H}(t) - i\hat{H}(t) \right) \hat{U}(t) = 0$$

• So $\hat{U}^{\dagger}(t)\hat{U}(t)=\hat{I}$ at all times t, and $\hat{U}(t)$ must always be unitary.

Single-Qubit Gates

- u gates
 - U gate $u3(\theta, \phi, \lambda) = u(\theta, \phi, \lambda)$
 - P gate $p(\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix} = u3(0,0,\lambda)$
- Identity gate $Id = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = u3(0,0,0)$
- Pauli gates

•
$$X$$
: bit-flip gate $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = u3(\pi, 0, \pi)$

- Y: bit- and phase-flip gate $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = u3(\pi, \pi/2, \pi/2)$
- Z: phase-flip gate $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = u3(0,0,\pi)$
- Clifford gates
 - Hadamard gate $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = u3(0,0,\pi)$
 - S gate $S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = u3(0,0,\pi/2)$

•
$$S^{\dagger}$$
 gate $S^{\dagger} = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} = u3(0,0,-\pi/2)$

• *C*3 gate

•
$$T$$
 gate $T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} = u3(0,0,\pi/4)$

•
$$T^{\dagger}$$
 gate $T^{\dagger} = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\pi/4} \end{pmatrix} = u3(0,0,-\pi/4)$

- Standart Rotations
 - Rotation around X-axis

$$R_{x}(\theta) = \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{pmatrix} = u3(\theta, -\pi/2, \pi/2)$$

Rotation around Y-axis

$$R_{y}(\theta) = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix} = u3(\theta,0,0)$$

Rotation around Z-axis

$$R_z(\phi) = \begin{pmatrix} e^{-i\phi/2} & 0\\ 0 & e^{i\phi/2} \end{pmatrix} \equiv u3(0,\phi,0)$$

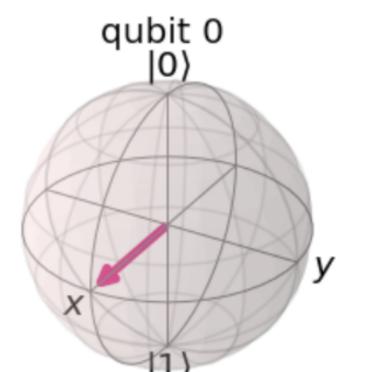
Hadamard Gate

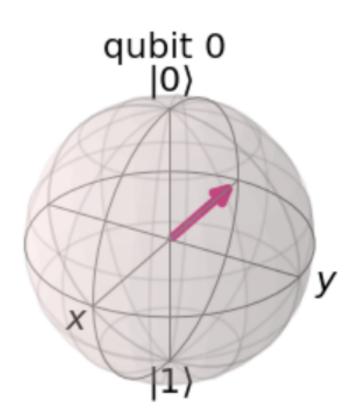
• Considering
$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
, and $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

• Let's apply H-gate on state vector $|0\rangle$:

$$H \mid 0 \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \mid 0 \rangle + \frac{1}{\sqrt{2}} \mid 1 \rangle$$

$$\Rightarrow \alpha = \frac{1}{\sqrt{2}}, \quad \beta = \frac{1}{\sqrt{2}} \quad \Rightarrow |\alpha|^2 = 0.5, \quad |\beta|^2 = 0.5$$





Demo Source

X-Gate

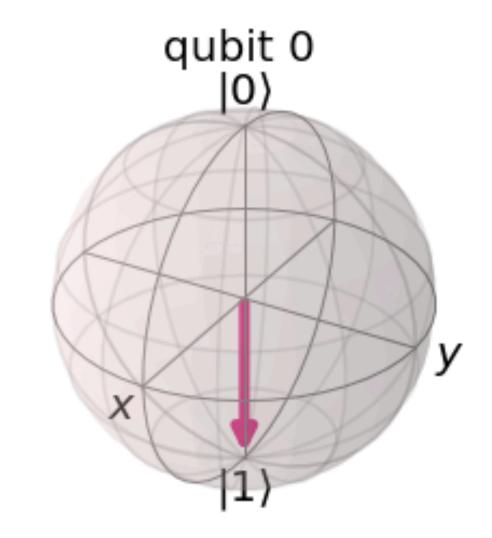
• Considering
$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
, and $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

• Let's apply X-gate on state vector $|0\rangle$:

$$X \mid 0 \rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 \mid 0 \rangle + 1 \mid 1 \rangle$$

$$\Rightarrow \alpha = 0, \quad \beta = 1$$

$$\Rightarrow |\alpha|^2 = 0, |\beta|^2 = 1$$



Demo Source

Multi and Two-qubit system

- For n qubits the complex vector space has dimensions $d=2^n$ grows exponentially with the number of qubits
- The basis vectors for the 2-qubit system are formed using the tensor product of basis vectors for a single qubit:

$$|0\rangle \otimes |0\rangle = |00\rangle = \begin{pmatrix} 1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |01\rangle = \begin{pmatrix} 1 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

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

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

$$|\psi\rangle = a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle = \begin{bmatrix} a_{00} \\ a_{01} \\ a_{10} \\ a_{11} \end{bmatrix}, |a_{00}|^2 + |a_{01}|^2 + |a_{10}|^2 + |a_{11}|^2 = 1$$
Demo Source

Two-qubit Gates - General Form

- Most of the two-qubit gates are of the controlled type (except for the SWAP gate)
- ullet Controlled type two-qubit gates applies U to one qubit, conditioned on the state of another qubit
- Lets apply on one qubit 1 the gate U on condition qubit 0 is equal to $|1\rangle$, where $U = \begin{pmatrix} u_{00} & u_{01} \\ u_{10} & u_{11} \end{pmatrix}$

Two-Qubit Gates

Controlled Pauli gates

• Controlled-X - flips the target qubit if the control qubit is in the state $|1\rangle$.

Controlled-bit MSB:
$$C_X = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$
, LSB: $C_X = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$

Controlled-Y gate

Controlled-bit MSB:
$$C_Y = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}$$
, LSB: $C_Y = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & 1 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}$

- Controlled-Z flips the phase of the target qubit if the control qubit is in the state $|1\rangle$. Controlled-bit MSB or LSB: $C_Z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$
- Hadamard gate LSB: $C_H = egin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}$

Controlled rotation gates

- Controlled rotation around Z-axis $C_{Rz}(\lambda) = egin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-i\lambda/2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\lambda/2} \end{pmatrix}$
- Controlled Phase rotation performs a phase rotation if both qubits are in the state $|11\rangle$

$$C_p(\lambda) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\lambda} \end{pmatrix}$$

Controlled-U rotation

$$C_{u}(\theta,\phi,\lambda) \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-i(\phi+\lambda)/2}\cos(\theta/2) & 0 & -e^{-i(\phi-\lambda)/2}\sin(\theta/2) \\ 0 & 0 & 1 & 0 \\ 0 & e^{i(\phi-\lambda)/2}\sin(\theta/2) & 0 & e^{i(\phi+\lambda)/2}\cos(\theta/2) \end{pmatrix}$$

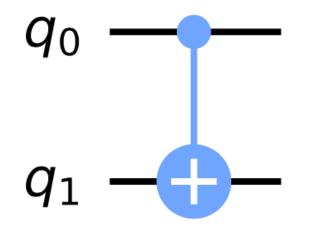
• SWAP gate - It transforms the basis vectors as

$$\begin{vmatrix} 00 \rangle \to |00\rangle , |01\rangle \to |10\rangle , |10\rangle \to |01\rangle , |11\rangle \to |11\rangle,$$

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

CNOT Gate

- CNOT (Controlled-X) Gate
- When the qubits are not in superposition of $|0\rangle$ and $|1\rangle$, they behave like classical bits and for the CNOT gate the following truth table is valid:



CNOT gate matrices:

CNOT _{MSB} =	[1	0	0	0		1	0	0	0
	0	1	0	0		0	0	0	1
	0	0	0	1		0	0	1	0
	0	0	1	0		0	1	0	$\begin{bmatrix} 0 \end{bmatrix}$

Input	Output				
00	00				
01	11				
10	10				
11	01				

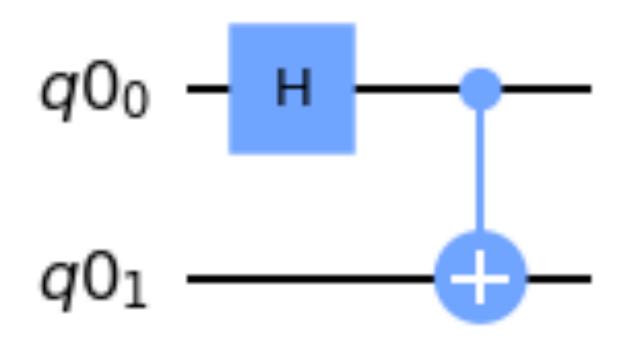
- The matrix swaps the amplitudes of $|\hspace{.06cm}01\rangle$ and $|\hspace{.06cm}11\rangle$ vectors

$$|a\rangle = \begin{bmatrix} a_{00} \\ a_{01} \\ a_{10} \\ a_{11} \end{bmatrix}, \quad \text{CNOT} |a\rangle = \begin{bmatrix} a_{00} \\ a_{11} \\ a_{10} \\ a_{01} \end{bmatrix} \leftarrow$$

Demo Source

Entanglement

Entanglement implements with the following circuit





Quantum Algorithms

- Quantum Fourier Tranformation
- Quantum Phase Estimation
- Shor's Algorithm
- Variational Quantum Eigensolver

Quantum Fourier Tranform (QFT)

• Quantum Fourier transform acts on a quantum state $|X\rangle = \sum_{j=0}^{\infty} x_j |j\rangle$ and

maps it to the quantum state
$$|Y\rangle = \sum_{k=0}^{N-1} y_k |k\rangle$$
, according to the formula:

$$y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j \omega_N^{jk}$$
, where $\omega_N^{jk} = e^{2\pi i \frac{jk}{N}}$

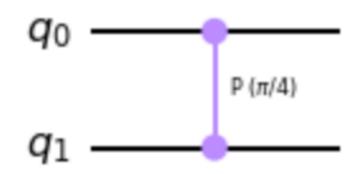
This can also be expressed as unitary matrix:

$$U_{QFT} = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \omega_N^{jk} |k\rangle\langle j|$$

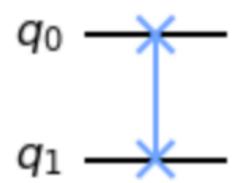
QFT implementation

- Needed operators:
 - H-Gate

Controlled Phase Gate



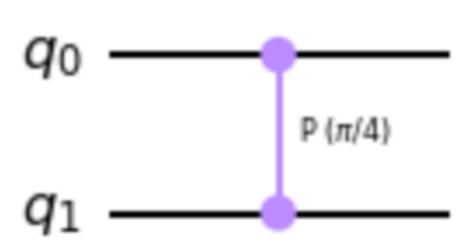
SWAP Gate



Controlled Phase Gate in two-qubit system

• Performs a phase rotation if both qubits are in the state $|11\rangle$

$$C_p(\lambda) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\lambda} \end{pmatrix}$$





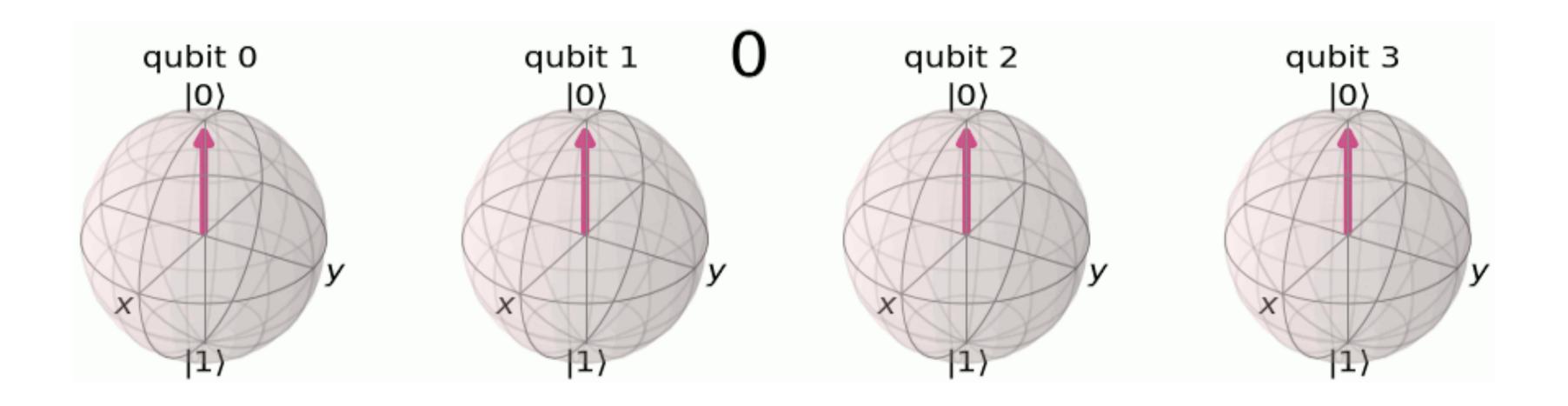
QFT Demos

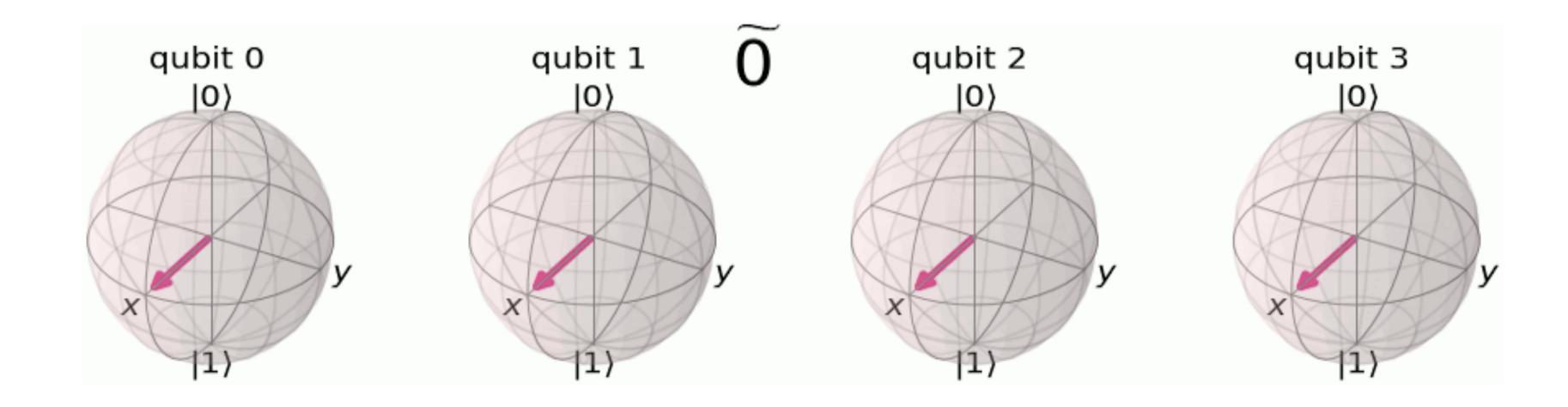
• QFT Example for 1-qubit system **Source**

• QFT Example for 2-qubit system **SOURCE**



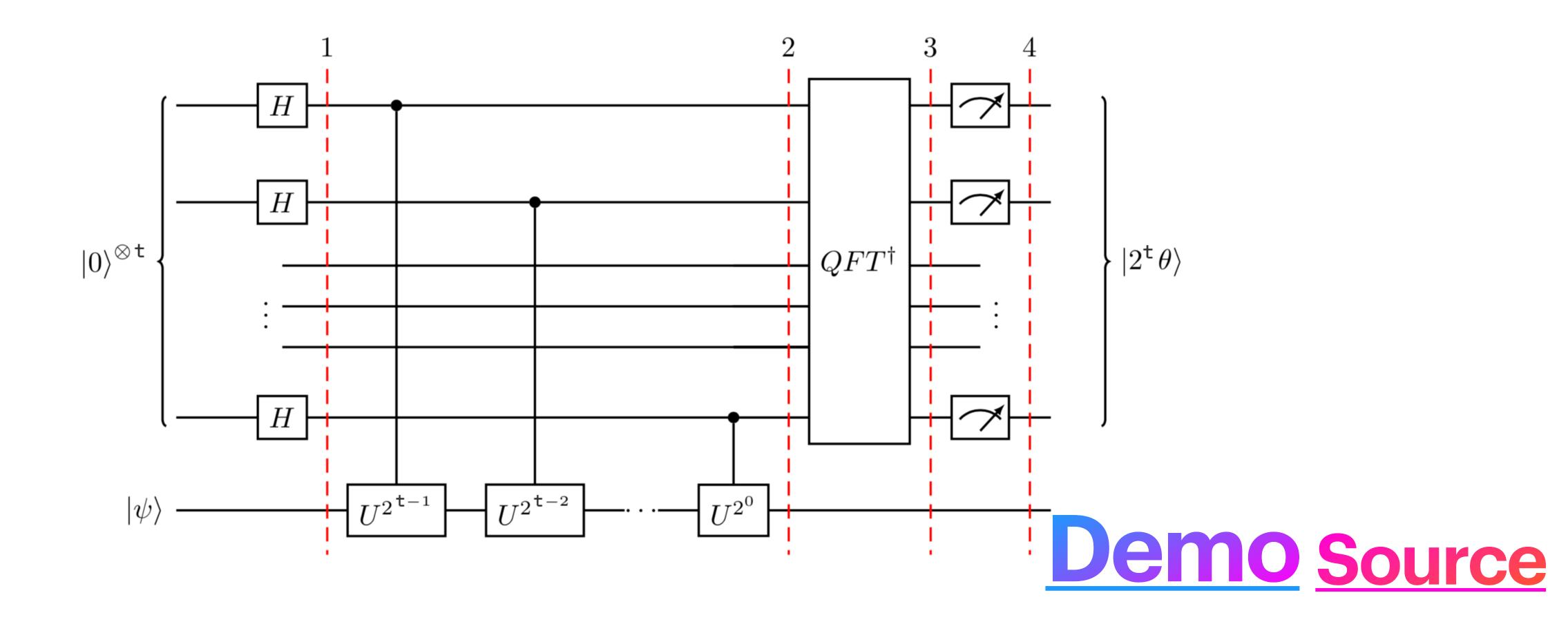
QFT with 4 qubits





Quantum Phase Estimation

• Given a unitary operator U, the algorithm estimates θ in $U|\psi\rangle=e^{2\pi i\theta}|\psi\rangle$, where $|\psi\rangle$ is an eigenvector and $e^{2\pi i\theta}$ is the corresponding eigenvalue



Simulating Molecules using VQE

- In the future Quantum Phase Estimation may be useful to find Eigen values of Hermitian matrix
- In 2014, Peruzzo et al. proposed Variational Quantum Eigensolver (VQE) method to estimate the ground state energy of molecule
- Given a Hermitian matrix H with unknown minimum eigenvalue λ_{min} and eigenstate $|\psi_{min}\rangle$, VQE provides an estimate λ_{θ} bounding λ_{min} :

$$\lambda_{min} \leq \lambda_{\theta} \equiv \langle \psi(\theta) | H | \psi(\theta) \rangle$$
where $| \psi(\theta) \rangle$ is eigenstate associated with λ_{θ} .

- If we apply $U(\theta)$ to some arbitrary starting state $|\psi\rangle$, we can obtain an estimate $U(\theta)\,|\psi\rangle\equiv|\psi(\theta)\rangle$ on $|\psi_{min}\rangle$
- Using classical controller the algorithm iteratively minimise the expectation value of $\langle \psi(\theta) | H | \psi(\theta) \rangle$ Demo Source

Resources

- The first part of the presentation is mostly based on:
 - https://qiskit.org/documentation/tutorials/circuits/
 3_summary_of_quantum_operations.html
- Second part is based on:
 - https://qiskit.org/textbook/ch-algorithms/index.html
- Useful Tutorial:
 - https://www.youtube.com/watch?v=a1NZC5rqQD8&list=PLOFEBzvs-Vvp2xg9-POLJhQwtVktlYGbY
- Find the presentation and examples on:
 - https://drive.google.com/drive/folders/
 1Dwh8zK2YD2cu3BWt-2HO0DQGvrYv2PfH?usp=sharing

Thank you!

