# Lecture 1 Intro to Implementations in Quantum Information Science

## I. *OUTLINE*

### A. Syllabus and overview

### B. Review of quantum circuits in the context of NISQ hardware

### C. In-class real-time tutorial to make sure everyone has access to qiskit and Microsoft Azure

### D. In class time for problem set

## II. *STATE PREPARATION AND MEASUREMENT*

### A. State preparation

At the start (and often in the middle) of any quantum algorithm is state preparation. Theoretically, we are able to define an arbitrary quantum state. For a single qubit initialized into the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + i|1\rangle\right)$$

we can code in qiskit

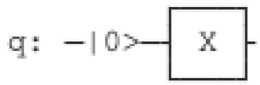
```
qc = QuantumCircuit(1)
initial_state = [1/np.sqrt(2)*complex(1,0),1/np.sqrt(2)*complex(0,1) ]
qc.initialize(initial_state, 0)
qc.draw()
```


But in experimental platforms, we cannot typically initialize into an arbitrary state, but typically into a single eigenstate of the computational basis. What are the ways in which initialization is experimentally performed?

Our standard way of thinking about initialization is the `reset` instruction in qiskit.

So experimentally what is likely happening is something more like

```
qc = QuantumCircuit(1)
qc.reset(0)
qc.x(0) qc.draw()
```




What is the consequence of having a single "reset" state on state preparation fidelity?

## B. Measurement

In a quantum algorithm measurement occurs at the end (and often in the middle). If we have a single qubit, *e.g.*

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + i|1\rangle\right)$$

we can measuring the state of the qubit in the computational basis. An important characteristic of the measurement process is the wavefunction collapse; Thus the output of a good quantum algorithm should give us a useful answer with high (enough) probability when measured.

Here we take a little time to understand (or review) the formulation of measurement. Projective measurements are described by an observable

$$M = \sum_m m P_m$$

in which $P_m$ is the projector on to the eigenspace of $M$ with eigenvalue $m$. The probability of getting measurement result $m$ is given by

$$p(m) = \langle\psi|P_m|\psi\rangle$$

and if outcome $m$ is measured, the quantum state immediately after measurement is

$$\frac{P_m|\psi\rangle}{\sqrt{p(m)}}$$

To make things concrete, in our computational basis for a single qubit we have the measurement observable

$$M = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

with $P_1 = |0\rangle\langle 0|$ (with measurement outcome 1)

$$P_{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

and $P_1 = |1\rangle\langle 1|$ or

$$P_{-1} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Here we follow NC's convention (p.xxix-xxx) If we take our single qubit above, we find measurement of $Z$ gives +1 with probability $\langle\psi|0\rangle\langle 0|\psi\rangle = 1/2$ and gives -1 with probability of 1/2.

Generally, we can define an observable:

$$\vec{v} \cdot \vec{\sigma} \equiv v_1\sigma_1 + v_2\sigma_2 + v_3\sigma_3$$

in which $\sigma_i$ is the the Pauli-$i$ operator.

$$\sigma_1 = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Measurement of this observable is sometimes referred to as 'measurement of spin along the $\vec{v}$ axis.

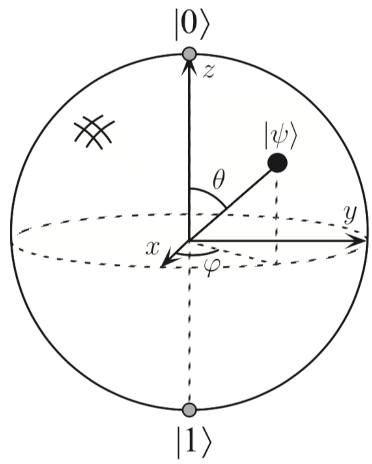
Algorithms may call for projective measurements along different axes (e.g. X,Y,Z). In fact, one paradigm of quantum computing, is measurement-based quantum computing in which a calculation is driven solely by single qubit measurements on an entangled network of qubits! However, a real quantum computer cannot only performs measurements in the computational basis. Physically, how might a measurement be performed?

If quantum computers can only measure in the computational (or Z) basis, how are measurements in other bases (e.g. X and Y) performed? We use this practical motivation to remind ourselves about about the Bloch sphere representations.

## C. Bloch sphere

An arbitrary qubit can be written in terms of two angles, $\theta$ and $\varphi$ which define a point on the unit sphere, called the Bloch sphere.

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




The Bloch vector is given by $(\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta)$. A measurement in the $\vec{v} = (\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta)$ basis would give $+1$ for a $|\psi\rangle$ and -1 for the wavevector pointing direction opposite to $|\psi\rangle$ (let $\varphi \to \phi + pi$ and $\theta \to \theta + \pi$. In order to effectively perform a measurement in the $\vec{v}$ basis, we need to perform a rotation to map $|\psi\rangle$ to $|0\rangle$.

The Pauli matrices give rise to the rotational operators about the $\hat{x}, \hat{y}, \hat{z}$ axis defined by the equations:

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

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

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

In the homework you can use these matrices to show how to perform a measurement in a non-computational basis.

# *III. DENSITY MATRIX AND STATE TOMOGRAPHY*

## A. Density matrix

Thus far we have only talked about pure states. The density matrix operator is used to describe a quantum system in whose state is not completely known. The density operator for such an ensemble is defined by

$$\rho \equiv = \sum_i p_1 |\psi\rangle_i \langle\psi|_i$$

in which $p_i$ is the probability of the quantum system being in pure state $\psi$.

In the context of quantum computing, what can make the state of the qubit unknown?

In the 2nd half of the course we will look more quantitatively benchmarking to determine the types of errors that happen in real quantum hardware. Here, we use the presence of errors to motivate the concepts of the density matrix and tomography. We do not go into a detail review of the density matrix, as it should be discussed in the first quarter of a QI course, however we do want to review the Bloch sphere representation of the density matrix. Specifically an arbitrary density matrix for a mixed state can be written as

$$\rho = \frac{I + \vec{r} \cdot \vec{\sigma}}{2} = \frac{I + r_1\sigma_1 + r_2\sigma_2 + r_3\sigma_3}{2}$$

in which the Bloch $\vec{r}$ is a real three-dimensional vector such that $|\vec{r}| \leq 1$.

The interested student is invited to show (Exercise 2.72 in NC)

1. The state $\rho$ is pure if an only if $|\vec{r}| = 1$.

2. For pure states, the description of the Bloch vector we have given coincides with our definition above.

In the problem set you will visualize $\rho$ for some pure states utilizing Qiskit.

The expectation value for an operator $A$ (e.g. a measurement operator) for a given $\rho$ is given by

$$\langle A \rangle = \mathrm{tr}(A\rho)$$

For example, the expectation value of $X$ for the pure state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ is

$$\mathrm{tr}(|\psi\rangle\langle\psi|X) = \mathrm{tr}\left(\frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right) = 1$$

## B. State tomography

Quantum state tomography is the method to determine an arbitrary quantum state $\rho$ from measurements. In real systems, $\rho$ will never be a pure state.

The Pauli matrices have the property of trace orthogonality,

$$\mathrm{tr}(\sigma_k \sigma_j) = 2\delta_{kj}$$

we find we can find the $r_k$ by finding the expectation value of $\sigma_k$, or

$$r_k = \langle\sigma_k\rangle = \mathrm{tr}(\rho\sigma_k)$$

Thus $\rho$ can be obtained by measuring me the expectation values of $X, Y$, and $Z$!

For an arbitrary density matrix of $n$ qubits, we have

$$\rho = \sum_{\vec{v}} \frac{\mathrm{tr}(\sigma_{v_1} \otimes \sigma_{v_2} \otimes \cdots \otimes \sigma_{v_n}\rho)\sigma_{v_1} \otimes \sigma_{v_2} \otimes \cdots \otimes \sigma_{v_n}}{2^n}$$

For n qubits, state tomography requires $4^n - 1$ measurements (see e.g. James, Kwiat, Munro and White, PRA 64, 052312 2001) making state tomography intractable for large quantum systems. Finding methods to estimate quantum states without doing full state tomography is an active area of research, e.g. utilizing modern mathematical optimization methods to determine the most likely state given a (much) smaller measurement set.

We can standard distance measure that we use to determine how close a given quantum state is to a target state is the fidelity. The fidelity of two quantum states $\rho$ and $\sigma$ is given by

$$F(\rho, \sigma) \equiv \mathrm{tr}\sqrt{\rho^{1/2}\sigma\rho^{1/2}}$$

You can verify that the fidelity between $\rho$ and a pure state $|\psi\rangle$ is thus

$$F(\rho, |\psi\rangle) = \sqrt{\langle\psi|\rho|\psi\rangle}$$

For quantum hardware, we are not interested in quantum state tomography but instead in quantum process tomography. The experimental procedure is as follows. If we have a $d$ dimensional system (e.g for a single qubit $d = 2$, for two qubits $d = 4$, etc.) we choose $d^2$ quantum states $|\psi_1\rangle, ..., |\psi_{d^2}\rangle$ chosen so that the corresponding density matrices $|\psi_1\rangle\langle\psi_1|, ..., |\psi_{d^2}\rangle\langle\psi_{d^2}|$ for a basis set for the space of matrices. Then we subject each $|\psi_j\rangle$ to the process we are evaluating (for example, an $X$ gate for a single qubit). We use quantum state tomography to determine the output state $\mathcal{E}(|\psi_j\rangle\langle\psi_j|)$. We then need to determine a useful representation of $\mathcal{E}$.

Beyond quantum process tomography is gate set tomography (which characterizes multiple gates) and randomized benchmarking.

## IV. SINGLE QUBIT GATES

As you learned in your prior quantum information course, there is a minimum gate set for universal quantum computation. Single qubit gates and the `CNOT` are one example of a universal set. Single qubit gates (i.e. gates taking one point on the bloch sphere to another point) do constitute a discrete gate set, but are actually closer to what is available in practice. For error correction purposes, a discrete gate set may be preferred. One example of a discrete gate set is `H, phase, CNOT + ` $\pi$`/8`.

While the `CNOT` gate is one we may commonly use in an algorithm, it may not be a native gate - i.e. the gates that are actually performed on the hardware. The IonQ native gate set are the following three single qubit gates

$$GZ(\theta) = R_z(\theta) = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}$$

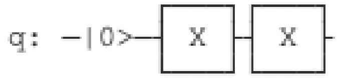
$$GPI(\phi) = \begin{bmatrix} 0 & e^{-i\phi/2} \\ e^{i\phi/2} & 0 \end{bmatrix}$$

$$GPI2\phi) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -ie^{-i\phi/2} \\ -ie^{i\phi/2} & 1 \end{bmatrix}$$

and the Molmer-Sorenson two qubit gate.

$$MS = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & -i \\ 0 & 1 & -i & 0 \\ 0 & -i & 1 & 0 \\ -i & 0 & 0 & 1 \end{bmatrix}$$

IonQ decomposes all gates into theses native gates. In addition, during this decomposition, the circuit is "optimized" for inefficiencies. As a simple example:




will simply be replaced with


This "optimization" makes general tomography impossible to perform via Azure Quantum at this time. However, later in the course we can directly access IonQ's system via the native gates to bypass their gate decomposition.