QUANTUM INFORMATION and COMPUTATION

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Understanding Quantum Information & Computation

Contents

Single Systems

Quantum Information

Simplified Description: Quantum states are represented by vectors; operations are represented by unitary matrices.

General Description: Quantum states are represented by density matrices; allows for a more general class of measurements and operations.

Classical Information

Consider a physical system "X" that stores information.

Assume X can be one of the <u>finite</u> number of classical states ($\sum$) at each moment.
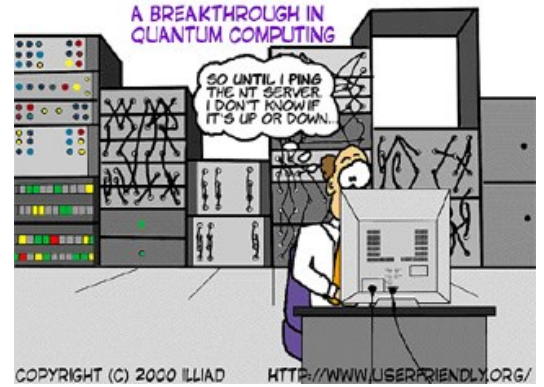
Example:

- o if X is a bit, $\sum$ = {0, 1} → binary alphabet
- o if X is six-sided dice, $\sum$ = {0, 1, 2, 3, 4, 5, 6}
- o if X is switch of an electric fan, $\sum$ = {high, medium, low, off}

Pr(x = 0) → **probabilistic state** → probability where it is in classical state "0"

Succinct way to represent is "column vector":

Example: if Pr(*x=0*) = 3/4 and Pr(*x=1*) = 1/4, then, column vector is:

$$\begin{pmatrix} 3/4 \\ 1/4 \end{pmatrix} \begin{matrix} \leftarrow entry\ corresponds\ to\ 0 \\ \leftarrow entry\ corresponds\ to\ 1 \end{matrix}$$

Probability vector:

- Entries are nonnegative real numbers and sum of all entries are "1"

Some Superposition Quantum States

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

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

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

$$|-i\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$$

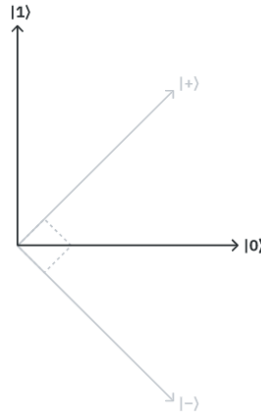**Dirac Notation**

$|\sum|$ = Number of elements in set $\sum$

➕ We denote by **| α ⟩** (called ket) the **column vector** having a 1 in the entry corresponding to $α \in \sum$ with 0 for all other entries.

Example: if $\sum$ = {0, 1}, then:

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

|0⟩ and |1⟩ are orthogonal[1], normalized (magnitude = length of arrow is 1) *and linearly independent* (one cannot be described in terms of another).

Note: This is a popular basis called *computational basis*. Also, other popular basis is |+⟩ and |-⟩ where:

$$|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \qquad |-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

❖ For probabilistic requirement, valid quantum state vectors should satisfy this:

$$\sum_{i=0}^{N-1} a_i^2 = 1$$

Representation of Popular Qubits

|0⟩		$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	**⟨0|**		$(1 \quad 0)$
|1⟩		$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$	**⟨1|**		$(0 \quad 1)$
|+⟩	$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	**⟨+|**	$\frac{1}{\sqrt{2}}\begin{pmatrix} \langle 0| \\ \langle 1| \end{pmatrix}$	$\frac{1}{\sqrt{2}}(1 \quad 1)$
|-⟩	$\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$	**⟨-|**	$\frac{1}{\sqrt{2}}\begin{pmatrix} \langle 0| \\ -\langle 1| \end{pmatrix}$	$\frac{1}{\sqrt{2}}(1 \quad -1)$
|i⟩	$\frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$	**⟨i|**	$\frac{1}{\sqrt{2}}\begin{pmatrix} \langle 0| \\ -i\langle 1| \end{pmatrix}$	$\frac{1}{\sqrt{2}}(1 \quad -i)$
|-i⟩	$\frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$	**⟨-i|**	$\frac{1}{\sqrt{2}}\begin{pmatrix} \langle 0| \\ i\langle 1| \end{pmatrix}$	$\frac{1}{\sqrt{2}}(1 \quad i)$

🞧 For 2 qubits:

$$|a\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \quad and \quad |b\rangle = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \;\Rightarrow\; |ab\rangle = \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix}$$

Here |ab⟩ is **product combined state** of |a⟩ and |b⟩ where |a⟩ represents the qubit on the left and |b⟩ is the one on the right. From probability perspective:

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[1] Orthogonal: geometrically perpendicular to each other

$$p_{|a\rangle}(|0\rangle) = p_{|ab\rangle}(|00\rangle + p_{|ab\rangle}(|01\rangle) = (a_0 b_0)^2 + (a_0 b_1)^2 = a_0^2 b_0^2 + a_0^2 b_1^2 = (b_0^2 + b_1^2)a_0^2 = a_0^2$$

Example:

$$|++\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle)$$

Samely:

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

Others:

$$|++\rangle = \frac{1}{2}\begin{pmatrix}1\\1\\1\\1\end{pmatrix} \quad |--\rangle = \frac{1}{2}\begin{pmatrix}1\\-1\\-1\\1\end{pmatrix} \quad |+-\rangle = \frac{1}{2}\begin{pmatrix}1\\-1\\1\\-1\end{pmatrix} \quad |-+\rangle = |-\rangle|+\rangle = \frac{1}{2}\begin{pmatrix}1\\1\\-1\\-1\end{pmatrix}$$

- We denote by ⟨α| (called bra) the **row vector** having a 1 in the entry corresponding to $\alpha \in \sum$ with 0 for all other entries.

Example: If $\sum$ = {0, 1} , then :   ⟨0| = (1 0)   ⟨1| = (0 1)

∴ ⟨ α | + | α ⟩ ≡ ⟨α||α⟩ ≡ ⟨α|α⟩→ bra-ket 😊 Its meaning may be expressed as follows: "How much does the second vector contain the first vector" (*If result is 1, it means both vector is completely same and if result is zero then vectors are completely opposite*)

Example:

$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \quad and \; \langle0| = (1 \quad 0) \quad \Rightarrow \quad \langle0|0\rangle = 1$$

$$|1\rangle = \begin{pmatrix}0\\1\end{pmatrix} \quad and \; \langle1| = (0 \quad 1) \quad \Rightarrow \quad \langle1|1\rangle = 0$$

In the same way: ⟨+|+⟩ = ⟨-|-⟩ = ⟨i|i⟩ = ⟨-i|-i⟩ = 1
and also ⟨0|1⟩ = ⟨1|0⟩ = 0
∴ If first vector is same as second vector in bra-ket, the result is 1 otherwise result is 0.

For |ψ⟩ = α|0⟩ + β|1⟩:
** ⟨0|ψ⟩ means "the amplitude of zero state of qubit ψ" = α⟨0|0⟩ + β⟨0|1⟩ = α
** |⟨0|ψ⟩|² means "probability of zero state of qubit ψ" = |α|²

Vectors of this form are called "**standard basis vectors**". It means, every vector can be expressed uniquely as a linear combination of standard basis vectors.

∴ |0⟩ *and* |1⟩ *are* **orthonormal[2] basis**.

Example:

$$\begin{pmatrix} 3/4 \\ 1/4 \end{pmatrix} = \frac{3}{4} \, |0\rangle + \frac{1}{4} \, |1\rangle$$

- To get ⟨α| from |α⟩, we need to take the conjugate transpose:

$$\langle \psi| = |\psi\rangle^\dagger = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}^\dagger = \begin{pmatrix} \alpha^\dagger & \beta^\dagger \end{pmatrix}$$

In other words, if |ψ⟩ = α|0⟩ + β|1⟩ ⇒ ⟨ψ| = α*⟨0| + β*⟨1|
   where α = x + iy ⇒ $\alpha^\dagger$ = α* = x - iy

- For U|ψ⟩ where U is a quantum gate: $(U|\psi\rangle)^\dagger = \langle\psi|U^\dagger$ *where* $U^\dagger \equiv complex\ transpose$

It means:

$$U = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \Rightarrow U^\dagger = \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix}$$

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha|0\rangle + \beta|1\rangle \Rightarrow (|\psi\rangle)^\dagger = \langle\psi| = \begin{pmatrix} \alpha^* & \beta^* \end{pmatrix}$$

$$U|\psi\rangle = (a\alpha + c\beta)|0\rangle + (b\alpha + d\beta)|1\rangle$$

$$(U|\psi\rangle)^\dagger = \begin{pmatrix} \alpha^* a^* + \beta^* c^* & \alpha^* b^* + \beta^* d^* \end{pmatrix}$$

** Gates are applied to "cat" from left and they are applied to "bra" from right.

** For any quantum gate U, $UU^\dagger = U^\dagger U = \mathbb{1}$ ∴ $\forall U \equiv unitary\ matrix$

** We know that, for any matrix M, $M.M^{-1}M^{-1}M = \mathbb{1}$ ⇒ $U^\dagger = U^{-1}$

** When we apply the inverse of gate(s), we get the same state before gate-application:
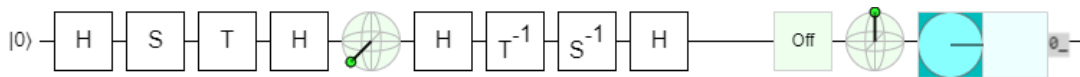
∴ All quantum gate operations are reversable!

Measuring Probabilistic States

If we measure a system X while it is in some probabilistic state, we see a classical state chosen at random according to the probabilities.
Suppose we see a classical state **α** ∈ ∑ . So:

$$\Pr(X = α) = 1$$

This probabilistic state is represented by the vector **| α ⟩**

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[2] two vectors in an inner product space are orthonormal if they are orthogonal (*or perpendicular along a line*) unit vectors.

For Pr(x=0) = 3/4 and Pr(x=1) = 1/4, measuring X reveals a transition, chosen at random:

$$\frac{3}{4}\,|0\rangle + \frac{1}{4}\,|1\rangle$$

To find the **probability of measuring a state** $|\psi\rangle$ in the state $|x\rangle$ we do:

$$p(|x\rangle) = |\langle x|\psi\rangle|^2$$

Example: If we look at the state $|q_0\rangle$, we can see the probability of measuring $|0\rangle$ is indeed 0,5: (*handled in py#2*)

$$|q_0\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{i}{\sqrt{2}}|1\rangle$$

$$\langle 0|q_0\rangle = \frac{1}{\sqrt{2}}\langle 0|0\rangle + \frac{i}{\sqrt{2}}\langle 1|1\rangle = \frac{1}{\sqrt{2}}1 + \frac{i}{\sqrt{2}}0 = \frac{1}{\sqrt{2}}$$

$$\langle 0|q_0\rangle^2 = \frac{1}{2}$$

The Implications of this Rule

1. Normalisation: The rule shows us that amplitudes are related to probabilities. We need the magnitude of the state vector to be 1 $\Rightarrow \langle\psi|\psi\rangle = 1$

Thus, for generalized state of a qubit $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ (*where* $\alpha, \beta \in \mathbb{C}$: *complex numbers*) $\Rightarrow |\alpha|^2 + |\beta|^2 = 1$

2. Alternative Measurement: The measurement rule gives us the probability $p(|x\rangle)$ that a state $|\psi\rangle$ is measured as $|x\rangle$. Nowhere does it tell us that $|x\rangle$ can only be either $|0\rangle$ or $|1\rangle$.

3. Global Phase: We know that measuring the state $|1\rangle$ will give us the output 1 with certainty. On the other hand,

$$\begin{bmatrix} 0 \\ i \end{bmatrix} = i|1\rangle$$

But, since:

$$|\langle x|(i|1\rangle)|^2 = |i\langle x|1\rangle|^2 = |\langle x|1\rangle|^2$$

$\Rightarrow$ This effect is completely independent of the measured state $|x\rangle$

Example: $e^{i\theta}$ is a global phase. Since $\left|e^{i\theta}\alpha\right|^2 = \left|e^{i\theta}\right|^2|\alpha|^2 = |\alpha|^2 \Rightarrow |\psi\rangle \equiv e^{i\theta}|\psi\rangle \therefore$ Multiplying a qubit state with a global phase does nothing in qubit's physical state.

4. The Observer Effect: The act of measuring changes the state of qubits (==*collapsing*== the state of the qubit).

$$|q\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \xrightarrow{measure\ |0\rangle} |q\rangle = |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

To achieve truly quantum computation, we must allow the qubits to explore more complex states. Measurements are therefore only used when we need to extract an output. This means that we often place all the measurements at the end of our quantum circuit.

x-measurement: Simply perform an h gate immediately before measurement.
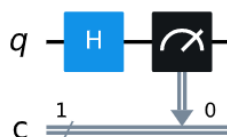
z-measurement: The standard form of measurement, which is done with just a measure gate.
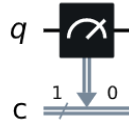
➕ Hadamard gate reverses the roles of the z measurement and x measurement. This leads to a simple effect in the visualization: it swaps the two lines.

The Uncertainty Principle: "*for certain pairs of attributes of a quantum system, it is impossible to know both with certainty.*" (Werner Heisenberg)

We could choose to encode a bit of information in a qubit.

- We can do it the normal way, using the |0⟩ and |1⟩ states to encode the bit values 0 and 1 and using the z measurement to read it out.
- Or we could do it an alternative way, using the |+⟩ and |-⟩ states to encode the bit values and the x measurement for read out.

But the uncertainty principle makes sure that we can't do both at once.

The Bloch Sphere

For generalized state of a qubit |q⟩ = α|0⟩ + β|1⟩ , we can only measure the difference in phase between the states **|0⟩** and **|1⟩.** Let's confine α, β to the real numbers and add a term to tell us the relative phase between them:

$$|q⟩ = α|0⟩ + e^{iΦ}β|1⟩ \quad α, β, Φ \in \mathbb{R}$$

According to the normalization in qubit state, $\sqrt{α^2 + β^2} = 1$ and using trigonometric identity $\sqrt{sin^2x + cos^2x} = 1$, we can obtain $α = \frac{\cos θ}{2}$ $β = \frac{\sin θ}{2}$. From this, we can describe the qubit state as:

$$|q⟩ = \cos\frac{θ}{2}|0⟩ + e^{iφ}Sin\frac{θ}{2}|1⟩ \quad θ, φ \in \mathbb{R}$$

Now, we can plot any single qubit state on the surface of a sphere, known as the *Bloch sphere*. A qubit in the state |+⟩ (*where θ=π/2 and Φ=0*)

```
from qiskit_textbook.widgets import plot_bloch_vector_spherical
coords = [pi/2,0,1] # [Theta, Phi, Radius]
plot_bloch_vector_spherical(coords) # Bloch Vector with spherical coordinates
```
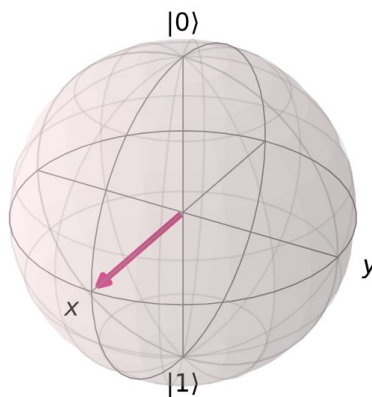
- **State vector** holds the amplitudes for the two states our qubit can be in. The **Bloch vector** is a visualization tool that maps the 2D, complex state vector onto real, 3D space.
- For **n** qubits, there are 2^n possible outcomes (*states*) and we can store these amplitudes in lists of length 2^{n3} which we call **state vectors** (*these vectors describe the state of qubits*).

State vector for two qubits:

$$|\psi\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle = \begin{pmatrix} c_{00} \\ c_{01} \\ c_{10} \\ c_{11} \end{pmatrix}$$

Example: This is an example of a state vector for a quantum computer with two qubits:

$$|x\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} amplitude\ of\ state\ 00 \\ amplitude\ of\ state\ 01 \\ amplitude\ of\ state\ 10 \\ amplitude\ of\ state\ 11 \end{pmatrix} = \sqrt{2}\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

and if we define:

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

then:

$$|x\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |01\rangle)$$

- For **n** qubits, there are 2^{n+1} transition amplitudes.

Example: The following matrix shows the transition amplitudes for CNOT operation:

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

Coordinate System Transformation for Qubit Vectors

$|\psi\rangle \quad = \alpha\,|0\rangle + \beta\,|1\rangle \quad$ and $\quad |\alpha|^2 + |\beta|^2 = 1 \quad \Rightarrow \quad r_\alpha^2 + r_\beta^2 = 1$

$= r_\alpha e^{i\psi_\alpha}|0\rangle + r_b e^{i\psi_b}|1\rangle$

$= e^{i\psi_\alpha}\,(r_\alpha|0\rangle + r_b e^{i(\psi_b-\psi_\alpha)}|1\rangle) = (r_\alpha|0\rangle + r_b e^{i(\psi_b-\psi_\alpha)}|1\rangle)$ since $e^{i\psi_\alpha}$ is a global phase and it is 1.

Since $\cos^2 \Theta/2 + \sin^2 \Theta/2 = 1 \Rightarrow$ *we can replace* $r_\alpha = \cos\frac{\theta}{2}$ *and* $r_\beta = \sin\frac{\theta}{2}$ *also* $\psi_\beta - \psi_\alpha = \phi$

Finally:

$|\psi\rangle \quad = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle \Rightarrow$ *spherical coordinate system representation*

Inverse transformation:

For z=x + iy:

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[3] To fully describe the state of qubits, we may need to keep track of up to 2^n amplitudes. But, if we begin in a product state, it is possible to keep track of everything with a very manageable **2n** amplitudes, rather than the full 2^n. Since anything that is not a product state is an entangled state, we find that entanglement is a necessary ingredient of any quantum advantage.

$$|r| = \sqrt{x^2 + y^2}$$
$$\theta = arctan\left(\frac{y}{x}\right)$$
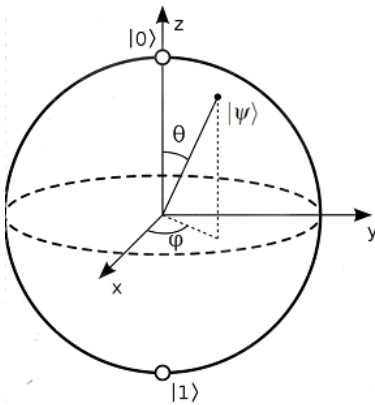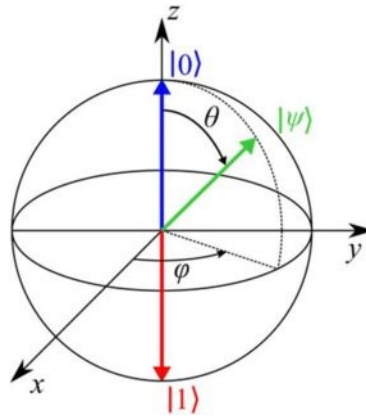
For $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$, we can transform the vector into spherical coordinates as:
$|\psi\rangle = \cos(\theta/2) |0\rangle + e^{i\Phi} \sin(\theta/2) |1\rangle$

with transform from cartesian coordinates to spherical coordinates and find the location of qubit in Bloch sphere:

 x = sin Θ cos Φ
 y = sin Θ sin Φ
 z = cos Θ

Example: $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \Rightarrow \theta = \frac{\pi}{2}$ and $\phi = 0$ *(corresponds to $x = 1, y = z = 0$ point in the bloch sphere)*

Example: To find the position of this qubit in Bloch sphere, find Θ and Φ values. (*Find the spherical coordinate system representation of this qubit*)

$$|\psi\rangle = \frac{3 + i\sqrt{3}}{4}|0\rangle - \frac{1}{2}|1\rangle$$

Answer:

For z=x + iy, $|r| = \sqrt{x^2 + y^2} \Rightarrow$ for our qubit $|r| = \frac{\sqrt{9+3}}{4} = \frac{\sqrt{12}}{4} = \frac{2\sqrt{3}}{4} = \frac{\sqrt{3}}{2}$

$$\theta = arctan\left(\frac{y}{x}\right) \Rightarrow \theta = \arctan\left(\frac{\sqrt{3}/4}{3/4}\right) = arctan\left(\frac{1}{\sqrt{3}}\right) = \frac{\pi}{6} \equiv 30°$$

$$\Rightarrow |\psi\rangle = \frac{\sqrt{3}}{2}e^{i\frac{\pi}{6}}|0\rangle - \frac{1}{2}|1\rangle = e^{i\frac{\pi}{6}}\left(\frac{\sqrt{3}}{2}|0\rangle - e^{-i\frac{\pi}{6}}\frac{1}{2}|1\rangle\right) = \frac{\sqrt{3}}{2}|0\rangle - e^{-i\frac{\pi}{6}}\frac{1}{2}|1\rangle = \frac{\sqrt{3}}{2}|0\rangle + e^{i\pi}e^{-i\frac{\pi}{6}}\frac{1}{2}|1\rangle$$

$$= \frac{\sqrt{3}}{2}|0\rangle + e^{i\frac{5\pi}{6}}\frac{1}{2}|1\rangle \Rightarrow \theta = \frac{\pi}{3} \text{ and } \phi = \frac{5\pi}{6}$$

$$\therefore |\psi\rangle = cos\left(\frac{\pi/3}{2}\right)|0\rangle + e^{i\frac{5\pi}{6}}sin\left(\frac{\pi/3}{2}\right)|1\rangle$$

Some complex number conversions:

- $e^{i\pi} = -1$ (*Euler's Formula*[4]: $e^{ix} = \cos x + i \sin x$)
- $e^{i\frac{\pi}{2}} = i$
- $e^{i\frac{\pi}{4}} = \sqrt{i}$
- $\left| e^{i\theta} \right|^2 = 1$

Deterministic[5] Operations

Every function $f : \sum \longrightarrow \sum$ describes a deterministic operation that performs the classical state **a** into **f(a)** for each **a $\in \sum$**

Given any function $f : \sum \longrightarrow \sum$, there is a unique matrix M satisfying:

$$M \,|a\rangle = |f(a)\rangle \qquad \qquad (for\ every\ a \in \textstyle\sum)$$

$$M(b,a) = \begin{cases} 1 & b = f(a) \\ 0 & b \neq f(a) \end{cases}$$

(b: row, a: column)

The action of this operation is described by matrix-vector multiplication:

$$v \longmapsto M\,v$$

$\longmapsto$ map sign

Example:

a	$f_1(a)$	a	$f_2(a)$	a	$f_3(a)$	a	$f_4(a)$
0	0	0	0	0	1	0	1
1	0	1	1	1	0	1	1

$$M_1 = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \quad M_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad M_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad M_4 = \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}$$

We see that:

      M_1: Constant zero function

      M_2: Identity function

      M_3: Negate function

      M_4: Constant one function

- The Dirac notation can be used for arbitrary vectors: Any name can be used in place of a classical state. Ket's are column vectors and bra's are row vectors.

Example: The notation $|\psi\rangle$ is commonly used to refer to an arbitrary vector:

$$|\psi\rangle = \frac{1+2i}{3}|0\rangle - \frac{2}{3}|1\rangle = \begin{pmatrix} \frac{1+2i}{3} \\ -\frac{2}{3} \end{pmatrix}$$

$|\psi\rangle$ is linear combination of $|0\rangle$ and $|1\rangle$ which is called "==*superposition*=="

$$\langle\psi| = \frac{1-2i}{3}\langle 0| - \frac{2}{3}\langle 1| = \begin{pmatrix} \dfrac{1-2i}{3} & -\dfrac{2}{3} \end{pmatrix}$$

where $|\psi\rangle$ is qubit's (ψ) state vector. For any column vector $|\psi\rangle$, the row vector $\langle\psi|$ is the conjugate transpose[6] of $|\psi\rangle$

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[4] https://en.wikipedia.org/wiki/Euler%27s_formula

[5] Deterministic: There is no randomness or uncertainty involved.

[6] Complex Conjugate: Invert (negate) only the complex part of the number.

Transpose: Rows become columns.

$$\langle\psi| = |\psi\rangle^{\dagger}$$

py#1: Sample Python code for: *set state of a qubit and it's measurement's drawing*

```
from qiskit import QuantumCircuit, assemble, Aer
from qiskit.visualization import plot_histogram, plot_bloch_vector
from math import sqrt, pi
qc = QuantumCircuit(1)
initial_state = [0,1]   # Define initial_state as |1⟩
qc.initialize(initial_state, 0) # Apply initialisation operation to the 0th qubit
sim = Aer.get_backend('aer_simulator')
qc.save_statevector()   # Tell simulator to save statevector
qobj = assemble(qc)     # Create a Qobj from the circuit for the simulator to run
result = sim.run(qobj).result() # Do the simulation and return the result
out_state = result.get_statevector()
print(out_state) # Display the output state vector
qc.measure_all()
qc.draw()
```

Output:

```
Statevector([0. + 0.j, 1. + 0.j], dims=(2,))
```
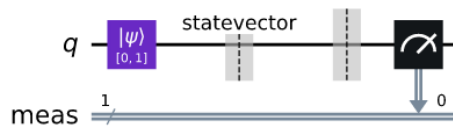

py#2: *Qubit in superposition*

```
from qiskit import QuantumCircuit, assemble, Aer
from qiskit.visualization import plot_histogram, plot_bloch_vector
from math import sqrt, pi

initial_state = [1/sqrt(2), 1j/sqrt(2)]  # Define state |q_0>
qc = QuantumCircuit(1) # Must redefine qc
qc.initialize(initial_state, 0) # Initialize the 0th qubit in the state `initial_state`
qc.save_statevector() # Save statevector
qobj = assemble(qc)
state = sim.run(qobj).result().get_statevector() # Execute the circuit
print(state)         # Print the result
qobj = assemble(qc)
results = sim.run(qobj).result().get_counts()
plot_histogram(results)
```

Output:

```
Statevector([0.70710678 + 0.j, 0. + 0.70710678j], dims=(2,))
```

Conjugate Transpose: First apply conjugate, then apply transpose.
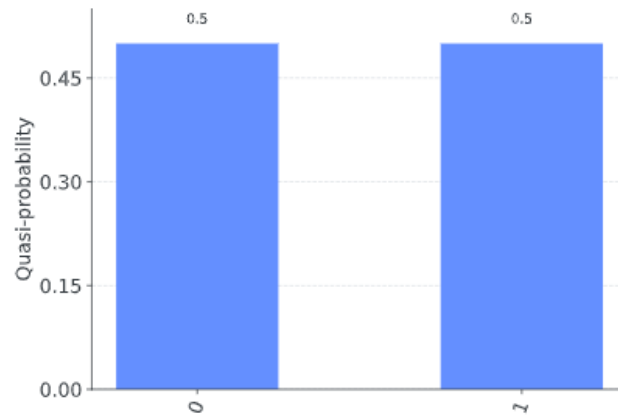
Multiplying row vector to column vector:

$$\langle a|b\rangle = \langle a| \, |b\rangle = \begin{cases} 1 & a = b \\ 0 & a \neq b \end{cases}$$

which is inner product. According to the definition, $\langle 1|0\rangle = \langle 0|1\rangle = 0$ and $\langle 0|0\rangle = \langle 1|1\rangle = 1$

Multiplying column vector to row vector:

Example:

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

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

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

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

∴ In general, **|a⟩⟨b|** has a **1** in the (a, b) entry and **0** for all other entries.

Result:

$$M = \sum_{b \in \Sigma} |f(b)\rangle \langle b|$$

$$M|a\rangle = \sum_{b \in \Sigma} |f(b)\rangle \langle b|a\rangle = |f(a)\rangle$$

Probabilistic Operations
Probabilistic operations are classical operations that may introduce randomness or uncertainty.

Example :
- If the classical state is 0, then do nothing.
- Otherwise flip the bit with probability ½.

Corresponding matrix is:

$$\begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

We see that this function is also equal to ½ probability of "constant zero function" and ½ probability of "identity function".

Probabilistic operations are described by stochastic matrices:
- All entries are nonnegative real numbers,
- The entries in every column sum to 1.

- If we want to find the probability of two unrelated events occurring, we multiply their probabilities together.

Example :
For qubits |a⟩ and |b⟩ with two-qubit states |ba⟩, what is the probability that the qubit on the right comes out 0 ?

$$|a\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \qquad |b\rangle = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \quad and \quad |ab\rangle = \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix}$$

where a_0 is the amplitude of state 0 and so on. So, probability of state |a⟩ as |0⟩ :

$$P_{|a\rangle}(|0\rangle) = P_{|ba\rangle}(|00\rangle) + P_{|ba\rangle}(|10\rangle) = (b_0 a_0)^2 + (b_1 a_0)^2 = b_0^2 a_0^2 + b_1^2 a_0^2 = (b_0^2 + b_1^2) a_0^2 = a_0^2$$

**$(b_0 a_0)^2$ is the probability of measuring 00 (*This is the amplitude of the state |00⟩ squared*)
** $b_0^2 + b_1^2 = 1$ because this is the probability of qubit b "being 1" and "being 0". Sum of them gives the total probability. Total probability of a qubit is always 1.

Composing Operations

Suppose **X** is a system and M_1, …. M_N are stochastic matrices representing probabilistic operations on **X**. Applying the first probabilistic operation to the probability vector v, then applying second probabilistic operation to the result yields this vector:

$$M_2.(M_1.v) = (M_2.M_1).v$$

The probabilistic operation obtained by composing the first and second probabilistic operation is represented by the matrix product M₂M₁.

Composing the probabilistic operations represented by the matrices M_1, … M_N (in that order) is represented by this matrix product:

$$M_n \dots\dots.. M_1$$

Important: Matrix multiplication is <u>NOT commutative</u> !

Quantum Information

A quantum state of a system is represented by a column vector whose indices are placed in correspondence with the classical state of that system:
- The entries are <u>complex</u> numbers,
- The sum of the absolute values squared of the entries (= **Euclidean norm**) must equal 1.

The **Euclidean Norm** ($\|v\|$) for vectors with complex number entries (α) is defined as:

$$v = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} \Rightarrow \|v\| = \sqrt{\sum_{k=1}^{n} |\alpha_k|^2}$$

Quantum state vectors are therefore unit vectors with respect to this norm.

Examples of qubit (quantum bit) states:
- Standard basis states: $|0\rangle$ and $|1\rangle$
- Plus / minus states:

$$|+\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle \quad and \quad |-\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle$$

- A state without a special name:

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

Measuring Quantum States
Measurements provide a mechanism for extracting classical information from quantum systems.

Standard basis measurements:
- The possible outcomes are the classical states.
- The probability for each classical state to be outcome is the absolute value squared of the corresponding quantum state vector entry.

Example: Measuring the quantum state for qubit in + state:

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

yields an outcome as follows:

$$\Pr(outcome\ is\ 0) = \left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2} \quad \Pr(outcome\ is\ 1) = \left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$$

Example: Measuring this qubit's quantum state:

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

yields an outcome as follows:

$$\Pr(outcome\ is\ 0) = \left|\frac{1+2i}{3}\right|^2 = \frac{5}{9} \quad \Pr(outcome\ is\ 1) = \left|-\frac{2}{3}\right|^2 = \frac{4}{9}$$

Measuring a system changes its quantum state: If we measure a system when it's in a quantum state, then the state will change as a result of having performed that measurement. ∴ if we obtain the classical state **a**, the new quantum state becomes **|a⟩.** For the state in the previous example, if we measure (with probability 5/9), we obtain the outcome "zero", in which case, the state transitions to $|0\rangle$. (It is referred to as "collapse of the quantum state")

Example: Measuring this qubit's quantum state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{2}|01\rangle + \frac{\sqrt{3}}{4}|10\rangle + \frac{1}{4}|11\rangle$$

$$Probability\ of\ |00\rangle = \left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$$

If we only measure the left qubit:

$$Probability\ of\ |0\rangle\ for\ left\ qubit = \left|\frac{1}{\sqrt{2}}\right|^2 + \left|\frac{1}{2}\right|^2 = \frac{3}{4}$$

$$Probability\ of\ |1\rangle\ for\ left\ qubit = \left|\frac{\sqrt{3}}{4}\right|^2 + \left|\frac{1}{4}\right|^2 = \frac{1}{4}$$

If we measure left qubit as "0", the qubit pair collapses to this new position:

$$|\psi\rangle \xrightarrow{collapses} \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{2}|01\rangle$$

The final state collapses to the kets where left-qubit is zero. But total probability of this new state is <u>not</u> one. So, we should normalize it:

$$A\left(\left|\frac{1}{\sqrt{2}}\right|^2 + \left|\frac{1}{2}\right|^2\right) = 1 \quad \Rightarrow \quad A = \frac{2}{\sqrt{3}}$$

Then normalized new state is:

$$|\psi\rangle = \frac{1}{\sqrt{3}}\left(\sqrt{2}|00\rangle + |01\rangle\right)$$

Unitary Operations

The set of allowable operations (*gates*) that can be performed on a quantum state is different than it is for classical information. <u>Operations on quantum state vectors are represented by unitary matrices.</u> (<u>Operations on probabilistic states are represented by stochastic matrices</u>)

To preserve the total probability in all cases, our operations need to be reversible. This means we can perform our quantum gates backwards to 'undo' them and be left with the state we started with. We say matrices with this property are ***unitary***.

Definition: A square matrix *U* having complex number entries is unitary if it satisfies the equalities:

$$U^\dagger U = \mathbb{1} = UU^\dagger \ (for\ square\ matrices)$$

* *For non-square matrix, one of the equations above is valid and enough.*

where $U^\dagger$ is the conjugate transpose of U and $\mathbb{1}$ is the identity matrix. Both equalities are equivalent to $U^{-1} = U^\dagger$

The condition that an $n\ x\ n$ matrix U is unitary is equivalent to:

$$\|Uv\| = \|v\|$$

For every n-dimensional column vector *v* with complex number entries.

If $\boldsymbol{v}$ is a quantum state vector, then $\boldsymbol{Uv}$ is also a quantum state vector.

Operations should be designed by matrices, transformations act linearly on vectors representing states.

Conditions of being a Quantum Gate

- A quantum gate U:
    - should be linear, means, $U(\alpha|0\rangle + \beta|1\rangle) = \alpha U|0\rangle + \beta U|1\rangle$

o should give an output such that $|\alpha'^2| + |\beta'^2| = 1$

o should be reversible, means, if you re-apply gate to the output vector of it, the original values should be obtained.
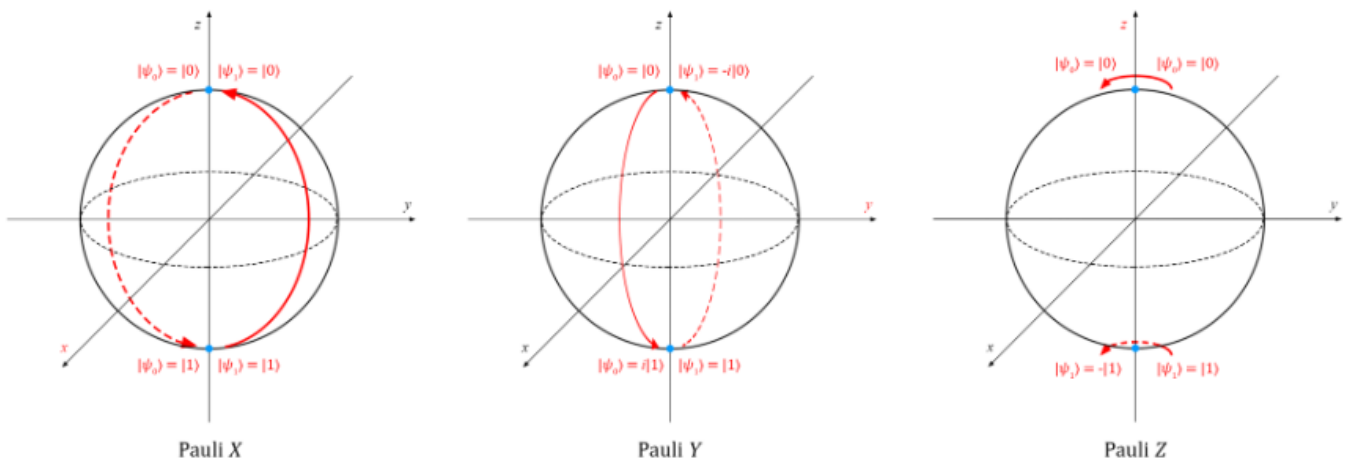
Qubit Unitary Operations

Pauli Operations: Pauli operations are ones represented by the <u>Pauli matrices</u> given below:

$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Common alternative notations: X = σ_x, Y = σ_y and Z = σ_z

The operation σ_x is called a **bit flip** (or a **NOT** operation), and the σ_z operation is called a **phase flip**:

$$\sigma_x |0\rangle = |1\rangle \qquad \sigma_z |0\rangle = |0\rangle$$
$$\sigma_x |1\rangle = |0\rangle \qquad \sigma_z |1\rangle = -|1\rangle$$


Pauli X   Pauli Y   Pauli Z

X gate is represented by "**.cx(in, in)**" in Quiskit.
Z gate is represented by "**.cz(in, in)**" in Quiskit.

- X*X = Y*Y = Z*Z = $\mathbb{1}$

```
from qiskit import QuantumCircuit, assemble, Aer
from math import pi, sqrt
from qiskit.visualization import plot_bloch_multivector, plot_histogram
sim = Aer.get_backend('aer_simulator')
# Let's do an X-gate on a |0⟩ qubit
qc = QuantumCircuit(1)
qc.x(0)
# Let's see the result
qc.save_statevector()
qobj = assemble(qc)
state = sim.run(qobj).result().get_statevector()
plot_bloch_multivector(state)
```
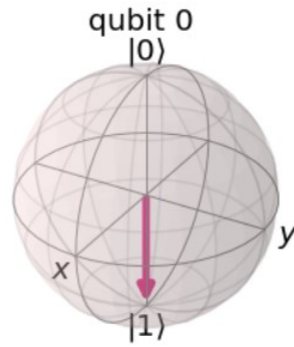
Hadamard Operation: This gate allows us to move away from the poles of the Bloch sphere and create a superposition of $|0\rangle$ and $|1\rangle$. It has the matrix:

$$H = \begin{pmatrix} \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \\ \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Checking that **H** is unitary is a straightforward calculation:

$$\begin{pmatrix} \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \\ \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \end{pmatrix}^{\dagger}\begin{pmatrix} \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \\ \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \\ \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \\ \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \dfrac{1}{2}+\dfrac{1}{2} & \dfrac{1}{2}-\dfrac{1}{2} \\ \dfrac{1}{2}-\dfrac{1}{2} & \dfrac{1}{2}+\dfrac{1}{2} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$H|0\rangle=|+\rangle \qquad H|1\rangle=|-\rangle \qquad H|+\rangle=|0\rangle \qquad H|-\rangle=|1\rangle$$

This can be thought of as a rotation around the Bloch vector [1,0,1] (the line between the x & z-axis) Hadamard gate is represented by "**.h(in, in)**" in Quiskit.

Example: We can show that: *X = HZH*

$$HZH = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = X$$
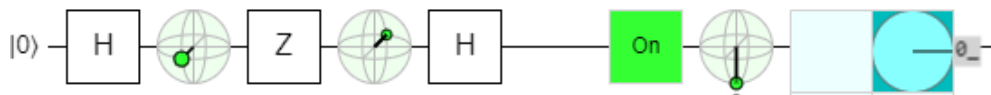
Phase Operations (*p-gate*): The P-gate performs a rotation of Θ around the Z-axis direction.

$$P_\theta = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}$$

for any choice of a real number θ.

The operations:

$$S = P_{\frac{\pi}{2}} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \qquad T = P_{\frac{\pi}{4}} = \begin{pmatrix} 1 & 0 \\ 0 & \dfrac{1+i}{\sqrt{2}} \end{pmatrix} \qquad P_0 = \mathbb{1} \qquad P_\pi = \sigma_z$$
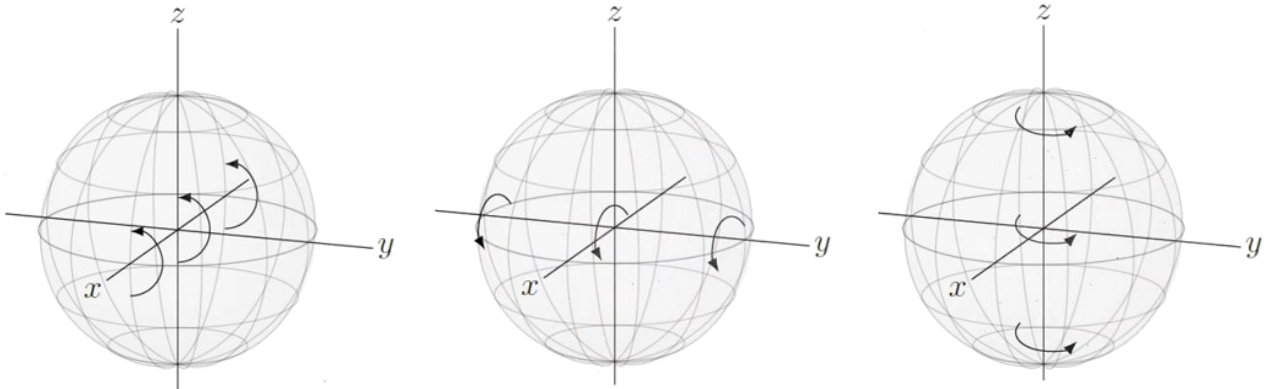
are important examples.

Example:

$$T|0\rangle = |0\rangle \quad and \ T|1\rangle = \frac{1+i}{\sqrt{2}}|1\rangle \quad where \ T = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1+i}{\sqrt{2}} \end{pmatrix}$$

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

$$HT|+\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1+i}{2}|-\rangle = \left(\frac{1}{2} + \frac{1+i}{2\sqrt{2}}\right)|0\rangle + \left(\frac{1}{2} - \frac{1+i}{2\sqrt{2}}\right)|1\rangle$$
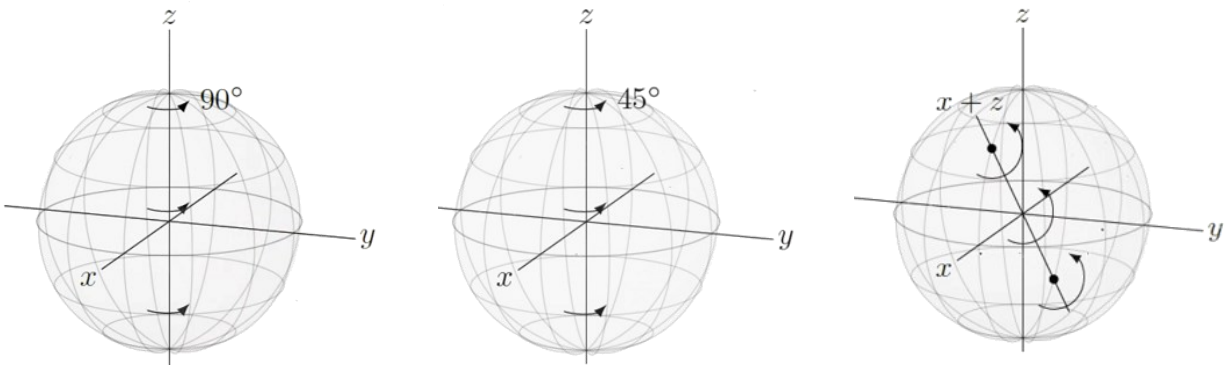
Gates Summary

X Gate provides 180° rotation	**Y Gate** provides 180° rotation	**Z Gate** provides 180° rotation
in X axis	in Y axis	in Z axis
X|0⟩=|1⟩	Y|0⟩= i|1⟩	Z|0⟩= i|1⟩
X|1⟩=|0⟩	Y|1⟩= -i|0⟩	Z|1⟩= -i|0⟩
X|+⟩=|+⟩	Y|+⟩= -i |-⟩	Z|+⟩=|-⟩
X|-⟩=-|-⟩	Y|-⟩= i |+⟩	Z|-⟩=|+⟩
X|i⟩=|-i⟩	Y|i⟩= |i⟩	Z|i⟩=|-i⟩
X|-i⟩=|i⟩	Y|-i⟩= -|-i⟩	Z|-i⟩=|i⟩

Some phase comments:

** The Z gate applied to a single qubit has the effect of doing nothing to |0⟩ and giving a **phase of -1** to the state |1⟩.

** For the Z gate, it only has any effect at all when <u>both qubits</u> are in state |1⟩.

S (*phase*) Gate	**T (*phase*) Gate**	**H Gate**
X|0⟩=|0⟩	T|0⟩= i|1⟩	H|0⟩= |+⟩

$X\|1\rangle = i\|1\rangle$	$T\|1\rangle = e^{i\pi/4}\|1\rangle$	$H\|1\rangle = \|-\rangle$
$X\|+\rangle = \|i\rangle$	$T\|+\rangle = \frac{1}{\sqrt{2}}(\|0\rangle + \sqrt{i}\|1\rangle)$	$H\|+\rangle = \|0\rangle$
$X\|-\rangle = -\|i\rangle$	$T\|-\rangle =$	$H\|-\rangle = \|1\rangle$
$X\|i\rangle =$	$T\|i\rangle =$	$H\|i\rangle =$
$X\|-i\rangle =$	$T\|-i\rangle =$	$H\|-i\rangle =$

- $T^2 = S$
- $S^2 = Z$
- $H^2 = \mathbb{1}$

Representation of Popular Gates

$$Pauli\ gates: \quad X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad T = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix} \quad S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} = T^2$$

$$X = HZH = HT^4H$$

$$Y = SXZS = T^2HT^4HT^6$$

$$Z = HXH = S^2 = T^4$$
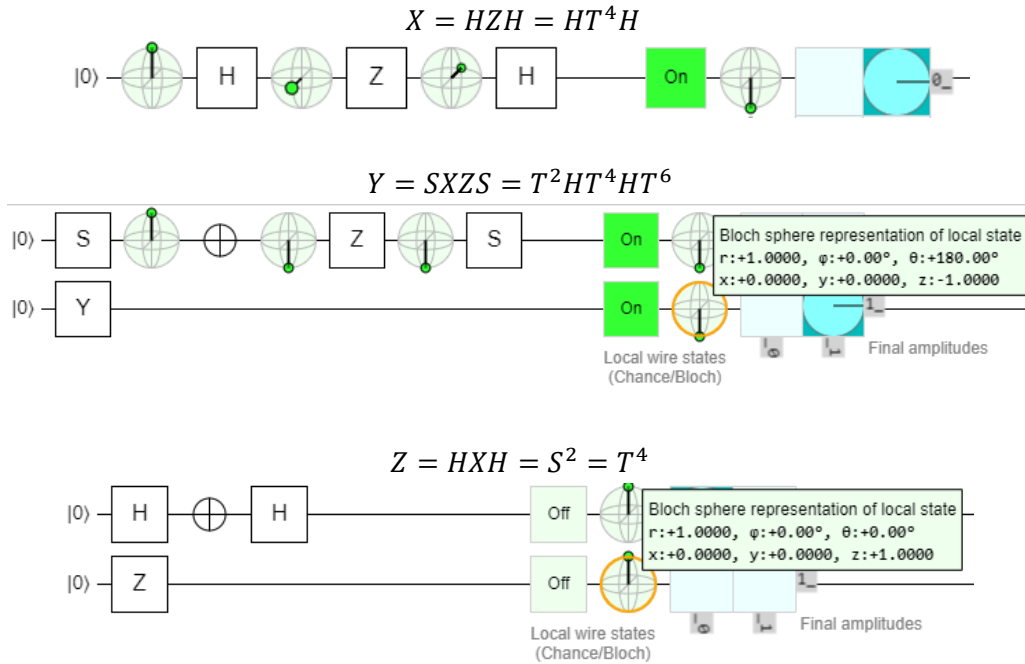
Theorem: Every single-qubit gate can be defined as a rotation over an axis in Bloch gate.

Proof: Let's define:

$$\hat{n} = n_x\hat{x} + n_y\hat{y} + n_z\hat{z} \quad where\ n_x^2 + n_y^2 + n_z^2 = 1$$

A general definition of a qubit is as follows:

$$U = e^{i\gamma}\left[\cos\left(\frac{\theta}{2}\right)I - i\sin\left(\frac{\theta}{2}\right)(n_xX + n_yY + n_zZ)\right]$$

where Θ is rotation angle, X, Y, Z are known gates and n_x, n_y, n_z are the coefficients that determines the rotation axis.

Let's see that Hadamard gate can be represented by U for:

$$\hat{n} = \frac{1}{\sqrt{2}}\hat{x} + \frac{1}{\sqrt{2}}\hat{z} \quad and \quad \theta = \pi$$

When we replace the variables into U, we get:

$$U = -ie^{i\gamma}\frac{1}{\sqrt{2}}(X + Z)$$

Now, let's apply generic qubit state to U and check if the result is same as Hadamard gate or not:

$$U|0\rangle = -ie^{i\gamma}\frac{1}{\sqrt{2}}(X + Z)|0\rangle = -ie^{i\gamma}\frac{1}{\sqrt{2}}(|1\rangle + |0\rangle) = -ie^{i\gamma}|+\rangle$$

(where we know that X|0⟩=|1⟩ and Z|0⟩=|0⟩)

$$U|1\rangle = -ie^{i\gamma}\frac{1}{\sqrt{2}}(X + Z)|1\rangle = -ie^{i\gamma}\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = -ie^{i\gamma}|-\rangle$$

when we get $\gamma = {}^{\pi}\!/_2 \Rightarrow -ie^{i\gamma} = -i.i = (-1)(-1) = 1$, and we see that U ≡ H

In the similar way, we can show that U≡S . We know that S gate rotates a qubit over Z axis π/2 degree. So:

$$\hat{n} = \hat{z} \qquad \theta = \frac{\pi}{2} \quad and \quad \gamma = \frac{\pi}{4}$$

Let's replace the variables over U, we get:
$$U = e^{i\frac{\pi}{4}}\frac{1}{\sqrt{2}}(I + iZ)$$

Then, apply this gate to generic qubit state:
$$U|0\rangle = e^{i\frac{\pi}{4}}\frac{1}{\sqrt{2}}(1 - i)|0\rangle = |0\rangle \qquad where \quad \frac{1-i}{\sqrt{2}} = e^{-i\frac{\pi}{4}}$$

$$U|1\rangle = e^{i\frac{\pi}{4}}\frac{1}{\sqrt{2}}(1 + i)|1\rangle = e^{i\frac{\pi}{2}}|1\rangle = i|1\rangle$$

So, we see that U ≡ S

Toffoli Gate: It is basic AND operation. It requires 2 inputs and it is represented by "*.ccx(in, in, out)*" in Quiskit.

CNOT Gate: The CNOT (*controlled-NOT*) gate acts on two qubits, which are known as the 'control' and the 'target'. If the control is in state |0⟩, the cx does nothing. If the control is in state |1⟩, the cx performs an X (not) on the target qubit.
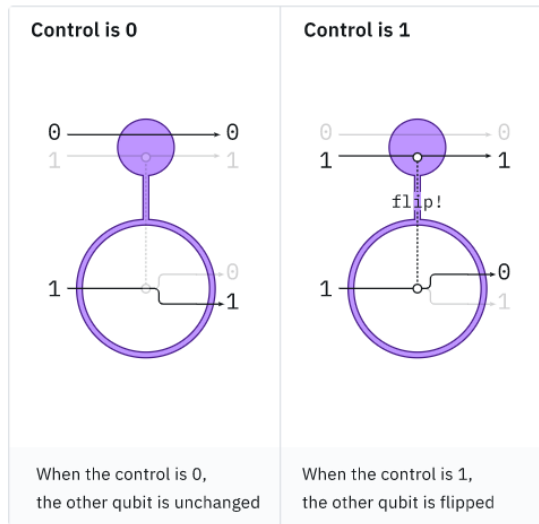
CNOT gate is represented by "*.cx(in, in)*" in Quiskit.

Compositions of qubit Unitary Operations
Compositions of unitary operations are represented by matrix multiplication (similar to the probabilistic setting).

$$R = HSH = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\sqrt{2} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\sqrt{2} \end{pmatrix} = \begin{pmatrix} \frac{1+i}{2} & \frac{1-i}{2} \\ \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix}$$

(The unitary matrices are closed under multiplication)

$$R^2 = \begin{pmatrix} \frac{1+i}{2} & \frac{1-i}{2} \\ \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = NOT\ operation = bit\ flip = X = \sigma_x$$

$\therefore$ R is square root of NOT operation. $(X = (HSH)^2)$
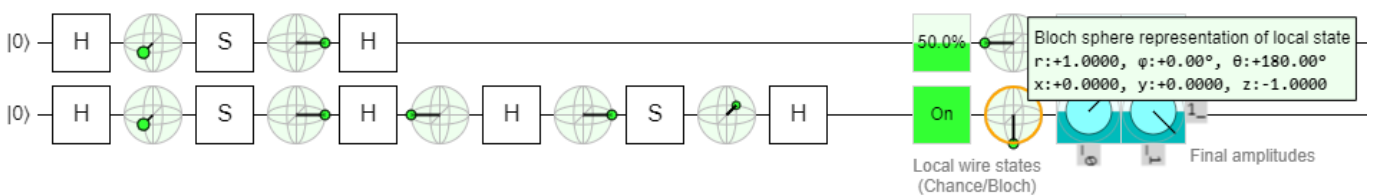
Multiple Systems

Classical States

Classical state of a system is a configuration of a system that can be recognized and described unambiguously without any uncertainty or error.

Suppose that we have two systems:

- X is a system having classical state set $\sum$.
- Y is a system having classical state set Γ.

Imagine that, X and Y are placed side-by-side with X on the left and Y on the right, and viewed together as if they form a single system. We denote this new compound system by (X, Y) or XY.

Classical state of XY is the cartesian product:

$$\sum x \, \Gamma \, = \, \{(a,b) : a \in \sum \ and \ b \in \Gamma\}$$

Example: If $\sum$ = {0, 1} and Γ = {a, b, c}, then:

$$\sum x \, \Gamma = \{ (0, a), (0, b), (0, c), (1, a), (1, b), (1, c) \}$$

This description generalizes to more than two systems in a natural way:

Suppose $X_1, \ldots, X_n$ are systems having classical state sets $\sum_1, \ldots \sum_n$ respectively. The classical state set of n-tuple $(X_1, \ldots X_n)$, viewed as a single compound system, is the Cartesian product:

$$\sum_1, \ldots \sum_n = \{ (a_1, \ldots a_n) : (a_1 \in \sum_1, \ldots a_n \in \sum_n \}$$

Example: if $\sum_1 = \sum_2 = \sum_3$ = {0, 1} , then the classical state set of (X_1, X_2, X_3) is:

$$\sum_1 x \sum_2 x \sum_3 = \{(0,0,0), (0,0,1), (0,1,0), (0,1,1), (1,0,0,), (1,0,1), (1,1,0), (1,1,1) \}$$

An n-tuple $(a_1, \ldots a_n)$ may also be written as a string $a_1 \ldots a_n$. (*drop parentheses and comma*)

Example: Suppose $X_1, \ldots X_{10}$ are bits, so this classical state sets are all the same:

$$\sum_1 = \sum_2 \ = \ldots = \sum_{10} = \{0,1\}$$

The classical state set of $(X_1, \ldots X_{10})$ is the Cartesian product:

$$\sum_1 x \sum_2 \ x \ldots x \sum_{10} = \{0,1\}^{10}$$

Written as strings, these classical states look like this (*1.024 lines*):

<div align="center">

0000000000
0000000001
0000000010
⋮

</div>

1111111111

Ordering Cartesian Product State Sets

Convention: Cartesian products of classical state sets are ordered lexicographically (*i.e., dictionary ordering*):

- We assume the individual classical state sets are already ordered.
- Significance decreases from left to right.

Example: The Cartesian product {1,2,3} x {0,1} is ordered like this:

(1,0), (1,1), (2,0), (2,1), (3,0), (3,1)

When n-tuples written as strings and ordered in this way, we observe familiar patterns, such as {0,1} x {0,1} being ordered as 00, 01, 10, 11.

Probabilistic States

Probabilistic states of compound systems associate probabilities with the Cartesian product of the classical state sets of the individual systems.

Example: This is a probabilistic state of a pair of bits (X,Y):

$$Pr((X,Y) = (0,0)) = ½$$
$$Pr((X,Y) = (0,1)) = 0$$
$$Pr((X,Y) = (1,0)) = 0$$
$$Pr((X,Y) = (1,1)) = ½$$

$$\begin{pmatrix} ½ \\ 0 \\ 0 \\ ½ \end{pmatrix} \begin{matrix} \leftarrow & probability\ associated\ with\ state\ 00 \\ \leftarrow & probability\ associated\ with\ state\ 01 \\ \leftarrow & probability\ associated\ with\ state\ 10 \\ \leftarrow & probability\ associated\ with\ state\ 11 \end{matrix}$$

Definition: For a given probabilistic state of (X, Y), we say that X and Y are **independent[7]**, if:

$$Pr((X, Y) = (a, b)) = Pr\ (X = a)\ Pr\ (Y = b)$$

for all $a \in \sum$ and $b \in \Gamma$.[8]

Suppose that a probabilistic state of (X, Y) is expressed as a vector:

$$|\pi\rangle = \sum_{(a,b) \in \sum x \Gamma} |ab\rangle$$

The systems X and Y are independent if there exist probability vectors:

$$|\emptyset\rangle = \sum_{a \in \Sigma} q_a |a\rangle \quad and \quad |\psi\rangle = \sum_{b \in \Gamma} r_b |b\rangle$$

---

[7] Statistical Independence = Absence or correlation

[8] It says that, the probability of X to be in any one classical state and the probability of Y to be in some other classical state have absolutely nothing to do with one another.

Such that $p_{ab} = q_a r_b$ for all $a{\in}\Sigma$ and $b{\in}\Gamma$. (*| Φ⟩ and |ψ⟩ probabilistic states of X and Y*)

Example : The probabilistic state of a pair of bits (X, Y) represented by the vector

$$|\pi\rangle = \frac{1}{6}|00\rangle + \frac{1}{12}|01\rangle + \frac{1}{2}|10\rangle + \frac{1}{4}|11\rangle$$

is one in which X and Y are independent. The required condition is true for these probabilistic vectors:

$$|\emptyset\rangle = \frac{1}{4}|0\rangle + \frac{3}{4}|1\rangle \quad and \quad |\psi\rangle = \frac{2}{3}|0\rangle + \frac{1}{3}|1\rangle$$

(*The probability for each possible setting for the two bits is given by the product of the corresponding probabilities for the individual bits*)

Example : For the probabilistic state

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

of two bits (X, Y), we have that X and Y are not independent. $\equiv$ The bits are correlated.
If they were, we would have numbers q_0, q_1, r_0, r_1 such that:

$$q_0 r_0 = \tfrac{1}{2} \quad q_0 r_1 = 0 \quad q_1 r_0 = 0 \quad q_1 r_1 = \tfrac{1}{2}$$

But $q_0 r_1$ is zero, then either q_0=0 or r_0=0 (or both), contradicting either the first or last equality.
(*$q_0 r_1$ cannot be 0 because at least q_0 or r_1 should be zero. If any of them is zero, $q_0 r_0$ or $q_1 r_1$ cannot be ½ . So, these four conditions cannot be obtained ∴ The probabilistic state is not independent*)

Tensor Products of Vectors

Definition: The tensor product of two vectors (*Φ and ψ*) where Σ and Γ are any choice of classical state sets:

$$|\Phi\rangle = \sum_{a\in\Sigma} \alpha_a |a\rangle \quad and \quad |\Psi\rangle = \sum_{b\in\Gamma} \beta_b |b\rangle$$

is the vector:

$$|\Phi\rangle \otimes |\Psi\rangle = |\Phi \otimes \Psi\rangle = |\Phi\rangle|\Psi\rangle = |\Phi\Psi\rangle = |\Phi,\Psi\rangle = \sum_{(a,b)\in\Sigma x\Gamma} \alpha_a \beta_b |ab\rangle$$

Equivalently, the vector $|\pi\rangle=|\Phi\rangle \otimes |\psi\rangle$ is defined by this condition:

$$\langle ab|\pi\rangle = \langle a|\Phi\rangle \langle b|\psi\rangle \qquad \text{(for all } a{\in}\Sigma \text{ and } b{\in}\Gamma)$$

Example:

$$|\phi\rangle = \frac{1}{4}|0\rangle + \frac{3}{4}|1\rangle \quad and \quad |\psi\rangle = \frac{2}{3}|0\rangle + \frac{1}{3}|1\rangle$$

$$|\Phi\rangle \otimes |\Psi\rangle = \frac{1}{6}|00\rangle + \frac{1}{12}|01\rangle + \frac{1}{2}|10\rangle + \frac{1}{4}|11\rangle$$

- Following out convention for ordering the elements of Cartesian product sets, we obtain this specification for the tensor product of two column vectors:

$$\begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_m \end{pmatrix} \otimes \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_k \end{pmatrix} = \begin{pmatrix} \alpha_1\beta_1 \\ \vdots \\ \alpha_1\beta_k \\ \alpha_1\beta_2 \\ \vdots \\ \alpha_1\beta_k \\ \vdots \\ \alpha_m\beta_1 \\ \vdots \\ \alpha_m\beta_k \end{pmatrix}$$

Important Properties of Tensor Products

** The tensor product of two vector is bilinear.

  1. Linearity in the first argument:

$$(|\Phi_1\rangle + |\Phi_2\rangle) \otimes |\Psi\rangle = |\Phi_1\rangle \otimes |\Psi\rangle + |\Phi_2\rangle \otimes |\Psi\rangle$$

$$(\alpha |\Phi\rangle) \otimes |\Psi\rangle = \alpha(|\Phi\rangle \otimes |\Psi\rangle)$$

  2. Linearity in the second argument:

$$|\Phi\rangle \otimes (|\Psi_1\rangle + |\Psi_2\rangle) = |\Phi\rangle \otimes |\Psi_1\rangle + |\Phi\rangle \otimes |\Psi_2\rangle$$

$$|\Phi\rangle \otimes (\alpha|\Psi\rangle) = \alpha(|\Phi\rangle \otimes |\Psi\rangle)$$

Tensor Products of Vectors

If we define $|\psi\rangle = |\Phi_1\rangle \otimes |\Phi_2\rangle \otimes \cdots \otimes |\Phi_n\rangle$ *then* $\langle a_1 \cdots a_n|\psi\rangle = \langle a_1|\phi\rangle \otimes \cdots \langle a_n|\phi\rangle$

- The tensor product of three or more vector is *multilinear*.

Measurements of Probabilistic States

Measurement of compound systems work in the same way as measurements of single systems – provided that all of the systems are measured.

Example: Suppose that two bits (X, Y) are in the probabilistic state $\frac{1}{2}|00\rangle + \frac{1}{2}|11\rangle$. Measuring both bits yields the outcome 00 with probability ½ and the outcome with the probability ½ . Because measuring all of the systems is equivalent to measuring the entire compound system.

If we measure just X but don't measure Y, then it means there is still could exist some uncertainty about the state of Y and this uncertainty is reflected by this formula:

$$\Pr(Y = b \mid X = a) = \frac{\Pr((X, Y = (a, b))}{\Pr(X = a)}$$

Example: Suppose (X, Y) is in the probabilistic state $\frac{1}{12}|00\rangle + \frac{1}{4}|01\rangle + \frac{1}{3}|10\rangle + \frac{1}{3}|11\rangle$, we write this vector as follows:

$$|0\rangle \otimes \left(\frac{1}{12}|0\rangle + \frac{1}{4}|1\rangle\right) + |1\rangle \otimes \left(\frac{1}{3}|0\rangle + \frac{1}{3}|1\rangle\right)$$

Case 1: The measurement outcome is zero:

$$Pr(outcome\ is\ zero) = \frac{1}{12} + \frac{1}{4} = \frac{1}{3}$$

Conditioned on this outcome, the probabilistic state of Y becomes:

$$\frac{\frac{1}{12}|0\rangle + \frac{1}{4}|1\rangle}{\frac{1}{3}} = \frac{1}{4}|0\rangle + \frac{3}{4}|1\rangle$$

Case 2: The measurement outcome is one:

$$Pr(outcome\ is\ one) = \frac{1}{3} + \frac{1}{3} = \frac{2}{3}$$

Conditioned on this outcome, the probabilistic state of Y becomes:

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

The same method can be used when Y is measured, rather than X. Suppose that (X, Y) is in some arbitrary probabilistic state:

$$\sum_{a,b\ \in\ \Sigma x \Gamma} p_{ab}|ab\rangle = \sum_{a,b\ \in\ \Sigma x \Gamma} p_{ab}|a\rangle \otimes |b\rangle = \sum_{b \in \Gamma} \left(\sum_{a\ \in\ \Sigma} p_{ab}|a\rangle \right) \otimes |b\rangle$$

1. The probability that a measurement of Y yields an outcome a ∈ Σ is:

$$Pr(Y = b) = \sum_{a\ \in\ \Sigma} p_{ab}$$

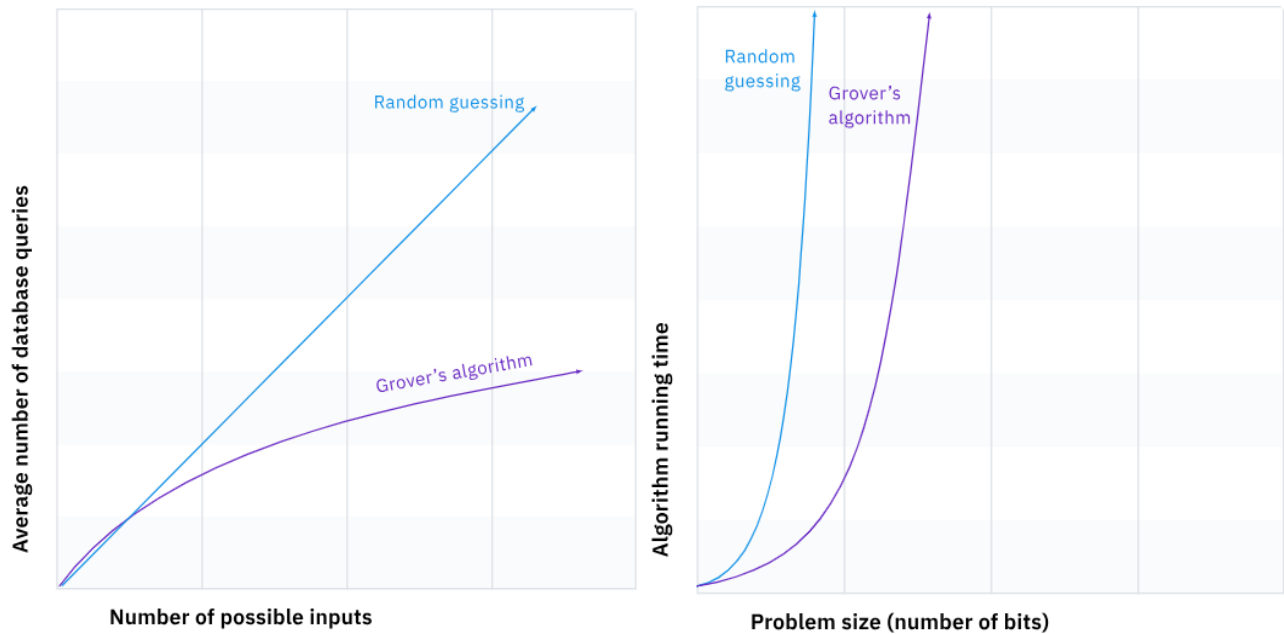2. Conditioned on the outcome b ∈ Γ, the probabilistic state of X becomes

$$\frac{\sum_{a\ \in\ \Sigma} p_{ab}|a\rangle}{\sum_{c\ \in\ \Sigma} p_{c,b}}$$

Operations on Probabilistic States

---

[9] Waterloo Üniversitesi'ndeki David R. Cheriton Bilgisayar Bilimleri Okulu'nda bilgisayar bilimi profesörü, Kuantum Hesaplama Enstitüsü'nün bir üyesi, Çevre Teorik Fizik Enstitüsü'nün bağlı bir üyesi ve Kanada Üyesidir.

Simulators

Bloch sphere simulators:
** https://attilakun.net/bloch/
** https://www.st-andrews.ac.uk/physics/quvis/simulations_html5/sims/blochsphere/blochsphere.html
** https://bits-and-electrons.github.io/bloch-sphere-simulator/#{%22blochSphereStateProperties%22:{%22theta%22:%220.0000%22,%22phi%22:%2290.0000%22},%22customGatesProperties%22:{},%22lambdaGatesProperties%22:{%22polarAngle%22:%220%22,%22azimuthAngle%22:%220%22}}

Quantum FlyTrap Virtual Lab - Simulator: https://lab.quantumflytrap.com/lab?mode=waves
Quantum Circuit Simulator: https://thequantumlaend.de/quantum-circuit-designer/
Quantum Circuit Designer: https://algassert.com/quirk

Other:
https://learn.microsoft.com/en-us/azure/quantum/concepts-the-qubit

Designing a new gate in Quirk Simulator Web Page
Let:

$$U = \begin{pmatrix} \dfrac{\sqrt{2}-i}{2} & \dfrac{1}{2} \\ -\dfrac{1}{2} & \dfrac{\sqrt{2}+i}{2} \end{pmatrix}$$

If we want to see this gate in Quirk simulation, do the followings:
- Enter Quirk web site (https://algassert.com/quirk).
- Click "Make Gate" button on top of the screen.
- Enter the coefficients of the gate into the "From Matrix" screen as follows:
  - (sqrt(2)-i)/2, 1/2
  - -1/2, (sqrt(2)+i)/2
- You will see the amplitude of each cell of the gate matrix and the gate rotation axis on the bloch sphere, in the bottom of "From Matrix".
- Give a name to the gate from "circuit symbol" text box.
- Click "Create Matrix Gate" button.
- You will see the new gate in the right most side of toolbox-2 at the bottom of the screen.

Quantum Computing: Search Algorithms
Grover's Quantum Search Algorithm

When searching any database, Grover's algorithm grows with the square root of the number of inputs, which for unstructured search (*search on unordered data*) is a quadratic improvement over the best classical algorithm.

Each extra variable (bit) in our SAT problem doubles the number of possible solutions (*i.e. entries to our database*), so the search space grows exponentially with the number of bits. Since random guessing grows linearly with N, the running time will grow by roughly 2^n.

SAT *(Boolean satisfiability problem)*

SAT is the problem of determining if there exists an interpretation that satisfies a given Boolean formula. The satisfiability problem considers the case in which N boolean variables are used to form a Boolean expression involving negation (NOT), conjunction (AND) and disjunction (OR). The problem is to determine whether there is any assignment of values to the Boolean variables which makes the formula **true**. For simplicity, it is common to require that the boolean expression be written in conjunction normal form or "CNF".

A formula in CNF consists of:
- clauses joined by AND;
- each clause, in turn, consists of literals joined by OR;
- each literal is either the name of a variable (*a positive literal*), or the name of a variable preceded by NOT (a negative literal).

Structure of CNF File:[10]
- The file may begin with comment lines. The first character of each comment line must be a lower case letter "c".
- The comment lines are followed by the "problem" line. This begins with a lower case "p" followed by a space, followed by the problem type, which for CNF files is "cnf", followed by the number of variables followed by the number of clauses.
- The remainder of the file contains lines defining the clauses, one by one.
- A clause is defined by listing the index of each positive literal, and the negative index of each negative literal. Indices are 1-based, and for obvious reasons the index 0 is not allowed.
- The definition of a clause is terminated by a final value of "0".

Example:
```
c example DIMACS-CNF 3-SAT
p cnf 3 5
-1 -2 -3 0
```

---

[10] https://people.sc.fsu.edu/~jburkardt/data/cnf/cnf.html

```
1 -2 3 0
1 2 -3 0
1 -2 -3 0
-1 2 3 0
```

According to this CNF file, the line "1 -2 3 0" means: if bit1 is 1, bit2 is 0 and bit3 is 1 then this clause is satisfied.

For tis CNF file, corresponding quantum circuit which is created by Quiskit's circuit library is as follows:

> *from qiskit.circuit.library import PhaseOracle*
> *oracle = PhaseOracle.from_dimacs_file('examples/3sat.dimacs')*
> *oracle.draw()*
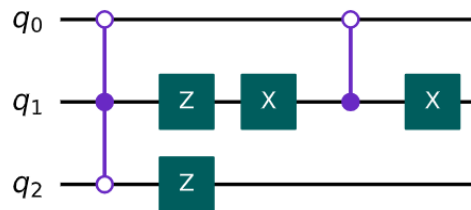
To use this circuit with Grover's algorithm, we want the oracle to change the phase of the output state by 180° (i.e. multiply by -1) if the state is a solution.

$$U_{oraacle}|x\rangle = \begin{cases} |x\rangle & \text{if } x \text{ is not a solution} \\ -|x\rangle & \text{if } x \text{ is a solution} \end{cases}$$

For example, the only solutions to this problem are 000, 011, and 101, so the circuit above has this matrix:

$$U_{oracle} = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Then, let's look at the steps of Grover's algorithm:

- **Step_1**: Create an equal superposition of every possible input to the oracle by applying H-gate to initial state $|0\rangle$ of each qubit. We'll call this equal superposition state $|s\rangle$.
- **Step_2:** The next step is to run the oracle circuit (U_{oracle}) on these qubits.
- **Step_3:** The final step is to run a circuit called the 'diffusion operator' or 'diffuser' (U_s) on the qubits.
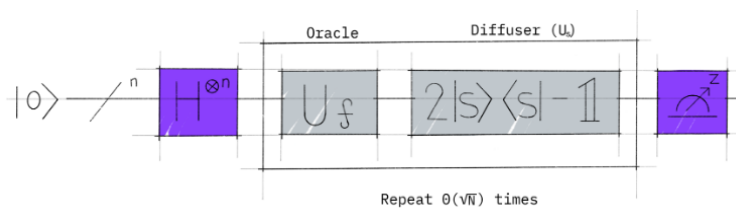
- We then need to repeat steps 2 & 3 a few times depending on the size of the circuit. For difficult problems (*if there is only one solution*), we need to repeat these steps $\sqrt{N}$ times.
    - For difficult problems, there are a lot of possible inputs and only a small number of solutions. In this case |s⟩ is much closed to |⊠⟩ (*all solution states*) rather than |√⟩ (*all other states*). Let say, the angle between |s⟩ and |⊠⟩ is θ at the beginning.
    - After each iteration (*running step 1 and step 2*), |s⟩ reaches towards |√⟩ by 2θ
    - We see that $Sin(\theta) = \frac{1}{\sqrt{N}}$
    - Since for small θ, we want to rotate |s⟩ around 90 degrees to reach |√⟩. So, we need $\sqrt{N}$ iterations for the solution.

```
from qiskit import QuantumCircuit
init = QuantumCircuit(3)
init.h([0,1,2])
# steps 2 & 3 of Grover's algorithm
from qiskit.circuit.library import GroverOperator
grover_operator = GroverOperator(oracle)
qc = init.compose(grover_operator)
qc.measure_all()
qc.draw()
```
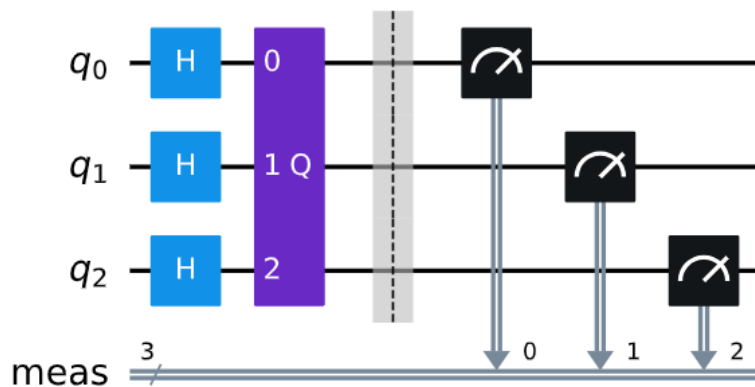

Then we can get the results from simulator:

```
# Simulate the circuit
from qiskit import Aer, transpile
sim = Aer.get_backend('aer_simulator')
t_qc = transpile(qc, sim)
counts = sim.run(t_qc).result().get_counts()

# plot the results
from qiskit.visualization import plot_histogram
plot_histogram(counts)
```
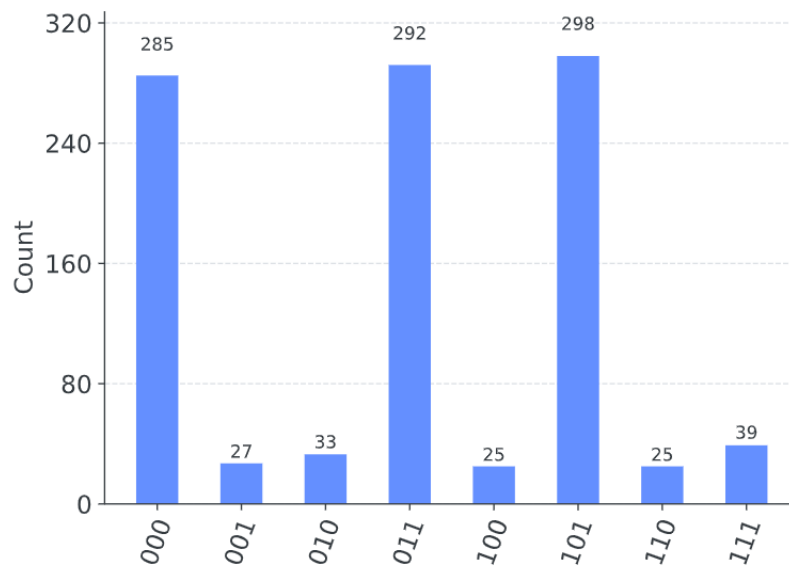
We can see that system gives high probabilities on three solutions of this SAT problem.

Circuits for Grover's algorithm

```
from qiskit import QuantumCircuit
oracle = QuantumCircuit(2)
oracle.cz(0,1)  # invert phase of |11>
def display_unitary(qc, prefix=""):
    """Simulates a simple circuit and display its matrix representation.
    Args:
        qc (QuantumCircuit): The circuit to compile to a unitary matrix
        prefix (str): Optional LaTeX to be displayed before the matrix
    Returns:
        None (displays matrix as side effect)
    """
    from qiskit import Aer
    from qiskit.visualization import array_to_latex
    sim = Aer.get_backend('aer_simulator')
    # Next, we'll create a copy of the circuit and work on
    # that so we don't change anything as a side effect
    qc = qc.copy()
    # Tell the simulator to save the unitary matrix of this circuit
    qc.save_unitary()
    unitary = sim.run(qc).result().get_unitary()
    display(array_to_latex(unitary, prefix=prefix))

display_unitary(oracle, "U_\\text{oracle}=")
```

$$U_{oracle} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

Creating the diffuser:

- Do the transformation $|s\rangle \rightarrow |11\rangle$ (i.e., x-gate)
- Reflect around $|11\rangle$ (i.e., the cz-gate)
- Do the transformation $|11\rangle \rightarrow |s\rangle$

```
diffuser = QuantumCircuit(2)
diffuser.h([0, 1])
diffuser.x([0,1])
diffuser.cz(0,1)
diffuser.x([0,1])
diffuser.h([0,1])
diffuser.draw()
```
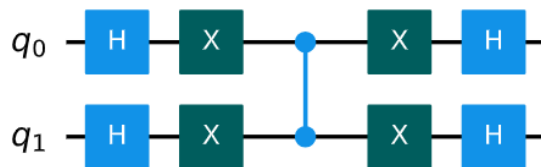

- Now perform oracle and perform diffuser to get Grover's algorithm:

```
grover = QuantumCircuit(2)
grover.h([0,1])  # initialise |s>
grover = grover.compose(oracle)
grover = grover.compose(diffuser)
grover.measure_all()
grover.draw()
```
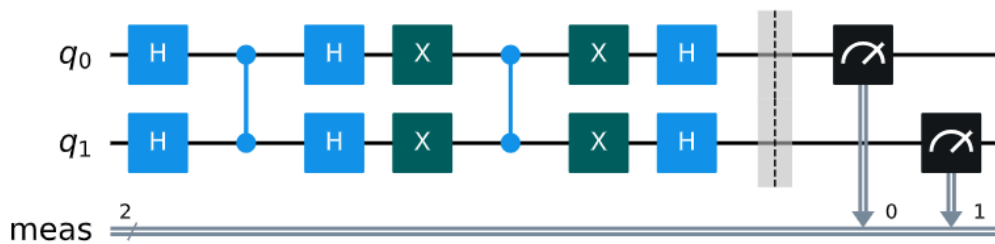

And finally, simulate the result:

```
from qiskit import Aer
sim = Aer.get_backend('aer_simulator')
sim.run(grover).result().get_counts()
```

RESULT: {'11': 1024} (*100% probability of measuring $|11\rangle$*)

** Same problem solution with Quirk[11]:
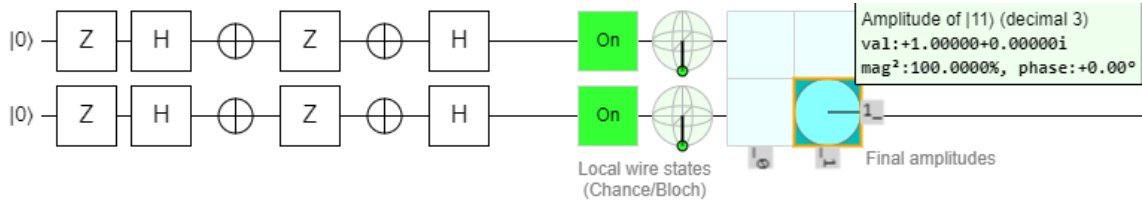
Schöning's Algorithm

Like random guessing, Schöning's algorithm chooses an input at random and checks if it works. If it does not work, algorithm picks an unsatisfied clause and toggles a bit in the string to satisfy that clause. On average it's beneficial to keep toggling bits in this manner a few times. If the initial guess was close enough, there's a fair chance we'll stumble upon the correct solution. If not, then after some number of steps, the computer starts again with a new completely random guess. Also, if you create a circuit that carries out the bit-toggling part of Schöning's algorithm, you can use this as the oracle and use Grover's algorithm to find the best "initial guess".

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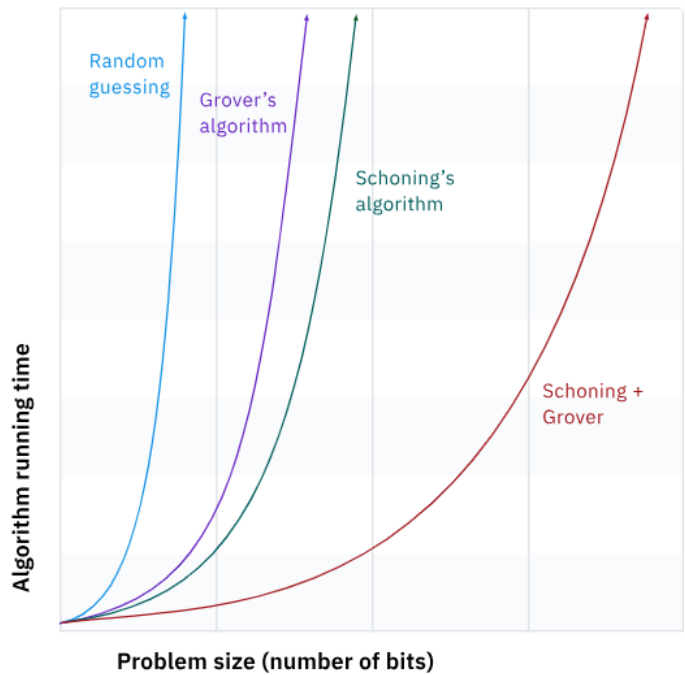
https://algassert.com/quirk#circuit={%22cols%22:[[%22Z%22,%22Z%22],[%22H%22,%22H%22],[%22X%22,%22X%22],[%22Z%22,%22Z%22],[%22X%22,%22X%22],[%22H%22,%22H%22]]}
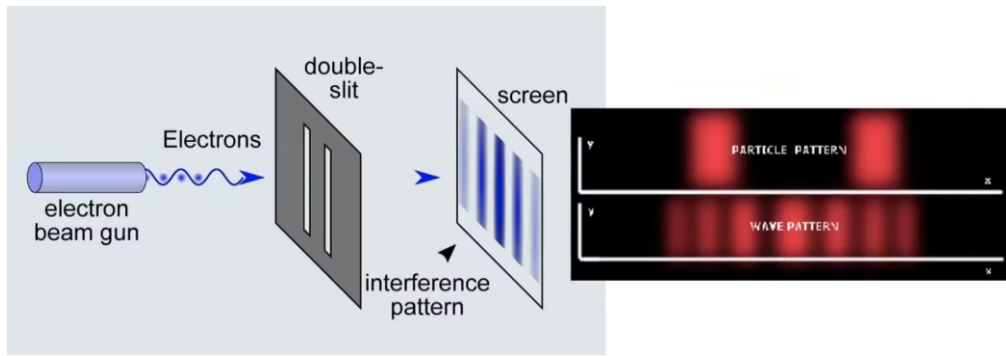
Qiskit Global Summer School – 2022[12]
Lesson Notes

History of Quantum Computing
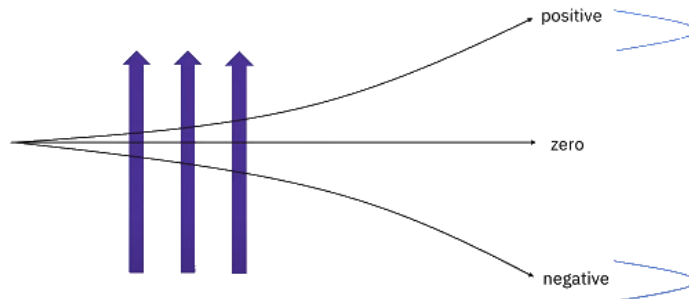
Magnetism of silver atoms – result: spin up or spin down.



anti aligned atoms

---
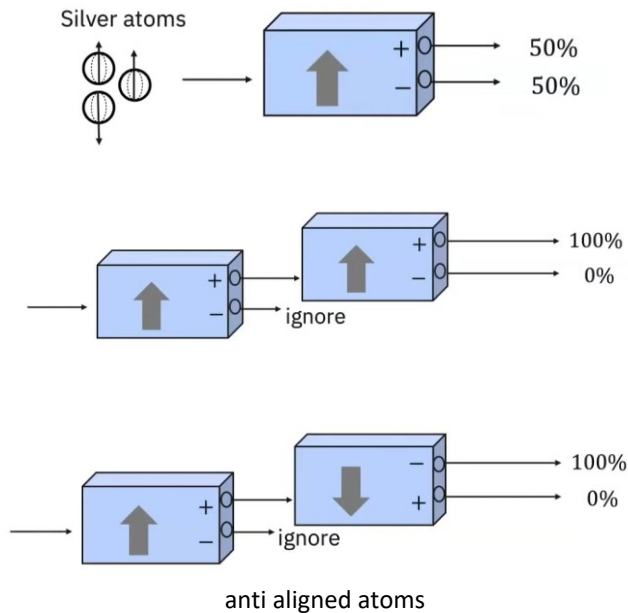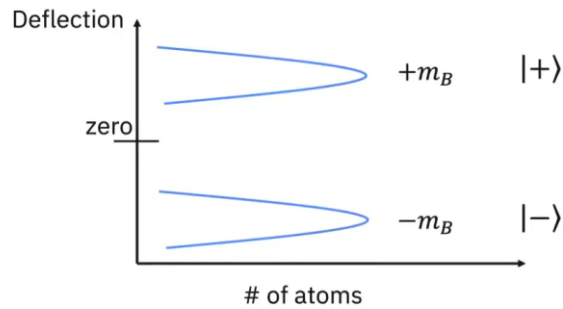
[12] Olivia Lanes (IBM), Maria Violaris (IBM), Jeffry Cohn (IBM Research Staff Member)

Measuring the double slit

(if you watch which slit the electrons go through, you'll see particle pattern, if you don't watch, then electrons will interfere with itself and go through both slits at the same time [*superposition principle of quantum mechanics*], then you'll see wave pattern)
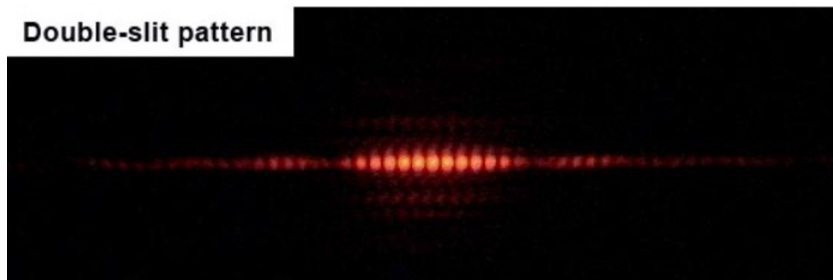
Superposition: Some combination of |+⟩ and |-⟩   This state can be written as: ψ= |+⟩ ∓ |-⟩

Popular superpositions and position of quit in bloch sphere for this veector:

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \quad (x = 1)$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \quad (x = -1)$$

$$|i\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle) \quad (y = 1)$$

$$|-i\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle) \quad (y = -1)$$

∴
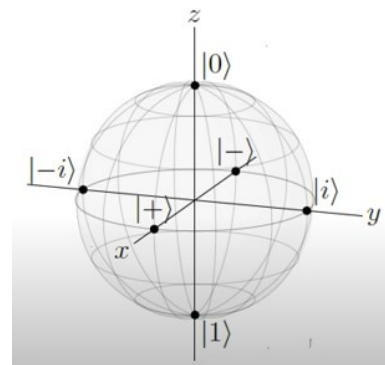
*"**Quantum mechanics forces us to the brink of implausibility … but not beyond**"*

- Single particles can exist in state of superposition, which combines multiple measurable states with certain probabilities associated with them.
- Single particles can interfere with themselves due to this nature.
- Upon measurement, only these definite states can be observed and the outcome is probabilistic, not determinate.
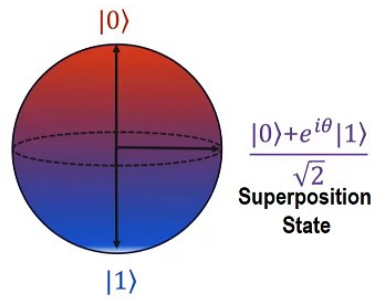
For quantum computer that is ready for quantum simulation:

- We should have quantum bits.
- They should be initialized into a well known states.
- These states will have relatively-long coherence times (*it will stay in the state we initialized in, and not just decay into the ground statebefore we can run quantum algorithms and quantum gates on it*).
- We need a universal set of quantum gates and a qubit-specific measurement capability (*we can individually measure every single qubit in the system without perturbing the other qubits as well*).

Superposition: $\Psi = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$: $|+\rangle$ and $|-\rangle$

Entanglement: To create entanglement, we need to apply multi-qubit gates, commonly **cx** (CNOT) or **cz**.

$$\Psi = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$

$|01\rangle$ is another way of writing a tensor product $|0\rangle \otimes |1\rangle$

Example:

$$Since\ |\psi\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle = \begin{pmatrix} c_{00} \\ c_{01} \\ c_{10} \\ c_{11} \end{pmatrix}$$

$$|+0\rangle = \left(\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\right)\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)$$

$|+0\rangle$ is a two qubit state vector that actually describes a pair of single qubit states: $|+\rangle$ and $|0\rangle$. We called $|+0\rangle$ product state[13] because the state of $|+0\rangle$ belongs to first (on the left qubit which is $+$). Because as we see in the state vector:

- $|00\rangle$: Both qubits are in the state $|0\rangle$.
- $|10\rangle$: The qubit states are $|1\rangle$ (*on the left*) and $|0\rangle$ (*on the right*).

$$|+0\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)$$

---

[13] In product state, each qubit can be independently described by a single qubit state with two amplitudes.

Complex Numbers Recap
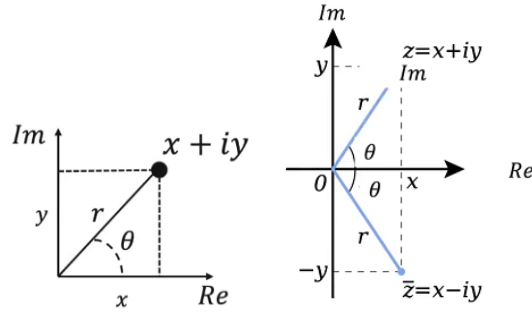
$$z = x + iy \qquad e^{i\theta} = \cos\theta + i\sin\theta \qquad |e^{i\theta}| = 1 \qquad (Euler's\ Equation)$$

$$z = re^{i\theta} = r\cos\theta + ir\sin\theta$$

$$x^2 + y^2 = r^2(cos^2\theta + sin^2\theta) = r^2$$

Complex Conjugates & Hermitian Conjugates

$$Complex\ conjugate: z^* = \bar{z} = x - iy = re^{-i\theta}$$

$$Norm\ squared: |z^2| = z^*z = r^2$$

$$|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow |\psi\rangle^\dagger = \langle\psi| = (a, b)$$

$$Hermitian\ conjugate: H = \begin{bmatrix} a & c \\ b & d \end{bmatrix} \Rightarrow H^\dagger = \begin{bmatrix} a^* & b^* \\ c^* & d^* \end{bmatrix}$$

* All quantum computations and quantum states live in a vector space we call the *Hilbert space*, where $H = C^{2^n}$

Orthogonality & Inner Products

$\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^* = a_1^* b_1 + a_2^* b_2 + \ldots + a_n^* b_n$: Inner Product

In the other words:

$$for\ |\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad and \quad |\phi\rangle = \begin{pmatrix} \gamma \\ \delta \end{pmatrix} \quad \Rightarrow \quad \langle\psi|\phi\rangle = \alpha^*\gamma + \beta^*\delta$$

- $\langle\psi|\psi\rangle = 1$
- $\langle\psi|\Phi\rangle = \langle\Phi|\psi\rangle^*$
- If $\langle\psi|\Phi\rangle = 0 \Rightarrow \psi$ and Φ are orthogonal each other. (completely opposite physical reality like heads & tails)

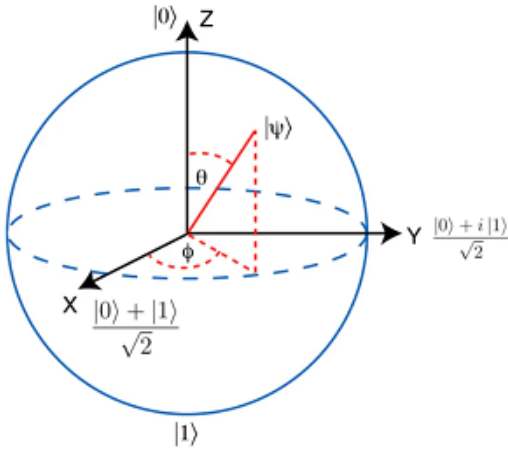*Example*:

$$|a\rangle = \frac{3 + i\sqrt{3}}{4}|0\rangle + \frac{1}{2}|1\rangle \qquad |b\rangle = \frac{1}{4}|0\rangle + \frac{\sqrt{15}}{2}|1\rangle \quad => calculate\ \langle a|b\rangle$$

Answer:

$$\langle a|b\rangle = \begin{pmatrix} \dfrac{3 - i\sqrt{3}}{4} & \dfrac{1}{2} \end{pmatrix} \begin{pmatrix} 1/4 \\ \sqrt{15}/2 \end{pmatrix} = \frac{3 - i\sqrt{3}}{16} + \frac{\sqrt{15}}{8} = \frac{3 + 2\sqrt{15} - i\sqrt{3}}{16}$$

Orthogonal & Orthonormal

- The two orthogonal z-basis states of a qubit are $|0\rangle$ and $|1\rangle$
- The two orthogonal x-basis states of a qubit are $|+\rangle$ and $|-\rangle$
- The two orthogonal y-basis states of a qubit are $|i\rangle$ and $|-i\rangle$

Example: The qubit state $|\psi\rangle = \frac{\sqrt{3}}{4}|0\rangle + \frac{1}{2}|1\rangle$ can be expressed in terms of $|+\rangle$ and $|-\rangle$ as follows:

$$|0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) \quad and \quad |1\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)$$

$$|\psi\rangle = \frac{\sqrt{3}}{4}|0\rangle + \frac{1}{2}|1\rangle = \frac{\sqrt{3}}{4}\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) + \frac{1}{2}\frac{1}{\sqrt{2}}(|+\rangle - |-\rangle) = \frac{1}{\sqrt{2}}\left(\frac{\sqrt{3}+2}{4}|+\rangle + \frac{\sqrt{3}-2}{4}|-\rangle\right)$$

- For two base qubit state Φ_1 and Φ_2: if $\langle\Phi_1|\Phi_1\rangle = 1$ and $\langle\Phi_1|\Phi_2\rangle = 0$, then they are said to be "orthogonal" and "orthonormal".
- Any qubit state can be expressed as : $|\psi\rangle = \langle 0|\psi\rangle |0\rangle + \langle 1|\psi\rangle |1\rangle = \langle +|\psi\rangle |+\rangle + \langle -|\psi\rangle |-\rangle$

Example: The qubit state $|\psi\rangle = \frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle$, find the $|+\rangle$ and $|-\rangle$ base representations and calculate α' (*amplitude of* $|+\rangle$)

Answer: For $|\psi\rangle = \alpha'|+\rangle + \beta'|-\rangle$, $\alpha' = \langle +|\psi\rangle$.

$$\alpha' = \langle +|\psi\rangle = \frac{1}{\sqrt{2}}(\langle 0| + \langle 1|)\left(\frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle\right) = \frac{\sqrt{3}}{2\sqrt{2}} + \frac{1}{2\sqrt{2}} = \frac{\sqrt{6}+\sqrt{2}}{4}$$

Example:

$$|a\rangle = cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}sin\left(\frac{\theta}{2}\right)|1\rangle$$

Find $|b\rangle$ such that $|a\rangle$ and $|b\rangle$ are orthonormal.

Answer:
For this antipod requests,
$\theta \rightarrow \pi - \theta$
$\Phi \rightarrow \pi + \Phi$

So:

$$|b\rangle = cos\left(\frac{\pi - \theta}{2}\right)|0\rangle + e^{i(\pi+\phi)}sin\left(\frac{\pi - \theta}{2}\right)|1\rangle$$

Example: Find $|b\rangle$ such that it is orthonormal with the following qubit $|a\rangle$:

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

Answer:

$$Cos\left(\frac{\pi}{6}\right) = \frac{\sqrt{3}}{2} \Rightarrow sin\left(\frac{\pi}{6}\right) = \frac{1}{2} \text{ and if we use } \phi = 0 \Rightarrow use \; \theta = \frac{\pi}{3} \; \phi = 0$$

Then, after we apply antipod requests ($\theta' \to \pi - \theta \; and \; \Phi' \to \pi + \Phi$) we get θ'=2π/3, Φ'= π
So:

$$|b\rangle = cos\left(\frac{\theta'}{2}\right)|0\rangle + e^{i\phi'}sin\left(\frac{\theta'}{2}\right)|1\rangle = \frac{1}{2}|0\rangle - \frac{\sqrt{3}}{2}|1\rangle$$

Outer Product

$$for \; |\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad and \quad |\phi\rangle = \begin{pmatrix} \gamma \\ \delta \end{pmatrix} \quad \Rightarrow \quad |\psi\rangle\langle\phi| = \begin{pmatrix} \alpha\gamma^* & \alpha\delta^* \\ \beta\gamma^* & \beta\delta^* \end{pmatrix}$$

$$(|\psi\rangle\langle\phi|)^\dagger = |\phi\rangle\langle\psi|$$

$$|0\rangle\langle0| + |1\rangle\langle1| = |00\rangle\langle00| + |01\rangle\langle01| + |10\rangle\langle10| + |11\rangle\langle11| = \mathbb{1} \quad \textit{completeness}$$

Tensor Product

$$|a\rangle \otimes |b\rangle = |ab\rangle$$

$$|\psi\rangle = c_0|00\rangle + c_1|01\rangle + c_2|10\rangle + c_3|11\rangle = \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{pmatrix} \quad and \quad \langle\psi| = \begin{pmatrix} c_0^* & c_1^* & c_2^* & c_3^* \end{pmatrix}$$

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_1\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \\ a_2\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a_1b_1 \\ a_1b_2 \\ a_2b_1 \\ a_2b_2 \end{pmatrix}$$

Example:

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

Example:
Rewrite the following two qubit states as a tensor product:

$$\frac{1}{\sqrt{6}}|00\rangle + \frac{1}{\sqrt{6}}|01\rangle + \frac{1}{3}|10\rangle + \frac{1}{3}|11\rangle$$

Answer:
The first vector of state comes from the first item of first states of tensor product and first item of second states, and so on.

$$\frac{1}{\sqrt{6}}|00\rangle \Rightarrow \frac{1}{\sqrt{3}}|0\rangle . \frac{1}{\sqrt{2}}|0\rangle$$

So, the result is:

$$\left(\frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle\right) \otimes \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right)$$

Example: Try to separate this state into a tensor product:

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

Answer:

It is impossible to separate these two states! Because this is an example of entangled qubits which by definition cannot be described by their individual parts alone (cannot be seperated). Entangled states can only be described by the sum component of all of the different states which make up the entangled state. So, you can not separate and measure each individual qubit any longer.

Quantum Calculation Basics

Amplitudes

Amplitudes are probabilities with **magnitude** and **phase** (direction). So, the result of phase is that, when we add two amplitudes they can cancel each other. This behaviour is called "*interference*" and this is what causes the unexplained behaviour. Amplitude is a complex number.
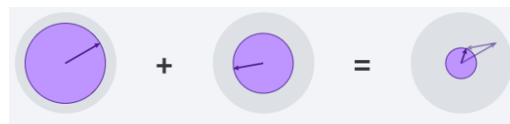
Magnitude: + 0,8 + 0,6 = 0,31
Phase: 30 + 190 = 70

To find the probability of measuring an outcome, we square the magnitude of that outcome's amplitude.
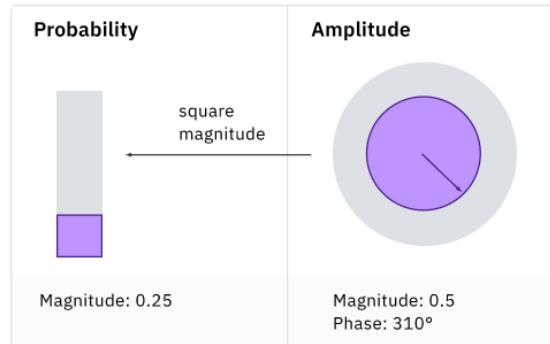
Quantum states are normalized, and probability is calculated by the norm squared of the amplitudes:

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

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

Example:

What is the probability of measuring $|1\rangle$ from the quantum state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{\frac{i\pi}{6}}|1\rangle\right)$$

Answer: We should take complex conjugate times the original coefficient of the number in front of the one state and multiply those together:

$$\left|\frac{e^{\frac{i\pi}{6}}}{\sqrt{2}}\right|^2 = \frac{e^{\frac{i\pi}{6}}}{\sqrt{2}} \cdot \frac{e^{-\frac{i\pi}{6}}}{\sqrt{2}} = \frac{e^0}{2} = \frac{1}{2}$$

Hint: Notice that probability of measuring |0⟩ is ½ so the probability of measuring |1⟩ should be ½ because total of them should be 1 due to normalization rules. So, $\frac{e^{\frac{i\pi}{6}}}{\sqrt{2}}$ is just a phase that does not actually end up mattering when you go to make a measurement.

Operators

Operators changes the state of qubits (*rotate, move, spin ...*). Operator is symbolized as "A" with a little triangle cap (*that means it is a quantum operator*), as shown below:

$$\hat{A} = \hat{A}^{\dagger} \quad (Hermitian\ operator)$$

Eigenvector Equation: $A|\psi\rangle = a|\psi\rangle$ *where* a: *Eigenvalue* $|\psi\rangle$: *Eigenvector* (*if* $|\psi\rangle$ *is an eigenvector of A*)

If $|\psi\rangle$ is not an eigenvector of A, then it has no specific associated eigenvalue of A, and the observable does not have a single definite value in that case. Instead, the measurements of the observable A will each yield an eigenvalue with a certain probability that's related to the decomposition of $|\psi\rangle$ relative to the orthonormal eigen basis of A.

Eigenvalue: Measurable and real value.

Summary:
- Quantum observables (*anything you want to measure in quantum mechanics*) are Hermitian operators (*A Hermitian operator is equal to its own complex conjugate*).
- They all have real eigenvalues.
- Eigenvectors with different eigen values are orthogonal (*so they don't overlap in the vector space*).
- Eigenvectors of an operator form a complete orthonormal basis (*you can write any state that you wish as a linear combination of the eigenvectors associated with a specific operator*).

Gates

Gates are another way of changing quantum state. We can enact on the quantum computer laboratory. Big series of gates approximately be equal to a theoretical operator. A gate is a linear map of the quantum system. Linear means that, it can be distributed across the state even as a superposition, but it still must be equal to that total probability of one.

Quantum gates are linear maps:
$$U(\alpha|0\rangle + \beta|1\rangle) = \alpha U|0\rangle + \beta U|1\rangle$$
(Total probability must remain equal to 1.)

Gates are represented by matrices which can be written as a combination of the <u>outer</u> products:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = |0\rangle\langle 1| + |1\rangle\langle 0| \Rightarrow \text{bit-flip gate}$$

$$X|0\rangle = |1\rangle \qquad X|1\rangle = |0\rangle$$

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

$$H|0\rangle=|+\rangle \qquad H|1\rangle=|-\rangle \qquad H|+\rangle=|0\rangle \qquad H|-\rangle=|1\rangle$$

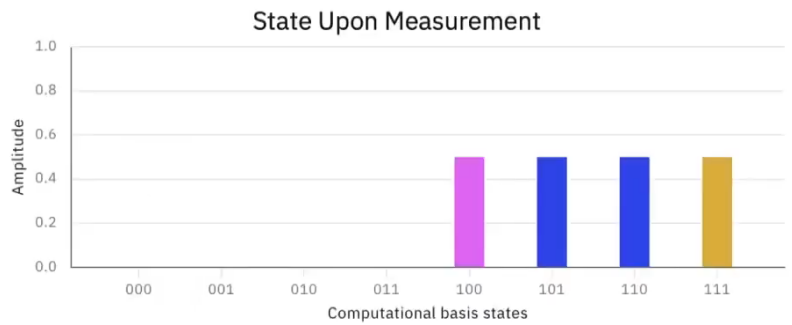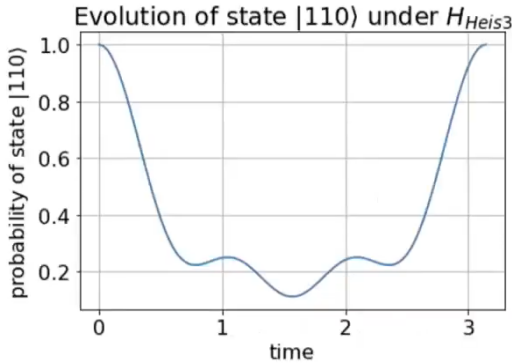** Gates must be unitary:
$$U^{\dagger}U=U\ U^{\dagger} = I$$
$$I|a\rangle = 1|a\rangle \qquad eigenvalue\ can\ only\ be\ 1$$

$$I_1 = [1] \quad I_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \ldots \quad I_n = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

$X*X = XX* = I^2 = I$ (*because* X *is a quantum gate, it must be unitary*)

Time Evolution

What happens if we wait to measure, and let $|\psi\rangle$ evolve naturally? (*examine 3 qubit state: 110 state*)

3 states of quantum simulation:

- Quantum state preparation: *let say, $|\psi\rangle = |110\rangle$*
- Time evolution (*let it evolve in time undisturbed*)
- Measurement (*collapses the state into the classical values zero and one, we will then try to make sense of and try to extract information from*)
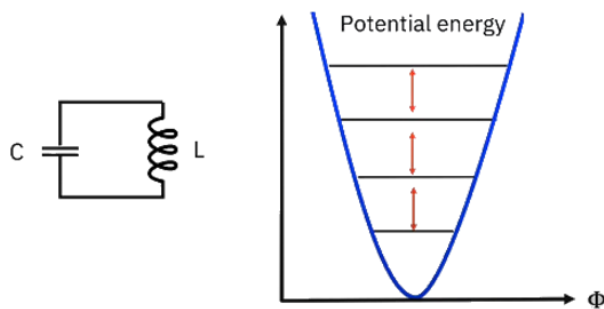
### Real World Hardware
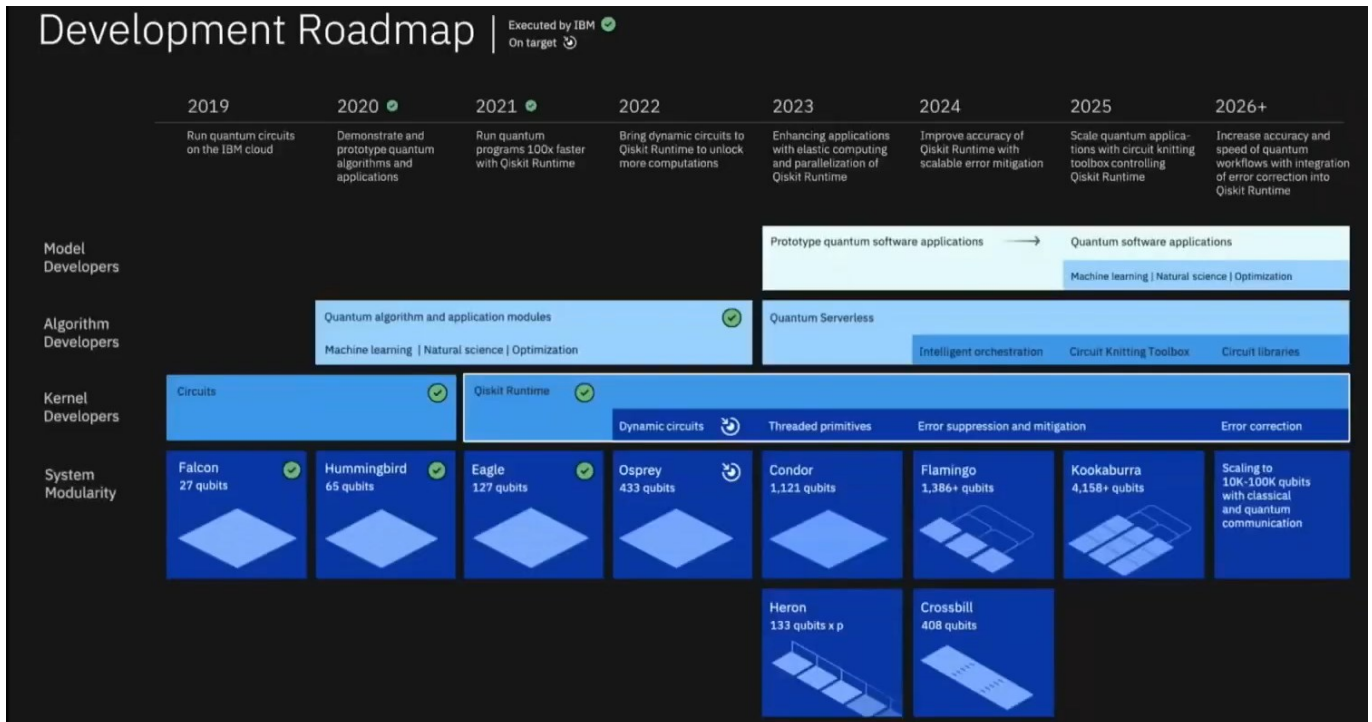
IBM Quantum Computer Development Roadmap
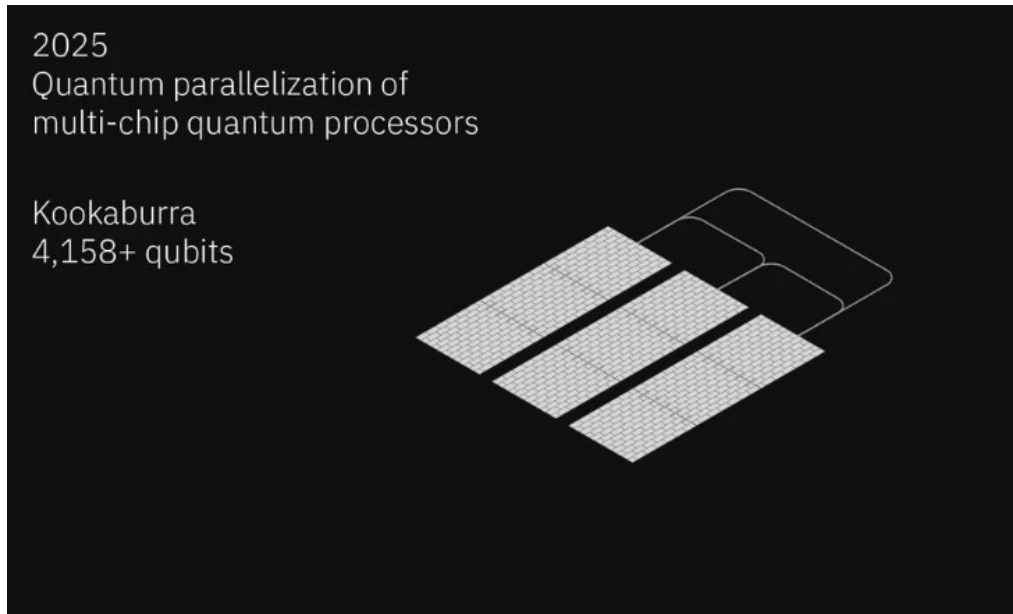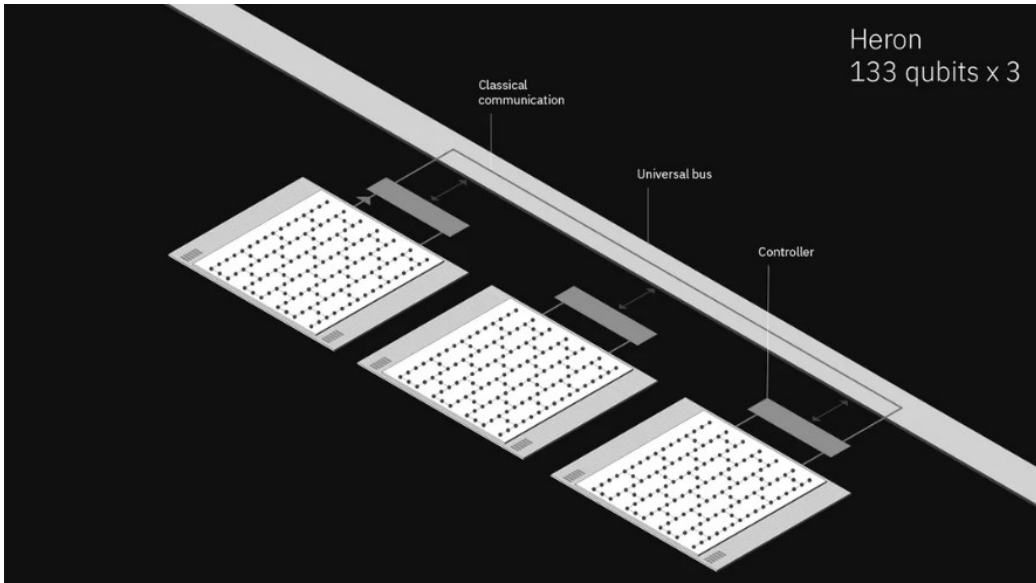
IBM Online Quantum Computer Access Address: https://www.ibm.com/quantum (*Create IBM ID and access to qubits are free*)
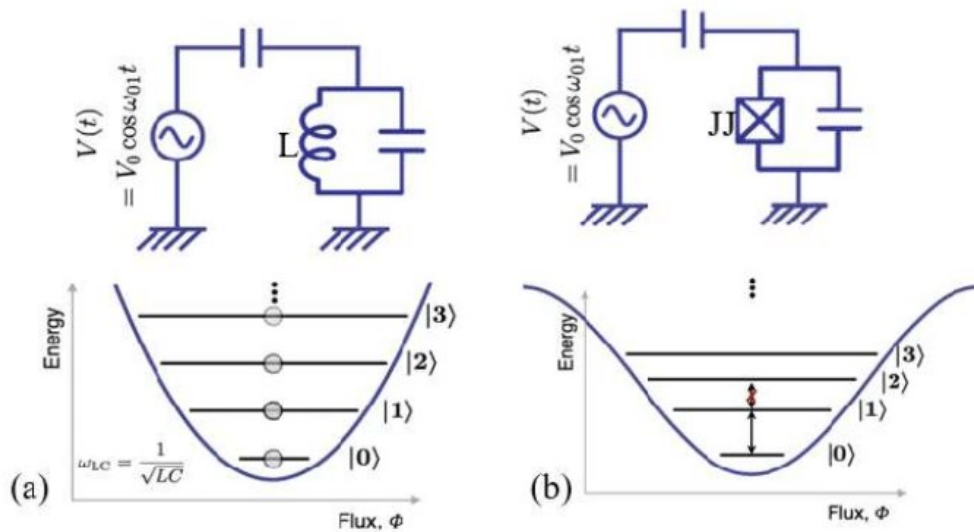
The Josephson Junction

Normal reaction (*potential energy*) of a circuit (*capacitor & inductor, harmonic oscillator[14]*) that represents equally spaced energy levels (*There is no way to isolate any two energy levels, they are evenly spaced*)

$$I = I_0 \sin(\phi)$$
$$E = E_J \cos(\phi)$$
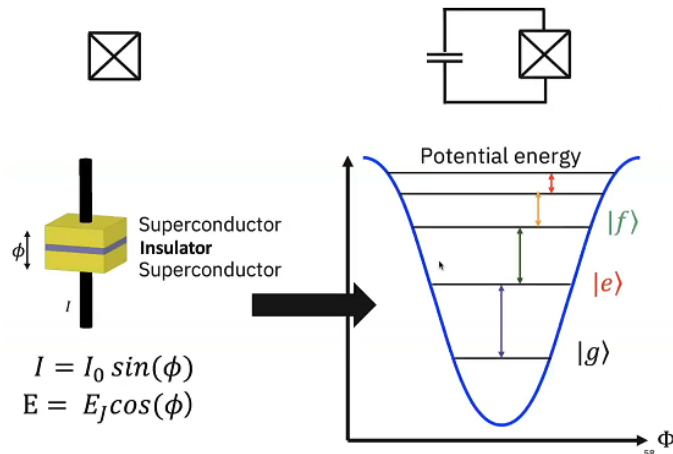
Josephson junction that stretches potential energy well in such a way that the rungs on the ladder no longer equidistant, so we can take the lowest two energy level (*ground state & excited state*), and isolate those with a specific pulse at that transition energy and call that our "qubit"

(a) LC oscillator circuit behaving a harmonic oscillator with equally spaced energy levels. (b) Equivalent LC oscillator with inductor replaced by Josephson junction behaving an anharmonic oscillator. [15]

How do we measure a qubit ?

- We never interact with it directly.
- We couple that qubit to a 2D or 3D resonator.
- Qubit will have an effect on that resonator.
- We can see that effect by interacting with that resonator. (*The qubit and the cavity are very far away from each other in terms of frequency, we'll able to see a shift in the resonator's frequency, depending on what state the qubit is in. For example, if the qubit is in the ground state or the excited state, this will affect the shift in the frequency of the resonator. So, by measuring the in-phase or the quadrature phase component of a microwave signal tone, it is just the same as*

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[14] A **resonator** is a device which exhibits resonance or resonant behavior (*it naturally oscillates with greater amplitude at some frequencies, called resonant frequencies*). An **oscillator** is an electronic device which produces periodic oscillating electronic signal. (*they both have the same working procedure & generate frequency oscillation as output*)

[15]https://www.researchgate.net/publication/358153899_Superconducting_Radio_Frequency_Resonators_for_Quantum_Computing_A_Short_Review
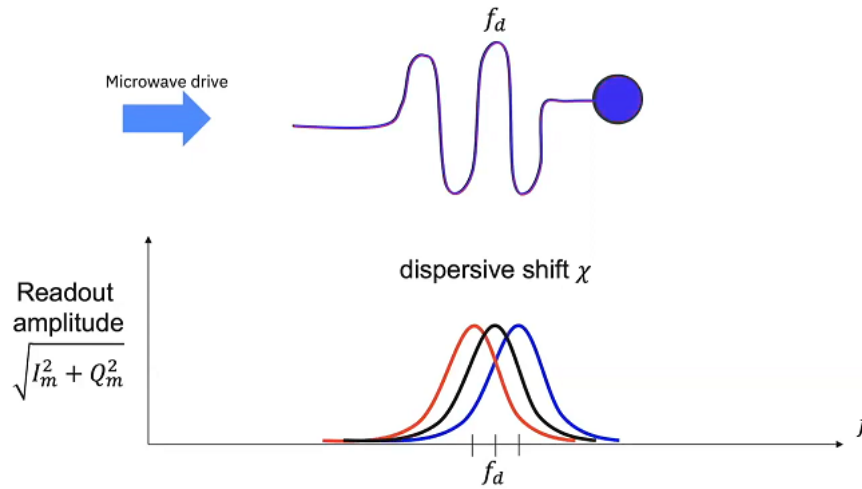
Measurement in room temperature:
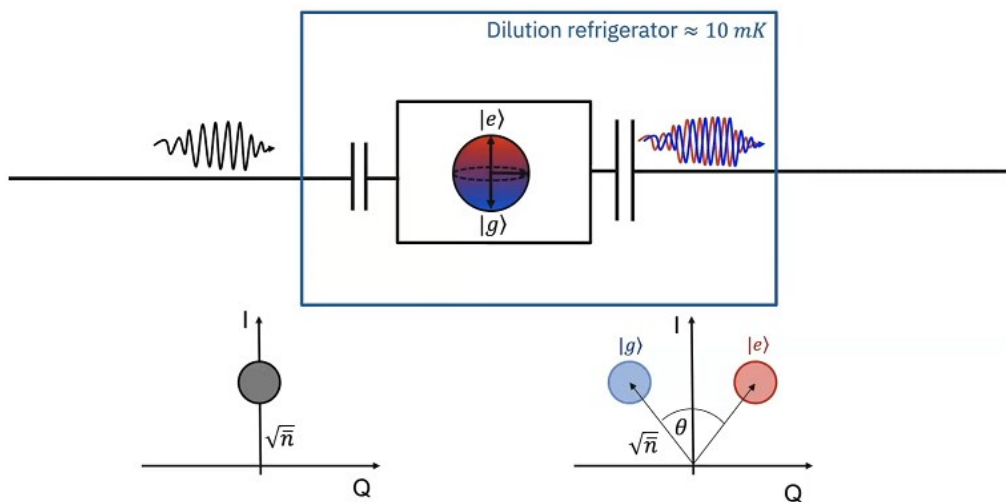
- Send a pulse of microwave light from a generator down into coaxial lines of the fridge.
- Pulse will interact with the qubit. When it leaves the resonator, it will be shifted either down or up, depending on if that qubit state is in "e" or "g".
- If you plot this microwave tone in the IQ space or the imaginary real space as a Gaussian blob, you would be able to see that blob shift left or right depending on if that qubit state is "e" or "g".[16]

Building Blocks of Quantum: From Linear Algebra to Quantum Circuits

Quantum Gates

X gate is 180-degree rotation on X axis in Bloch sphere.

$$\hat{X}|+\rangle = \frac{1}{\sqrt{2}}X(|1\rangle + |0\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$$

$\therefore |+\rangle$ is eigenvector of X with eigenvalue 1.

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[16] Animation of this progress: https://youtu.be/zG1ZxZhMjpQ?list=PLOFEBzvs-Vvo5o97bYt8o1l8Ra1poMASQ&t=2174

$$\hat{X}|-\rangle = \frac{1}{\sqrt{2}}X(|0\rangle - |1\rangle) = -\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = -|-\rangle$$

(where − is the global phase of |-). It is a factor that multiplies the entire state. It doesn't affect measurement outcomes, because when we take the modular squared of the minus state, it's not going to affect the measurement. But if we apply X to a combination of plus and minus, we obtain measurable outcome)

∴ |-⟩ is eigenvector of X with eigenvalue -1.

Example: For combination of plus and minus, global phase affects measurement outcomes as follows (*which is called relative phase*):

$$\hat{X}|0\rangle = \frac{1}{\sqrt{2}}X(|+\rangle + |-\rangle) = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle) = |1\rangle$$

Y gate is 180° rotation on Y axis in Bloch sphere. **Z gate** is same for Z axis.

Related matrix is: $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ for Y gate and $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ for Z gate.

General value for eigenvectors for unitary matrices is: $a = e^{i\psi}$:
$$U|\psi\rangle = a|\psi\rangle \quad \Rightarrow \quad (U|\psi\rangle)^{\dagger} = \langle\psi|U^{\dagger} = \langle\psi|a^{*}$$

$$\langle\psi|U^{\dagger}U|\psi\rangle = aa^{*}\langle\psi|\psi\rangle = |a^{2}| = 1$$

For generalized state of a qubit |ψ⟩ = α|0⟩ + β|1⟩:
  Z |ψ⟩ = α|0⟩ - β|1⟩
  X |ψ⟩ = α|1⟩ + β|0⟩
  XZ |ψ⟩ = α|1⟩ - β|0⟩

Hadamard gate: We can use this gate to create superposition from single qubit. (*does rotation between X and Z axis*)

H|0⟩=|+⟩   H|1⟩=|-⟩   H|+⟩=|0⟩   H|-⟩=|1⟩
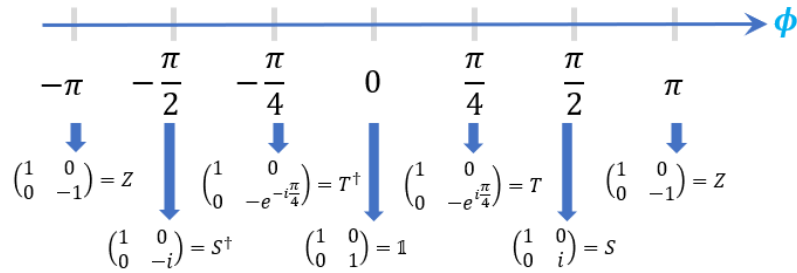

Hadamard Gate
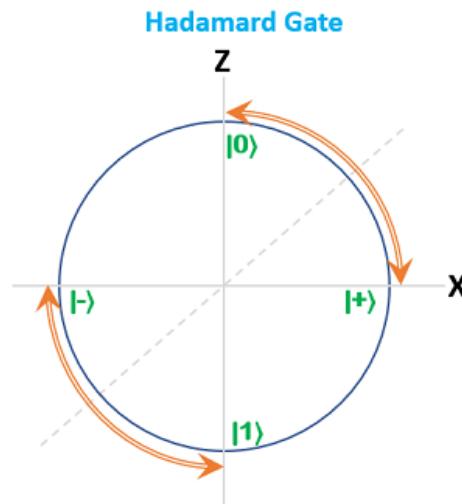
$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \qquad H = H^{-1} \qquad HH|\psi\rangle = \mathbb{1}|\psi\rangle = |\psi\rangle$$

Phase Gate:

$$P = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$

Important Single Qubit Gates

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = Z \qquad \begin{pmatrix} 1 & 0 \\ 0 & -e^{-i\frac{\pi}{4}} \end{pmatrix} = T^\dagger \qquad \begin{pmatrix} 1 & 0 \\ 0 & -e^{i\frac{\pi}{4}} \end{pmatrix} = T \qquad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = Z$$

$$\begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} = S^\dagger \qquad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1} \qquad \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = S$$

Bra-ket for Gates

Outer product: $|a\rangle\langle b| \equiv |a \text{ X } b|$

$$|0X0| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}(1 \quad 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad |0X1| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad |1X0| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad |1X1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

So, we can express any matrix in terms of our bra-ket notation.

$$\alpha|0X0| + \beta|0X1| + \gamma|1X0| + \delta|1X1| = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

$$\alpha|+X+| + \beta|+X-| + \gamma|-X+| + \delta|-X-| = \begin{pmatrix} \alpha^2 & \beta^2 \\ \gamma^2 & \delta^2 \end{pmatrix}$$

(we are doing with the assumption that the basis of the matrix is plus minus basis)

Example:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |0X1| + |1X0| \qquad\qquad X|0\rangle = |0X1||0\rangle + |1X0|\,|0\rangle = |1\rangle$$

Inner product: $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^* = a_1{}^*b_1 + a_2{}^*b_2 + \ldots + a_n{}^*b_n$

Example: the inner product of $|x_1\rangle$ and $|x_2\rangle$ is:

$$\langle x_1|x_2\rangle = \begin{pmatrix} \alpha_0^\dagger & \beta_0^\dagger \end{pmatrix}\begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} = \alpha_0^\dagger\beta_0 + \alpha_1^\dagger\beta_1$$

** The inner product of a qubit state vector with itself is always 1:

$$\langle x_1|x_1\rangle = \begin{pmatrix} \alpha_0^\dagger & \beta_0^\dagger \end{pmatrix}\begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} = \alpha_0^\dagger\alpha_0 + \alpha_1^\dagger\alpha_1 = |\alpha_0|^2 + |\alpha_1|^2 = 1$$

Example:

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

Multiple Qubits

Tensor product:

$$|a\rangle \otimes |b\rangle = |ab\rangle$$

$$if\ |a\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}\ and\ |b\rangle = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix},\ then\ |a\rangle \otimes |b\rangle = \begin{pmatrix} a_1 \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \\ a_2 \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ a_1 b_2 \\ a_2 b_1 \\ a_2 b_2 \end{pmatrix} : states\ of\ both\ qubits$$

$$(A \otimes B)(\ |a\rangle \otimes |b\rangle) = A|a\rangle \otimes B|b\rangle$$

Example:
(X ⊗ Z) (|01⟩) = X |0⟩ Z |1⟩ = |1⟩ (-1) = - |1⟩

Example:
(X ⊗ Z) (|0+⟩) = X |0⟩ Z |+⟩ = |1⟩ |-⟩ = |1-⟩

Example: For qubits $|x\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$ and $|y\rangle = \beta_0 |0\rangle + \beta_1 |1\rangle$:
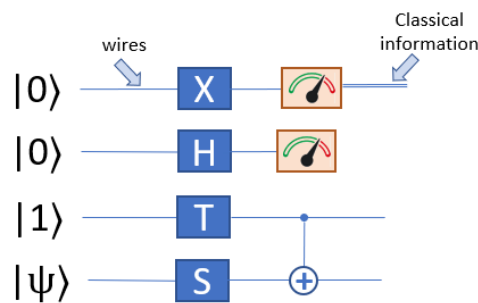
|x⟩⊗|y⟩   = (α₀ |0⟩ + α₁ |1⟩) ⊗ (β₀ |0⟩ + β₁ |1⟩)
            = α₀ β₀ |0⟩⊗|0⟩ + α₀ β₁ |0⟩⊗|1⟩ + α₁ β₀ |1⟩⊗|0⟩ + α₁ β₁ |1⟩⊗|1⟩
            = α₀ β₀ |00⟩ + α₀ β₁ |01⟩ + α₁ β₀ |10⟩ + α₁ β₁ |11⟩

Definition:

$$for\quad |a\rangle = \sum_j \alpha_j |a_j\rangle \quad and \quad |b\rangle = \sum_k \beta_k |b_k\rangle \quad we\ have:$$

$$|a\rangle \otimes |b\rangle = \sum_j \sum_k \alpha_j \beta_k \left(|a_j\rangle \otimes |b_k\rangle\right) = \sum_j \sum_k \alpha_j \beta_k \left(|a_j b_k\rangle\right)$$

Quantum Circuits

2-Qubit Gates
C-NOT (CX) gate (controlled-NOT gate) : Creates entanglements between qubits.

CX |00⟩ = |00⟩
CX |01⟩ = |01⟩
CX |10⟩ = |11⟩
CX |11⟩ = |10⟩

> CX gate is controlled on the first qubit and targets on the second qubit. If the first qubit is zero, then it does nothing to the second. If first qubit is 1, then it applies the X gate to the second and flips it to whichever state it adds up it after applying the X gate.

$$|00\rangle \overset{H}{\rightarrow} (|0\rangle + |1\rangle)|0\rangle \equiv |00\rangle + |10\rangle \xrightarrow{C-NOT} |00\rangle + |11\rangle \equiv \textbf{\textit{Maximally entangled}} \equiv |++\rangle + |--\rangle$$

Because if we measure the first qubit and get "zero" value, we know the second bit is "zero". If we measure the first qubit and get "one" value, we know the second bit is "one". The corresponding circuit is as follows:
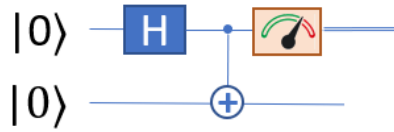
In order to measure in plus minus basis *(instead of zero − one basis)*:
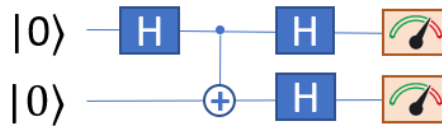
Bell states

These are important entangled states. By using previous circuit with different input pairs such as $|0\rangle$ & $|0\rangle$, $|0\rangle$ & $|1\rangle$, $|1\rangle$ & $|0\rangle$ and $|1\rangle$ & $|1\rangle$, we obtain the following outputs that are called as bell states:

$$|\emptyset^+\rangle = |00\rangle + |11\rangle$$

$$|\emptyset^-\rangle = |01\rangle + |10\rangle$$

$$|\psi^+\rangle = |00\rangle - |11\rangle$$

$$|\psi^-\rangle = |01\rangle - |10\rangle$$

These bell states form an orthonormal basis:
$$\langle\phi_i|\phi_j\rangle = 0 \quad \textit{They are all orthogonal}$$

Each bell states are maximally entangled.

Pure and Mixed States

For entangled qubit pair, if we want to describe the state of one of the qubits, we need to introduce ***density matrix:***

Let say: $|\psi\rangle = |00\rangle + |11\rangle$

$$\varrho = |\psi X\psi| = (|00\rangle + |11\rangle)(\langle00| + \langle11|) = |00\rangle\langle00| + |00\rangle\langle11| + |11\rangle\langle00| + |11\rangle\langle11| = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

This means, we can represent our overall state of the two qubits this matrix called "*density matrix*" instead of the ket notation, which we called the state vector.

Partial trace: If we call overall state ϱ_{12}, then to get ϱ_1, we do the partial trace over the second qubit of ϱ_{12}:

$$\varrho_1 = tr_2\varrho_{12}$$

So the way that a trace works is that for a matrix, the trace is the sum of the diagonal elements. And in the bra-ket notation, we do the bra of each basis state and ket of each basis state on either side of our state to extract the diagonal elements. And then, we add them together to get the trace of a matrix.

$$\sum_j \langle \psi_j | \varrho_{12} | \psi_j \rangle$$

If we do partial trace, this means that we are only doing this for one of the qubits:

$$|00\rangle\langle00| + |00\rangle\langle11| + |11\rangle\langle00| + |11\rangle\langle11| = |0\rangle\langle0| \otimes |0\rangle\langle0| + |0\rangle\langle1| \otimes |0\rangle\langle1| + |1\rangle\langle0| \otimes |1\rangle\langle0| + |1\rangle\langle1| \otimes |1\rangle\langle1|$$

So, the density matrix for first qubit is:

$$\varrho_1 = tr_2 \varrho_{12} = |0X0| + |1X1| \ after \ normalizaton \ = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

For the second qubit:

$$\varrho_2 = tr_1 \varrho_{12} = |0X0| + |1X1| \ after \ normalizaton \ = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Result: If we look at the each individual qubit on its own, it's as though it had half probability of being prepared in the "zero state" and half probability in the "one state" but it is a statistical mixture of "zero" and "one" (*instead of being a superposition of zero and one*) because we do not know which is which. So, it's different to having the state being zero plus one ($|0\rangle + |1\rangle$).

Because we see statistical mixture of zero and one, ϱ_1 and ϱ_2 are ***mixed states***.
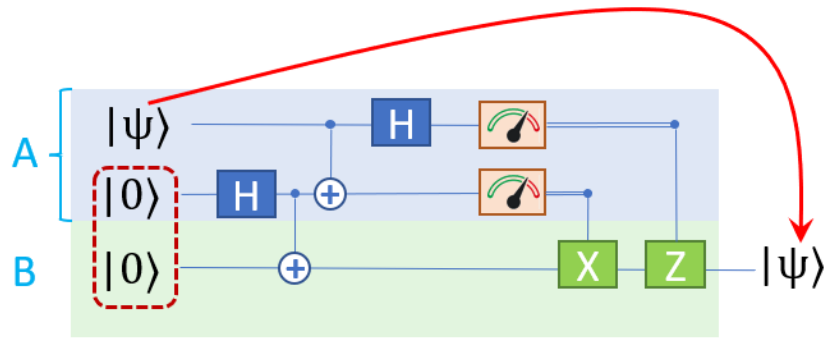- They do not have a definite state that we can write out using a state vector.
- To write it using a state vector, we need to look up both systems together and then we have this overall entangled state ($|\psi\rangle = |00\rangle + |11\rangle$). So the individual states we have here (ϱ_1 *and* ϱ_2), they don't tell us whether these qubits are entangled or not, they just mean that will get outcomes as though we have a statistical mixture of the state zero and state one.
- The significance of mixed states on the Bloch sphere is that pure states are all **on the surface** of the sphere whereas mixed states are inside. Every point **inside** the Bloch sphere can be represented by a mixed state.

Quantum Teleportation

IT allows us to get a quantum state and then by doing some interactions between that state and another quantum state, which we know is entangled with a far away quantum state that someone else has, we can make out two qubits interact, send that person some classical information. They can use that to reconstruct our quantum state, which was unknown on wherever they are in the universe. It is **transport of the state** of some unknown quantum system from one place to another, by only sending classical information from one place to another.

Example: A and B are in different cities, and they have only a telephone line for communication. A and B has one entangled qubit and A want to transport the unknown state of qubit ψ to B:

Answer: The quantum circuit is as follows. A only informs B for the measured state of the first qubit and B then applies X and/or Z gate to obtain the state of ψ.

For $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$:

$|\psi\rangle|00\rangle \Rightarrow (\alpha|0\rangle + \beta|1\rangle)(|00\rangle + |11\rangle) = \alpha|000\rangle + \alpha|011\rangle + \beta|100\rangle + \beta|111\rangle$

After applying CNOT gate $\Rightarrow \alpha|000\rangle + \alpha|011\rangle + \beta|110\rangle + \beta|101\rangle$
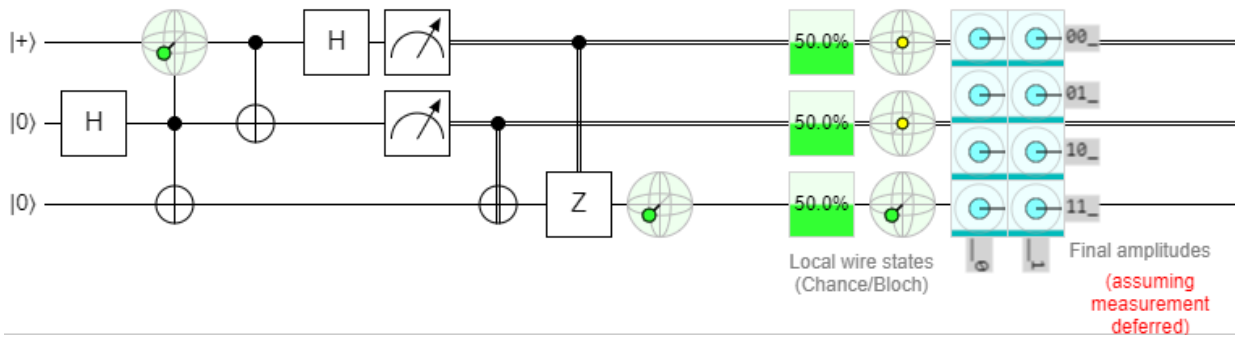
After applying H gate $\Rightarrow \alpha|000\rangle + \alpha|100\rangle + \alpha|011\rangle + \alpha|111\rangle + \beta|010\rangle - \beta|110\rangle + \beta|001\rangle - \beta|101\rangle$

$\quad = |00\rangle\,(\alpha|0\rangle + \beta|1\rangle) + |10\rangle\,(\alpha|0\rangle - \beta|1\rangle) + |01\rangle\,(\alpha|1\rangle + \beta|0\rangle) + |11\rangle\,(\alpha|1\rangle - \beta|0\rangle)$

$\quad = |00\rangle\,|\psi\rangle + |10\rangle\,Z\,|\psi\rangle + |01\rangle\,X\,|\psi\rangle + |11\rangle\,X\,Z\,|\psi\rangle$

Now:
- if A informs that measured state is $|00\rangle$, then B directly gets ψ.
- if A informs that measured state is $|10\rangle$, then B applies Z gate to get ψ.
- if A informs that measured state is $|01\rangle$, then B applies X gate to get ψ.
- if A informs that measured state is $|11\rangle$, then B applies XZ gates to get ψ.

Related quantum circuit diagram[17]

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[17] Use this link to open related quantum circuit design and simulation:
https://algassert.com/quirk#circuit={%22cols%22:[[1,%22H%22],[%22Bloch%22,%22%E2%80%A2%22,%22X%22],[%22%E2%80%A2%22,%22X%22],[%22H%22],[%22Measure%22,%22Measure%22],[1,%22%E2%80%A2%22,%22X%22],[%22%E2%80%A2%22,1,%22Z%22],[1,1,%22Bloch%22]],%22init%22:[%22+%22]}

Hamiltonian Time Evolution

The Hamiltonian of a system is an operator corresponding to the total energy of that system, including both kinetic energy and potential energy.[18]

The Hamiltonian of a system represents the total energy of the system; that is, the sum of the kinetic and potential energies of all particles associated with the system. The Hamiltonian takes different forms and can be simplified in some cases by taking into account the concrete characteristics of the system under analysis, such as single or several particles in the system, interaction between particles, kind of potential energy, time varying potential or time independent one.

Schrödinger Equation

Schrödinger Hamiltonian:

By analogy with classical mechanics, the Hamiltonian is commonly expressed as the sum of operators corresponding to the kinetic and potential energies of a system in the form:

Single particle:

$$\hat{H} = \hat{T} + \hat{V} \quad where\ \hat{V} = V(r,t) : potential\ energy\ operator \quad \hat{T} = \frac{\hat{p}^2}{2m} : kinetic\ energy\ operator$$

$$(m : mass\ of\ particle \quad \hat{p} = i\bar{h}\nabla : momentum\ operator)$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} : Laplace\ Operator$$

$$\Rightarrow \hat{H} = \frac{\bar{h}^2}{2m}\nabla^2 + V(r,t)$$

Many Particles:

$$\hat{H} = \sum_{n=1}^{N} \widehat{T_n} + \hat{V} \quad where\ \hat{V} = V(r_1, r_2, \cdots r_N, t) \quad \widehat{T_n} = \frac{\bar{h}^2}{2m_n}\nabla^2{}_n$$

So, Schrödinger Hamiltonian for the N-particle case:

$$\hat{H} = -\frac{\bar{h}^2}{2}\sum_{n=1}^{N}\frac{1}{m_n}\nabla^2{}_n + V(r_1, r_2, \cdots r_N, t)$$

and general form of the Hamiltonian: the Hamiltonian of the system is the sum of the separate Hamiltonians for each particle:

$$\hat{H} = \sum_{i=1}^{N} \hat{H}_i$$

This is an idealized situation—in practice the particles are almost always influenced by some potential, and there are many-body interactions.

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[18] https://en.wikipedia.org/wiki/Hamiltonian_(quantum_mechanics)

Schrödinger Equation:

The Hamiltonian generates the time evolution of quantum states.

$$i\bar{h}\frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi\rangle \quad where \; \bar{h}: Planck's \; constant, \hat{H}: Hamiltonian \; operator$$

Planck's constant: defines the quantum nature of energy and relates the energy of a photon to its frequency:

h= 6.62607015×10^{-34} joule-hertz^{-1} (*to simplify the equations h=1*)

Hermitian: H† = H *where $\dagger \equiv$ transpose & complex conjugate*

E_x: eigenvalue $\equiv$ energy of system $\Rightarrow$
$$\begin{bmatrix} E_1 & \cdots & \cdots & 0 \\ \vdots & E_2 & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & & E_n \end{bmatrix} \Rightarrow H = \sum_k E_k|k\rangle\langle k| \equiv diagonal \; matrix$$

where k: energy eigenstates

Ground state energy: Lowest possible energy $\equiv$ lowest eigenvalue in the matrix

Example: $\hat{H} = \bar{h}\omega X$ *where $X = X - gate$ and $\omega = coefficient$*

Eigenstates: |+⟩ : +hω , |-⟩ : -hω $\Rightarrow$ lowest eigenvalue = -hω $\equiv$ ground state energy $\equiv$ |-⟩

Exponential of a Matrix

In a matrix in a diagonal form:

$$for \; M = \sum_k e_k|k\rangle\langle k| \quad f(M) = f(e_k)|k\rangle\langle k|$$

(*means, doing some function to the matrix is same as doing the function on the individual eigenvalues, if the matrix is diagonal*.)

So, if we apply this rule to exponential function:

$$exp(M) = exp(e_k)|k\rangle\langle k|$$

Run this result in a Z gate:

$$for \; Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad exp(\theta Z) = \begin{pmatrix} exp(\theta) & 0 \\ 0 & exp(-\theta) \end{pmatrix}$$

Solving Schrodinger Equation

Given the state at some initial time (t=0), we can solve it to obtain the state at any subsequent time. In particular, if H is independent of time, then:

$$|\psi(t)\rangle = exp\left[-\frac{iHt}{\bar{h}}\right]|\psi(0)\rangle$$

$$i\bar{h}\frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi\rangle$$

$$i\bar{h}\frac{\partial}{\partial t}|\psi(t)\rangle = i\bar{h}\frac{\partial}{\partial t}\left(exp\left[\frac{-iHt}{\bar{h}}\right]|\psi(0)\rangle\right) = -i\bar{h}\frac{i}{\bar{h}}H\,exp\left[\frac{iHt}{\bar{h}}\right]|\psi(0)\rangle = H|\psi(t)\rangle$$

For time t_1 to t_2:

$$|\psi(t_2)\rangle = exp\left[-\frac{iH(t_2-t_1)}{\bar{h}}\right]|\psi(t_1)\rangle$$

$$U(t_1,t_2) = exp\left[-\frac{iH(t_2-t_1)}{\bar{h}}\right] : unitary\ quantum\ gate$$

By using this unitary gate, we can find $|\psi(t_2)\rangle$ = U$|\psi(t_1)\rangle$

Checking Unitarity

$$U = exp\left[-\frac{iH(t_2-t_1)}{\bar{h}}\right]$$

$$U^\dagger U = exp\left[-\frac{iH(t_2-t_1)}{\bar{h}}\right]^\dagger exp\left[-\frac{iH(t_2-t_1)}{\bar{h}}\right] = exp\left[\frac{iH^\dagger(t_2-t_1)}{\bar{h}}\right]exp\left[-\frac{iH(t_2-t_1)}{\bar{h}}\right] = exp[0] = \mathbb{1}\ where\ H^\dagger = H$$

Commutativity

For operators A and B we can say A and B **commute** if AB = BA . It is named as '*commutator*' and shown as {A, B]

It means if we apply first A and then B to a state, it gives same result if we first apply A and then B operator.

If AB = - BA then they are **anti-commute** and shown as {A, B}

Exponentials with Commutativity

Diagonalizable: If any two matrices that can both be written in the "same" basis are simultaneously diagonalizable.

If the matrices commute:

$$\exp(A)\exp(B) = \exp(A+B)$$

Proof:

$$for\ \ A = \sum_k a_k|k\rangle\langle k|\ \ and\ B = \sum_k b_k|k\rangle\langle k|$$

$$\exp(A)\exp(B) = \exp\left(\sum_k a_k|k\rangle\langle k|\right)\exp\left(\sum_k b_k|k\rangle\langle k|\right) = \sum_k \exp(a_k)|k\rangle\langle k|\sum_k \exp(b_k)|k\rangle\langle k|$$

$$= \sum_k \exp(a_k+b_k)|k\rangle\langle k| = \exp(A+B)$$

Example: The Z gate is diagonal in the computational basis |0⟩ and |1⟩ whereas X gate is diagonal in |+⟩ and |-⟩ basis. So, they don't commute, and they are not simultaneously diagonalizable.

Unitary Gates ⇔ Hamiltonians
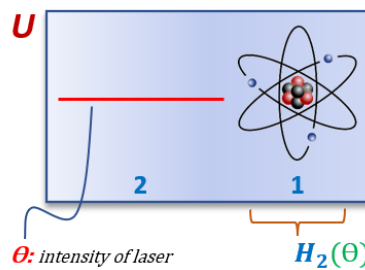
For any unitary gate *U = exp (iK)* where K is some Hermitian operator ⇒

$$K = -i \log U = -i \log \sum_k U_u |k\rangle\langle k| \quad \textit{where } \sum_k U_u |k\rangle\langle k| \textit{ is the diagonal form representation}$$

$$= -\mathrm{i} \sum_k \log U_u |k\rangle\langle k| = -\mathrm{i} \sum_k \log e^{i\psi_k} |k\rangle\langle k| \quad \textit{since eigenvalues of unitary} \equiv e^{i\psi_k}$$

$$= -\mathrm{i} \sum_k i\psi_k |k\rangle\langle k| = \sum_k \psi_k |k\rangle\langle k| = K^\dagger \equiv \textit{hermitian}$$

Evolutions of Subsystems

Atom interacting with laser beam with varying intensity of θ ≡ open system:

We can describe them altogether by a joint Hamiltonian to describe the system as a whole. We can consider the Hamiltonian just for the atom so this will be an approximation to the actual evolution of the atom, and this will correspond to a unitary gate. So, we can approximately model the dynamics of this atom by a unitary gate. This is important because if we can model it by unitary gates, then we can start to think about how to simulate it on a quantum computer because everything there is unitary apart from measurements.

Simulating Hamiltonians

🔸 Simulating Hamiltonians classically are very inefficient.

Remember that Hamiltonians are described by the Schrodinger equation:

$$i\bar{h} \frac{\partial |\psi\rangle}{\partial t} = \widehat{H} |\psi\rangle$$

Let's define the state of a particle as a function of its position using the inner product ⟨x|ψ⟩ = ψ(x)

Then, Hamiltonian of a single particle is:

$$i\bar{h} \frac{\partial}{\partial t} \psi(x) = \left[-\frac{1}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) \quad : \textit{Hamiltanian} \rightarrow \textit{kinetic energy} + \textit{potential energy}$$

If we have one qubit, we need to solve two equations: we need to know how |0⟩ and |1⟩ evolves and then we know how any linear combination of them evolves.

If we have two qubits, we need to know how all 4 computational basis states (*|00, |01)), |10) and |11)*) evolve. So, we need to solve four equations.

Similarly, for n qubits, we need to solve 2^n equations which increases exponentially. That's why classical simulation is slow (*and impossible to solve the n qubit equations for big n values*)

Local Interactions

We can make the assumption that they are interacting locally rather than distant parts of the system are interacting.

In the previous interaction example, notice that $H_2(\theta)$ varies over time. Here, we first assume that Hamiltonian that is NOT varying over time. So, H is time independent. In this case, we can use the earlier Schrodinger equation:

$$|\psi(t)\rangle = exp\left[-\frac{iHt}{\hbar}\right]|\psi(0)\rangle$$

For simplification of this equation, we can split our system we've assumed local interactions as mentioned before. So, we can split Hamiltonian into small a sum of smaller Hamiltonians (let say, L parts) that are each acting on only a few qubits:

$$H = \sum_{k=1}^{L} H_k$$

Such that, let say if $H_1 = X_3X_4$, it means that an X gate is applied to qubit 3 and another X gate is applied to qubit 4. Again, if $H_2 = Z_5$, it means that Z gate is applied to qubit 5. So, we can have Hamiltonians corresponding to interactions between different qubits or just acting on a single qubit as well.

For smaller subsystems, e^{-iH_kt}, it is easier to approximate quantum circuits, but we can't rely on out operators commuting the H case. It means:

$$e^{iHt} = e^{-i\sum_k H_k t} \neq e^{iH_1} + e^{iH_2} \cdots e^{iH_L} = \sum e^{iH_k t}$$

Trotter Formula

Let say we've Hermitian operators A and B:

$$\lim_{n\to\infty}\left(e^{\frac{iAt}{\hbar n}}e^{\frac{iBt}{\hbar n}}\right)^n = e^{\frac{i(A+B)t}{\hbar}}$$

or

$$\lim_{n\to\infty}\left(e^{\frac{iAt}{n}}e^{\frac{iBt}{n}}\right)^n = e^{i(A+B)t} \ \ with \ \bar{h} = 1$$

So, if we use the approximation previously mentioned:

$$e^{i(A+B)\Delta t} = e^{iA\Delta t}e^{iB\Delta t} + O(\Delta t^2) \quad where \ O(\Delta t^2): error$$

Simulating Schrödinger Equation

$$H = \frac{p^2}{2m} + V(x) : Hamiltonian \ of \ a \ single \ particle$$

$$|\psi\rangle = \int_{-\infty}^{\infty}|x\rangle\langle x|\psi\rangle \, \partial x \Rightarrow approximate \ as \ discrete \ sum \ \Rightarrow |\psi\rangle = \sum_{k=-\frac{d}{\Delta x}}^{\frac{d}{\Delta x}} a_k|k\Delta x\rangle$$

where d: total distance, Δx: space steps, particles moves from $|-d\rangle$ (*when k=-d/Δx*) to $|+d\rangle$ (*when k=d/Δx*).

Total length (*total # of points*) from -d to +d (*including zero*) is (2d/Δx)+1. So lets find the number of computational basis states (*# of qubits : n*):

$$\frac{2d}{\Delta x} + 1 = 2^n \Rightarrow n = \log\left(\frac{2d}{\Delta x} + 1\right)$$

∴ Advantage of using qubits → we can remove exponentials in classical states.

We know that, [V(x), p/2m] ≠0

and then, let's compute the exponentials of the Hamiltonian individually and combine them as shown previously:

V(x) → $e^{-iV(k\Delta x)\Delta t}$ and $\frac{p}{2m}$ → $U_{FFT} x U_{FFT}^t = p$ ⇒ $|k\rangle \to U_{FFT} e^{-\frac{ix^2}{2m}} U_{FFT}^t |k\rangle$

∴ So, we reduce our simulation of the Schrödinger equation to simulating these individual Hamiltonians of the different subparts of the overall Hamiltonian.

Fourier Transform (FT)

QFT: Performs the Fourier Transform of amplitudes of a quantum state in a way that is much faster than what a classical computer could do. It does not allow us to perform usual Fourier Transforms that we can do any faster than a classical computer, because of the difficulty in retrieving the information from measuring quantum state. But we can use this technique of the QFFT within various other algorithms and it's actually extremely useful for that reason. (*i.e., factoring large numbers, shamed by Shores algorithm, phase estimation which is where you can approximate the eigenvalues of a unit tree operator …*)

Discrete FT:

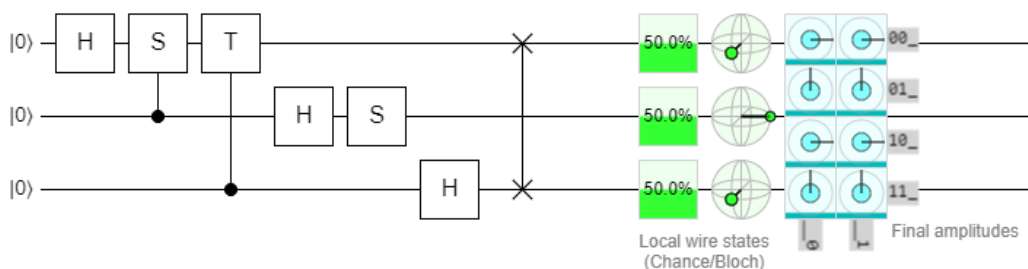$$a_1, a_2 \dots a_N \to b_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} a_j e^{\frac{2\pi i j_k}{N}}$$

⇒ QDFT:
|0⟩, … |N-1⟩→|j⟩ where:

$$|j_k\rangle \to \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} b_j e^{\frac{2\pi i j_k}{N}} |k\rangle$$

FT of an overall state:

$$\sum_{j=0}^{N-1} a_j |j\rangle \xrightarrow{unitary} \sum_{k=0}^{N-1} b_j |k\rangle$$

Example:

Three qubits Fourier Transform

An application Area of FT: Phase Estimation

$$U|u\rangle = e^{2\pi i\varphi}|u\rangle \quad \textit{we want to know the parameter in the eigen value}$$

Phase estimation happens in a few stages:

Stage-1:

Register-1: # of t register (*set of qubits, in zero state*) depends on how well we want to estimate the accuracy of ψ (in eigenvalue) and what probability we want to get a correct answer.

Register-2: Consists of many qubits we need to characterize U state.

* Then we apply Hadamard gate to each qubits in register-1 and we do a series of controlled gates from the first register to the second register.

* We do our first control gate from the bottom qubit (*of the register-1*) is a control of U^{2^0} (*of register-2*) and then we continue this pattern where we go, next qubit U^{2^1} up to $U^{2^{t-1}}$

* We find that the outcome of the second register is still U because we've just been adding phases.

* So, overall phase estimation: When we measure the first register at the end, in the computational basis, what we get out are the digits of the phase. It means, if $\varphi = 0.\varphi_0\varphi_1\cdots\varphi_t$ and we can know φ if we know all of these t bits and the states that our qubits end up in after the first stage. It means, after applying Hadamard and control gates and work through the state of qubits, we will get:

$$1^{st}\ stage:\ \frac{1}{2}(|0\rangle + e^{2\pi i 0.\varphi_t}|1\rangle) + (|0\rangle + e^{2\pi i 0.\varphi_{t-1}\varphi_t}|1\rangle)\cdots$$

and then after we apply the inverse Fourier transform, it simplifies this expression $\rightarrow |\varphi_1\varphi_2\cdots\varphi_t\rangle$

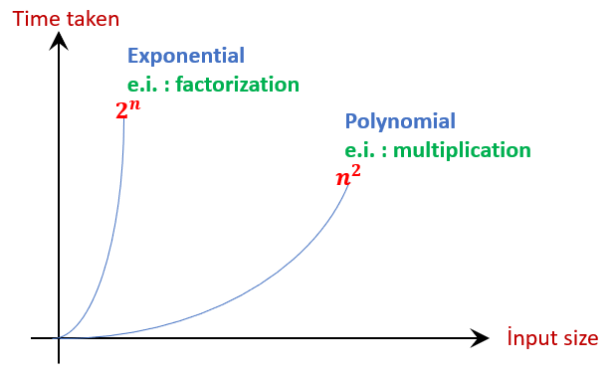Then we can measure all qubits in the first register in the computational basis and we know the value of φ exactly.
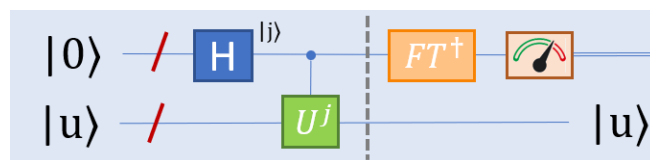
If we cannot prepare the state U directly, we can prepare other state:

$$|\Psi\rangle = \sum_u c_u|u\rangle \ \textit{where}\ |c_u|^2: \textit{probability of correct outcome}$$

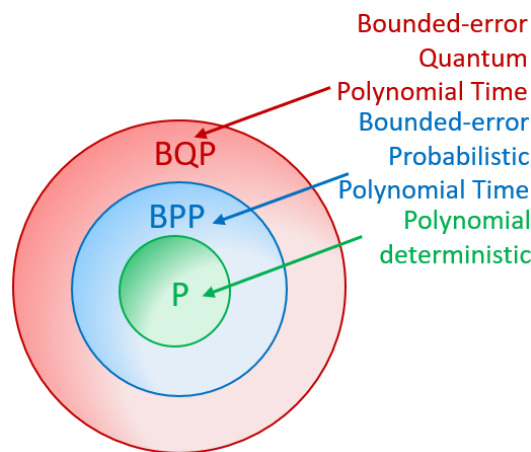to obtain the approximate of φ value (*if we can't prepare U*)

Complexity

For classical algorithms:

For exponential, we need exponential time in classical computers. But in quantum, the complexity is shifted from 2^n to n^2 (*shift from exponential to polynomial*) with Shores algorithm.

Complexity Classes

BQP: BQP is the class of decision problems solvable by a <u>quantum computer</u> in polynomial time, with an error probability of at most 1/3 for all instances.

BPP: BPP is the class of decision problems solvable by a <u>probabilistic Turing machine</u> in polynomial time with an error probability bounded by 1/3 for all instances.

Simulation Problems

For a particular model of a quantum system its simulation consists of the ability to emulate how the state of the system changes in time. A simulation with the ability to track the wave function as a function in time precisely can also estimate observables[19].

The models we examine will be described by a Hamiltonian *H* (which describes how the pieces within that system interact) as long as our systems are closed.

If *H* is time-independent, then its time-evolution propagator is given by:

$$|\Psi(t)\rangle = U(t,0)|\Psi_0\rangle = e^{-iHt}|\psi(0)\rangle \ where \ e^{-iHt}: propagator$$

If *H(t)* is time-dependent, then the propagator is given by:

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[19] Observables are the types of things that would be measured in a lab setting and we want to understand how those expectation values change with time as the wave function evolves.

$$|\Psi(t)\rangle = \mathcal{T} \, exp\left[\int_0^t dt' H(t')\right] = 1 - i \int_0^t dt_1 H(t_1) + (-i)^2 \int_0^t \int_0^{t_1} dt_1 dt_2 H(t_1)H(t_2) + \cdots$$

Why Simulation?

- Model validation with experiment
- Model to model validation
- Savings in terms of time and resources compared to running experiments
- Emergence of states and phases

Gibbs State: It is an equilibrium probability distribution which remains invariant under future evolution of the system. For example, a stationary or steady-state distribution of a Markov chain, such as that achieved by running a Markov chain Monte Carlo iteration for a sufficiently long time, is a Gibbs state.[20]

Probability Distribution: It is the mathematical function that gives the probabilities of occurrence of different possible outcomes for an experiment.[21]
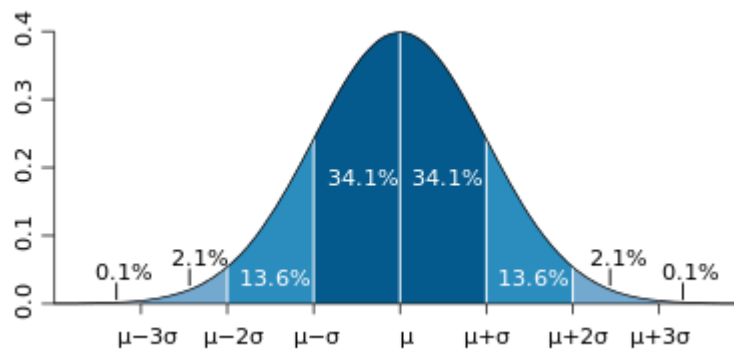
Markov Chain: It is a stochastic model describing a sequence of possible events in which the probability of each event depends only on the state attained in the previous event.[22]

Two-state Markov Process

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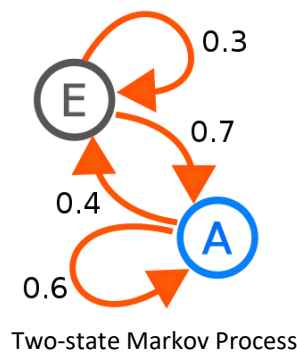
[20] https://en.wikipedia.org/wiki/Gibbs_state
[21] https://en.wikipedia.org/wiki/Probability_distribution
[22] https://en.wikipedia.org/wiki/Markov_chain