

# Motivation

Quantum theory is a mathematical model of the physical world.

physics of the atomic and subatomic world

many behaviors have no analog in the classical world

GOAL:

Comfort level with the mathematics and concepts that determine behavior and interactions of qubits.

Understanding of the constraints and opportunities of quantum computation.

# Linear Algebra

$$\begin{bmatrix} \cos 90^\circ & \sin 90^\circ \\ -\sin 90^\circ & \cos 90^\circ \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \Omega \\ \Omega \end{bmatrix}$$

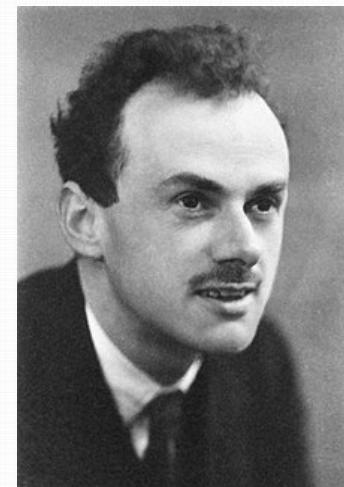
<https://xkcd.com/184/>

# Vectors and Dirac (bra-ket) Notation

We are going to be working with ***n*-dimensional vectors of complex numbers.**

A **ket** is a column vector:  $|a\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix}$

A **bra** is a row vector,  
with the complex conjugates of  
the corresponding ket:



Paul Dirac

A bra is the **adjoint (complex conjugate transpose)** of a ket.

# Vector Space

A **vector space** is a collection of vectors that is closed under addition and scalar multiplication.

Can add vectors together, or multiply any vector by a scalar, and the result is still in the set.

# Vector Space Properties

A vector space with vectors A, B, and C has the following properties:

- Commutativity:  $A+B=B+A$
- Associativity of vector addition:  $(A+B)+C=A+(B+C)$
- Additive identity:  $0+A=A+0=A$ , for all A
- Existence of additive inverse:  
For any A, there exists a  $(-A)$  such that  $A+(-A)=0$
- Scalar multiplication identity:  $1A=A$
- Given scalars r and s
  - Associativity of scalar multiplication:  $r(sA)=(rs)A$
  - Distributivity of scalar sums:  $(r+s)A=rA+sA$
  - Distributivity of vector sums:  $r(A+B)=rA+rB$

# Basis Vectors

A set of elements (vectors) in a vector space ( $V$ ) is called a **basis**, or a set of **basis vectors**, if:

- a) The vectors are linearly independent, and
- b) Every vector in  $V$  is a linear combination of these vectors.

Linearly independent = no vector in the set can be written as a linear combination of other vectors in the set.

## Example: Standard Basis

For a 4-dimensional vector space over complex numbers, these vectors are known as the **standard basis**:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad |2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Any vector can be written as:  $|a\rangle = c_0|0\rangle + c_1|1\rangle + c_2|2\rangle + c_3|3\rangle$

# Hilbert Space: Inner Product

A Hilbert space is a vector space over complex numbers with an inner product  $\langle b|a \rangle$ .



David Hilbert

$$|a\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix}$$

$$|b\rangle = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$$

$$\langle b|a \rangle = (\beta_0^* \quad \beta_1^*) \cdot \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} = \alpha_0\beta_0^* + \alpha_1\beta_1^*$$

# Properties of the Inner Product

Conjugate symmetric:  $\langle b|a \rangle = \langle a|b \rangle^*$

Linear:  $\langle b|(\alpha|x\rangle) = \alpha\langle b|x\rangle$

Positive definite:  $\langle a|a \rangle > 0$ , for  $|a\rangle \neq 0$

Norm:  $\|a\| = \sqrt{\langle a|a \rangle}$

# Inner Product and Basis Vectors

For orthonormal basis vectors, inner product is either 0 or 1.

$$\langle e_i | e_j \rangle = \delta_{ij}$$

Any vector can be expressed as a linear combination of basis vectors:

$$|\psi\rangle = \sum_i \alpha_i |e_i\rangle$$

Coefficients are derived from the inner products:

$$|\psi\rangle = \sum_i \langle \psi | e_i \rangle |e_i\rangle$$

# Outer Product

$$|a\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix}$$

$$|a\rangle\langle b| = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} \begin{pmatrix} \beta_0^* & \beta_1^* \end{pmatrix} = \begin{pmatrix} \alpha_0\beta_0^* & \alpha_0\beta_1^* \\ \alpha_1\beta_0^* & \alpha_1\beta_1^* \end{pmatrix}$$

$$|b\rangle = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$$

Can be viewed as an operator that transforms  $|b\rangle$  to  $|a\rangle$ .

# Unitary Matrix

A unitary matrix is a square complex matrix whose adjoint equals its inverse.

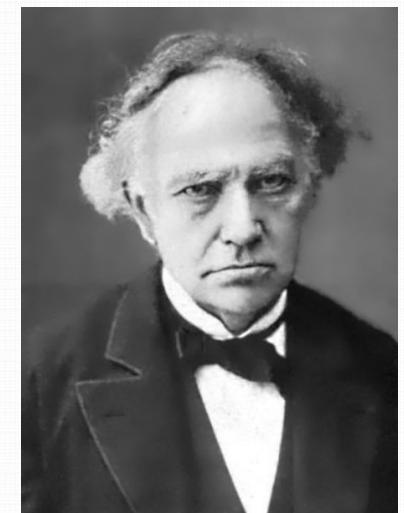
$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

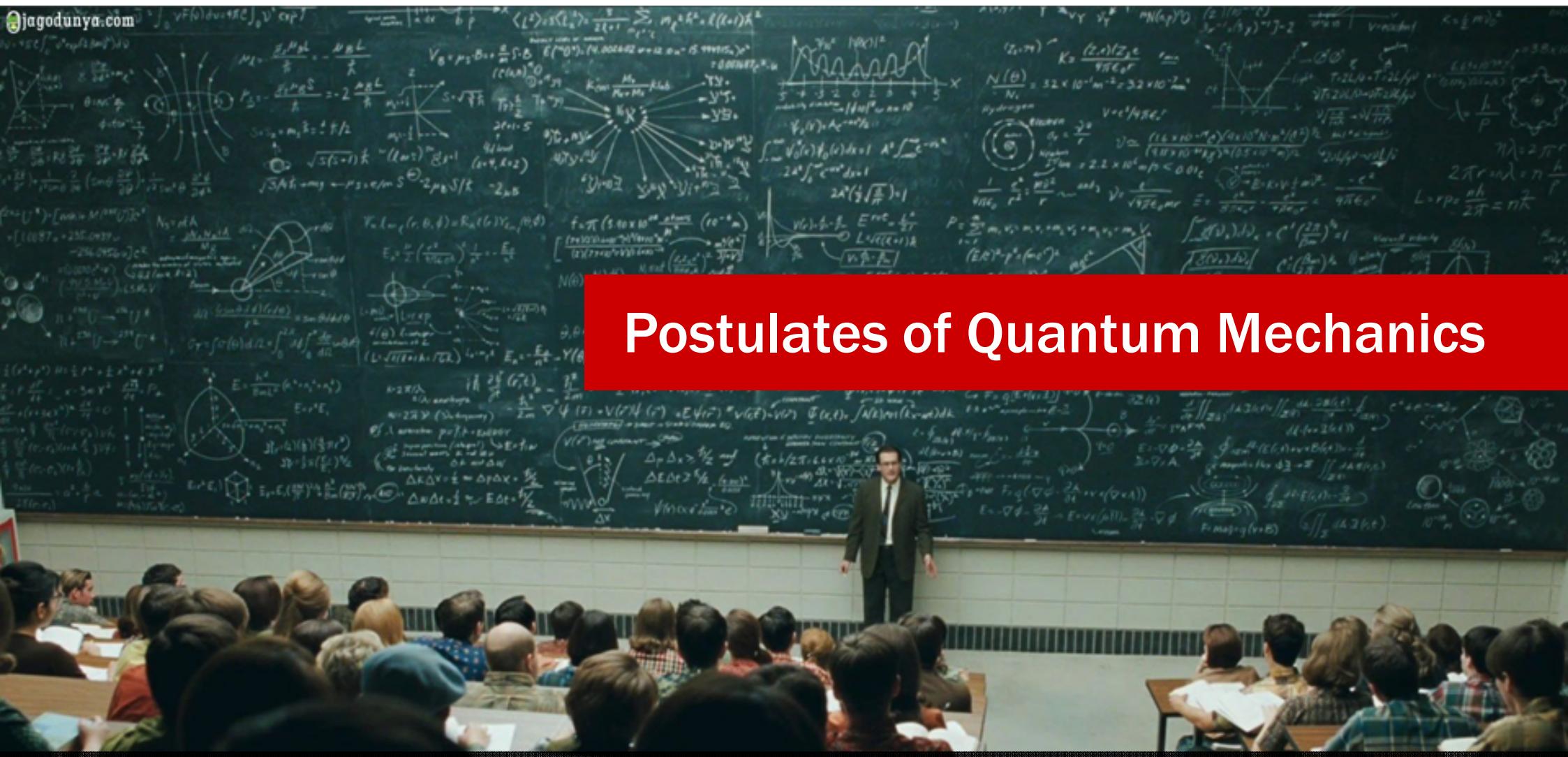
$$U^\dagger = \begin{pmatrix} a^* & b^* \\ c^* & d^* \end{pmatrix}$$

Also called the  
*conjugate transpose* or the  
*Hermitian transpose*.

Unitary if  $UU^\dagger = U^\dagger U = I$

Unitary transform preserves the norm of a vector.





## Postulates of Quantum Mechanics

NC STATE  
UNIVERSITY

Electrical &  
Computer Engineering

Computer  
Science

@NCStateECE  
@cscnccsu

# Postulate 1

Associated to any *isolated* physical system is a Hilbert space known as the system's **state space**.

The system is completely specified by its **state vector**, which is a unit vector in the state space.

Also known as  
its *wave function*.

$$|\psi\rangle = \sum_i \alpha_i |e_i\rangle$$

$$\sum_i |\alpha_i|^2 = 1$$

# Single Qubit

The two standard basis vectors represent distinct states.

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

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

A superposition of these two states is also a state:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \text{ where } |\alpha|^2 + |\beta|^2 = 1$$

# Composite System

Suppose system A has Hilbert space  $H_A$ .

Suppose system B has Hilbert space  $H_B$ .

The state space of the two systems together is  $H_A \otimes H_B$   
where  $\otimes$  represents the tensor product, also called the Kronecker  
product.

# Tensor Product

$$A \otimes B = \begin{pmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{pmatrix} \otimes \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix}$$

$$= \begin{pmatrix} a_{00} \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} & a_{01} \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} \\ a_{10} \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} & a_{11} \begin{pmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a_{00}b_{00} & a_{00}b_{01} & a_{01}b_{00} & a_{01}b_{01} \\ a_{00}b_{10} & a_{00}b_{11} & a_{01}b_{10} & a_{01}b_{11} \\ a_{10}b_{00} & a_{10}b_{01} & a_{11}b_{00} & a_{11}b_{01} \\ a_{10}b_{10} & a_{10}b_{11} & a_{11}b_{10} & a_{11}b_{11} \end{pmatrix}$$

# Standard Basis for 2-qubit System

$$|0\rangle_A \otimes |0\rangle_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0 & \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |00\rangle_{AB}$$

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

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

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

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

## Standard Basis for 2-qubit System

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

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

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

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

State space for n qubits has  $2^n$  dimensions.

Basis states = {  $|j\rangle$  }, where  $j = 0..2^n-1$

# State Vector for n-qubit System

$$|\psi\rangle_n = \alpha_0|...000\rangle + \alpha_1|...001\rangle + \alpha_2|...010\rangle + \alpha_3|...011\rangle + \dots$$

$$|\psi\rangle_n = \alpha_0|0\rangle + \alpha_1|1\rangle + \alpha_2|2\rangle + \alpha_3|3\rangle + \dots$$

$$|\psi\rangle_n = \sum_j \alpha_j |j\rangle$$

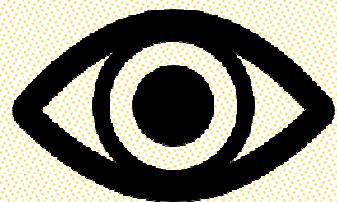
# Separable vs. Entangled States

There are states that cannot be expressed as the tensor product of independent qubit states.

Separable	Entangled
$\frac{1}{\sqrt{2}} 01\rangle + \frac{1}{\sqrt{2}} 11\rangle$ $= \frac{1}{\sqrt{2}}( 0\rangle +  1\rangle) \otimes  1\rangle$	$\frac{1}{\sqrt{2}} 00\rangle + \frac{1}{\sqrt{2}} 11\rangle$

## Postulate 2

Every **observable** attribute of a physical system is described by an **operator** that acts on the kets that describe the system.



Observable is something that can be measured.  
E.g., spin, position, polarization, charge, ...

Operator is described by a Hermitian matrix.

# Eigenstate and Eigenvalue

In general, applying an operator to a state will change the state.

There are some states that are not changed, except for a scalar multiplier:

$$M|a_j\rangle = \lambda_j|a_j\rangle$$

These are called **eigenstates**, and the scalar value  $\lambda$  is the **eigenvalue** that corresponds to that eigenstate.

# Postulate 3

When an observable is **measured**, the only possible outcome will be an **eigenvalue** of the operator for that observable.



Physical measurements are always real numbers.

Operator is described by a Hermitian matrix, which has real eigenvalues!

# Measurement Eigenstates

This postulate is the basis for the “quantized” (discrete) nature of measured quantities.

The eigenstates  $a_j$  of a Hermitian operator form a basis:

They are orthogonal --  $\langle a_j | a_k \rangle = \delta_{jk}$

Any state can be expressed as a linear combination (with complex coefficients) of the eigenstates.

# Measuring in the Standard Basis

Consider this measurement operator:

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

Two eigenstates,  $|0\rangle$  and  $|1\rangle$ , with eigenvalues +1 and -1.

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

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

## Postulate 4

For a system in state  $|\psi\rangle$ , when an observable is measured, the probability of obtaining eigenvalue  $\lambda_j$  (corresponding to eigenstate  $|a_j\rangle$ ) is:

$$|\langle a_j | \psi \rangle|^2$$

The complex number  $\langle a_j | \psi \rangle$  is a “probability amplitude.” It cannot be directly measured. Must be squared to get a real value.

# Measuring in the Standard Basis

If we measure  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$  in the standard basis...

$\langle 0|\psi\rangle = \alpha$ , and  $\langle 1|\psi\rangle = \beta$ , so:

Probability of measuring +1 =  $|\alpha|^2$

Probability of measuring -1 =  $|\beta|^2$

Suppose  $|\psi\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$ . The probability of measuring +1 or -1 would be 0.5 for each.

# Expected Value

A system prepared in state  $|\psi\rangle$  and measured repeated using operator  $A$  will yield a variety of results, each with probability  $|\langle a_j|\psi\rangle|^2$ .

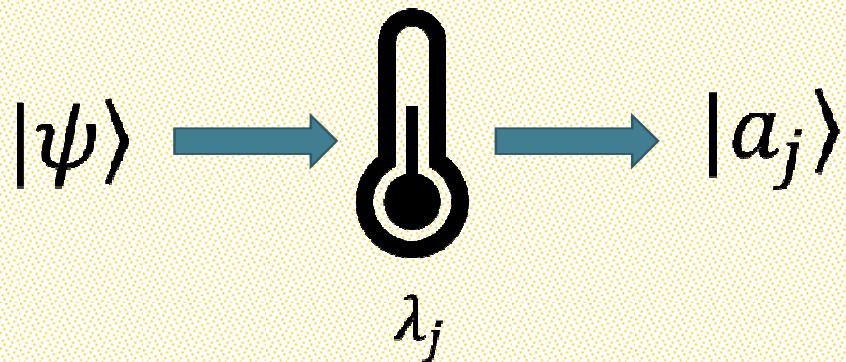
Running the same experiment (computation) twice is not expected to yield the same result!

Expected value:

$$\langle\psi\rangle \equiv \sum_j \lambda_j \cdot \Pr(|a_j\rangle) = \langle\psi|A|\psi\rangle$$

## Postulate 5

When an observable is **measured**, obtaining eigenvalue  $\lambda_j$ ,  
the state of the system is **changed** to become the corresponding  
eigenstate  $|a_j\rangle$ .



# Collapse of the Wave Function

This postulate describes the “collapse” of the wave function that occurs when a measurement occurs.

All information that was embodied in the superposition is lost.  
Permanently!

# Implications

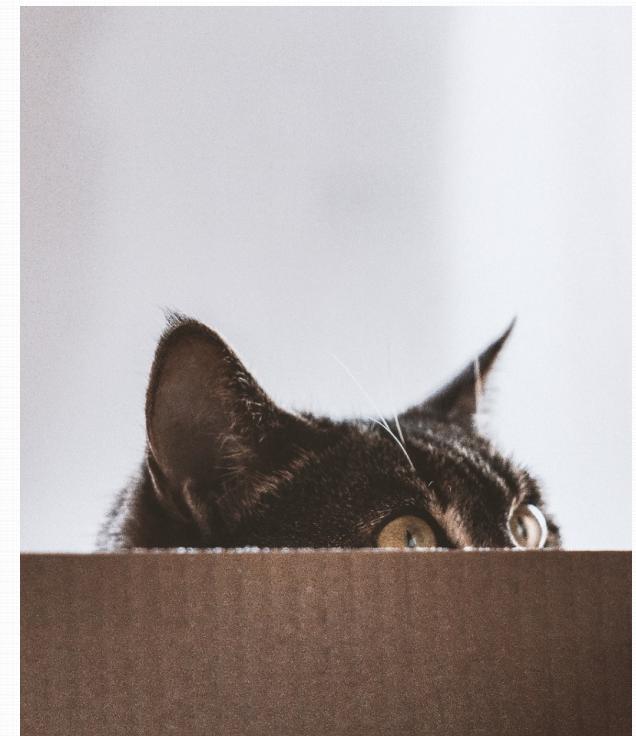
We never have access to the complete quantum state.

Any measurement/observation extracts one classical value  
and destroys the quantum state.

Can't probe or insert print statements.

Can't pause, probe, and resume to debug.

Can't checkpoint and restart.



# Partial Measurement

What happens if we measure one qubit in a multi-qubit system?

- (1) Forces that qubit to  $|0\rangle$  or  $|1\rangle$ , based on probability amplitudes.
- (2) “Removes” other cases where qubit is not the measured value.
- (3) Renormalizes the remaining components.

$$|\psi\rangle = \frac{|00\rangle + |01\rangle + |10\rangle + |11\rangle}{2} \rightarrow \begin{array}{l} \text{Measure: Qubit 0 = 1} \\ \text{Prob = 1/2} \end{array}$$

↓

$$|\psi\rangle = \frac{|01\rangle + |11\rangle}{\sqrt{2}}$$

# Another Example

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

Prob = 1/16

Prob = 2/16

Prob = 10/16

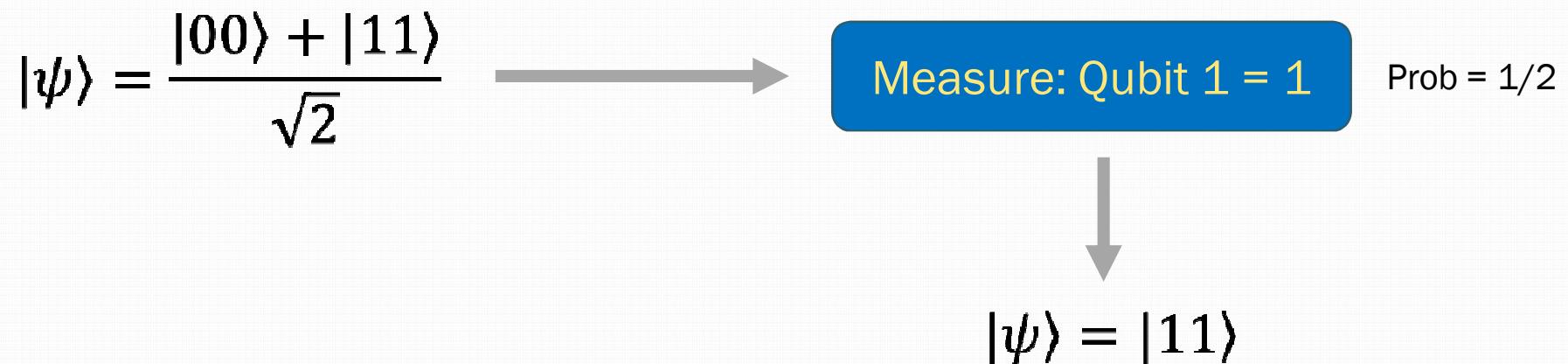
Prob = 3/16

Measure: Qubit 1 = 1

Prob = 13/16

$$|\psi\rangle = \frac{3+i}{\sqrt{16}} |10\rangle - \frac{i\sqrt{3}}{\sqrt{16}} |11\rangle$$

# Entanglement Revisited



When we measure qubit 1 = 1, we know (without measuring!) that qubit 0 = 1, with 100% certainty. But... there was a 50/50 chance that qubit 0 was 0 or 1 before measurement.

This is true even when the two entangled qubits are separate in space.

## Postulate 6

The evolution of a closed quantum system over time is described by a **unitary transformation**.

The state  $|\psi\rangle$  of the system at time  $t_1$  is related to the state  $|\psi'\rangle$  of the system at time  $t_2$  by a unitary  $U$  which depends only on times  $t_1$  and  $t_2$ .

$$|\psi'\rangle = U|\psi\rangle$$

# Implications for Quantum Computing

Program = step by step evolution from initial state to end state

Each step **must be unitary**.

Preserves norm, so sum of probabilities = 1.

Has an inverse, so reversible.

System must be closed: no interaction with environment.  
(Measurement is not reversible.)

Unitary transform is a “rotation” of the vector.

# Bloch Sphere Representation

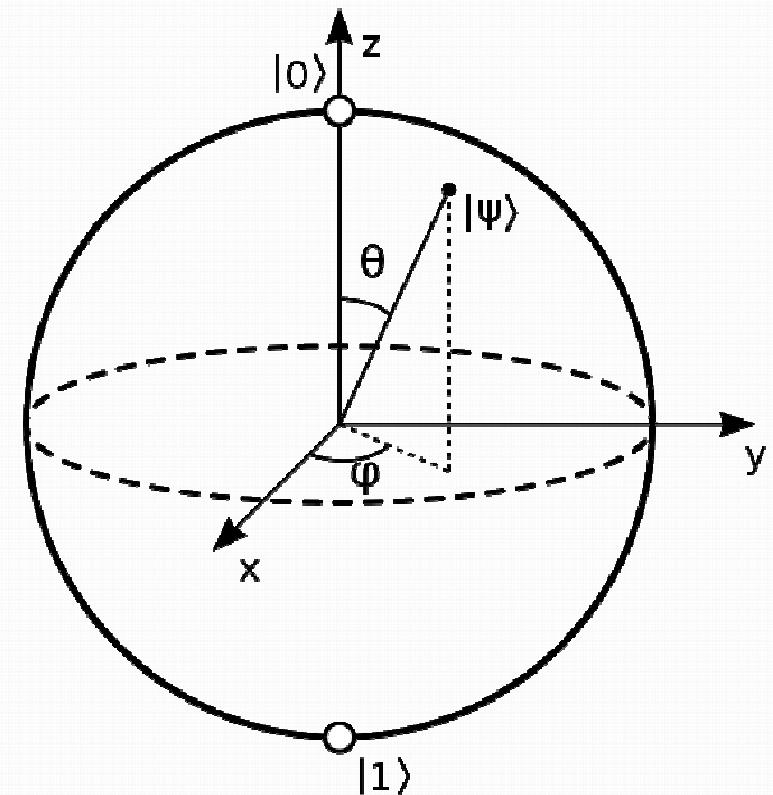
$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\varphi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$

Two parameters:

$\theta$  is angle of rotation around X-axis.

$\varphi$  is angle of rotation around Z-axis.

Reminder:  $e^{i\varphi} = \cos\varphi + i\sin\varphi$



# Some Unitary Transformations

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

Rotation around the X axis.  
(swaps  $|0\rangle$  and  $|1\rangle$  coefficients,  $\theta = \pi$ )

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

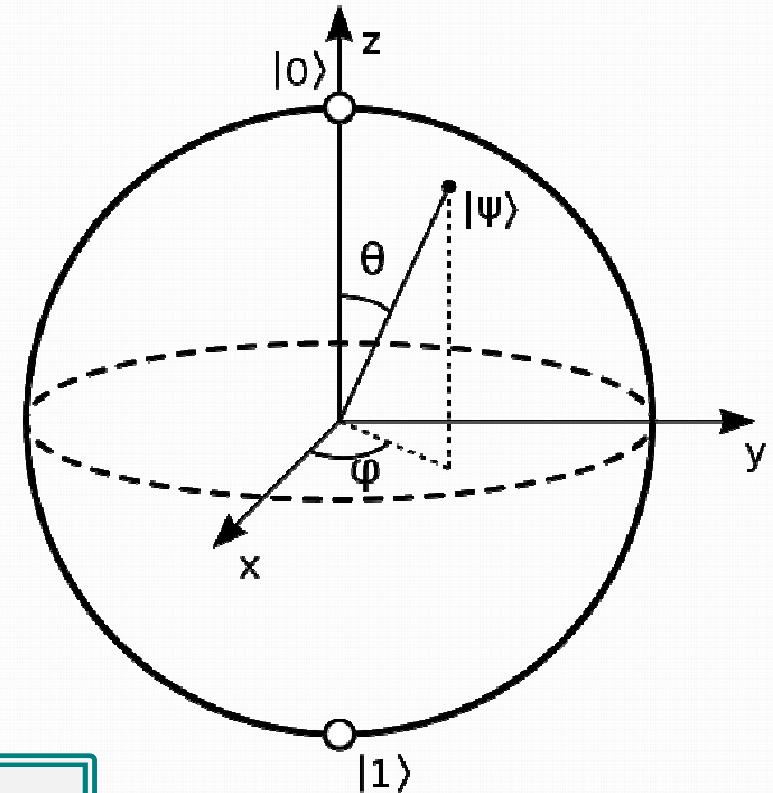
Rotation around the Z axis.  
(negates  $|1\rangle$  coefficient,  $\varphi = \pi$ )

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Rotation around the Y axis.  
( $Y = iXZ$ )

*Pauli matrices*

Quirk demo:  
<https://algassert.com/quirk>



# Two-Qubit Transform

Perform X on qubit<sub>1</sub> = 1, and Z on qubit<sub>0</sub>.

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

<i>Start</i>	<i>End</i>
$ 00\rangle$	$ 10\rangle$
$ 01\rangle$	$- 11\rangle$
$ 10\rangle$	$ 00\rangle$
$ 11\rangle$	$- 01\rangle$

# Two-Qubit Transform

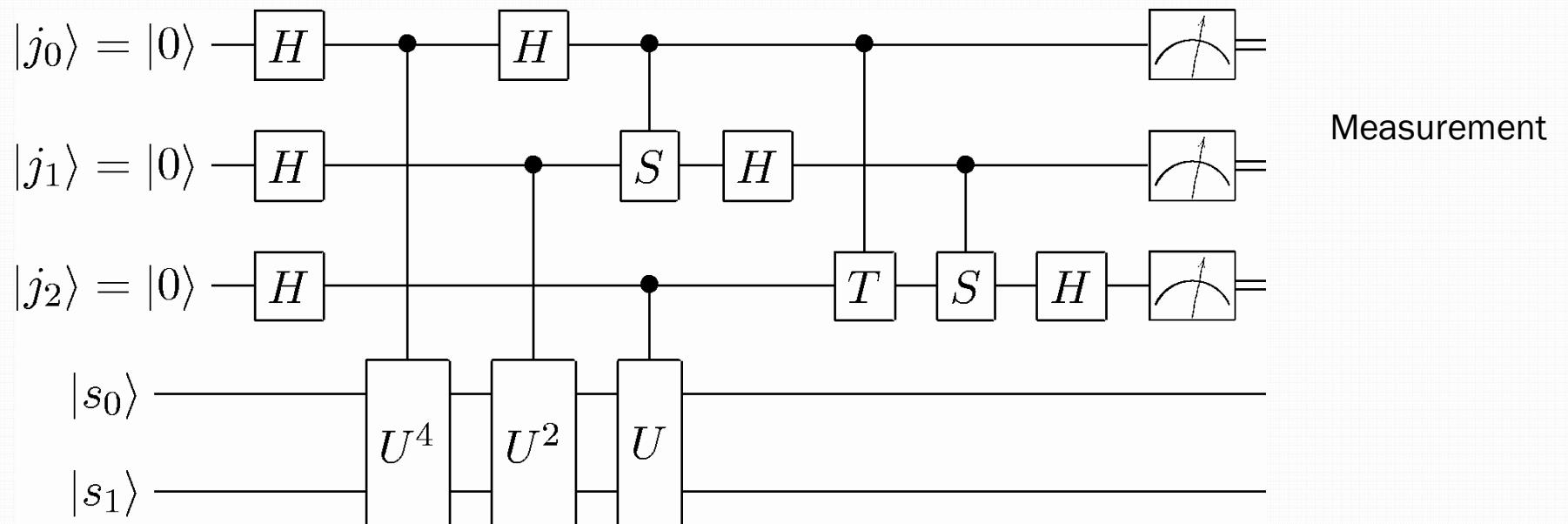
$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

If  $qubit_1 = 1$ , flip  $qubit_0$ .

<i>Start</i>	<i>End</i>
$ 00\rangle$	$ 00\rangle$
$ 01\rangle$	$ 01\rangle$
$ 10\rangle$	$ 11\rangle$
$ 11\rangle$	$ 10\rangle$

# Gate-Model Program = Circuit

Program = step-by-step evolution from initial state to final state  
Each step (gate) is unitary.



# Summary

# Qubits

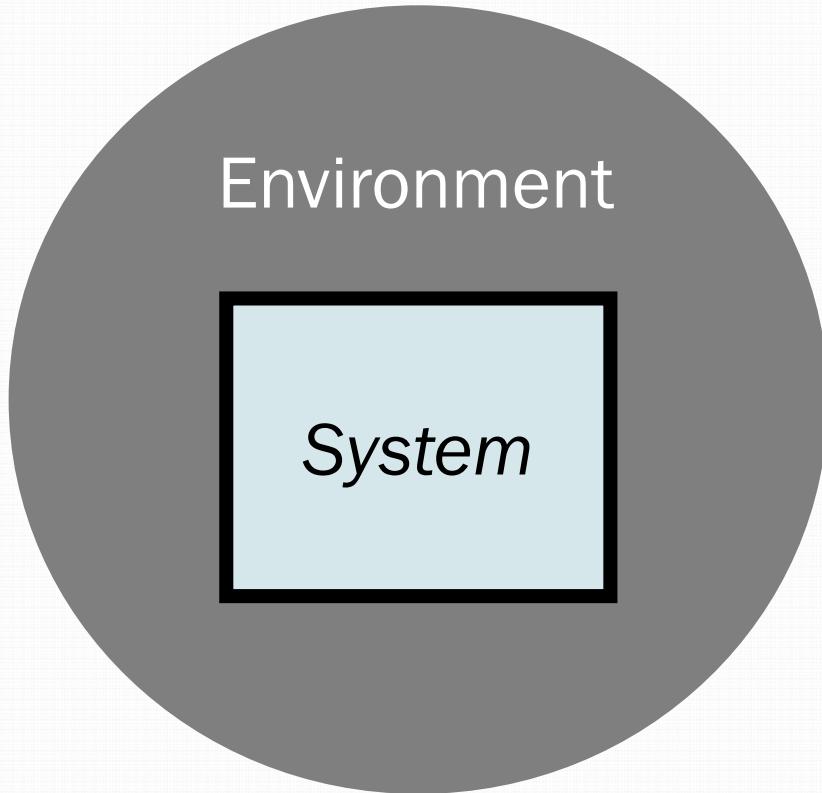
Qubit is represented by a vector in a complex Hilbert space.

Systems are composed using tensor product.

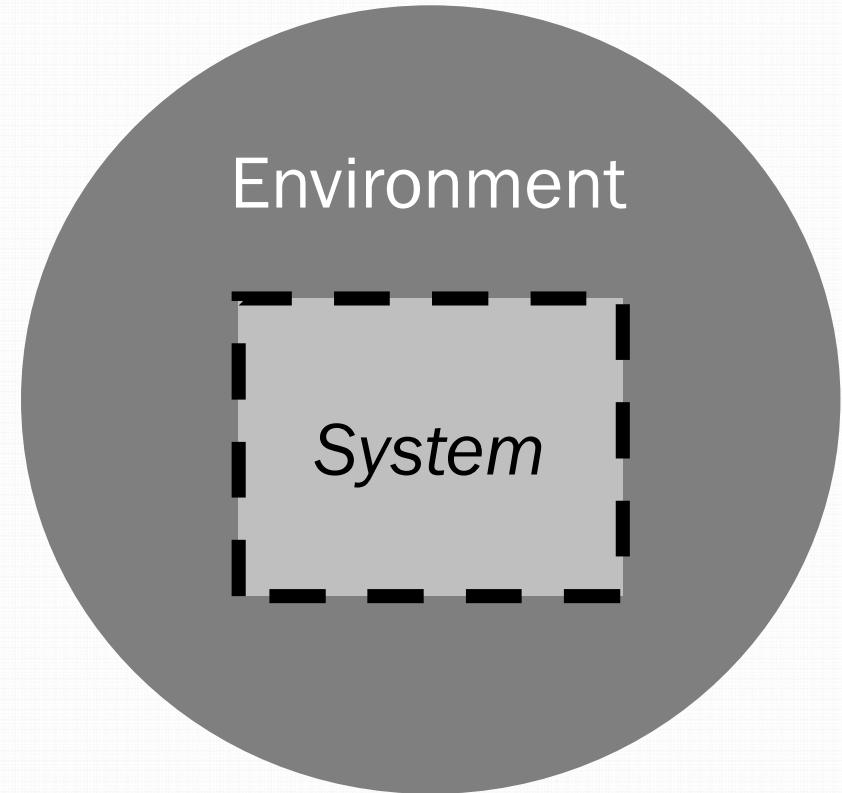
State evolves by unitary transforms (rotations).

Measurement projects state to an eigenstate of the measurement operator.

# Decoherence



Theory: closed system



Reality: not closed