

# Mathematical Tools for Quantum Computing

CPSC 4470/5470

Introduction to Quantum Computing

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# Mathematical Model of Quantum Systems

**Four Principles** to model quantum systems mathematically:

### 1. Superposition:

The state of a qubit is a unit complex vector in the two-dimensional *Hilbert Space*.

### 2. Composition:

The joint state of many (independent) quantum systems is the tensor product of component states.

#### 3. Transformation:

Time evolution of a quantum system is a *unitary process*.

#### 4. Measurement:

Measuring a quantum state causes its superposition to *collapse/project* to one of its basis states randomly.

Von Neumann: "In mathematics, you don't understand things. You just get used to them."



# Superposition State of A Qubit

The **state of a qubit** is represented by a unit vector in the two-dimensional complex vector space (**Hilbert Space**  $\mathbb{C}^2$ ). In the Dirac notation:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

where  $\alpha, \beta \in \mathbb{C}$ , satisfying that its 2-norm:  $|\alpha|^2 + |\beta|^2 = 1$ .

Here,  $\alpha$  and  $\beta$  are called the **probability amplitudes** on the (classical) basis,  $|0\rangle$  and  $|1\rangle$ , respectively.

(can be negative, even complex numbers)

$$|\psi\rangle = 0.6|0\rangle - 0.8|1\rangle = \begin{bmatrix} 0.6\\ -0.8 \end{bmatrix}$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{i}{\sqrt{2}}|1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\i\end{bmatrix}$$

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

Not valid: 
$$\frac{1}{4}|0\rangle + \frac{i}{2}|1\rangle = \begin{bmatrix} 1/4\\i/2 \end{bmatrix}$$

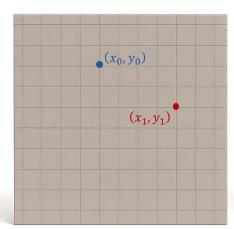
# **Vector Spaces**

**Vector space**: a (special) set of vectors.

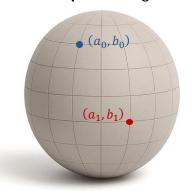
**Example:** Position vectors for points on a 2D surface.

 $\mathbb{R}^2$ : Two-dimensional real vector space

Position on a flat surface: X-y plane



Surface of a sphere: Longitude-latitude



Two real-valued coordinates.

**Algebra**: that allows us to take linear combinations.

- Scalar multiplication:  $c \cdot \vec{a} = \begin{bmatrix} ca_0 \\ ca_1 \end{bmatrix}$  for some  $c \in \mathbb{R}$
- Vector addition:  $\vec{a} + \vec{b} = \begin{bmatrix} a_0 + b_0 \\ a_1 + b_1 \end{bmatrix}$

"Vectors after algebra remain in the same space."

 $\mathbb{R}^n$ : n-dimensional real vector space:

all vectors with n real components:  $\vec{a} = \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{bmatrix} \in \mathbb{R}^n$ 

### More about Vectors

Properties (derive on board):

• Length of a vector (as in  $\ell_2$ -norm or Euclidean norm):  $\vec{a} = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix}$ 

$$\|\vec{a}\|_2^2 = \vec{a}^T \vec{a}$$

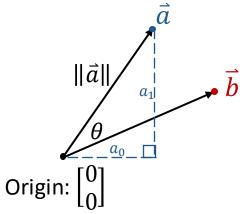
• Angle between two vectors:  $\vec{a} = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix}$  and  $\vec{b} = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix}$ 

$$\|\vec{a}\| \cdot \|\vec{b}\| \cos \theta = \vec{a}^T \vec{b}$$

Hilbert space: inner-product vector space.

Well-defined "geometry" (incl. length and angle).

 $\vec{a}^T$ : Transpose of  $\vec{a}$ 



Inner product of  $\vec{a}$  and  $\vec{b}$ :  $\vec{a}^T \vec{b}$ 

Do they work for complex vectors?

# What about Complex Vectors?

### A **complex number** $\alpha \in \mathbb{C}$ is of form:

$$\alpha = a_0 + a_1 i$$
Real component

Where  $a_0$ ,  $a_1 \in \mathbb{R}$  and  $i^2 = -1$ .

A vector in a two-dimensional complex vector space:

$$|\psi\rangle = \begin{bmatrix} \alpha_0 \\ \alpha_1 \end{bmatrix} \in \mathbb{C}^2$$

### Can we use the same definition for length and angle?

• Length:

$$\vec{a}^T \vec{a} = \|\vec{a}\|_2^2$$

Angle:

$$\vec{a}^T \vec{b} = \|\vec{a}\| \cdot \|\vec{b}\| \cos \theta$$

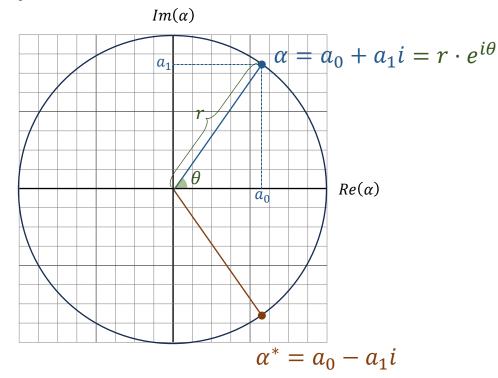
What could be problematic?

Example: Length of  $|\psi\rangle = \begin{bmatrix} 1 \\ i \end{bmatrix}$ ?

# Complex Numbers

A **complex number**  $\alpha \in \mathbb{C}$  is of form:  $\alpha = a_0 + a_1 i$ , where  $a_0, a_1 \in \mathbb{R}$  and  $i^2 = -1$ .

### **Complex Plane:**



Cartesian coordinate 
$$(a_0, a_1)$$
: (real, imaginary)  $\alpha = a_0 + a_1 i$ 

Euler's formula  $e^{i\theta} = \cos \theta + i \sin \theta$ 

**Polar coordinate** 
$$(r, \theta)$$
: (magnitude, phase)  $\alpha = r \cos \theta + r \sin \theta \ i = r \cdot e^{i\theta}$  "length" "angle"

"Length": Magnitude 
$$r=|\alpha|=\sqrt{a_0^2+a_1^2}=\sqrt{\alpha^*\alpha}$$
 "Angle": Complex phase  $\theta=\arctan\frac{a_1}{a_0}$ 

**Notation**: 
$$\alpha^*$$
 is the complex conjugate of  $\alpha$  
$$\alpha^* = a_0 - a_1 i = r \cdot e^{-i\theta}$$

# Back to Complex Vectors

For a quantum state  $|\psi\rangle = \begin{bmatrix} \alpha_0 \\ \alpha_1 \end{bmatrix}$ : What are  $\langle \psi | \psi \rangle$ ,  $\langle 0 | \psi \rangle$  and  $\langle 1 | \psi \rangle$ ?

### Algebra:

- Scalar multiplication:  $c \cdot |\psi\rangle = \begin{bmatrix} c\alpha_0 \\ c\alpha_1 \end{bmatrix}$  for some  $c \in \mathbb{C}$
- Vector addition:  $|\psi\rangle + |\varphi\rangle = \begin{bmatrix} \alpha_0 + \beta_0 \\ \alpha_1 + \beta_1 \end{bmatrix}$

### **Properties** (derive on board):

• Length of a vector:  $|\psi\rangle = \frac{\alpha_0}{\alpha_1}$ 

$$\||\psi\rangle\|_2^2 = \begin{bmatrix} \alpha_0^* & \alpha_1^* \end{bmatrix} \cdot \begin{bmatrix} \alpha_0 \\ \alpha_1 \end{bmatrix}$$

Example: Length of  $|\psi\rangle = \begin{bmatrix} 1 \\ i \end{bmatrix}$ 

• Angle between two vectors:  $|\psi\rangle = \begin{bmatrix} \alpha_0 \\ \alpha_1 \end{bmatrix}$  and  $|\varphi\rangle = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$ 

$$\cos \theta = \begin{bmatrix} \alpha_0^* & \alpha_1^* \end{bmatrix} \cdot \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

### **Dirac Notation:**

$$\langle \psi | = (|\psi\rangle)^{\dagger} = (|\psi\rangle^*)^T = [\alpha_0^* \quad \alpha_1^*]$$

Adjoint of a vector: conjugate transpose

Inner product: "Bra-ket"

$$\rightarrow \langle \psi | \cdot | \varphi \rangle = \langle \psi | \varphi \rangle$$

# What about more qubits?

Two coins:

3

?

$$Pr(0_A) = 0.36$$
,  $Pr(1_A) = 0.64$ 

$$Pr(0_B) = 0.5$$
,  $Pr(1_B) = 0.5$ 

Assuming they are independent:  $Pr(0_A 0_B) = Pr(0_A) \cdot Pr(0_B)$ 

$$Pr(0_A 0_B) = 0.36 \cdot 0.5,$$
  $Pr(0_A 1_B) = 0.36 \cdot 0.5,$   $Pr(1_A 0_B) = 0.64 \cdot 0.5,$   $Pr(1_A 1_B) = 0.64 \cdot 0.5,$ 

We use a "joint state" to fully characterize the system:

**Tensor product:** 

$$\begin{bmatrix} 0.36 \\ 0.64 \end{bmatrix} \otimes \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} = \begin{bmatrix} 0.36 \cdot \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \\ 0.64 \cdot \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 0.36 \cdot 0.5 \\ 0.36 \cdot 0.5 \\ 0.64 \cdot 0.5 \\ 0.64 \cdot 0.5 \end{bmatrix} \stackrel{\Pr(0_A 0_B)}{\Pr(1_A 0_B)}$$

Two qubits:



$$|\psi_A\rangle = 0.6|0\rangle + 0.8|1\rangle$$

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

Assuming they are independent:  $\langle 0_A 0_B | \psi_{AB} \rangle = \langle 0_A | \psi_A \rangle \cdot \langle 0_B | \psi_B \rangle$ 

$$|\psi_{AB}\rangle = 0.6 \cdot \frac{1}{\sqrt{2}}|00\rangle - 0.6 \cdot \frac{1}{\sqrt{2}}|01\rangle + 0.8 \cdot \frac{1}{\sqrt{2}}|10\rangle - 0.8 \cdot \frac{1}{\sqrt{2}}|11\rangle$$

$$\begin{bmatrix} 0.6 \\ 0.8 \end{bmatrix} \otimes \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 0.6 \cdot 1/\sqrt{2} \\ -0.6 \cdot 1/\sqrt{2} \\ 0.8 \cdot 1/\sqrt{2} \\ -0.8 \cdot 1/\sqrt{2} \end{bmatrix}_{ \begin{vmatrix} 1_A 0_B \rangle \\ |1_A 0_B \rangle \\ |1_A 1_B \rangle }$$

# High-Dimensional Complex Hilbert Space

The **joint state of n qubit** is a  $2^n$ -dimensional complex vector in the **Hilbert Space**  $\mathcal{H}$ , described by complex numbers,  $\alpha_i \in \mathbb{C}$ , for  $i \in \{0,1\}^n$ , satisfying that its 2-norm:  $\sum_{i \in \{0,1\}^n} |\alpha_i|^2 = 1$ . In the Dirac notation:

$$|\psi\rangle = \alpha_{00\dots 0}|00\dots 0\rangle + \alpha_{00\dots 1}|00\dots 1\rangle + \dots + \alpha_{11\dots 1}|11\dots 1\rangle = \begin{bmatrix} \alpha_{00\dots 0} \\ \alpha_{00\dots 1} \\ \vdots \\ \alpha_{11\dots 1} \end{bmatrix} \in \mathcal{H} = \mathbb{C}^{2^n}$$

Inner product: 
$$\langle \psi | \psi \rangle = [\alpha_{00...0}^* \quad \alpha_{00...0}^* \quad ... \quad \alpha_{00...0}^*] \begin{bmatrix} \alpha_{00...0} \\ \alpha_{00...1} \\ \vdots \\ \alpha_{11...1} \end{bmatrix} = \sum_{i \in \{0,1\}^n} \alpha_i^* \alpha_i = 1$$
 Normalized.

This is a linear combination over  $2^n$  basis states:  $|00 \dots 0\rangle$ ,  $|00 \dots 1\rangle$ , ...,  $|11 \dots 1\rangle$ .

# Change of Basis?



$$|\psi\rangle = 0.6|0\rangle + 0.8|1\rangle$$

$$|\psi\rangle=0.6|0\rangle+0.8|1\rangle$$
 Standard basis: 
$$\left\{ \begin{array}{l} |0\rangle=\begin{bmatrix}1\\0\end{bmatrix}\\ |1\rangle=\begin{bmatrix}0\\1 \end{array} \right]$$

Define an alternative basis:

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

Derive on board:

$$|\psi\rangle = ?|+\rangle + ?|-\rangle$$

What about the following basis for  $|\psi\rangle$ ?

$$\begin{cases} |v\rangle = |0\rangle + i|1\rangle \\ |w\rangle = |0\rangle - i|1\rangle \end{cases}$$

What are the criteria for a "good" basis?

### Orthonormal Basis

**Span:** A set of vectors  $|v_0\rangle, |v_1\rangle, ..., |v_{n-1}\rangle$  spans the vector space S, if for any vector  $|w\rangle \in S$ , there exists  $\alpha_0, ..., \alpha_{n-1} \in \mathbb{C}$ :

$$|w\rangle = \alpha_0|v_0\rangle + \alpha_1|v_1\rangle + \dots + \alpha_{n-1}|v_{n-1}\rangle$$

Linear combination (with complex coefficients)

**Linear dependence**: A set of (non-zero) vectors are *linearly* dependent if there exists  $\alpha_0, \dots, \alpha_{n-1}$  not all zero:

$$0 = \alpha_0 |v_0\rangle + \alpha_1 |v_1\rangle + \dots + \alpha_{n-1} |v_{n-1}\rangle$$

**Basis**: *linearly independent* vectors *spans* the vector space *S*.

#### Orthonormal basis:

- Length: A set of unit vectors
- Angle: mutually orthogonal

$$\langle v_j | v_k \rangle = \begin{cases} 1, & \text{if } j = k \text{ (unit length)} \\ 0, & \text{if } j \neq k \text{ (orthogonal)} \end{cases}$$

**Examples:** two-qubit basis

$$|00\rangle = \begin{bmatrix} 1\\0\\0\\0 \end{bmatrix}, |01\rangle = \begin{bmatrix} 0\\1\\0\\0 \end{bmatrix}, |10\rangle = \begin{bmatrix} 0\\0\\1\\0 \end{bmatrix}, |11\rangle = \begin{bmatrix} 0\\0\\0\\1 \end{bmatrix}$$

$$|++\rangle = \frac{1}{2} \begin{bmatrix} 1\\1\\1\\1 \end{bmatrix}, |+-\rangle = \frac{1}{2} \begin{bmatrix} 1\\-1\\1\\-1 \end{bmatrix}, |-+\rangle = \frac{1}{2} \begin{bmatrix} 1\\1\\-1\\-1 \end{bmatrix}, |--\rangle = \frac{1}{2} \begin{bmatrix} 1\\-1\\-1\\1 \end{bmatrix}$$

# The Process of Evolving a Probabilistic State

A **Markov Process** is a stochastic process over a state space S such that:

$$\Pr[S_{t+1} = s' | S_t = s, S_{t-1} = s_{t-1}, \dots, S_0 = s_0] = \Pr[S_{t+1} = s' | S_t = s]$$
 For all state  $s_t \in S$  at time  $t$ .

**Transition probability** (from s to s'):

$$\Pr[S_{t+1} = s' | S_t = s]$$

### **Example:**

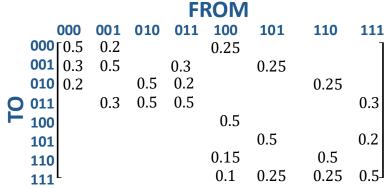
A 3-bit Markov Model for CPSC 4470 student:

- P Phone out? (0 = away, 1 = out)
- D Discussing? (0 = quiet, 1 = participating)
- U Understanding now? (0 = lost, 1 = get)

### Eight possible states ( $s \in S$ ):

- O PDU Silently lost
- $1 \stackrel{(P)}{(D)} \stackrel{(U)}{(U)}$  Zen absorber
- 2 PDU Eager-but-lost
- 3 (P) (D) (U) Classroom king
- 4 P D U Doomscrolling
- 5 PDU Overconfident texter
- 6 PDU Clueless chaos
- 7 PDU Mythical Multitasker

# A **transition matrix** to fully characterize the process.



### Col-k, Row-j of the matrix:

$$T[k,j] = \Pr[S_{t+1} = k | S_t = j]$$

- Non-negative elements.
- Columns sum to 1.

# The Process of Evolving a Probabilistic State

 $\lceil \Pr[S_t = 0] \rceil$ 

 $Pr[S_t = 1]$ 

 $\Pr[S_t = 2]$ 

 $Pr[S_t = 3]$ 

 $\Pr[S_t = 4]$ 

 $\Pr[S_t = 5]$ 

 $\Pr[S_t = 6]$ 

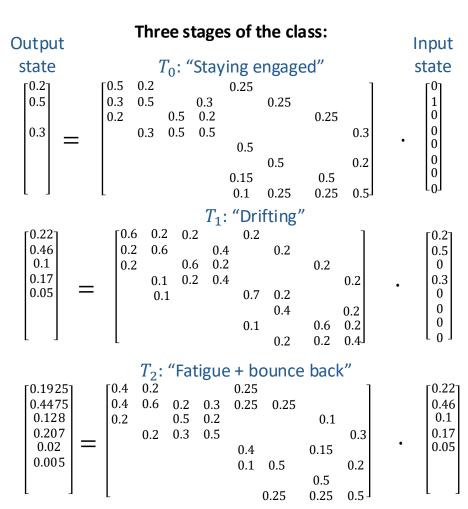
 $\lfloor \Pr[S_t = 7] \rfloor$ 

### **Probabilistic mixture** of possible states:

### **Evolution** of probabilistic state:

$$\overrightarrow{p_{t+1}} = T \cdot \overrightarrow{p_t}$$

**Transition matrix** 



# The Process of Evolving a Superposition State

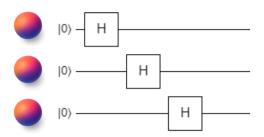
**Superposition** of possible states:

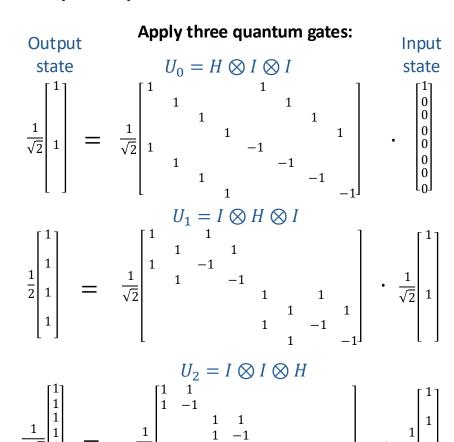
$$|\psi_t\rangle = \begin{bmatrix} \alpha_{00\dots 0} \\ \alpha_{00\dots 1} \\ \vdots \\ \alpha_{11\dots 1} \end{bmatrix}$$

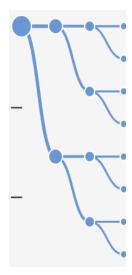
**Evolution** of superposition state:

$$|\psi_{t+1}\rangle = U \cdot |\psi_t\rangle$$

Unitary matrix







# Geometry-Preserving Transformations

**Inner product** gives the length and angle of vectors:

Real vectors:  $\overrightarrow{v_i}^T \overrightarrow{v_k}$ 

Complex vectors:  $\langle v_j | v_k \rangle$ 

Transformations that preserves "geometry": lengths and angles.

- Orthonormal basis stays orthonormal.
- Shapes don't get stretched.

	Orthogonal Matrix	Unitary Matrix
Definition	$Q^TQ = I$	$U^{\dagger}U = I$
Inverse	$Q^{-1} = Q^T$	$U^{-1} = U^{\dagger}$
Columns	Real orthonormal vectors	Complex orthonormal vectors
Example	2D rotation matrix	Quantum gates

**Principle #3: Transformation** 

(More details in Lecture 5.)

# **Understanding Projections**

<u>Derive on board</u>:

$$\Pi_0 = \frac{|0\rangle\langle 0|}{\langle 0|0\rangle}$$
, What is  $\Pi_0 |\psi\rangle$ ?

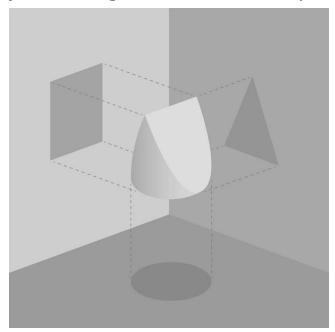
**Principle #4: Measurements** 

(More details in Lecture 6.)

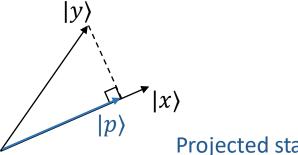
**Projection** (as a "linear operator": mapping from one vector space to another)

Example:

3D object casting shadows onto 2D plane.



Projecting  $|y\rangle$  onto the line direction of  $|x\rangle$ .



Projected state:  $|p\rangle = ?$ 

**Projection is a matrix:** 

$$|p\rangle = \Pi_x |y\rangle, \Pi_x = \frac{|x\rangle\langle x|}{\langle x|x\rangle}$$

Outer product: a matrix

Inner product: a scalar

### **Properties:**

- 1.  $\Pi$  is symmetric. (Hermitian:  $\Pi^{\dagger} = \Pi$ )
- 2. Project twice is the same as once.  $(\Pi^2 = \Pi)$

### Hermitian Matrix in QM

**Symmetric matrix** (real):

$$S^T = S$$

**Hermitian matrix** (complex):

$$H^{\dagger} = H$$

- Hermitian matrix has real eigenvalues. -
- Corresponding to *physical observable* with real-valued quantity.

Why?

Eigenvalue equation for a linear operator A:

$$A|v_i\rangle = \lambda_i|v_i\rangle$$

where  $|v_i\rangle$  is the (non-zero) **eigenvector**, and  $\lambda_i$  is a complex number known as the **eigenvalue**. <u>Derive on board</u> (Pauli Matrices):

"Pauli Z operator" 
$$\sigma_Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
 Standard basis!  $\{|0\rangle, |1\rangle\}$ 

- Eigenvalues:  $\lambda_0=1$  and  $\lambda_1=-1$  Eigenvectors:  $|v_0\rangle=\begin{bmatrix}1\\0\end{bmatrix}$  and  $|v_1\rangle=\begin{bmatrix}0\\1\end{bmatrix}$

"Pauli Y operator" 
$$\sigma_Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

 $\{|+i\rangle, |-i\rangle\}$  basis!

- Eigenvalues:  $\lambda_0 = 1$  and  $\lambda_1 = -1$
- Eigenvectors:  $|v_0\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1\\i \end{bmatrix}$  and  $|v_1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1\\-i \end{bmatrix}$

"Pauli X operator" 
$$\sigma_{\chi} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

 $\{|+\rangle, |-\rangle\}$  basis!

- Eigenvalues:  $\lambda_0 = 1$  and  $\lambda_1 = -1$
- Eigenvectors:  $|v_0\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1\\1 \end{bmatrix}$  and  $|v_1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1\\1 \end{bmatrix}$

# Spectral Theorem

For a linear operator that is normal ( $A^{\dagger}A = AA^{\dagger}$ ), we can write it in the **spectral decomposition**:

$$A = \sum_{i} \lambda_{j} |v_{j}\rangle\langle v_{j}|$$

where  $\lambda_i$  are the eigenvalues, and  $|v_i\rangle$  are the corresponding (orthonormal) eigenvectors.

### **Examples:**

$$\sigma_Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = (+1)|0\rangle\langle 0| + (-1)|1\rangle\langle 1| \qquad \sigma_X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = (+1)|+\rangle\langle +|+(-1)|-\rangle\langle -|$$

### **Applications:**

Power of a matrix:

$$A^{8} = \left(\sum_{j} \lambda_{j} |v_{j}\rangle\langle v_{j}|\right)^{8} = \sum_{j} \lambda_{j}^{8} |v_{j}\rangle\langle v_{j}|$$

Exponential of a matrix:

$$e^A \equiv \sum_{k=0}^{\infty} \frac{1}{k!} A^k = \sum_j e^{\lambda_j} |v_j\rangle\langle v_j|$$

### **Example:**

$$e^{i\theta\sigma_z} = e^{i\theta}|0\rangle\langle 0| + e^{-i\theta}|1\rangle\langle 1| = \begin{bmatrix} e^{i\theta} & 0\\ 0 & e^{-i\theta} \end{bmatrix}$$