130B Quantum Physics

Part I. Matrix Mechanics

Introduction

■ Everything is a Vector

■ What is Quantum Mechanics?

Quantum mechanics is a *physics theory* that describes the behavior of *quantum systems* (microscopic particles, strings, qubits ...).

What does **physics theory** do in general?

- Describe the **state** of the system: a set of variables encoding the relevant *information* of the system.
- Predict (i) the **observables** (measurement outcomes) and (ii) their **dynamics** (time evolution).

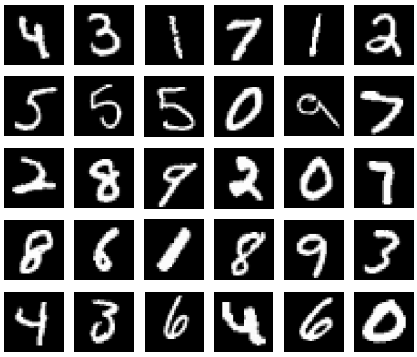
Physics theory is about encoding the physical reality in the form of **information** and generating predictions about the reality based on such information.

■ How to Encode Information?

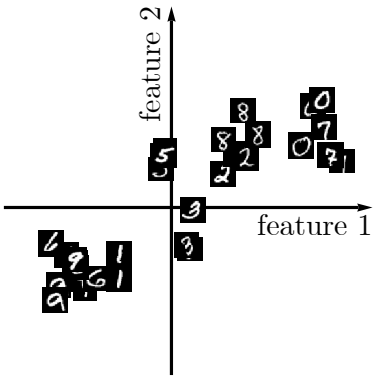
State variables encode the information about the system. They are *inferred* from observations.

- State variables may not have "physical meaning".
- Choice of state variables may not be unique. (There can be more than one way to describe a system.)

Example: how to describe the following images?



- Image file: brightness of each pixel. - describe a state by all possible observables.
- Human: digits 0, 1, 2, ..., 9. - describe a state by a *name*.
- Machine learning: feature vectors in the latent space. - describe a state by a *vector* in a vector space. [This is the most close to what we do in quantum mechanics.]



In quantum mechanics, every **state** of a quantum system is *described* by a **complex vector** (an array of *complex* numbers).

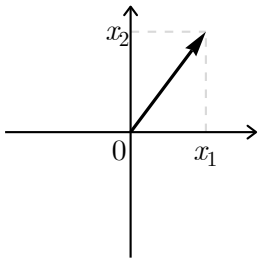
- The vector components are the state variables, and they may not need to have physical meanings. [They are also called **probability amplitudes** or **wave amplitudes**, but I don't explain what is "waving" here.]
- This particular (vector-based) approach of describing quantum states is not the only way. There are other ways to formulate quantum mechanics, just to name a few: density matrix formulation (matrix-based), classical shadow formulation (probability-based) [1], quantum bootstrap (observable-based) [2].
- However, the vector description is a simple and efficient way to describe a (pure) state of a quantum system. So we will start from state vectors.
- Information encoded in a quantum state is called **quantum information**. It provides the foundation for quantum computation/communication.

[1] Hsin-Yuan Huang, Richard Kueng, John Preskill. arXiv:2002.08953.

[2] Xizhi Han, Sean A. Hartnoll, Jorrit Kruthoff. arXiv:2004.10212.

▪ What is a Vector?

- *Geometric* interpretation: a vector (in high-school physics) is an *arrow*, used to represent a physical quantity that has both **magnitude** and **direction**.
  - Example: the displacement vector $\boldsymbol{x}$ in a two-dimensional coordinate space

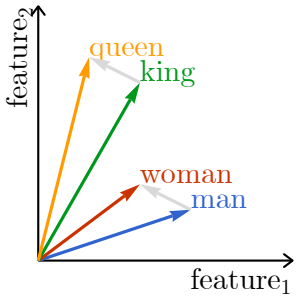


$\boldsymbol{x} = (x_1, x_2) = (0.6, 0.8)$

- *Algebraic* interpretation: a vector (in computer science) is an *array* of *numbers*, serves as a **data structure** for storing and representing **information**.
  - Example 1: Color vector (the red/green/blue values form a vector)

```
.rgb = [1., 0.5, 0.25] # [r, g, b]
.rgb = [0.25, 0.5, 1.]
```

  - Example 2: Word vector (in natural language processing), vector representations of words that encode the meaning and semantics of the words.



Use semantic relationship by vector arithmetic [3]:

$$|\text{king}\rangle - |\text{man}\rangle + |\text{woman}\rangle = |\text{queen}\rangle. \tag{1}$$

Vector in Quantum Mechanics:

- The notion of **state vector** in **quantum mechanics** is closer to the *algebraic* interpretation --- it is used to encode the *state* of a quantum system, or to store the *data* of quantum information. There is no direct physical meaning associated with its amplitude and direction.
- Real and complex vectors:
  - **Real vector**: an array of *real* numbers --- the space of n-component real vectors is denoted as $\mathbb{R}^n$

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n. \tag{2}$$

- **Complex vector**: an array of *complex* numbers --- the space of n-component complex vectors is denoted as $\mathbb{C}^n$

$$\boldsymbol{z} = (z_1, z_2, \ldots, z_n) \in \mathbb{C}^n. \tag{3}$$

They are just arrays of different *data types*. Compare to real vectors, *complex* vectors are more powerful data structures that can describe the *wave* behavior conveniently, and is therefore widely used in quantum mechanics.

[3] Ekaterina Vylomova, Laura Rimell, Trevor Cohn, Timothy Baldwin. arXiv:1509.01692

■ Complex Algebra

■ Complex Number

A **complex number** z is made of two real numbers (x, y) that combine with the **real unit** 1 and the **imaginary unit** $i = \sqrt{-1}$ respectively,

$$x \in \mathbb{R},\ y \in \mathbb{R} \to z = x + i\, y \in \mathbb{C}. \tag{4}$$

The real and imaginary units obey the following multiplication rules

$$1 \times 1 = 1,\ 1 \times i = i \times 1 = i,\ i \times i = -1. \tag{5}$$

- **Addition**:

$$\left\{ \begin{array}{l} z = x + i\, y \\ w = u + i\, v \end{array} \right. \to z + w = (x + u) + i\,(y + v) \tag{6}$$

- **Multiplication**:

$$\left\{ \begin{array}{l} z = x + i\, y \\ w = u + i\, v \end{array} \right. \to z\, w = (x\, u - y\, v) + i\,(x\, v + y\, u) \tag{7}$$

- **Complex conjugate**:

$$z = x + i\, y \to z^* = x - i\, y. \tag{8}$$

Real and imaginary parts can be extracted from

$$\begin{aligned} \mathrm{Re}\, z &= \frac{1}{2}\,(z + z^*) = x, \\ \mathrm{Im}\, z &= \frac{1}{2\,i}\,(z - z^*) = y. \end{aligned} \tag{9}$$

■ Complex Number in *Mathematica*

The imaginary unit i can be typeset in *Mathematica* by ESC i ESC. For example, here is a complex number

```
3 + 1 i
```

```
3 + i
```

Multiplying two complex numbers together (*Mathematica* treats the space between two numbers as a multiplication operator just as $a\, b = a \times b$ in algebra)

```
(3 + i) (4 + 2 i)
```

```
10 + 10 i
```

Complex conjugation is given by

```
Conjugate[3 + i]
```

```
3 - i
```

Extract real and imaginary part by

```
Re[3 + i]
Im[3 + i]
```

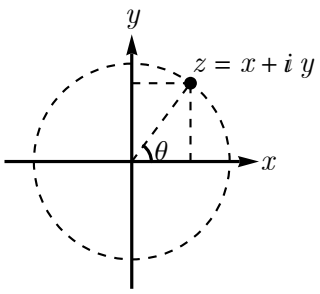
```
3
```

```
1
```

■ Polar Complex Form

Through the Euler formula, a complex number $z = x + i\, y$ may be written in a polar-coordinate form

$$z = |z| \cos\theta + i\, |z| \sin\theta = |z|\, e^{i\,\theta}. \tag{10}$$



- $|z|$ - **complex modulus** (or **magnitude**)

$$|z|^2 = z^*\, z = x^2 + y^2. \tag{11}$$

(The complex conjugate is needed here to ensure $|z|^2 \geq 0$.)

- θ - **complex argument** (or **phase**)

$$\arg z \ = \theta = \mathrm{Im} \ln z = \arctan \frac{y}{x}. \tag{12}$$

Complex numbers make it convenient to express the phase *rotation* by *multiplication* of phase factors $e^{i\theta}$, or *addition* of phase angles θ,

$$\boxed{e^{i\theta_1} e^{i\theta_2} = e^{i(\theta_1+\theta_2)}.} \tag{13}$$

Complex conjugation simply flips the phase angle ($\theta \to -\theta$),

$$\boxed{\left(e^{i\theta}\right)^* = e^{-i\theta}.} \tag{14}$$

■ Linear Algebra

■ Matrix and Vector

- A **matrix** is a two-dimensional array of numbers,

$$M = \begin{pmatrix} M_{11} & M_{12} & \cdots \\ M_{21} & M_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \in \mathbb{C}^{m\times n}. \tag{15}$$

  - Matrix elements (components) M_{ij} are labeled by a *row index* $i = 1, \ldots, m$ and a *column index* $j = 1, \ldots, n$. Each component itself is a number. Let us consider $M_{ij} \in \mathbb{C}$ to be general, such that the space of m-row n-column matrices will be denoted as $\mathbb{C}^{m\times n}$.
  - If $m = n$, the matrix is said to be a **square matrix**. In quantum mechanics, we will be mostly dealing with square matrices.
- A **vector** can be viewed as a special case of a *matrix*.
  - *Column* vectors (multi-row single-column)

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix} \in \mathbb{C}^{n\times 1} \cong \mathbb{C}^n. \tag{16}$$

  - *Row* vectors (single-row multi-column)

$$\langle v| = \begin{pmatrix} v_1^* & v_2^* & \cdots \end{pmatrix} \in \mathbb{C}^{1\times n} \cong \mathbb{C}^n. \tag{17}$$

  - *Column v.s. row*: In terms of encoding information in n numbers, it doesn't matter whether they are arranged in a column or a row. But when it comes to matrix-vector multiplication (to be discussed soon), there is a difference. So we use the $|v\rangle$ and $\langle v|$ notation to distinguish them, instead of writing both as $\boldsymbol{v}$.

■ Linear Superposition

Matrix (or vector) space. All $m \times n$ matrices forms a matrix space $\mathbb{C}^{m\times n}$. Its defining

property is that any linear combination of matrices in the space is still a matrix in the same space (same applies to vectors)

$$\forall\, A,\, B \in \mathbb{C}^{m\times n};\, \alpha, \beta \in \mathbb{C}:\\ \alpha\, A + \beta\, B \in \mathbb{C}^{m\times n} \tag{18}$$

A **linear combination** can be broken down into two types of basic operations:

- **Scalar multiplication**:

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \to \alpha\, A = \begin{pmatrix} \alpha\, A_{11} & \alpha\, A_{12} & \cdots \\ \alpha\, A_{21} & \alpha\, A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \tag{19}$$

meaning that

$$\boxed{(\alpha\, A)_{ij} = \alpha\, A_{ij}.} \tag{20}$$

- **Addition**:

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix},\, B = \begin{pmatrix} B_{11} & B_{12} & \cdots \\ B_{21} & B_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}\\ \to A + B = \begin{pmatrix} A_{11} + B_{11} & A_{12} + B_{12} & \cdots \\ A_{21} + B_{21} & A_{22} + B_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \tag{21}$$

meaning that

$$\boxed{(A + B)_{ij} = A_{ij} + B_{ij}.} \tag{22}$$

All these rules applies to vectors when matrices are single-column or single-row.

■ Matrix Multiplication

Matrix multiplication is an *associative binary* operation:

$$\mathbb{C}^{m\times n} \times \mathbb{C}^{n\times l} \to \mathbb{C}^{m\times l}, \tag{23}$$

meaning that two matrices can multiply if and only if the *column* dimension of the *left* matrix matches the *row* dimension of the *right* matrix.

- Explicitly, when we write

$$\begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} & \cdots \\ B_{21} & B_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & \cdots \\ C_{21} & C_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \tag{24}$$

we mean that

$$C_{ij} = \sum_k A_{ik}\, B_{kj}, \tag{25}$$

where $k = 1, \ldots, n$ is the index to be **contracted** (to be summed over).

- We can denote Eq. (24) on the matrix level simply as

$$A\, B = C. \tag{26}$$

Matrix-vector multiplication: If one of the matrix is reduced to a vector, the above rules still apply. A matrix can left-multiply a column vector or right-multiply a row vector, if their contracted dimensions matches.

- Left-multiplication

$$\begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix} \\ \Rightarrow v_i = \sum_j A_{ij}\, u_j, \tag{27}$$

- Right-multiplication

$$\begin{pmatrix} u_1 & u_2 & \cdots \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} v_1 & v_2 & \cdots \end{pmatrix} \\ \Rightarrow v_j = \sum_i u_i\, A_{ij}, \tag{28}$$

Vector-vector multiplication: If both matrices are reduced to vectors of the same dimension, we can define a **inner product** and a **outer product** between them.

- Inner product

$$\begin{pmatrix} u_1 & u_2 & \cdots \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix} = \sum_i u_i\, v_i = \text{"a scalar (number)"}, \tag{29}$$

- Outer product

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix} \begin{pmatrix} u_1 & u_2 & \cdots \end{pmatrix} = \begin{pmatrix} v_1\, u_1 & v_1\, u_2 & \cdots \\ v_2\, u_1 & v_2\, u_2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}. \tag{30}$$

- Multiplying two row vectors or two column vectors are illegal (because dimensions do not match).

$$(\,u_1\;\;u_2\;\;\cdots\,)\,(\,u_1\;\;u_2\;\;\cdots\,)\to\text{No!}$$

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix}\to\text{No!} \tag{31}$$

■ Identity Matrix and Kronecker Symbol

Identity matrix: a special $n\times n$ *square* matrix whose *diagonal* are all 1's and *off-diagonal* are all 0's. It looks like

$$\mathbb{1}=\begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \ddots \\ 0 & 0 & 1 & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{32}$$

- The matrix element of an identity matrix can be expressed using the **Kronecker delta** symbol δ_{ij},

$$\boxed{\mathbb{1}_{ij}=\delta_{ij}\equiv\begin{cases} 1 & i=j, \\ 0 & i\neq j. \end{cases}} \tag{33}$$

- Identity matrix multiplying on any vector keeps the vector unchanged, i.e. $\forall\,\boldsymbol{u}\in\mathbb{C}^n:\boldsymbol{u}\,\mathbb{1}=\mathbb{1}\,\boldsymbol{u}=\boldsymbol{u}$. This implies that the Kronecker delta has the following property

$$\sum_i u_i\,\delta_{ij}=u_j,$$
$$\sum_j \delta_{ij}\,u_j=u_i. \tag{34}$$

  - Rule of thumb: when δ_{ij} appears in a summation of i (or j), it annihilates with the summation symbol and replaces summation index i by j (or j by i) in the summand.

■ Matrix Algebra in *Mathematica*

Construct two matrices

```
A = {{1, 2, 3}, {4, 5, 6}, {7, 8, 9}};
B = {{9, 8, 7}, {6, 5, 4}, {3, 2, 1}};
A // MatrixForm
B // MatrixForm
```

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

$$\begin{pmatrix} 9 & 8 & 7 \\ 6 & 5 & 4 \\ 3 & 2 & 1 \end{pmatrix}$$

- Linear combine them simply as

```
A + B // MatrixForm
α A + β B // MatrixForm
```

$$\begin{pmatrix} 10 & 10 & 10 \\ 10 & 10 & 10 \\ 10 & 10 & 10 \end{pmatrix}$$

$$\begin{pmatrix} \alpha + 9\,\beta & 2\,\alpha + 8\,\beta & 3\,\alpha + 7\,\beta \\ 4\,\alpha + 6\,\beta & 5\,\alpha + 5\,\beta & 6\,\alpha + 4\,\beta \\ 7\,\alpha + 3\,\beta & 8\,\alpha + 2\,\beta & 9\,\alpha + \beta \end{pmatrix}$$

- Multiply them using "." symbol, standing for the "dot product".

```
A.B // MatrixForm
```

$$\begin{pmatrix} 30 & 24 & 18 \\ 84 & 69 & 54 \\ 138 & 114 & 90 \end{pmatrix}$$

```
B.A // MatrixForm
```

$$\begin{pmatrix} 90 & 114 & 138 \\ 54 & 69 & 84 \\ 18 & 24 & 30 \end{pmatrix}$$

Unlike multiplying two number ($a\,b = b\,a$, which is *commutative*), matrix multiplication is **non-commutative**, meaning that

$$A\,B \neq B\,A, \tag{35}$$

for two square matrices A, $B \in \mathbb{C}^{n\times n}$ *in general*.

■ Matrix as a Machine

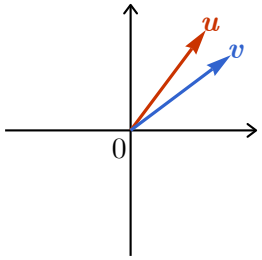
A *matrix* can be viewed as a machine that takes in a *vector*, acts (multiplies) on it, and returns a *new vector*.

Examples of 2×2 matrix M acting on 2-component vectors.

$$\boldsymbol{u} \xrightarrow{M} \boldsymbol{v} = M\,\boldsymbol{u}. \tag{36}$$

- Exchanging the two components in the vector by

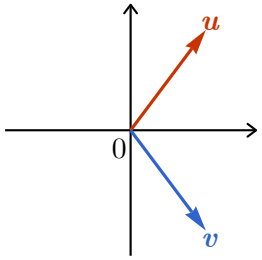
$$M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{37}$$



$$\boldsymbol{u} = \begin{pmatrix} 0.6 \\ 0.8 \end{pmatrix} \xrightarrow{M} \boldsymbol{v} = \begin{pmatrix} 0.8 \\ 0.6 \end{pmatrix}$$

- Reflecting the vector with respect to an axis by

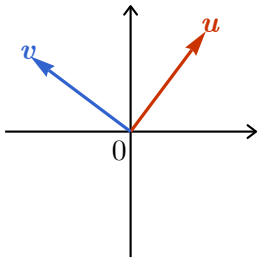
$$M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{38}$$



$$\boldsymbol{u} = \begin{pmatrix} 0.6 \\ 0.8 \end{pmatrix} \xrightarrow{M} \boldsymbol{v} = \begin{pmatrix} 0.6 \\ -0.8 \end{pmatrix}$$

- Rotating the vector by 90° counterclockwise by

$$M = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{39}$$



$$\boldsymbol{u} = \begin{pmatrix} 0.6 \\ 0.8 \end{pmatrix} \overset{M}{\to} \boldsymbol{v} = \begin{pmatrix} -0.8 \\ 0.6 \end{pmatrix}$$

■ Eigen System of a Matrix

An **eigen system** of a $n \times n$ *square* matrix M refers to the set of **eigenvalues** $\lambda^{(k)}$ and the corresponding **eigenvectors** $\boldsymbol{u}^{(k)}$ for $k = 1, \ldots, n$ such that

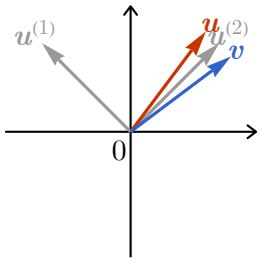
$$M\, \boldsymbol{u}^{(k)} = \lambda^{(k)}\, \boldsymbol{u}^{(k)}, \tag{40}$$

meaning that the multiplication of the matrix M to its eigenvector $\boldsymbol{u}^{(k)}$ can be reduced to the scalar multiplication by $\lambda^{(k)}$.

Examples eigen systems of 2×2 matrices M.

- Exchanging the two components in the vector by

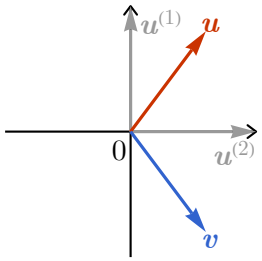
$$M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{41}$$



k	$\lambda^{(k)}$	$\boldsymbol{u}^{(k)}$
1	-1	$\begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$
2	1	$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$

- Reflecting the vector with respect to an axis by

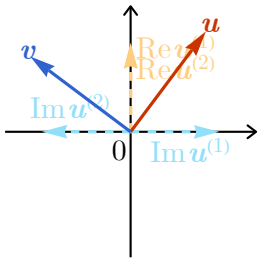
$$M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{42}$$



k	$\lambda^{(k)}$	$\boldsymbol{u}^{(k)}$
1	-1	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$
2	1	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

- Rotating the vector by 90° counterclockwise by

$$M = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{43}$$



k	$\lambda^{(k)}$	$\boldsymbol{u}^{(k)}$
1	i	$\begin{pmatrix} \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$
2	$-i$	$\begin{pmatrix} -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$

▫ Finding eigen systems in *Mathematica*

```
M = {{0, 1}, {1, 0}};
M // MatrixForm
```

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

```
Eigensystem[M]
```

```
{{-1, 1}, {{-1, 1}, {1, 1}}}
```

```
M.{-1, 1}
```

```
{1, -1}
```

```
M.{1, 1}
```

```
{1, 1}
```

Quantum States

■ Ket and Bra

■ Ket Vector

Postulate 1 (States): **States** of a quantum system are described as **vectors** in the associated Hilbert space.

In quantum mechanics, every **state** of a quantum system is described by a *complex column vector*, denoted by a **ket** (or ket state, ket vector) $|v\rangle$ in *Dirac's notation*,

$$|v\rangle \doteq \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix}, \tag{44}$$

where $v_1, v_2, \ldots \in \mathbb{C}$. The *length* of the vector depends on the **dimension** of the vector space.

- Note: "$\doteq$" implies the vector representation is *basis dependent* and the values of vector components may change if we view the same state in a different basis.
- To write down the vector representation, we must specified a set of (orthonormal) **basis vectors** in the vector space, and represent them as one-hot unit vectors:

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix}, |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ \vdots \end{pmatrix}, \ldots. \tag{45}$$

- Such that $|v\rangle$ can be expressed as a linear combination of basis vectors

$$\boxed{\begin{aligned} |v\rangle &= v_1 |1\rangle + v_2 |2\rangle + \ldots \\ &= \sum_i v_i |i\rangle. \end{aligned}} \tag{46}$$

- The ith vector component v_i is the linear combination coefficient in front of the ith basis vector $|i\rangle$.

Superposition Principle: any linear combination of quantum states of a given quantum

system is still a valid quantum state of the same system.

■ Bra Vector

Every **ket** $|v\rangle$ has a **dual vector**, called **bra** $\langle v|$, a *complex row vector*. They are related by *conjugate transpose* with respect to each other.

$$|v\rangle \doteq \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix} \overset{\text{dual}}{\longleftrightarrow} \langle v| = \begin{pmatrix} v_1^* & v_2^* & \cdots \end{pmatrix}. \tag{47}$$

The name comes from the fact that they combine into a **bracket**, which represents a scalar product [to be introduced later].

- Every basis vector $|i\rangle$ also has a **dual basis vector** $\langle i|$, the are represented as

$$\begin{aligned} &\langle 1| \doteq \begin{pmatrix} 1 & 0 & \cdots \end{pmatrix}, \\ &\langle 2| \doteq \begin{pmatrix} 0 & 1 & \cdots \end{pmatrix}, \\ &\cdots. \end{aligned} \tag{48}$$

- The dual basis vectors form a set of basis for the bra vector. In terms of basis vectors,

$$\begin{aligned} \langle v| &= v_1^* \langle 1| + v_2^* \langle 2| + \ldots \\ &= \sum_i v_i^* \langle i|. \end{aligned} \tag{49}$$

- The ith vector component v_i^* is the linear combination coefficient in front of the ith dual basis vector $\langle i|$.

■ Qubit System

A **qubit** (or **quantum-bit**) is a quantum system that has two distinct states.

- The two distinct states are $|0\rangle$ and $|1\rangle$.
- We can *choose* $|0\rangle$ and $|1\rangle$ to be the **basis** vectors (like choosing a *coordinate system*) and write:

$$|0\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \; |1\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{50}$$

  - The *vector representation* of a *quantum state* is also called a **state vector**.
  - By saying that a qubit is a **two-state system**, its *state vector* has *two components*.
- A generic quantum state of a qubit is a complex *linear superposition* of the basis states

$$|\psi\rangle = \psi_0 |0\rangle + \psi_1 |1\rangle \doteq \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}. \tag{51}$$

  - $\psi_0, \psi_1 \in \mathbb{C}$ are complex numbers. They parameterize the state $|\psi\rangle$.

- Conversely, every two-component complex vector describes a qubit state.
- **Statistical interpretation**: $|\psi_0|^2$ and $|\psi_1|^2$ are respectively the probabilities to observe the qubit in the 0 and the 1 states.

- There is a dual bra vector $\langle\psi|$ associated with each ket vector $|\psi\rangle$,

$$\langle\psi| = \psi_0^* \langle 0| + \psi_1^* \langle 1| \doteq \begin{pmatrix} \psi_0^* & \psi_1^* \end{pmatrix}, \tag{52}$$

which, the bra state, encodes the *same* information about the qubit as the ket state. They are equally good description of the quantum state of a qubit (but play different roles in defining the scalar product, as to be discussed soon).

■ Scalar Product

■ Definition

Scalar product (or **inner product**) is a function that takes two ket vectors, $|u\rangle$ and $|v\rangle$,

$$|u\rangle \doteq \begin{pmatrix} u_1 \\ u_2 \\ \vdots \end{pmatrix}, |v\rangle \doteq \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix}, \tag{53}$$

and returns a complex number, denoted by the bracket $\langle u|v\rangle$,

$$\begin{aligned} \langle u|v\rangle &\doteq \begin{pmatrix} u_1^* & u_2^* & \cdots \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix} \\ &= u_1^* v_1 + u_2^* v_2 + \ldots \\ &= \sum_i v_i^* w_i. \end{aligned} \tag{54}$$

- Exchanging the two states in a scalar product lead to a complex conjugation of result

$$\langle v|u\rangle = \langle u|v\rangle^*. \tag{55}$$

- Scalar product of any vector $|v\rangle$ with itself is *real* and *positive definite*,

$$\langle v|v\rangle \geq 0. \tag{56}$$

More specifically,

$$\langle v|v\rangle \begin{cases} = 0 & \text{if } |v\rangle = 0 \\ > 0 & \text{otherwise} \end{cases}. \tag{57}$$

- This implies the **Cauchy-Schwarz inequality**

$$|\langle u|v\rangle|^2 \leq \langle u|u\rangle \langle v|v\rangle. \tag{58}$$

Exc 1 Prove Eq. (58).

Hilbert space: the space of all ket vectors together with their scalar product structure, denoted as $\mathcal{H}$, which is the space of all possible quantum states of a system.

■ Normalization

Squared norm of a vector $|v\rangle$ is the *scalar product* of the vector with itself, denoted as

$$\|v\|^2 = \langle v|v\rangle. \tag{59}$$

Taking off the square, $\|v\| = \sqrt{\langle v|v\rangle}$ is the **norm** of $|v\rangle$.

Normalized state: a state $|v\rangle$ is **normalized** ⇔ Its *norm* is *one*, i.e.

$$\boxed{\|v\|^2 = \langle v|v\rangle = \sum_i |v_i|^2 = 1.} \tag{60}$$

- Example: Consider a qubit state

$$|v\rangle \doteq \begin{pmatrix} v_0 \\ v_1 \end{pmatrix}, \tag{61}$$

the normalization condition means

$$\langle v|v\rangle = v_0^* \, v_0 + v_1^* \, v_1 = 1. \tag{62}$$

- In general, the normalization condition means

$$\langle v|v\rangle = \sum_i |v_i|^2 = 1. \tag{63}$$

According to the statistical interpretation of quantum state, $|v_i|^2$ is the *probability* to observe the system in the ith basis state. The normalization condition is simply a requirement that the probabilities must *sum up to unity*.

- **Normalization** of a state: if a state $|v\rangle$ was *not* normalized, it can be normalized by

$$|v\rangle \to \frac{|v\rangle}{\|v\|} = \frac{1}{\sqrt{\langle v|v\rangle}} \, |v\rangle, \tag{64}$$

unless $\|v\|$ is zero or infinity.

Exc 2 Normalize the vector $|v\rangle \doteq \begin{pmatrix} 1 \\ 2\,i \end{pmatrix}$.

■ Orthogonality

Orthogonal states: two states $|u\rangle$ and $|v\rangle$ are **orthogonal** to each other ⇔ their *scalar product* is *zero*, i.e.

$$\boxed{\langle u|\, v\rangle = \sum_i u_i^* \, v_i = 0.} \tag{65}$$

- For example, the qubit states $|0\rangle$ and $|1\rangle$ (see Eq. (50)) are *orthogonal*, as

$$\langle 0|1\rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0. \tag{66}$$

  $|0\rangle$ and $|1\rangle$ are *orthogonal* for a good reason: they are **distinct** states of a qubit, i.e. if the qubit is in state 0, it is definitely not in state 1, vice versa.

■ Basis and Hilbert Space

■ Orthonormal Basis

Orthonormal basis: a (ordered) set of kets

$$\mathcal{B} = \{|i\rangle : i = 1, 2, \ldots, n\}, \tag{67}$$

in which the vectors are **normalized** by themselves and **orthogonal** to each other:

$$\langle i|j\rangle = \delta_{ij} \equiv \begin{cases} 1 & i = j, \\ 0 & i \neq j. \end{cases} \tag{68}$$

- Each orthogonal basis state describes a distinct reality of the quantum system.
- Orthonormal basis states are *represented* by **one-hot vectors**, as they are normalized and orthogonal to each other

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \; |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \; |3\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}, \; \ldots. \tag{69}$$

Choosing a basis is always a helpful practice in quantum mechanics. But quantum mechanics can be formulated in a basis independent manner.

■ Hilbert Space

A set of orthonormal basis spans a **Hilbert space** (the vector space of kets), denoted as

$$\mathcal{H} = \text{span}\, \mathcal{B} = \text{span}\, \{|i\rangle : i = 1, 2, \ldots, n\}. \tag{70}$$

- The **dimension** of the vector space $\dim \mathcal{H}$ = the number n of basis vectors = the *maximal* number of *linearly independent* vectors in the space.
  - The Hilbert space dimension of a quantum system can be *finite* or *infinite*. Example: a qubit - $\dim \mathcal{H} = 2$, ten qubits - $\dim \mathcal{H} = 2^{10} = 1024$, a particle in a continuous space - $\dim \mathcal{H} = \infty$.

- Dimension of the Hilbert space is often a *choice*: we don't really know how many independent states are there in a quantum system. We only care about the states that are *relevant* to us.

- Example: $|0\rangle$ and $|1\rangle$ form an *orthonormal basis* of the qubit Hilbert space. They represent two distinct realities: if the qubit is in state $|0\rangle$, it is definitely not in state $|1\rangle$ (and vice versa).

State Basis Expansion

Completeness: Any *full* set of *distinct* states in the Hilbert space $\mathcal{H}$ forms a *complete* set of orthonormal basis $\mathcal{B}$, such that *every* state $|v\rangle \in \mathcal{H}$ can be expanded as a *linear superposition* of the basis states,

$$|v\rangle = v_1 |1\rangle + v_2 |2\rangle + \ldots = \sum_i v_i |i\rangle. \tag{71}$$

- Each basis state $|i\rangle$ describes a distinct reality that the quantum system can realize under observation.

- The *superposition coefficient* v_i are the **components** of the state vector, which can be extracted by the *scalar product* with the basis state,

$$v_i = \langle i|v\rangle. \tag{72}$$

Eq. (71) and Eq. (72) can be written in a more elegant form in terms of bras and kets only

$$|v\rangle = \sum_i |i\rangle \langle i|v\rangle. \tag{73}$$

- **Statistical interpretation**: If a quantum system is known to be in a superposition state $|v\rangle = \sum_i v_i |i\rangle$ of distinct realities described by orthogonal states $|i\rangle$ ($i = 1, 2, \ldots$), an observation designed to discern which reality the system is really in will find the system in the state $|i\rangle$ with the probability

$$p(i \mid v) = |v_i|^2 = |\langle i|v\rangle|^2. \tag{74}$$

Born's Rule

Fidelity

The **fidelity** $F(u, v)$ between two quantum states $|u\rangle$ and $|v\rangle$ quantifies the similarity (overlap) between two states. It is given by the squared absolute value of their scalar product (assuming the normalization of state vectors)

$$F(u, v) = |\langle u|v\rangle|^2. \tag{75}$$

- Fidelity is *symmetric*: $F(u, v) = F(v, u)$.
- Fidelity takes values in the range of

$$0 \le F(u, v) \le 1. \tag{76}$$

This follows from the Cauchy-Schwarz inequality of scalar product Eq. (58) that $|\langle u|v\rangle|^2 \le \langle u|u\rangle \langle v|v\rangle$.

▪ Statistical Interpretation

Hypothesis testing: If a quantum system is prepared in a state $|v\rangle$, an observation designed to check whether the system is in the state $|u\rangle$ will return a confirmative result with probability

$$\boxed{p(u \mid v) = |\langle u|v\rangle|^2.} \tag{77}$$

Detailed balance: the probability to observe one state given another is the same as the other way round, both are given by their fidelity

$$p(u \mid v) = p(v \mid u) = F(u, v) = |\langle u|v\rangle|^2. \tag{78}$$

- **Identical states**. Two states $|u\rangle$ and $|v\rangle$ are *identical* iff the fidelity between them is *one* (fully overlap)

$$|\langle u|v\rangle|^2 = 1. \tag{79}$$

  - This is only achievable when

$$|u\rangle = e^{i\varphi} |v\rangle, \tag{80}$$

    i.e. the two states are the same up to phase ambiguity.

  - **Reality** must be *confirmable* by *repeated* observations: if a quantum system is known to be in a state $|v\rangle$, observing the system again will certainly confirm the state $|v\rangle$ (with probability 1).

- **Distinct states**. Two states $|u\rangle$ and $|v\rangle$ are *distinct* iff the fidelity between them is *zero* (no overlap)

$$|\langle u|v\rangle|^2 = 0. \tag{81}$$

  - *Orthogonal* states $\Leftrightarrow$ *distinct* realities.
  - **Distinct realities** are *distinguishable* by *repeated* observations: if a quantum system is known to be in a state $|v\rangle$, observing the system again will certainly not find the system in another orthogonal state $|u\rangle$.

- **Overlapping states**. In general, two different states $|u\rangle$ and $|v\rangle$ may have partial overlap (they don't need to be orthogonal), i.e. their fidelity falls between zero and one

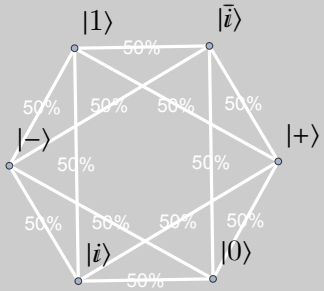
$$0 < |\langle u|v\rangle|^2 < 1. \tag{82}$$

  - Realities can overlap: if two quantum states are more similar to (more overlapped with) each other, the probability to confuse them is higher.

|"3"⟩ ≐  , |"5"⟩ ≐  .

HW 1

{|0⟩, |1⟩}, {|+⟩, |−⟩}, and {|i⟩, |ī⟩} are three pairs of distinct states of a *qubit* (i.e. 2-dimensional Hilbert space). Within each pair, the two states are orthogonal. However, any two states from different pairs have 50% overlap (i.e. 1/2 fidelity). Their overlapping relations can be visualized as the following graph.



Can you figure out an assignment of 2-component vector representation for these states that is consistent with their overlapping relations?
[Hint: read Lecture 2 of [4]]
[Comment: This result shows how it is possible to embed so many different realities just in a 2-dimensional Hilbert space.]

[4] Leonard Susskind, Art Friedman. *Quantum Mechanics - the Theoretical Minimum*. Publisher: Basic Books (2014).

Quantum Operators

■ Matrix Representation

■ Definition

Operator: an operator acts on a state and returns a new state.

$$\begin{aligned} \hat{O} : \mathcal{H} &\to \mathcal{H} \\ |v\rangle &\mapsto |w\rangle = \hat{O}\,|v\rangle \end{aligned} \tag{83}$$

- **Identity operator** is a special operator that maps any state to itself (the do-nothing operator), denoted as $\mathbb{1}$.

$$\forall\, |v\rangle : \mathbb{1}\,|v\rangle = |v\rangle. \tag{84}$$

■ Operator Acting on State

Recall: a matrix *multiplying* on a vector produces a new vector. If every **quantum state** is described by a **vector**, one may conjecture that every **quantum operator** should be described

by a (square) **matrix**. --- This is indeed a basic assumption of quantum mechanics: states are to be operated (transformed) *linearly*.

Applying an *operator* to a *state* ≐ multiplying a *matrix* to a *vector*.

$$\begin{array}{ccc} |w\rangle & = & \hat{O} \quad\quad |v\rangle \\ \downarrow\doteq & & \downarrow\doteq \quad\quad \downarrow\doteq \\ \begin{pmatrix} w_1 \\ w_2 \\ \vdots \end{pmatrix} & = & \begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix} \end{array} \tag{85}$$

or equivalently

$$w_i = \sum_j O_{ij}\, v_j. \tag{86}$$

- The **matrix element** O_{ij} tells how the operator should act on each basis states: the operator $\hat{O}$ will turn a basis state $|j\rangle$ to a superposition state of basis states $|i\rangle$ with superposition coefficients O_{ij}.

$$\hat{O}\,|j\rangle = \sum_i O_{ij}\,|i\rangle. \tag{87}$$

Exc 3 Show Eq. (87) as a result of Eq. (85) using one-hot representation for basis vectors.

- In other words, O_{ij} is the **amplitude** to transform basis state $|j\rangle$ to basis state $|i\rangle$ under the action of the operator $\hat{O}$. It is sufficient to specify the operator by specifying its action on basis states, as all possible states are just linear combination of basis states, and the operator acts linearly.

■ Operator Basis Expansion

Given an *orthonormal* basis $\mathcal{B} = \{|i\rangle : i = 1, 2, ...\}$ of the Hilbert space $\mathcal{H}$, every *operator* $\hat{O}$ acting in $\mathcal{H}$ can be expanded as a *linear combination* of **basis operators** $|i\rangle\langle j|$,

$$\hat{O} = \sum_{ij} |i\rangle\, O_{ij}\, \langle j|, \tag{88}$$

- $|i\rangle\langle j|$ denotes the operator that targets the state $|j\rangle$ and transforms it to the state $|i\rangle$, because

$$\begin{aligned} &(|i\rangle\langle j|)\,|k\rangle = |i\rangle\langle j|k\rangle = |i\rangle\,\delta_{jk} \\ &= \begin{cases} |i\rangle & \text{if } k = j, \\ 0 & \text{if } k \neq j. \end{cases} \end{aligned} \tag{89}$$

  Thus Eq. (88) is consistent with the Eq. (87) in describing how the operator $\hat{O}$ acts on the state.

- $O_{ij} \in \mathbb{C}$ are *complex* coefficients, which can be extracted by

$$O_{ij} = \langle i| \hat{O} |j\rangle. \tag{90}$$

Exc 4 Prove Eq. (90) from Eq. (88) using the orthonormal property of the basis vectors, without representing them as on-hot vectors explicitly.

- Alternatively, $|i\rangle\langle j|$ can be represented as an **one-hot matrix** that is zero everywhere with a single 1 at the row-i column-j. For example, in a 2-dimensional Hilbert space [recall Eq. (30) for how to outer product two vectors]

$$\begin{aligned}
|1\rangle\langle 1| &\doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \\
|1\rangle\langle 2| &\doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \\
|2\rangle\langle 1| &\doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \\
|2\rangle\langle 2| &\doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.
\end{aligned} \tag{91}$$

Therefore, Eq. (88) indeed reconstructs the matrix representation

$$\begin{aligned}
&O_{11}|1\rangle\langle 1| + O_{12}|1\rangle\langle 2| + O_{21}|2\rangle\langle 1| + O_{22}|2\rangle\langle 2| \\
&\doteq \begin{pmatrix} O_{11} & O_{12} \\ O_{21} & O_{22} \end{pmatrix}.
\end{aligned} \tag{92}$$

The above can be generalized to larger matrices (higher dimensions).

Matrix representation. Every operator $\hat{O}$ can be represented as a matrix

$$\hat{O} \doteq \begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}. \tag{93}$$

The ith row jth column matrix element O_{ij} describes:

- The linear combination coefficient in front of the basis operator $|i\rangle\langle j|$, as in Eq. (88).
- The amplitude to transform state $|j\rangle$ to state $|i\rangle$ under the action of the operator $\hat{O}$, as in Eq. (87).

■ Examples of Operators

Example I: Identity operator

Identity operator is universally represented by the **identity matrix** in any orthonormal basis (independent of the basis choice).

According to Eq. (90),

$$\mathbb{1}_{ij} = \langle i|\,\mathbb{1}\,|j\rangle = \langle i|j\rangle = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}. \tag{94}$$

- In matrix representation Eq. (93),

$$\mathbb{1} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & \ddots \end{pmatrix}. \tag{95}$$

- Using Dirac notation Eq. (88),

$$\boxed{\mathbb{1} = \sum_{ij} |i\rangle\, \mathbb{1}_{ij}\, \langle j| = \sum_{i} |i\rangle\, \langle i|.} \tag{96}$$

This is also call the **resolution of identity**.

Example II: Pauli operators

Pauli operators are a set of operators acting on a qubit.

$$\begin{aligned} \hat{\sigma}^x &= |1\rangle\langle 0| + |0\rangle\langle 1|, \\ \hat{\sigma}^y &= i\,|1\rangle\langle 0| - i\,|0\rangle\langle 1|, \\ \hat{\sigma}^z &= |0\rangle\langle 0| - |1\rangle\langle 1|, \end{aligned} \tag{97}$$

Sometimes the identity operator

$$\mathbb{1} = |0\rangle\langle 0| + |1\rangle\langle 1|, \tag{98}$$

is also included as the 0th Pauli operator.

Pauli matrices - matrix representations of Pauli operators on the qubit basis $\{|0\rangle, |1\rangle\}$:

$$\boxed{\mathbb{1} \doteq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \hat{\sigma}^x \doteq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \hat{\sigma}^y \doteq \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \hat{\sigma}^z \doteq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.} \tag{99}$$

■ Operator Algebra

■ Operator Product

Product (or **composition**) of two **operators** $\hat{O}$ and $\hat{P}$ is a combined operator $\hat{O}\,\hat{P}$ that first applies $\hat{P}$ to the sate then applies $\hat{O}$ (from *right* to *left*):

$$\left(\hat{O}\,\hat{P}\right)|v\rangle = \left(\hat{O}\left(\hat{P}\,|v\rangle\right)\right). \tag{100}$$

- Composing two *operators* $\doteq$ multiplying two *matrices*.

$$\hat{O}\,\hat{P} \doteq \begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} P_{11} & P_{12} & \cdots \\ P_{21} & P_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}. \tag{101}$$

Exc 5 Prove Eq. (101) using Eq. (88).

- Operator product is *non-commutative* in general, i.e.

$$\hat{O}\,\hat{P} \neq \hat{P}\,\hat{O}. \tag{102}$$

■ Single-Qubit Pauli Operators

Example: product of Pauli operators

Multiplication table

	$\mathbb{1}$	$\hat{\sigma}^x$	$\hat{\sigma}^y$	$\hat{\sigma}^z$
$\mathbb{1}$	$\mathbb{1}$	$\hat{\sigma}^x$	$\hat{\sigma}^y$	$\hat{\sigma}^z$
$\hat{\sigma}^x$	$\hat{\sigma}^x$	$\mathbb{1}$	$i\,\hat{\sigma}^z$	$-i\,\hat{\sigma}^y$
$\hat{\sigma}^y$	$\hat{\sigma}^y$	$-i\,\hat{\sigma}^z$	$\mathbb{1}$	$i\,\hat{\sigma}^x$
$\hat{\sigma}^z$	$\hat{\sigma}^z$	$i\,\hat{\sigma}^y$	$-i\,\hat{\sigma}^x$	$\mathbb{1}$

(103)

Exc 6 Verify Eq. (103) by multiplying Pauli matrices defined in Eq. (99).

- The table Eq. (103) can be summarized in a single formula: the product of Pauli matrices (as the defining property of Pauli matrices)

$$\hat{\sigma}^a\,\hat{\sigma}^b = \delta^{ab}\,\mathbb{1} + i\,\epsilon^{abc}\,\hat{\sigma}^c, \tag{104}$$

where a, b, $c = x$, y, z.

- δ^{ab} denotes the Kronecker delta symbol, defined as

$$\delta^{ab} = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{if } a \neq b \end{cases} \tag{105}$$

- ϵ^{abc} denotes the Levi-Civita symbol, defined as

$$\epsilon^{abc} = \begin{cases} 1 & \text{if } (a\ b\ c) \text{ is a cyclic of } (x\ y\ z) \\ -1 & \text{if } (a\ b\ c) \text{ is a cyclic of } (z\ y\ x) \\ 0 & \text{otherwise} \end{cases} \tag{106}$$

- Another version of Eq. (104) using vector notation

$$(\boldsymbol{m}\cdot\hat{\boldsymbol{\sigma}})\,(\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}}) = (\boldsymbol{m}\cdot\boldsymbol{n})\,\mathbb{1} + i\,(\boldsymbol{m}\times\boldsymbol{n})\cdot\hat{\boldsymbol{\sigma}}, \tag{107}$$

where $\boldsymbol{m}$, $\boldsymbol{n}$ are three-component vectors (each component is a scalar).

- The generalized vector $\hat{\boldsymbol{\sigma}}$ should be understood as a vector of matrices, or as a three-dimensional tensor (shape: $3 \times 2 \times 2$).
- Here $\boldsymbol{m} \cdot \hat{\boldsymbol{\sigma}}$ means

$$\begin{aligned} \boldsymbol{m} \cdot \hat{\boldsymbol{\sigma}} &= m_x\, \hat{\sigma}^x + m_y\, \hat{\sigma}^y + m_z\, \hat{\sigma}^z \\ &\doteq \begin{pmatrix} m_z & m_x - i\, m_y \\ m_x + i\, m_y & -m_z \end{pmatrix}. \end{aligned} \tag{108}$$

  As we contract a 3-component vector $\boldsymbol{m}$ with a $3 \times 2 \times 2$-component tensor $\hat{\boldsymbol{\sigma}}$ along the first index (the dimension 3 index), the result is a 2×2 matrix.
- Repeatedly applying Eq. (107) enables us to product more Pauli operators together. For example

$$(\boldsymbol{l} \cdot \hat{\boldsymbol{\sigma}})\, (\boldsymbol{m} \cdot \hat{\boldsymbol{\sigma}})\, (\boldsymbol{n} \cdot \hat{\boldsymbol{\sigma}}) = i\, \boldsymbol{l} \cdot (\boldsymbol{m} \times \boldsymbol{n})\, \mathbb{1} + ((\boldsymbol{m} \cdot \boldsymbol{n})\, \boldsymbol{l} - (\boldsymbol{l} \cdot \boldsymbol{n})\, \boldsymbol{m} + (\boldsymbol{l} \cdot \boldsymbol{m})\, \boldsymbol{n}) \cdot \hat{\boldsymbol{\sigma}}\,. \tag{109}$$

Exc 7 Derive Eq. (109).

■ Commutator

Commutator of two operators $\hat{O}$ and $\hat{P}$

$$\boxed{\left[\hat{O},\, \hat{P}\right] = \hat{O}\, \hat{P} - \hat{P}\, \hat{O}.} \tag{110}$$

- Commutator is *antisymmetric*, $\left[\hat{O},\, \hat{P}\right] = -\left[\hat{P},\, \hat{O}\right]$.
- As a result, *commutator* of an operator with *itself* always *vanishes* $\left[\hat{O},\, \hat{O}\right] = 0$.
- If the commutator vanishes $\left[\hat{O},\, \hat{P}\right] = 0$, we say that the two operators $\hat{O}$ and $\hat{P}$ **commute**, i.e. $\hat{O}\, \hat{P} = \hat{P}\, \hat{O}$ (operators can *pass though* each other as if they were *numbers*) ⇒ it does not matter which operator is applied first, the consequence will be the same.

Example: dressing up to school.

- A: put on the socks,
- B: put on the shoes,
- C: put on the hat,

A and B do *not commute* (changing the order leads to different result). But A and C *commute*, B and C also *commute* (changing the order does not affect the result).

Useful *rules* to evaluate commutators

- **Bi-linearity**:

$$\begin{aligned} \left[\hat{O},\, \hat{P} + \hat{Q}\right] &= \left[\hat{O},\, \hat{P}\right] + \left[\hat{O},\, \hat{Q}\right], \\ \left[\hat{O} + \hat{P},\, \hat{Q}\right] &= \left[\hat{O},\, \hat{Q}\right] + \left[\hat{P},\, \hat{Q}\right]. \end{aligned} \tag{111}$$

Exc 8 Prove Eq. (111).

- **Product rules**:

$$\begin{aligned}\left[\hat{O}, \hat{P}\,\hat{Q}\right] &= \left[\hat{O}, \hat{P}\right]\hat{Q} + \hat{P}\left[\hat{O}, \hat{Q}\right],\\ \left[\hat{O}\,\hat{P}, \hat{Q}\right] &= \left[\hat{O}, \hat{Q}\right]\hat{P} + \hat{O}\left[\hat{P}, \hat{Q}\right].\end{aligned} \tag{112}$$

Exc 9 Prove Eq. (112).

Example: Commutators of Pauli operators

$$\begin{aligned}\left[\hat{\sigma}^x, \hat{\sigma}^y\right] &= 2\,i\,\hat{\sigma}^z,\\ \left[\hat{\sigma}^y, \hat{\sigma}^z\right] &= 2\,i\,\hat{\sigma}^x,\\ \left[\hat{\sigma}^z, \hat{\sigma}^x\right] &= 2\,i\,\hat{\sigma}^y.\end{aligned} \tag{113}$$

Or more compactly as

$$\boxed{\left[\hat{\sigma}^a, \hat{\sigma}^b\right] = 2\,i\,\epsilon^{abc}\,\hat{\sigma}^c,} \tag{114}$$

for $a, b, c = x, y, z$, using the Levi-Civita symbol ϵ^{abc} defined in Eq. (106).

- Eq. (114) can be considered as the defining algebraic properties of *single-qubit operators* (Pauli matrices). Or even more compactly expressed using the **cross product** of vectors

$$\boxed{\hat{\boldsymbol{\sigma}} \times \hat{\boldsymbol{\sigma}} = 2\,i\,\hat{\boldsymbol{\sigma}}.} \tag{115}$$

■ Operator Function

Operator power. nth power of an operator $\hat{O}$ is the composition of $\hat{O}$ by n times.

$$\hat{O}^n = \hat{O}\,\hat{O}\,\ldots(n\,\text{times})\ldots\,\hat{O}. \tag{116}$$

Operator function. Given a function $f(x)$ that admits Taylor expansion

$$f(x) = \sum_n c_n\,x^n, \tag{117}$$

the corresponding operator function is defined as

$$\boxed{f(\hat{O}) = \sum_n c_n\,\hat{O}^n,} \tag{118}$$

with the same set of coefficients c_n.

- $f(\hat{O})$ is still an operator that can act on states in $\mathcal{H}$.
- **Operator exponential**. Given the exponential function

$$e^x = 1 + x + \frac{x^2}{2!} + \ldots = \sum_{n=0}^{\infty} \frac{1}{n!}\, x^n, \tag{119}$$

the exponential of an operator is defined as

$$e^{\hat{O}} = \mathbb{1} + \hat{O} + \frac{\hat{O}^2}{2!} + \ldots = \sum_{n=0}^{\infty} \frac{1}{n!}\, \hat{O}^n, \tag{120}$$

- Note: exponentiating an matrix is NOT exponentiating each of the matrix element.

Example: exponentiating a Pauli matrix

Exc 10

Given $\hat{\sigma}^y \doteq \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$,
show that the matrix representation of $e^{i\,\theta\,\hat{\sigma}^y}$ is
$e^{i\,\theta\,\hat{\sigma}^y} \doteq \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$.

HW 2

Use the definition Eq. (120) to prove that
$\exp(i\,\theta\,\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}}) = \cos(\theta)\,\mathbb{1} + i\sin(\theta)\,\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}}$
given that $\boldsymbol{n}$ is a 3-component *real unit vector*.

■ Operator Trace

The **trace** of an operator $\hat{O}$ is defined as

$$\boxed{\mathrm{Tr}\ \hat{O} = \sum_i \langle i|\ \hat{O}\ |i\rangle.} \tag{121}$$

The result is a scalar.

- On the matrix level, taking the trace is simply *summing* over *diagonal* matrix elements

$$\mathrm{Tr}\begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} = O_{11} + O_{22} + \ldots = \sum_i O_{ii}. \tag{122}$$

- **Linear property**: trace is a *linear functional* of operators.

$$\mathrm{Tr}\left(\alpha\ \hat{O} + \beta\ \hat{P}\right) = a\,\mathrm{Tr}\ \hat{O} + \beta\,\mathrm{Tr}\ \hat{P}. \tag{123}$$

- **Cyclic property**: the trace of a product of operators is invariant under the cyclic permutation of the operators.

$$\begin{aligned}&\mathrm{Tr}\left(\hat{O}\,\hat{P}\right) = \mathrm{Tr}\left(\hat{P}\,\hat{O}\right),\\&\mathrm{Tr}\left(\hat{O}\,\hat{P}\,\hat{Q}\right) = \mathrm{Tr}\left(\hat{P}\,\hat{Q}\,\hat{O}\right) = \mathrm{Tr}\left(\hat{Q}\,\hat{O}\,\hat{P}\right),\\&\cdots\end{aligned} \tag{124}$$

Exc 11 Prove Eq. (124).

The operator trace is *useful* in computing **scalar product** or **fidelity**:

- Scalar product

$$\boxed{\langle u|v\rangle = \mathrm{Tr}\,|v\rangle\langle u|.} \tag{125}$$

- Fidelity

$$|\langle u|v\rangle|^2 = \langle u|v\rangle\langle v|u\rangle = \mathrm{Tr}\,|v\rangle\langle v|\,|u\rangle\langle u|. \tag{126}$$

Example: trace of Pauli operators

Pauli operators are *traceless*.

$$\mathrm{Tr}\,\hat{\sigma}^x = \mathrm{Tr}\,\hat{\sigma}^y = \mathrm{Tr}\,\hat{\sigma}^z = 0. \tag{127}$$

This is true for a Pauli operator along any direction

$$\boxed{\mathrm{Tr}\,\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}} = 0.} \tag{128}$$

Measurement

■ Hermitian Operators

■ Hermitian Conjugate

We have explained how an operator $\hat{O}$ acts on a *ket* state $|v\rangle$, what about its action on the *bra* state $\langle v|$?

	ket	bra (dual)
Hilbert space	$\mathcal{H}$	$\mathcal{H}^*$
basis	$\mathcal{B} = \{\|i\rangle\}$	$\mathcal{B}^* = \{\langle i\|\}$
state	$\|v\rangle = \sum_i v_i\,\|i\rangle$	$\langle v\| = \sum_i v_i^*\,\langle i\|$
vector	$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix}$	$\begin{pmatrix} v_1^* & v_2^* & \cdots \end{pmatrix}$
component	$v_i = \langle i\|v\rangle$	$v_i^* = \langle v\|i\rangle$

(129)

operator	$\hat{O} = \sum_{ij} \lvert i\rangle\, O_{ij}\, \langle j\rvert$	$\hat{O}^\dagger = \sum_{ij} \lvert i\rangle\, O^*_{ji}\, \langle j\rvert$
matrix	$\begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$	$\begin{pmatrix} O^*_{11} & O^*_{21} & \cdots \\ O^*_{12} & O^*_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$
component	$O_{ij} = \langle i\rvert\, \hat{O}\, \lvert j\rangle$	$O^*_{ij} = \langle j\rvert\, \hat{O}^\dagger\, \lvert i\rangle$
action	$\lvert w\rangle = \hat{O}\, \lvert v\rangle$	$\langle w\rvert = \langle v\rvert\, \hat{O}^\dagger$

- Just like the *bra* $\langle v|$ is the **dual** of the *ket* $|u\rangle$, the **Hermitian conjugate** operator $\hat{O}^\dagger$ is the **dual** of the original operator $\hat{O}$, such that
  - if the operator $\hat{O}$ takes $|v\rangle$ to $|w\rangle$:

$$\begin{aligned} \hat{O} : \mathcal{H} &\to \mathcal{H} \\ |v\rangle &\mapsto |w\rangle = \hat{O}\,|v\rangle \end{aligned} \tag{130}$$

  - then the operator $\hat{O}^\dagger$ takes $\langle v|$ to $\langle w|$:

$$\begin{aligned} \hat{O}^\dagger : \mathcal{H}^* &\to \mathcal{H}^* \\ \langle v| &\mapsto \langle w| = \langle v|\, \hat{O}^\dagger \end{aligned} \tag{131}$$

- Given an *orthonormal* basis $\mathcal{B} = \{|i\rangle : i = 1, 2, \ldots\}$ of the Hilbert space $\mathcal{H}$, if $\hat{O}$ is given by

$$\hat{O} = \sum_{ij} |i\rangle\, O_{ij}\, \langle j|, \tag{132}$$

then $\hat{O}^\dagger$ should be given by

$$\boxed{\hat{O}^\dagger = \sum_{ij} |i\rangle\, O^*_{ji}\, \langle j|.} \tag{133}$$

Exc 12 Verify that Eq. (133) is consistent with the definition Eq. (131).

- In terms of *matrix* representation, the **Hermitian conjugate** acts as
  - **matrix transpose** (interchanges the rows and columns),
  - followed by **complex conjugation** of each matrix element.

$$\begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}^\dagger = \begin{pmatrix} O^*_{11} & O^*_{21} & \cdots \\ O^*_{12} & O^*_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}. \tag{135}$$

How to think of it: Hermitian conjugate ~ a generalization of *complex conjugate* from complex *numbers* to *matrices*.

Hermitian conjugate has the following properties:

- **Duality**: suppose $\hat{O}$ is an operator

$$\hat{O}^{\dagger\dagger} = \hat{O}. \tag{136}$$

- **Linearity**: suppose $\hat{O}$ and $\hat{P}$ are operators, α and β are complex numbers,

$$\left(\alpha\, \hat{O} + \beta\, \hat{P}\right)^{\dagger} = \alpha^*\, \hat{O}^{\dagger} + \beta^*\, \hat{P}^{\dagger}. \tag{137}$$

- **Transpose Property**: suppose $\hat{O}$ and $\hat{P}$ are operators

$$\boxed{\left(\hat{O}\, \hat{P}\right)^{\dagger} = \hat{P}^{\dagger}\, \hat{O}^{\dagger}.} \tag{138}$$

Exc 13 Prove the property Eq. (138).

■ Hermitian Operator

Real numbers play a special role in physics. The results of any measurements are real. If in quantum mechanics, physical observables are represented by *operators*, how do we impose the "real" condition on operators?

- A **real number** is a number whose *complex conjugation* is itself.

$$z = z^* \Leftrightarrow z \in \mathbb{R}. \tag{139}$$

- A ~~real operator~~ **Hermitian operator** is an linear operator whose *Hermitian conjugate* is itself.

An operator $\hat{O} = \sum_{ij} |i\rangle\, O_{ij}\, \langle j|$ is call **Hermitian**, if

$$\boxed{\hat{O} = \hat{O}^{\dagger},} \tag{140}$$

or in terms of matrix elements,

$$O_{ij} = O_{ji}^*. \tag{141}$$

■ Eigensystem (General)

Given an operator $\hat{O}$, the **eigenvectors** $|O_k\rangle$ are a set of special vectors, on which the operator $\hat{O}$ acts as a *scalar* multiplication

$$\boxed{\hat{O}\, |O_k\rangle = O_k\, |O_k\rangle, \;\; (k = 1, 2, \ldots)} \tag{142}$$

and the corresponding scalars O_k are called the **eigenvalues** (of the corresponding eigenvectors).

- Eq. (142) is called the **eigen equation** of an operator $\hat{O}$.
  - The eigenvalues can be found by solving the algebraic (polynomial) equation for O

$$\det\left(\hat{O} - O\,\mathbb{1}\right) = 0. \tag{143}$$

- For each solution of eigenvalue $O = O_k$, the corresponding eigenvector $|O_k\rangle$ is found by solving the linear equation

$$\left(\hat{O} - O_k\,\mathbb{1}\right)|O_k\rangle = 0. \tag{144}$$

- Use *Mathematica* to solve the eigen problem (recommended)

```
Eigensystem[{{0, 1}, {1, 0}}]
```

```
{{-1, 1}, {{-1, 1}, {1, 1}}}
```

■ Eigensystem (Hermitian Operators)

What is special about Hermitian operators?

Suppose $\hat{O} = \hat{O}^\dagger$ is a Hermitian operator and

$$\hat{O}\,|O_k\rangle = O_k\,|O_k\rangle,\ (k = 1, 2, \ldots). \tag{145}$$

- **Eigenvalues** are **real**.

$$\hat{O} = \hat{O}^\dagger \Rightarrow O_k \in \mathbb{R}. \tag{146}$$

- **Eigenvectors** form a **complete** set of basis. (Any vector can be expanded as a sum of these eigenvectors.)
  - Eigenvectors of *different* eigenvalues are *orthogonal* (automatically)

$$O_k \neq O_l \Rightarrow \langle O_k|O_l\rangle = 0. \tag{147}$$

  - Eigenvectors of the *same* eigenvalue can be *made orthogonal* (by orthogonalization, e.g. Gram-Schmidt procedure).

```
Orthogonalize[{{1, 2}, {3, 4}}]
```

$$\left\{\left\{\frac{1}{\sqrt{5}}, \frac{2}{\sqrt{5}}\right\}, \left\{\frac{2}{\sqrt{5}}, -\frac{1}{\sqrt{5}}\right\}\right\}$$

  - For *bounded* Hermitian operators (e.g. finite matrices in finite dimensional Hilbert space), eigenvectors can be *normalized*.

Exc 14 Prove Eq. (146) and Eq. (147).

Therefore each **Hermitian operator** $\hat{O}$ generates a *complete* set of *orthonormal* basis $\{|O_k\rangle : k = 1, 2, \ldots\}$ for the Hilbert space $\mathcal{H}$, also called the **eigenbasis** of $\hat{O}$.

- The completeness of the basis implies

$$\sum_k |O_k\rangle \langle O_k| = \mathbb{1}. \tag{149}$$

- Hermitian operator $\hat{O}$ can always be represented in its own eigenbasis, leading to the **spectral decomposition**

$$\hat{O} = \sum_k |O_k\rangle \, O_k \, \langle O_k|. \tag{150}$$

  - Note: unlike a generic matrix representation $\hat{O} = \sum_{ij} |i\rangle \, O_{ij} \, \langle j|$, in the spectral decomposition Eq. (150), the summation only run through the eigenbasis once.
  - In the eigenbasis, the Hermitian operator is represented as a **diagonal matrix**.

$$\hat{O} \simeq \begin{pmatrix} O_1 & & \\ & O_2 & \\ & & \ddots \end{pmatrix}. \tag{151}$$

    So the procedure of bring the *matrix* representation to its *diagonal* form by transforming to its *eigenbasis* is called **diagonalization**. (We will discuss more about it later.)

Diagonalization is particularly useful in constructing the operator function. For example, the operator function $f(\hat{O})$ defined in Eq. (118) can be constructed by

$$f(\hat{O}) = \sum_k |O_k\rangle \, f(O_k) \, \langle O_k|, \tag{152}$$

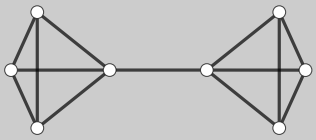
Exc 15 Prove Eq. (152).

or in the matrix form as

$$f(\hat{O}) \simeq \begin{pmatrix} f(O_1) & & \\ & f(O_2) & \\ & & \ddots \end{pmatrix}.$$

HW 3

A particle can travel on a graph.



Let $|i\rangle$ denotes the state that the particle stays on the ith vertex of the graph. The following operator

$\hat{H} = -\sum_{i \rightarrowtail j} (|i\rangle\langle j| + |j\rangle\langle i|)$

describes the quantum process for the particle to tunnel from one vertex to the adjacent vertex (the summation sums over all links $i \rightarrowtail j$ on the graph).

(i) Represent the operator $\hat{H}$ as a matrix in the basis of $\{|i\rangle\}$.

(ii) Write a computer program to compute the lowest and second lowest eigenvalues.

(iii) Visualizing the corresponding eigen vectors by marking the vector components on the graph. What do you find?

[Comment: quantum mechanics can be applied to classify vertices on a graph --- an algorithm known as the **spectral clustering**.]

■ Eigensystem (Pauli Operators)

Example: Eigenvalues and eigenvectors of Pauli operators

Pauli matrices are 2×2 Hermitian matrices. Each one has two distinct eigenvalues, and two corresponding orthogonal eigenvectors.

opertor	$\hat{\sigma}^x$		$\hat{\sigma}^y$		$\hat{\sigma}^z$	
(matrix)	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$		$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$		$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	
eigenvalue	$+1$	-1	$+1$	-1	$+1$	-1
eigenvector	$\|+\rangle$	$\|-\rangle$	$\|i\rangle$	$\|\bar{i}\rangle$	$\|0\rangle$	$\|1\rangle$
(vector)	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$
projector	$\|+\rangle\langle+\|$	$\|-\rangle\langle-\|$	$\|i\rangle\langle i\|$	$\|\bar{i}\rangle\langle\bar{i}\|$	$\|0\rangle\langle 0\|$	$\|1\rangle\langle 1\|$
(matrix)	$\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

(153)

Spectral decompositions:

- Pauli-x

$$\hat{\sigma}^x = |+\rangle\langle+| - |-\rangle\langle-|, \tag{154}$$

with projection operators

$$|+\rangle\langle+| = \frac{\mathbb{1}+\hat{\sigma}^x}{2},$$
$$|-\rangle\langle-| = \frac{\mathbb{1}-\hat{\sigma}^x}{2}. \tag{155}$$

- Pauli-y

$$\hat{\sigma}^y = |i\rangle\langle i| - |\bar{i}\rangle\langle\bar{i}|, \tag{156}$$

with projection operators

$$|i\rangle\langle i| = \frac{\mathbb{1}+\hat{\sigma}^y}{2},$$
$$|\bar{i}\rangle\langle\bar{i}| = \frac{\mathbb{1}-\hat{\sigma}^y}{2}. \tag{157}$$

- Pauli-z

$$\hat{\sigma}^z = |0\rangle\langle 0| - |1\rangle\langle 1|, \tag{158}$$

with projection operators

$$|0\rangle\langle 0| = \frac{\mathbb{1}+\hat{\sigma}^z}{2},$$
$$|1\rangle\langle 1| = \frac{\mathbb{1}-\hat{\sigma}^z}{2}. \tag{159}$$

In general, the Pauli operator $\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}}$ along the direction of the unit vector $\boldsymbol{n}$ has the following spectral decomposition

$$\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}} = |\boldsymbol{n}\cdot\boldsymbol{\sigma}{=}{+}1\rangle\langle\boldsymbol{n}\cdot\boldsymbol{\sigma}{=}{+}1| - |\boldsymbol{n}\cdot\boldsymbol{\sigma}{=}{-}1\rangle\langle\boldsymbol{n}\cdot\boldsymbol{\sigma}{=}{-}1|, \tag{160}$$

with the projection operators

$$\boxed{|\boldsymbol{n}\cdot\boldsymbol{\sigma}{=}{\pm}1\rangle\langle\boldsymbol{n}\cdot\boldsymbol{\sigma}{=}{\pm}1| = \frac{\mathbb{1}\pm\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}}}{2}.} \tag{161}$$

Exc 16 Prove Eq. (160) and Eq. (161).

■ Observables

■ Physical Observable

Postulate 2 (Observables): **Physical observables** of a quantum system are described by **Hermitian operators** (represented as Hermitian matrices) acting on the associated Hilbert space.

Consider a Hermitian operator $\hat{O}$ with eigenvalues O_k and eigenvectors $|O_k\rangle$ ($m = 1, 2, \ldots, g_k$), i.e.

$$\hat{O} = \sum_k |O_k\rangle\, O_k\, \langle O_k|. \tag{162}$$

The operator $\hat{O}$ corresponds to a physical observable O in the sense that

- All possible **measurement outcomes** (or **observation values**) of the observable O are given by (and only by) the *eigenvalues* O_k.
- The **measurement** projects (collapses) the quantum state to the eigenspace $\mathcal{H}_k$ spanned by the eigenstates of the corresponding measurement outcome O_k.

■ Measurement Postulate

Postulate 3 (Measurement): Given a quantum system in the **state** $|\psi\rangle$ and the **observable** O to be measured:
(i) the **probability** to observe the measurement outcome O_k is $p(O_k\,|\,\psi) = |\langle O_k|\psi\rangle|^2$,
(ii) if O_k is observed, the state will **collapse** to $|O_k\rangle$.

- In quantum measurement, there is no way to tell for certain which outcome will be observed. There is only a **conditional probability** $p(O_k\,|\,\psi)$ that we can predict.
- Upon observing the measurement outcome O_k, the quantum state will be updated --- a process known as **quantum state collapse**.

$$|\psi\rangle \xrightarrow[\text{observe } O_k]{\text{measure } O} |O_k\rangle. \tag{163}$$

  - $|\psi\rangle$ is called the **prior state** (pre-measurement state)
  - $|O_k\rangle$ is called the **posterior state** (post-measurement state)
  - **Bayesian view** of quantum state collapse:
    - The quantum state represents our *subjective* knowledge or belief about the system, not (necessarily) an *objective* physical reality.
    - Measurements provide new information that forces us to *update* our beliefs → the "collapse" happens in our knowledge.
    - The measurement postulate tells us how to update the quantum state given the observation, in a logically consistent manner.
- How to deal with **degeneracy**?

  An eigenvalue O_k is n-fold degenerated ⇔ there exists n orthonormal eigenstates (their choices are not unique) of $\hat{O}$ corresponding to the same eigenvalue:

$$\hat{O}\,|O_k,1\rangle = O_k\,|O_k,1\rangle,$$
$$\hat{O}\,|O_k,2\rangle = O_k\,|O_k,2\rangle, \tag{164}$$

...

$\hat{O}\,|O_k,n\rangle = O_k\,|O_k,n\rangle$.

Then if the measurement outcome O_k is observed in measuring O on state $|\psi\rangle$, how to compute $p(O_k\,|\,\psi)$ and the posterior state?

- Step I: Compute the scalar products $\alpha_m = \langle O_k,m|\psi\rangle$, meaning that

$$|\psi\rangle = \sum_{m=1}^{n} \alpha_m\,|O_k,m\rangle + \ldots \text{(other states)}. \tag{165}$$

- Step II: Aggregate the probability:

$$\boxed{p(O_k\,|\,\psi) = \sum_{m=1}^{n} |\alpha_m|^2 = \sum_{m=1}^{n} |\langle O_k,m|\psi\rangle|^2.} \tag{166}$$

- Step III: Renormalize the amplitudes α_m

$$\tilde{\alpha}_m = \frac{\alpha_m}{\sqrt{p(O_k\,|\,\psi)}} = \frac{\langle O_k,m|\psi\rangle}{\sqrt{p(O_k\,|\,\psi)}}, \tag{167}$$

and reconstruct the posterior state

$$\boxed{|\psi\rangle \xrightarrow[\text{observe } O_k]{\text{measure } O} |\psi'\rangle = \sum_{m=1}^{n} \tilde{\alpha}_m\,|O_k,m\rangle.} \tag{168}$$

Note: it is always a good practice to normalize the state (i.e. ensuring $\langle\psi'|\psi'\rangle = 1$) after quantum state collapse.

HW 4

Let $\{|1\rangle, |2\rangle, |3\rangle\}$ be a set of orthonormal basis of a three-state system. Suppose the system is in the prior state $|\psi\rangle = \frac{1}{\sqrt{3}}\,(|1\rangle + |2\rangle + |3\rangle)$.

Consider measuring the observable $\hat{O} = |1\rangle\langle 2| + |2\rangle\langle 1| - |3\rangle\langle 3|$.
(i) What are the possible measurement outcomes (observation values)?
(ii) What are the probabilities to observe each outcome?
(iii) What posterior states will the system collapse to after observing each outcome?

■ Expectation Value

The **expectation value** of an observable O, denoted as $\langle O\rangle$, is the *averaged* measurement outcome of O over many repeated experiments (with the same prior state $|\psi\rangle$ prepared each time).

According to the measurement postulate

$$\langle O\rangle := \sum_k O_k\,p(O_k\,|\,\psi)$$

$$= \sum_k O_k \, |\langle O_k|\psi\rangle|^2$$

$$= \sum_k \langle\psi|O_k\rangle \, O_k \, \langle O_k|\psi\rangle$$

Given $\hat{O} = \sum_k |O_k\rangle \, O_k \, \langle O_k|$, we conclude

$$\boxed{\langle O\rangle = \langle\psi| \, \hat{O} \, |\psi\rangle.} \tag{170}$$

- The answer is a *real* scalar (as $\hat{O}$ is Hermitian).
- Represented as *vectors* and *matrices*,

$$\langle O\rangle = (\psi_1^* \;\; \psi_2^* \;\; \cdots) \begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix}. \tag{171}$$

Alternatively, the expectation value can also be written as a trace of the product of the observable operator $\hat{O}$ and the state projector $|\psi\rangle\langle\psi|$

$$\langle O\rangle = \text{Tr} \; \hat{O} \, |\psi\rangle\langle\psi|. \tag{172}$$

- The advantage of this approach is to circumvent solving for $|\psi\rangle$ explicitly (sometimes the state projector is easier to construct than the state vector).

HW 5

Let $\boldsymbol{m}$ and $\boldsymbol{n}$ be three-component real unit vectors. For a qubit, consider measuring $\boldsymbol{n}\cdot\boldsymbol{\sigma}$ on the $|\boldsymbol{m}\cdot\boldsymbol{\sigma}{=}{+}1\rangle$ state.
(i) What is the probability to observe $\boldsymbol{n}\cdot\boldsymbol{\sigma} = +1$?
(ii) What is the expectation value of the operator $\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}}$ on the state $|\boldsymbol{m}\cdot\boldsymbol{\sigma}{=}{+}1\rangle$?
[Express your results in terms of $\boldsymbol{m}$ and $\boldsymbol{n}$. Hint: using Eq. (172) and Eq. (161) can simplify the calculation.]

■ Variance

The **variance** of an observable O on a state $|\psi\rangle$ is defined as

$$\boxed{\text{var} \; O = \left\langle (O - \langle O\rangle)^2 \right\rangle = \left\langle O^2 \right\rangle - \langle O\rangle^2.} \tag{173}$$

where $\left\langle O^2 \right\rangle = \langle\psi| \, \hat{O}^2 \, |\psi\rangle$ and $\langle O\rangle = \langle\psi| \, \hat{O} \, |\psi\rangle$. The square root of the variance defines the **standard deviation**:

$$\text{std} \; O = \sqrt{\text{var} \; O}\,. \tag{174}$$

Uncertainty Relation: for any pair of *observables* A and B measured on any given *state* (repeatedly),

$$\boxed{(\text{std } A)\,(\text{std } B) \geq \frac{1}{2}\,|\langle [A,\, B]\rangle|.} \tag{175}$$

Exc 17 Prove Eq. (175).

- In words, the product of the *uncertainties* cannot be smaller than half of the magnitude of the expectation value of the *commutator*.
- For *commuting* observables ($[A,\, B] = 0$), $(\text{std } A)\,(\text{std } B) \geq 0$, it is possible to have $\text{std } A = \text{std } B = 0$ simultaneously, i.e. A and B can be jointly measured with perfect certainty.
- For *non-commuting* observables, there exists a state on which $|\langle [A,\, B]\rangle| \neq 0$. Then on such state, it is impossible to have $\text{std } A = \text{std } B = 0$ simultaneously, i.e. A and B can not be jointly measured with certainty.

Dynamics

■ Unitary Operators

■ Basis Transformation

Suppose we have two sets of orthonormal basis of the same Hilbert space $\mathcal{H}$

$$\begin{aligned} \mathcal{B} &= \{|i\rangle : i = 1,\, 2,\, \ldots,\, \dim \mathcal{H}\}, \\ \mathcal{B}' &= \{|i\rangle' : i = 1,\, 2,\, \ldots,\, \dim \mathcal{H}\}. \end{aligned} \tag{176}$$

For example, the eigen basis of $\hat{\sigma}^x$ v.s. that of $\hat{\sigma}^z$.

- The *same state* $|v\rangle$ can have *different vector* representations in different bases

$$v_i = \langle i|\, |v\rangle,\;\; v'_i = \langle i|'\, |v\rangle. \tag{177}$$

- The *same operator* $\hat{O}$ can have *different matrix* representations in different bases

$$O_{ij} = \langle i|\, \hat{O}\, |j\rangle,\;\; O'_{ij} = \langle i|'\, \hat{O}\, |j\rangle'. \tag{178}$$

How are representations in different bases related? - **Basis transformation**. Basis transformation from $\mathcal{B}$ to $\mathcal{B}'$ is describe by a matrix U with the matrix element

$$\boxed{U_{ij} = \langle i|'\, |j\rangle.} \tag{179}$$

such that the representation in the new basis is related to that in the old basis by

$$\begin{aligned} v'_i &= \sum_j U_{ij}\, v_j, \\ O'_{ij} &= \sum_{kl} U_{ik}\, O_{kl}\, U^*_{jl}. \end{aligned} \tag{180}$$

Exc 18 Using Eq. (179) to prove that Eq. (180) is compatible with Eq. (177) and Eq. (178).

In quantum mechanics, every operator is a matrix, and every matrix is an operator. So does the basis transformation matrix.

$$\hat{U} = \sum_i |i\rangle \langle i|'. \tag{181}$$

Exc 19 Check that the matrix element of $\hat{U}$ in Eq. (181) is indeed given by Eq. (179), regardless of represented in the basis $\mathcal{B}$ or $\mathcal{B}'$.

$\hat{U}$ in Eq. (181) is an example of the **unitary operator**.

A operator $\hat{U}$ is **unitary**, iff

$$\hat{U}^\dagger\, \hat{U} = \hat{U}\, \hat{U}^\dagger = \mathbb{1}. \tag{182}$$

Exc 20 Check that Eq. (181) satisfies the defining property Eq. (182) for unitary operator.

- The *inverse* of a unitary operator is its *Hermitian conjugate*

$$\hat{U}^{-1} = \hat{U}^\dagger. \tag{183}$$

The operator (basis transformation) implemented by $\hat{U}$ is *reversed* by that of $\hat{U}^\dagger$, and vice versa.

- When the two sets of basis $|i\rangle$ and $|i\rangle'$ are identical, $U = \mathbb{1}$ becomes the identity operator (which is also unitary).

In terms of the unitary operator, the basis transformation Eq. (180) can be written as

$$\begin{aligned} &\text{for ket state}: \quad |v\rangle \to \hat{U}\, |v\rangle, \\ &\text{for bra state}: \quad \langle v| \to \langle v|\, \hat{U}^\dagger, \\ &\text{for operator}: \quad \hat{O} \to \hat{U}\, \hat{O}\, \hat{U}^\dagger. \end{aligned} \tag{184}$$

- The operator $\hat{O}$ is also made of ket and bra states, so the unitary operator must be applied from both sides, when transforming an operator.
- The *expectation value* of an observable is *invariant* under *basis transformation*. (Physical reality should be *basis-independent*.)

$$\langle O\rangle = \langle\psi|\,\hat{O}\,|\psi\rangle \to \langle\psi|\,\hat{U}^\dagger\,\hat{U}\,\hat{O}\,\hat{U}^\dagger\,\hat{U}\,|\psi\rangle = \langle\psi|\,\mathbb{1}\,\hat{O}\,\mathbb{1}\,|\psi\rangle = \langle O\rangle. \tag{185}$$

■ Matrix Diagonalization

Diagonalization of a *Hermitian operator*: find a unitary operator $\hat{U}$ to bring the Hermitian operator $\hat{O}$ to *diagonal form* by transforming to its *eigenbasis*.

$$\begin{aligned}\hat{O} &= \sum_k |O_k\rangle\, O_k\, \langle O_k|,\\ \hat{U} &= \sum_k |k\rangle\, \langle O_k|,\end{aligned} \tag{186}$$

such that under $\hat{O} \to \hat{U}\,\hat{O}\,\hat{U}^\dagger$,

$$\hat{\Lambda} = \hat{U}\,\hat{O}\,\hat{U}^\dagger = \sum_k |k\rangle\, O_k\, \langle k| \doteq \begin{pmatrix} O_1 & & \\ & O_2 & \\ & & \ddots \end{pmatrix} \tag{187}$$

is diagonal in the basis of **one-hot vectors** $|k\rangle$.

- Every *Hermitian* matrix can be written as

$$\hat{O} = \hat{U}^\dagger\,\hat{\Lambda}\,\hat{U}, \tag{188}$$

with $\hat{\Lambda}$ being *diagonal* and $\hat{U}$ being *unitary*.

- Or equivalently, the *unitary* transformation $\hat{U}$ brings the *Hermitian* matrix to its *diagonal* form,

$$\hat{U}\,\hat{O}\,\hat{U}^\dagger = \hat{\Lambda}. \tag{189}$$

Example: diagonalization of Pauli matrix

The Pauli matrix $\hat{\sigma}^x$ can be diagonalized by the following unitary transformation (whose row vectors are bra eigenvectors of $\hat{\sigma}^x$)

$$\hat{U}_{\mathsf{H}} = \begin{pmatrix}\langle +|\\ \langle -|\end{pmatrix} \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}. \tag{190}$$

- This unitary operation $\hat{U}_{\mathsf{H}}$ is also known as the **Hadamard gate** in quantum information, an example of single-qubit gate.
- Under the unitary transformation, $\hat{\sigma}^x$ is brought to its diagonal form, which is $\hat{\sigma}^z$

$$\begin{aligned}\hat{U}_{\mathsf{H}}\,\hat{\sigma}^x\,\hat{U}_{\mathsf{H}}^\dagger &\doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\\ &= \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \doteq \hat{\sigma}^z.\end{aligned} \tag{191}$$

■ Hermitian Generators

If **Hermitian operators** are generalization of **real numbers**, then **unitary operators** are generalization of **phase factors**.

- A complex number $z \in \mathbb{C}$ is a phase factor, iff $|z| = 1$. Any phase factor can be written as $z = e^{i\theta}$, where $\theta \in \mathbb{R}$ is a *real* phase angle.

$$z^* z = z z^* = |z|^2 = 1 \Leftrightarrow z = e^{i\theta} \tag{192}$$

- Similar ideas apply to unitary operators: every **unitary operator** can be **generated** by a **Hermitian operator** $\hat{\Theta}$ in the form of

$$\boxed{\hat{U} = e^{i\hat{\Theta}}.} \tag{193}$$

Given a Hermitian operator $\hat{\Theta}$

$$\hat{\Theta} = \sum_k |\Theta_k\rangle\, \Theta_k\, \langle\Theta_k|, \tag{194}$$

by $e^{i\hat{\Theta}}$ we mean

- either by operator Taylor expansion Eq. (120)

$$e^{i\hat{\Theta}} = \mathbb{1} + i\hat{\Theta} + \frac{(i\hat{\Theta})^2}{2!} + \frac{(i\hat{\Theta})^3}{3!} + \ldots. \tag{195}$$

- or by spectral decomposition (HW 2)

$$e^{i\hat{\Theta}} = \sum_k |\Theta_k\rangle\, e^{i\Theta_k}\, \langle\Theta_k| \tag{196}$$

Don't do element-wise exponentiation on the matrix!

Exc 21 Use Eq. (196) to show that $\hat{U} = e^{i\hat{\Theta}}$ is unitary as long as $\hat{\Theta}$ is Hermitian.

Example: unitary generated by Pauli matrix. Recall $\hat{U}(\theta) = e^{i\theta\hat{\sigma}^y}$ in (Exc 10).

$$\hat{U}(\theta) = e^{i\theta\hat{\sigma}^y} \doteq \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}. \tag{197}$$

It implements a **basis rotation** with θ being the **rotation angle**:

$$\hat{U}(\theta)\,|0\rangle \doteq \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\theta \\ -\sin\theta \end{pmatrix}. \tag{198}$$

Special case: when $\theta = 0$, $\hat{U}(0) = \mathbb{1} \Rightarrow$ no rotation is performed.

More generally, let $\hat{U}(\theta)$ be the **unitary operator** that implements certain *basis rotation* by a real **angle** θ. When $\theta = \Delta\theta$ is **small**, we can Taylor expand

$$\hat{U}(\Delta\theta) = \hat{U}(0) + \hat{U}'(0)\,\Delta\theta + \ldots = \mathbb{1} + \hat{U}'(0)\,\Delta\theta + \ldots, \tag{199}$$

where $\hat{U}'(0)$ is $\partial_\theta \hat{U}(\theta)$ evaluated at $\theta = 0$.

- $\hat{U}'(0)$ is also an operator (matrix), usually denoted as $\hat{U}'(0) = i\,\hat{G}$. We call $\hat{G}$ the **generator** of the rotation/unitary operator, because it *generates* an **infinitesimal rotation**

$$\hat{U}(\Delta\theta) = \mathbb{1} + i\,\Delta\theta\,\hat{G} + ... \tag{200}$$

- $\hat{U}(\Delta\theta)$ is **unitary** ⇒ $\hat{G}$ is **Hermitian**.

$$\begin{aligned} & U(\Delta\theta)^{\dagger}\, U(\Delta\theta) \\ &= \left(\mathbb{1} - i\,\Delta\theta\,\hat{G}^{\dagger} + ...\right)\left(\mathbb{1} + i\,\Delta\theta\,\hat{G} + ...\right) \\ &= \mathbb{1} + i\,\Delta\theta\left(\hat{G} - \hat{G}^{\dagger}\right) + \ldots = \mathbb{1}. \end{aligned} \tag{201}$$

- *Large* rotations can be *accumulated* from *small* rotations.

$$\hat{U}(N\,\Delta\theta) = \hat{U}(\Delta\theta)^{N} = \left(\mathbb{1} + i\,\Delta\theta\,\hat{G}\right)^{N}. \tag{202}$$

As $\Delta\theta$ is small (but N can be large, s.t. $\theta = N\,\Delta\theta$ is finite),

$$\ln \hat{U}(N\,\Delta\theta) = N \ln\left(\mathbb{1} + i\,\Delta\theta\,\hat{G}\right) = i\,N\,\Delta\theta\,\hat{G}, \tag{203}$$

So $\hat{U}(N\,\Delta\theta) = e^{i\,N\,\Delta\theta\,\hat{G}}$, we obtain the *exponential* form

$$\boxed{\hat{U}(\theta) = e^{i\,\theta\,\hat{G}}.} \tag{204}$$

Conclusion: every *Hermitian* operator $\hat{\Theta} = \theta\,\hat{G}$ generates a *unitary* operator $e^{i\,\hat{\Theta}}$ by the exponential map.

■ Time Evolution

■ Time-Evolution is Unitary

Unitarity: *information* is never lost!

Basic assumption: quantum *information* is preserved under quantum *dynamics*, i.e. two *identical* and isolated systems

- start out in **different** states ⇒ **remains** in **different** states (towards both future and past).
- start out in the **same** state ⇒ follow **identical evolution** (towards both future and past).

Although **measurement** seems to be **non-deterministic**, evolution of quantum **state** is **deterministic**: suppose you know the *state* at one time, then the quantum *equation of motion* tell you what it will be later.

$$\boxed{|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle,} \tag{205}$$

$|\psi(0)\rangle$ is the initial state, and $|\psi(t)\rangle$ is the state at time t. $\hat{U}(t)$ is the **time-evolution operator** that takes $|\psi(0)\rangle$ to $|\psi(t)\rangle$. ☝ We will show that $\hat{U}(t)$ should be *unitary*.

- *Distinct* states remain *distinct*:

$$\langle \phi(0) \mid \psi(0) \rangle = 0 \Rightarrow \langle \phi(t) \mid \psi(t) \rangle = \langle \phi(0) | \, \hat{U}(t)^\dagger \, \hat{U}(t) \, | \psi(0) \rangle = 0. \tag{206}$$

- *Identical* states remain the *identical*:

$$\langle \psi(0) \mid \psi(0) \rangle = 1 \Rightarrow \langle \psi(t) \mid \psi(t) \rangle = \langle \psi(0) | \, \hat{U}(t)^\dagger \, \hat{U}(t) \, | \psi(0) \rangle = 1. \tag{207}$$

Or, the fact that the probability adds up to 1 must be preserved.

Treat $|\psi(0)\rangle$ and $|\phi(0)\rangle$ as members of any orthonormal basis, then Eq. (206) and Eq. (207) implies

$$\langle i | \, \hat{U}(t)^\dagger \, \hat{U}(t) \, | j \rangle = \delta_{ij} \Rightarrow \hat{U}(t)^\dagger \, \hat{U}(t) = \mathbb{1}. \tag{208}$$

Therefore, the **time-evolution** operator $\hat{U}(t)$ is **unitary**.

■ Hamiltonian

Hamiltonian *generates* time-evolution!

As a *unitary* operator, the *time-evolution* operator is also *generated* by a *Hermitian* operator, called the **Hamiltonian**,

$$\hat{H} = i \, \hat{U}'(0) = i \, \partial_t \, \hat{U}(t) \, |_{t=0} \, . \tag{209}$$

For small Δt, *infinitesimal* evolution is given by

$$\hat{U}(\Delta t) = \mathbb{1} - i \, \hat{H} \, \Delta t + ..., \tag{210}$$

therefore the state evolves as

$$|\psi(\Delta t)\rangle = \hat{U}(\Delta t) \, |\psi(0)\rangle = |\psi(0)\rangle - i \, \Delta t \, \hat{H} \, |\psi(0)\rangle, \tag{211}$$

meaning that

$$i \, \partial_t |\psi(0)\rangle = i \, \frac{|\psi(\Delta t)\rangle - |\psi(0)\rangle}{\Delta t} = \hat{H} \, |\psi(0)\rangle. \tag{212}$$

There is nothing special about $t = 0$. Eq. (212) should hold at any time.

$$i \, \partial_t |\psi(t)\rangle = \hat{H} \, |\psi(t)\rangle. \tag{213}$$

This is the **Schrödinger equation**, the *equation of motion* for the quantum state.

- The Hamiltonian $\hat{H}(t) = i \, \hat{U}'(t)$ can be **time-dependent** in general.
- But in many cases, we consider $\hat{H}$ to be **time-independent**, by assuming the **time-translation symmetry**.

What happens to Planck's constant?

$$\hbar = \frac{h}{2\,\pi} = 1.0545718\,(13) \times 10^{-34} \, \text{J s}. \tag{214}$$

In quantum mechanics, the *observable* associated with the **Hamiltonian** is the **energy**. To balance the *dimensionality* across the Schrödinger equation, *Planck's constant* is inserted for Eq. (213):

$$i\,\hbar\,\partial_t|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle. \tag{215}$$

Why is $\hbar$ so small? Well, the answer has more to do with biology than with physics ⇒ Why we are so big, heavy and slow? A natural choice for quantum mechanics is to set the units such that $\hbar = 1$. It is a common practice in theoretical physics (we will also use this convention sometimes).

■ Schrödinger Equation: State Dynamics

Postulate 4 (Dynamics): The **time-evolution** of the *state* of a quantum system is governed by the **Hamiltonian** of the system, according to the time-dependent **Schrödinger equation**.

$$\boxed{i\,\hbar\,\partial_t|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle.} \tag{216}$$

If the Hamiltonian $\hat{H}$ is **time-independent**, we can first find its eigenvalues (or **eigen energies**) and eigenvectors (or **energy eigenstates**).

$$\boxed{\hat{H}\,|E_k\rangle = E_k\,|E_k\rangle.} \tag{217}$$

This is also called the *time-independent* **Schrödinger equation**. Without solving a *differential equation*, we just need to *diagonalize* a *Hermitian matrix* in this case.

Each *energy eigenstate* will evolve in time simply by a *rotating overall phase*,

$$|E_k(t)\rangle = e^{-\frac{i}{\hbar}E_k\,t}\,|E_k\rangle. \tag{218}$$

- $|E_k\rangle$ form a complete set of orthonormal basis, called **energy eigenbasis**.

Exc 22 Verify that Eq. (218) is a solution of Eq. (216):

Any initial state $|\psi(0)\rangle$ will evolve in time by first *representing* the initial state in the *energy eigenbasis*, and attaching to each energy eigenstate by its rotating overall phase,

$$\begin{aligned}|\psi(t)\rangle &= \sum_i e^{-\frac{i}{\hbar}E_i\,t}\,|E_i\rangle\,\langle E_i\,|\,\psi(0)\rangle \\ &= e^{-\frac{i}{\hbar}\hat{H}\,t}\,|\psi(0)\rangle.\end{aligned} \tag{219}$$

A *time-independent* Hamiltonian generates the time-evolution via *matrix exponentiation*

$$\boxed{\hat{U}(t) = \exp\left(-\frac{i}{\hbar}\,\hat{H}\,t\right).} \tag{220}$$

However, for *time-dependent* Hamiltonian, there no such a clean formula. Evolution must be carried out step by step, denoted as a *time-ordered* exponential

$$\hat{U}(t) = \mathcal{T} \exp\left(-\frac{i}{\hbar} \int_0^t \hat{H}(t')\, d t'\right). \tag{221}$$

▫ Larmor Precession and Rabi Oscillation

How to write down a Hamiltonian?

- derive it from experiment,
- borrow it from some theory we like,
- pick one and see what happens.☜

Hamiltonian must be *Hermitian* anyway. For a single spin (qubit), the most general Hamiltonian takes the form of

$$\begin{aligned} \hat{H} &= h_0 \mathbb{1} + h_x \hat{\sigma}^x + h_y \hat{\sigma}^y + h_z \hat{\sigma}^z \\ &= h_0 \mathbb{1} + \boldsymbol{h} \cdot \hat{\boldsymbol{\sigma}}, \end{aligned} \tag{222}$$

where h_0, h_x, h_y, $h_z \in \mathbb{R}$ are all *real* coefficients.

- The time-evolution operator (set $\hbar = 1$ in the following)

$$\begin{aligned} \hat{U}(t) &= e^{-i \hat{H} t} \\ &= e^{-i h_0 t}\left(\cos(|\boldsymbol{h}|\, t)\, \mathbb{1} - i \sin(|\boldsymbol{h}|\, t)\, \tilde{\boldsymbol{h}} \cdot \hat{\boldsymbol{\sigma}}\right), \end{aligned} \tag{223}$$

where $|\boldsymbol{h}| = \sqrt{\boldsymbol{h} \cdot \boldsymbol{h}}$ and $\tilde{\boldsymbol{h}} = \boldsymbol{h} / |\boldsymbol{h}|$.

Exc 23 Derive Eq. (223) from Eq. (222).

- A state $|\psi(0)\rangle$ will evolve with time following

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}(t)\, |\psi(0)\rangle \\ &= e^{-i h_0 t}\left(\cos(|\boldsymbol{h}|\, t)\, \mathbb{1} - i \sin(|\boldsymbol{h}|\, t)\, \tilde{\boldsymbol{h}} \cdot \hat{\boldsymbol{\sigma}}\right) |\psi(0)\rangle. \end{aligned} \tag{224}$$

- If we measure $\boldsymbol{\sigma}$ on the state $|\psi(t)\rangle$, the expectation value will be given by

$$\begin{aligned} \langle \boldsymbol{\sigma} \rangle_t &= \langle \psi(t)|\, \hat{\boldsymbol{\sigma}}\, |\psi(t)\rangle \\ &= \cos(2\, |\boldsymbol{h}|\, t)\, \langle \boldsymbol{\sigma} \rangle_0 + \sin(2\, |\boldsymbol{h}|\, t)\, \tilde{\boldsymbol{h}} \times \langle \boldsymbol{\sigma} \rangle_0 + (1 - \cos(2\, |\boldsymbol{h}|\, t))\, \tilde{\boldsymbol{h}}\left(\tilde{\boldsymbol{h}} \cdot \langle \boldsymbol{\sigma} \rangle_0\right). \end{aligned} \tag{225}$$

which also evolves with time.

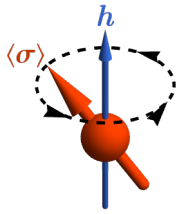
Exc 24 Derive Eq. (225) from Eq. (224).
Hint: Eq. (107) can make life much more easier.

Larmor precession: assume $\boldsymbol{h} = (0, 0, h_z)$ along the z-direction, and parameterize the expectation of the spin vector by $\langle \boldsymbol{\sigma} \rangle = (\sin\theta \cos\varphi, \sin\theta \sin\varphi, \cos\theta)$.

$$\langle \boldsymbol{\sigma} \rangle_t = (\sin\theta_0 \cos(\varphi_0 + 2\, h_z\, t),\ \sin\theta_0 \sin(\varphi_0 + 2\, h_z\, t), \cos\theta_0), \tag{226}$$

where θ_0 and φ_0 are the initial azimuthal and polar angles.

- The solution describes the *spin* $\langle \boldsymbol{\sigma} \rangle$ *precessing* around the axis of the *Zeeman field* $\boldsymbol{h}$.



- The precession frequency $\omega = 2\,|\boldsymbol{h}|$ is called the **Larmor frequency**. It can be used to probe the local Zeeman field strength, which has applications in nuclear magnetic resonance (NMR) and nitrogen-vacancy (NV) center.
- *Energy* of a spin in the Zeeman field is $\langle H \rangle = -\boldsymbol{h} \cdot \langle \boldsymbol{\sigma} \rangle$ (up to some constant energy shift h_0).

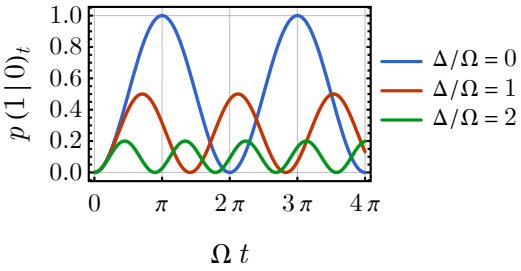
Rabi oscillation: a qubit initially prepared in state $|0\rangle$, evolved under the Hamiltonian

$$\hat{H} = \Omega\,\hat{\sigma}^x + \Delta\,\hat{\sigma}^z \doteq \begin{pmatrix} \Delta & \Omega \\ \Omega & -\Delta \end{pmatrix}, \tag{227}$$

where Ω is the *driving field* and Δ is called *detuning*. The probability to find the qubit in state $|1\rangle$ at time t is given by

$$p(1\,|\,0)_t = \langle \mathcal{P}_1 \rangle_t = \frac{1 - \langle \sigma^z \rangle_t}{2} = \frac{\sin^2(\omega\, t/2)}{1 + (\Delta/\Omega)^2}, \tag{228}$$

with the **Rabi frequency** $\omega = 2\,\sqrt{\Omega^2 + \Delta^2}$.



- **Rabi π-Pulse**: flipping $|0\rangle$ to $|1\rangle$ (and vice versa) by a π-pulse (turn on the driving field Ω for time $t = \pi/\Omega$ and turn off) at resonance $\Delta = 0$. This implements a NOT gate (or X gate) on a single qubit.

■ Heisenberg Equation: Operator Dynamics

Two *pictures* of the **quantum dynamics**:

- **Schrödinger picture**: state evolves in time, operator remains fixed,

$$\langle O(t) \rangle = \langle \psi(t) |\, \hat{O}\, | \psi(t) \rangle. \tag{229}$$

- **Heisenberg picture**: operator evolves in time, state remains fixed,

$$\langle O(t)\rangle = \langle\psi|\ \hat{O}(t)\,|\psi\rangle. \tag{230}$$

The two pictures are consistent, if

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi\rangle \Rightarrow \hat{O}(t) = \hat{U}(t)^{\dagger}\ \hat{O}\ \hat{U}(t), \tag{231}$$

such that Eq. (229) and Eq. (230) are consistent, as they both implies

$$\langle O(t)\rangle = \langle\psi|\ \hat{U}(t)^{\dagger}\ \hat{O}\ \hat{U}(t)\,|\psi\rangle. \tag{232}$$

Note: one should only apply one picture at a time, i.e. either the state or the operator is time-dependent, **but not both**.

In the *Heisenberg picture*, the time-evolution of an operator

$$\hat{O}(t) = \hat{U}(t)^{\dagger}\ \hat{O}\ \hat{U}(t), \tag{233}$$

described by the **Heisenberg equation**

$$i\,\hbar\,\partial_t\,\hat{O}(t) = \left[\hat{O}(t),\,\hat{H}\right]. \tag{234}$$

Exc 25

Derive Eq. (234) from Eq. (233).

Correspondingly, its expectation value evolves as

$$i\,\hbar\,\partial_t\langle O(t)\rangle = \left\langle\left[\hat{O}(t),\,\hat{H}\right]\right\rangle. \tag{235}$$

If $\left[\hat{O},\,\hat{H}\right] = 0$, the *Heisenberg equation* Eq. (234) implies that $\partial_t\langle O\rangle = 0$, i.e. O will be invariant in time. The observable O is a **conserved quantity** (or an **integral of motion**) if $\hat{O}$ *commutes* with the Hamiltonian $\hat{H}$.

HW 6

Consider a single-qubit Hamiltonian $H = \boldsymbol{h}\cdot\hat{\boldsymbol{S}}$, where $\hat{\boldsymbol{S}} = \frac{\hbar}{2}\,\hat{\boldsymbol{\sigma}}$ is the spin operator.
(i) Show that the expectation values of the spin operator evolves as $\partial_t\langle\boldsymbol{S}\rangle = \boldsymbol{h}\times\langle\boldsymbol{S}\rangle$.
(ii) Show that
$\langle\boldsymbol{S}\,(t)\rangle = \cos(|\boldsymbol{h}|\,t)\,\langle\boldsymbol{S}\,(0)\rangle + \sin(|\boldsymbol{h}|\,t)\,\tilde{\boldsymbol{h}}\times\langle\boldsymbol{S}\,(0)\rangle + (1-\cos(|\boldsymbol{h}|\,t))\,\tilde{\boldsymbol{h}}\left(\tilde{\boldsymbol{h}}\cdot\langle\boldsymbol{S}\,(0)\rangle\right)$
is a solution of $\partial_t\langle\boldsymbol{S}\rangle = \boldsymbol{h}\times\langle\boldsymbol{S}\rangle$, where $\tilde{\boldsymbol{h}} = \boldsymbol{h}/|\boldsymbol{h}|$.
This describes the dynamics of a spin in a Zeeman field $\boldsymbol{h}$.
(iii) Show that the spin component along the Zeeman field $\tilde{\boldsymbol{h}}\cdot\boldsymbol{S}$ is a conserved quantity.