Quantum Mechanics

Part I. State and Operator

Quantum States

■ Ket and Bra

■ State as a Vector

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

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

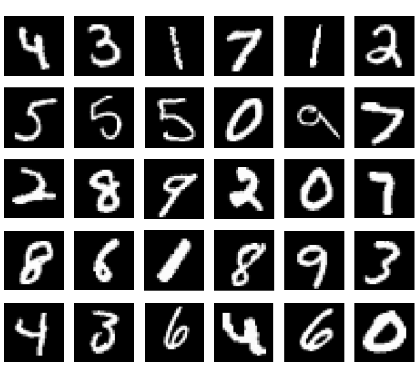
- Describe the **state** of the system: a set of variables encoding the relevant *information* of the system.
- Predict (i) the **observables** (measurement outcomes) and (ii) their **dynamics** (time evolution).

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

State variables are *inferred* from observations.

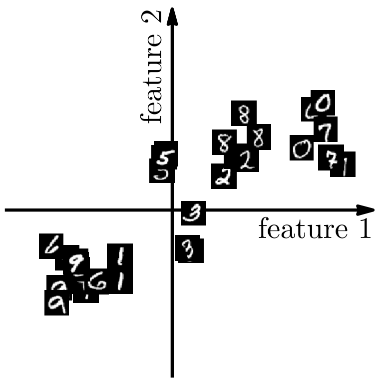
- State variables may not have "physical meaning".
- Choice of state variables may not be unique. (There can be more than one way to describe a system.)

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).

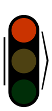
- The vector components are the state variables, and they may not need to have physical meanings. [They are also called **probability amplitudes** or **wave amplitudes**, but I don't explain what is "waving" here.]
- This particular (vector-based) approach of describing quantum states is not the only 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.

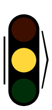
[1] Hsin-Yuan Huang, Richard Kueng, John Preskill. arXiv:2002.08953.

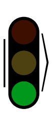
[2] Xizhi Han, Sean A. Hartnoll, Jorrit Kruthoff. arXiv:2004.10212.

Example: a (quantum) traffic light system.

One-hot Encoding: A traffic light system has three *distinct* states: red, yellow and green. In quantum mechanics, they can be described by three *orthogonal one-hot* vectors:

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

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

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

- **Distinct states**. Two states are *distinct*, if they can be be distinguished by the different *observation values* of an observable.
- **Quantum superposition**. What is peculiar about quantum states is that quantum mechanics allows us to write down *linear combinations* of states, which has no classical correspondence.

$$\frac{1}{\sqrt{6}}\begin{pmatrix}1\\ i\\ -2\end{pmatrix}=\frac{1}{\sqrt{6}}\Big(\Big|$$  $$\Big\rangle+i\Big|$$  $$\Big\rangle-2\Big|$$  $$\Big\rangle\Big). \quad (1)$$

Mathematically this is ok, but physically what does it mean?

- Well, the **norm square** of the superposition *coefficients* has the statistical interpretation of **probability**.

state	coeffient	probability
$\vert$  $\rangle$	$\frac{1}{\sqrt{6}}$	$\left\vert\frac{1}{\sqrt{6}}\right\vert^2=\frac{1}{6}$
$\vert$  $\rangle$	$\frac{i}{\sqrt{6}}$	$\left\vert\frac{i}{\sqrt{6}}\right\vert^2=\frac{1}{6}$
$\vert$  $\rangle$	$\frac{-2}{\sqrt{6}}$	$\left\vert\frac{-2}{\sqrt{6}}\right\vert^2=\frac{2}{3}$

  (2)

  The traffic light has 1/6 of the probability to be observed in red, and 1/6 in to be in yellow, and 2/3 to be in green.

- But what about the relative **sign** or **phase** of the superposition coefficients? - The complex nature of the state vector component is a feature that enables *quantum interference*.

To better understand the meaning of the state vector, we need to understand how quantum mechanics predicts *observables* from the *state*. This is the only way decode the *quantum information* back to the *physical reality*.

▪ Ket Vector

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

In **Dirac's notation**, a quantum state will be denoted by a **ket** (or ket state, ket vector) $|v\rangle$, which is an element in a complex vector space $\mathcal{H}$

$$|v\rangle \in \mathcal{H}. \quad (3)$$

- **Vector space**. The defining property of a vector space is that linear combinations of vectors are still in the vector space

$$\forall\ |u\rangle, |v\rangle \in \mathcal{H};\ \alpha, \beta \in \mathbb{C}: \\ \alpha\,|u\rangle + \beta\,|v\rangle \in \mathcal{H}. \tag{4}$$

- The fact that $\mathcal{H}$ is a *complex* vector space is reflected in the fact that α and β are *complex* numbers.
- This can be generalized to many vectors: any linear combinations of vectors is still a vector

$$\forall\ \{|u_n\rangle\} \subset \mathcal{H};\ \{\alpha_n\} \subset \mathbb{C}: \\ \sum_n \alpha_n\,|u_n\rangle \in \mathcal{H}. \tag{5}$$

Superposition Principle: any linear combination of quantum states of a given quantum system is still a valid quantum state of the same system.

- **Vector representation**: Each *ket* can be *represented* as a *column* vector

$$|v\rangle \doteq \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix}. \tag{6}$$

- 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.

Exc 1 If $|v\rangle \doteq \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$, $|w\rangle \doteq \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$, what is the vector representation of the state $|v\rangle + |w\rangle$ and $\lambda\,|v\rangle$ ($\lambda \in \mathbb{C}$ is a complex scalar).

- To write down the vector representation, we must specified a set of (orthonormal) **basis vectors** in the vector space $\mathcal{H}$, and represent them as one-hot unit vectors:

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix}, |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ \vdots \end{pmatrix}, \ \ldots. \tag{9}$$

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

$$|v\rangle = v_1\,|1\rangle + v_2\,|2\rangle + \ldots \\ = \sum_i v_i\,|i\rangle. \tag{10}$$

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

Example: a 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:

$$|0\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix},\ |1\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{11}$$

  - 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

$$\boxed{|\psi\rangle = \psi_0\,|0\rangle + \psi_1\,|1\rangle \doteq \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}.} \tag{12}$$

  - $\psi_0, \psi_1 \in \mathbb{C}$ 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.

HW 1

> Define the following qubit states:
> $|+\rangle = \frac{1}{\sqrt{2}}\,(|0\rangle + |1\rangle)$,
> $|-\rangle = \frac{1}{\sqrt{2}}\,(|0\rangle - |1\rangle)$,
> $|i\rangle = \frac{1}{\sqrt{2}}\,(|0\rangle + i\,|1\rangle)$.
> Express the state $|i\rangle$ as a quantum superposition of states $|+\rangle$ and $|-\rangle$ (i.e. find the linear combination coefficients).

▪ Bra Vector (I)

In **Dirac's notation**, a **bra** $\langle u|$ is a **dual vector** of a **ket** $|u\rangle$. The name comes from the fact that they combine into a **bracket**, which represents a scalar product [to be introduced later].

- If $|u\rangle$ is a linear combination of $|v\rangle$ and $|w\rangle$

$$|u\rangle = \alpha\,|v\rangle + \beta\,|w\rangle, \tag{13}$$

  then its dual is

$$\boxed{\langle u| = \alpha^*\,\langle v| + \beta^*\,\langle w|.} \tag{14}$$

  Under duality: (i) ket is flipped to bra (and vice versa), (ii) every *scalar* coefficient gets *complex conjugated*.

- **Vector representation**: Each *bra* can be *represented* as a *row* vector. If the ket vector (column vector) is

$$|v\rangle \doteq \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix}, \tag{15}$$

then the bra vector (dual row vector) is simply the **conjugate transpose** of the ket vector

$$\langle v| \doteq (\, v_1^* \;\; v_2^* \;\; \cdots \,). \tag{16}$$

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

$$\begin{aligned} \langle 1| &\doteq (\,1 \;\; 0 \;\; \cdots\,), \\ \langle 2| &\doteq (\,0 \;\; 1 \;\; \cdots\,), \\ &\cdots. \end{aligned} \tag{17}$$

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

$$\begin{aligned} \langle v| &= v_1^* \langle 1| + v_2^* \langle 2| + \ldots \\ &= \sum_i v_i^* \langle i|. \end{aligned} \tag{18}$$

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

▪ Scalar Product

Scalar product (or **inner product**) is a function that takes two vectors, $|u\rangle$ and $|v\rangle$, and returns a complex number, denoted as $\langle u|v\rangle$.

$$\begin{aligned} \langle\cdot|\cdot\rangle \,:\, \mathcal{H}\times\mathcal{H} &\to \mathbb{C} \\ |u\rangle, |v\rangle &\mapsto \langle u|v\rangle \end{aligned} \tag{19}$$

It must satisfy the following defining properties:

- Complex conjugation

$$\forall\, |u\rangle, |v\rangle \in \mathcal{H},\; \langle u|v\rangle = \langle v|u\rangle^* \tag{20}$$

Note: $\langle u|v\rangle \neq \langle v|u\rangle$ in general, unless $\langle u|v\rangle \in \mathbb{R}$.

- Linearity of the ket vector

$$\begin{aligned} &\forall\, |u\rangle, |v\rangle, |w\rangle \in \mathcal{H};\, \alpha, \beta \in \mathbb{C}: \\ &\langle u|(\alpha\,|v\rangle + \beta\,|w\rangle) = \alpha\,\langle u|v\rangle + \beta\,\langle u|w\rangle. \end{aligned} \tag{21}$$

- (Anti)linearity of the bra vector: using Eq. (20), Eq. (21), one can show

$$(\alpha^* \langle v| + \beta^* \langle w|)\,|u\rangle = \alpha^* \langle v|u\rangle + \beta^* \langle w|u\rangle. \tag{22}$$

Note: we follow the convention in Eq. (14) to denote the linear combination of bra vectors, which is different from the textbook notation (2.23).

Exc 2 Show that Eq. (22) is implied by Eq. (20) and Eq. (21).

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

$$\langle v|v\rangle \geq 0. \tag{24}$$

More specifically,

$$\langle v|v\rangle \begin{cases} = 0 & \text{if } |v\rangle = 0 \\ > 0 & \text{otherwise} \end{cases}. \tag{25}$$

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

$$|\langle u|v\rangle|^2 \leq \langle u|u\rangle\, \langle v|v\rangle. \tag{26}$$

Exc 3 Prove Eq. (26).

In the **vector representation** (assuming an orthonormal basis), take two states

$$|v\rangle \doteq \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix}, \; |w\rangle \doteq \begin{pmatrix} w_1 \\ w_2 \\ \vdots \end{pmatrix}, \tag{32}$$

the scalar product can be taken as

$$\begin{aligned} \langle v|w\rangle &\doteq (\, v_1^* \;\; v_2^* \;\; \cdots \,) \begin{pmatrix} w_1 \\ w_2 \\ \vdots \end{pmatrix} \\ &= v_1^*\, w_1 + v_2^*\, w_2 + \ldots \\ &= \sum_i v_i^*\, w_i. \end{aligned} \tag{33}$$

Exc 4 Verify that Eq. (33) is consistent with the defining properties of the scalar product in Eq. (20), Eq. (21), Eq. (22).

Hilbert space: a vector space equipped with a scalar product.

- Every quantum system is associated with a Hilbert space. Its different quantum states are different vectors in the same Hilbert space.

Bra Vector (II)

Linear functional Φ on a vector space $\mathcal{H}$ is a *linear* map that associates each vector in $\mathcal{H}$ with a complex number.

$$\begin{aligned} \Phi : \mathcal{H} &\to \mathbb{C} \\ |v\rangle &\mapsto \Phi(|v\rangle) = z \end{aligned} \tag{37}$$

Linearity requires Φ to satisfy

$$\forall\, |v\rangle, |w\rangle \in \mathcal{H};\ \alpha, \beta \in \mathbb{C}: \\ \Phi(\alpha\,|v\rangle + \beta\,|w\rangle) = \alpha\,\Phi(|v\rangle) + \beta\,\Phi(|w\rangle) \tag{38}$$

Example: "take the first component" functional

Let Φ_1 be a function that maps any vector $|v\rangle$ to its first component v_1

$$\Phi_1(|v\rangle) = v_1. \tag{39}$$

- This is a linear functional on the vector space.

$$\Phi_1(\alpha\,|v\rangle + \beta\,|w\rangle) = \alpha\, v_1 + \beta\, w_1 = \alpha\,\Phi_1(|v\rangle) + \beta\,\Phi_1(|w\rangle). \tag{40}$$

- Denote the first basis vector as $|1\rangle$, Φ_1 can be written as the scalar product:

$$\Phi_1(|v\rangle) = \langle 1|v\rangle. \tag{41}$$

In general, every ket vector $|u\rangle$ defines a corresponding *linear functional* through the scalar product:

$$\boxed{\Phi_{|u\rangle}(|v\rangle) = \langle u|v\rangle.} \tag{42}$$

- Conversely, in mathematics, this corresponding linear functional is treated as the definition of the dual bra vector $\langle u| = \Phi_{|u\rangle}$ of the original ket vector $|u\rangle$.
- **Riesz theorem**: any bounded linear functional acting on a Hilbert space $\mathcal{H}$ can be represented as a scalar product of the form in Eq. (42).
- **Dual vector space**. The space of such functionals (bra vectors) is called the dual vector space of $\mathcal{H}$, denoted as $\mathcal{H}^*$. The dual vector space $\mathcal{H}^*$ is the space of bra vectors.

▪ Norm and Orthogonality

▪ Norm

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

$$\|v\|^2 = \langle v|v\rangle. \tag{43}$$

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.

$$\boxed{\|v\|^2 = \langle v|v\rangle = 1.} \tag{44}$$

- Example: Consider a qubit state

$$|v\rangle \doteq \begin{pmatrix} v_0 \\ v_1 \end{pmatrix}, \tag{45}$$

the normalization condition means

$$\langle v|v\rangle = v_0^* \, v_0 + v_1^* \, v_1 = 1. \tag{46}$$

- In general, the normalization condition means

$$\langle v|v\rangle = \sum_i |\langle i|v\rangle|^2 = \sum_i |v_i|^2 = 1. \tag{47}$$

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

$$|v\rangle \to \frac{|v\rangle}{\|v\|} = \frac{1}{\sqrt{\langle v|v\rangle}} \, |v\rangle, \tag{48}$$

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

Exc 5 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.

$$\boxed{\langle u|\, v\rangle = 0.} \tag{51}$$

- For example, the qubit states $|0\rangle$ and $|1\rangle$ (see Eq. (11)) are *orthogonal*, as

$$\langle 0|1\rangle = (\,1 \;\; 0\,)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0. \tag{52}$$

$|0\rangle$ 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.

Orthogonal subspaces: two subspaces $\mathcal{H}_1$ and $\mathcal{H}_2$ in $\mathcal{H}$ are orthogonal if

$$\forall\ |u\rangle \in \mathcal{H}_1,\ |v\rangle \in \mathcal{H}_2 : \langle u|\, v\rangle = 0. \tag{53}$$

- **Complementary subspace**: $\mathcal{H}_{1,\perp}$ is the complementary subspace of $\mathcal{H}_1$, if $\mathcal{H}_1$ and $\mathcal{H}_{1,\perp}$ are orthogonal and $\mathcal{H}_1 \oplus \mathcal{H}_{1,\perp} = \mathcal{H}$.
  - For each $|v\rangle \in \mathcal{H}$, there is a unique decomposition:

    $$|v\rangle = |v_\parallel\rangle + |v_\perp\rangle, \tag{54}$$

    such that $|v_\parallel\rangle \in \mathcal{H}_1$ and $|v_\perp\rangle \in \mathcal{H}_{1,\perp}$.
  - $|v_\parallel\rangle$ is the **projection** of $|v\rangle$ in $\mathcal{H}_1$.

Exc 6

Consider a Hilbert space $\mathcal{H}$ spanned by three vectors $|x\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|y\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, $|z\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

(i) Let $\mathcal{H}_{\parallel} = \text{span}\{|x\rangle, |y\rangle\}$ and $\mathcal{H}_{\perp} = \text{span}\{|z\rangle\}$. Show that $\mathcal{H}_{\parallel}$ and $\mathcal{H}_{\perp}$ are orthogonal subspaces.

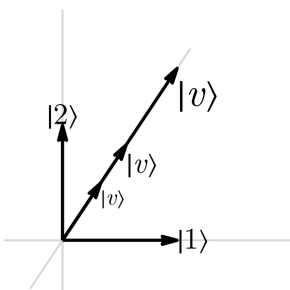
(ii) For $|v\rangle = v_x |x\rangle + v_y |y\rangle + v_z |z\rangle$, find the unique decomposition $|v\rangle = |v_{\parallel}\rangle + |v_{\perp}\rangle$, such that $|v_{\parallel}\rangle \in \mathcal{H}_{\parallel}$ and $|v_{\perp}\rangle \in \mathcal{H}_{\perp}$.

Ray and Phase Ambiguity

If $|v\rangle$ and $|v'\rangle$ are related by a scalar multiplication (for $\lambda \in \mathbb{C}$)

$$|v'\rangle = \lambda |v\rangle, \tag{63}$$

they describe the *identical* physical state of the quantum system. A picture in the real vector space would be like: (the vectors on a ray are all equivalent)



Precisely speaking, quantum states are described by **rays** of vectors in the Hilbert space, i.e. only the "direction" of state vector matters.

- The square **norm** of the state vector does not affect the *physical* property of the quantum system, because it represent the total probability of observation outcomes, which can always be taken to 1.
  - To fix the norm ambiguity, we will always require a state vector to be normalized, i.e. $\langle v|v\rangle = 1$.
- The **overall phase** of the state vector also does not matter, as it turns out that all *physical* properties about the quantum system is always unchanged under $|v\rangle \to e^{i\varphi} |v\rangle$.
  - But there is no canonical way to fix the phase ambiguity. We must ensure that any prediction about the quantum system must not rely on the overall phase on the formulation level.

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)

$$F(u, v) = |\langle u|v\rangle|^2. \tag{64}$$

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

  $$0 \leq F(u, v) \leq 1. \tag{65}$$

  This follows from the Cauchy-Schwarz inequality of scalar product Eq. (26) that $|\langle u|v\rangle|^2 \leq \langle u|u\rangle \langle v|v\rangle$.
- **Statistical interpretation**: If a quantum system is known to be in a state $|v\rangle$, observing the system again may find the system in another state $|u\rangle$ with probability

  $$p(u \mid v) = |\langle u|v\rangle|^2. \tag{66}$$

  - **Detailed balance**: the probability to observe one state on another is the same as the other way round

    $$p(u \mid v) = p(v \mid u) = F(u, v) = |\langle u|v\rangle|^2. \tag{67}$$

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

  $$|\langle u|v\rangle|^2 = 1. \tag{68}$$

  - This is only achievable when

    $$|u\rangle = e^{i\varphi} |v\rangle, \tag{69}$$

    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)

  $$|\langle u|v\rangle|^2 = 0. \tag{70}$$

  - *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

  $$0 < |\langle u|v\rangle|^2 < 1. \tag{71}$$

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

  $|3\rangle \doteq$ , $|5\rangle \doteq$ .

  Therefore, there is generally some probability to observe one state given another state, if the two states has some similarity.

Basis

General Basis

A set of vectors $\{|e_i\rangle : i = 1, 2 \ldots\}$ are said to be **linearly independent**, if

$$\sum_i c_i\, |e_i\rangle = 0 \Leftrightarrow \forall\ i : c_i = 0, \tag{72}$$

i.e. none of the vectors in the set can be written as a linear combination of the others.

Basis: a basis $\mathcal{B}$ of a vector space $\mathcal{H}$ is a set of *linearly independent* vectors $\mathcal{B} = \{|e_i\rangle : i = 1, 2 \ldots\}$ that *span* the full space of $\mathcal{H}$, denoted as

$$\mathcal{H} = \operatorname{span} \mathcal{B}, \tag{73}$$

i.e. any vector in $\mathcal{H}$ can be expanded as a linear combination of the basis vectors

$$\forall\ |v\rangle \in \mathcal{H},\ \exists\ \{v_i\} \subset \mathbb{C} : |v\rangle = \sum_i v_i\, |e_i\rangle. \tag{74}$$

- The coefficients v_i depend on what vector $|v\rangle$ is being expanded.
- The **dimension** of the vector space $\dim \mathcal{H}$ = the number 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 - $\dim \mathcal{H} = \infty$.
  - The summation in Eq. (74) becomes a infinite sum (countable) or an integration (uncountable) when the Hilbert space dimension is infinite.
  - 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.

Orthonormal Basis

Orthonormal basis: a basis $\mathcal{B} = \{|i\rangle : i = 1, 2, \ldots\}$ in which the basis vectors are **normalized** and **orthogonal** to each other.

$$\langle i|j\rangle = \delta_{ij} = \begin{cases} 1 & i = j, \\ 0 & i \neq j. \end{cases} \tag{75}$$

- Each orthogonal basis state describes a distinct reality of the quantum system.
- 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).
- **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,

$$|v\rangle = v_1\,|1\rangle + v_2\,|2\rangle + \ldots = \sum_{|i\rangle\in\mathcal{B}} v_i\,|i\rangle. \tag{76}$$

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

$$v_i = \langle i|v\rangle. \tag{77}$$

Eq. (76) and Eq. (77) can be written in a more elegant form in terms of bras and kets only

$$|v\rangle = \sum_{|i\rangle\in\mathcal{B}} |i\rangle\,\langle i|v\rangle. \tag{78}$$

- The squared norm of a state $|v\rangle$ is the sum of squared norm of its components on (any) orthonormal basis.

$$\langle v|v\rangle = \sum_i |\langle i|v\rangle|^2 = \sum_i |v_i|^2. \tag{79}$$

Exc 7 Using the orthonormal property $\langle i|j\rangle = \delta_{ij}$ to evaluate the norm of $|v\rangle = \sum_i |i\rangle\,\langle i|v\rangle$.

- Orthonormal basis states are *represented* by **one-hot vectors**, as they are normalized and orthogonal to each other

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix},\; |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix},\; |3\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix},\; \ldots. \tag{81}$$

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

HW 2

> Let $\{|0\rangle, |1\rangle\}$ be an orthonormal basis of a qubit, consider the following linear combinations
> $|0'\rangle = e^{i\varphi/2}\cos(\theta/2)\,|0\rangle + e^{-i\varphi/2}\sin(\theta/2)\,|1\rangle$,
> $|1'\rangle = -e^{i\varphi/2}\sin(\theta/2)\,|0\rangle + e^{-i\varphi/2}\cos(\theta/2)\,|1\rangle$,
> where θ and φ are arbitrary real angles. Show that $|0'\rangle$ and $|1'\rangle$ also form an orthonormal basis (for any choices of θ and φ).

■ Summary

- States are vectors.
- Ket and bra:

	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	$v_i = \langle i|v\rangle$	$v_i^* = \langle v|i\rangle$

(82)

- Scalar product

$$\langle u|v\rangle = \sum_i \langle u|i\rangle\,\langle i|v\rangle = \sum_i u_i^*\,v_i. \tag{83}$$

  - Normalized state $\langle v|v\rangle = 1$. To normalize a state:

$$|v\rangle \to \frac{|v\rangle}{\sqrt{\langle v|v\rangle}}. \tag{84}$$

  - Orthogonal states $\langle u|v\rangle = 0$.
  - Orthonormal basis $\mathcal{B} = \{|i\rangle : \langle i|j\rangle = \delta_{ij}\}$.
- Fidelity (similarity between quantum states)

$$F(u, v) = |\langle u|v\rangle|^2 \begin{cases} = 1 & \text{identical states} \\ = 0 & \text{distinct states} \\ \in (0, 1) & \text{overlapping states} \end{cases}. \tag{85}$$

  - Statistical interpretation: $p(u\,|\,v) = p(v\,|\,u) = F(u, v)$.

Quantum Operators

Operator and Matrix

Operator

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

$$\begin{aligned} \hat{O} : \mathcal{H} &\to \mathcal{H} \\ |v\rangle &\mapsto |w\rangle = \hat{O}\,|v\rangle \end{aligned} \tag{86}$$

- Distinction: *operator* is a vector-to-vector mapping, while *functional* is a vector-to-scalar mapping.
- **Linear operator**: an operator $\hat{O}$ is say to be *linear* if it satisfies the linear property

$$\begin{aligned} &\forall\, |u\rangle, |v\rangle \in \mathcal{H};\ \alpha, \beta \in \mathbb{C}: \\ &\hat{O}(\alpha\,|u\rangle + \beta\,|v\rangle) = \alpha\,\hat{O}\,|u\rangle + \beta\,\hat{O}\,|v\rangle. \end{aligned} \tag{87}$$

In quantum mechanics, all operators are linear operators (we will omit the adjective "linear" from now on).

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

$$\forall\, |v\rangle : \mathbb{1}\,|v\rangle = |v\rangle. \tag{88}$$

Operator as a Matrix

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

$$\boxed{\hat{O} = \sum_{ij} |i\rangle\, O_{ij}\, \langle j|,} \tag{89}$$

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

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

Exc 8 Prove Eq. (90) from Eq. (89).

- $|i\rangle\langle j|$ denotes the operator that take the system from state $|j\rangle$ to state $|i\rangle$, because

$$\begin{aligned} (|i\rangle\langle j|)\,|k\rangle &= |i\rangle\langle j|k\rangle = |i\rangle\,\delta_{jk} \\ &= \begin{cases} |i\rangle & \text{if } k = j, \\ 0 & \text{if } k \neq j. \end{cases} \end{aligned} \tag{92}$$

- **Matrix representation**. Every operator 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} is the linear combination coefficient in front of the basis operator $|i\rangle\langle j|$.

Exc 9 Use the vector representation of ket and bra basis to show Eq. (93) is the corresponding representation of Eq. (89).

Example: Identity operator

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

According to Eq. (90),

$$\mathbb{1}_{ij} = \langle i|\mathbb{1}|j\rangle = \langle i|j\rangle = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}. \tag{95}$$

- In matrix representation Eq. (93),

$$\mathbb{1} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & \ddots \end{pmatrix}. \tag{96}$$

- Using Dirac notation Eq. (89),

$$\mathbb{1} = \sum_{ij} |i\rangle \mathbb{1}_{ij} \langle j| = \sum_{i} |i\rangle\langle i|. \tag{97}$$

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

Example: Pauli operators

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

$$\begin{aligned} \hat{\sigma}^x &= |1\rangle\langle 0| + |0\rangle\langle 1|, \\ \hat{\sigma}^y &= i\,|1\rangle\langle 0| - i\,|0\rangle\langle 1|, \\ \hat{\sigma}^z &= |0\rangle\langle 0| - |1\rangle\langle 1|, \end{aligned} \tag{98}$$

Sometimes the identity operator

$$\mathbb{1} = |0\rangle\langle 0| + |1\rangle\langle 1|, \tag{99}$$

is also included as the 0th Pauli operator.

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

$$\mathbb{1} \doteq \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \hat{\sigma}^x \doteq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{\sigma}^y \doteq \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \hat{\sigma}^z \doteq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{100}$$

Operator Acting on State

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

- Consider an operator $\hat{O}$ acting on a state $|v\rangle$ resulting in a state $|w\rangle$

$$|w\rangle = \hat{O}\,|v\rangle, \tag{101}$$

where states and operators are expanded as

$$\begin{aligned} |v\rangle &= \sum_i v_i\,|i\rangle,\ |w\rangle = \sum_i w_i\,|i\rangle, \\ \hat{O} &= \sum_{ij} |i\rangle\, O_{ij}\,\langle j|. \end{aligned} \tag{102}$$

- The expansion coefficients are related by the matrix-vector multiplication

$$\begin{array}{ccccc} |w\rangle & = & \hat{O} & & |v\rangle \\ \downarrow\doteq & & \downarrow\doteq & & \downarrow\doteq \\ \begin{pmatrix} w_1 \\ w_2 \\ \vdots \end{pmatrix} & = & \begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} & & \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix} \end{array} \tag{103}$$

or equivalently

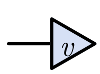
$$w_i = \sum_j O_{ij}\, v_j. \tag{104}$$

Exc 10 Prove the statement Eq. (103) using Eq. (102).

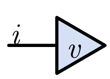
Tensor Network*

Tensor network: a diagrammatic representation of tensor contractions

- Each object (either state or operator) is a **tensor** (multi-dimensions array).
- **Vectors** are *rank-1 tensors*, represented by an object with *one* leg

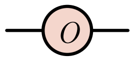


In component form:

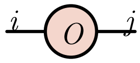


$= v_i$

- **Matrices** are *rank-2 tensors*, represented by an object with *two* legs



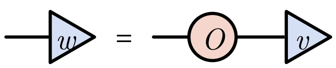
In component form:



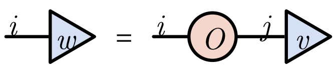
$= O_{ij}$

- **Tensor contraction**: indices on *internal legs* are automatically summed over. For example, matrix-vector multiplication can be expressed as a tensor contraction.

$|w\rangle = \hat{O}\,|v\rangle$



In component form:



$$w_i = \sum_j O_{ij}\, v_j$$

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*):

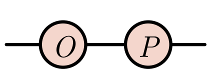
$$\left(\hat{O}\,\hat{P}\right)|v\rangle = \left(\hat{O}\left(\hat{P}\,|v\rangle\right)\right). \tag{109}$$

- Composing two *operators* ≃ multiplying two *matrices*.

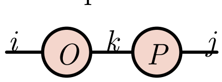
$$\boxed{\hat{O}\,\hat{P} \simeq \begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} P_{11} & P_{12} & \cdots \\ P_{21} & P_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}.} \tag{110}$$

Exc 11 Prove Eq. (110) using Eq. (89).

- Tensor network representation



In component form:



$$(O\,P)_{ij} = \sum_k O_{ik}\,P_{kj}$$

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

$$\hat{O}\,\hat{P} \neq \hat{P}\,\hat{O}. \tag{112}$$

Example: product of Pauli operators

Multiplication table

$$\begin{array}{c|cccc} & \mathbb{1} & \hat{\sigma}^x & \hat{\sigma}^y & \hat{\sigma}^z \\ \hline \mathbb{1} & \mathbb{1} & \hat{\sigma}^x & \hat{\sigma}^y & \hat{\sigma}^z \\ \hat{\sigma}^x & \hat{\sigma}^x & \mathbb{1} & i\,\hat{\sigma}^z & -i\,\hat{\sigma}^y \\ \hat{\sigma}^y & \hat{\sigma}^y & -i\,\hat{\sigma}^z & \mathbb{1} & i\,\hat{\sigma}^x \\ \hat{\sigma}^z & \hat{\sigma}^z & i\,\hat{\sigma}^y & -i\,\hat{\sigma}^x & \mathbb{1} \end{array} \tag{113}$$

Exc 12 Verify Eq. (113) by multiplying Pauli matrices defined in Eq. (100).

- The table Eq. (113) can be summarized in a single formula: the product of Pauli matrices (as the defining property of Pauli matrices)

$$\boxed{\hat{\sigma}^a\,\hat{\sigma}^b = \delta^{ab}\,\mathbb{1} + i\,\epsilon^{abc}\,\hat{\sigma}^c,} \tag{114}$$

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

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

$$\delta^{ab} = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{if } a \neq b \end{cases} \tag{115}$$

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

$$\epsilon^{abc} = \begin{cases} 1 & \text{if } (a\,b\,c) \text{ is a cyclic of } (x\,y\,z) \\ -1 & \text{if } (a\,b\,c) \text{ is a cyclic of } (z\,y\,x) \\ 0 & \text{otherwise} \end{cases} \tag{116}$$

- Another version of Eq. (114) using vector notation

$$\boxed{(\boldsymbol{m}\cdot\hat{\boldsymbol{\sigma}})\,(\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}}) = (\boldsymbol{m}\cdot\boldsymbol{n})\,\mathbb{1} + i\,(\boldsymbol{m}\times\boldsymbol{n})\cdot\hat{\boldsymbol{\sigma}},} \tag{117}$$

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: $3\times2\times2$).
- Here $\boldsymbol{m}\cdot\hat{\boldsymbol{\sigma}}$ means

$$\boldsymbol{m}\cdot\hat{\boldsymbol{\sigma}} = m_x\,\hat{\sigma}^x + m_y\,\hat{\sigma}^y + m_z\,\hat{\sigma}^z \doteq \begin{pmatrix} m_z & m_x - i\,m_y \\ m_x + i\,m_y & -m_z \end{pmatrix}. \tag{118}$$

As we contract a 3-component vector $\boldsymbol{m}$ with a $3\times2\times2$-component tensor $\hat{\boldsymbol{\sigma}}$ along the first index (the dimension 3 index), the result is a 2×2 matrix.

HW 3

Use Eq. (117) to show that the product of three Pauli operators follows
$(\boldsymbol{l}\cdot\hat{\boldsymbol{\sigma}})\,(\boldsymbol{m}\cdot\hat{\boldsymbol{\sigma}})\,(\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}}) = i\,\boldsymbol{l}\cdot(\boldsymbol{m}\times\boldsymbol{n})\,\mathbb{1} + ((\boldsymbol{m}\cdot\boldsymbol{n})\,\boldsymbol{l} - (\boldsymbol{l}\cdot\boldsymbol{n})\,\boldsymbol{m} + (\boldsymbol{l}\cdot\boldsymbol{m})\,\boldsymbol{n})\cdot\hat{\boldsymbol{\sigma}}$
[Hint: the vector triple product formula will be useful
$\boldsymbol{l}\times(\boldsymbol{m}\times\boldsymbol{n}) = (\boldsymbol{l}\cdot\boldsymbol{n})\,\boldsymbol{m} - (\boldsymbol{l}\cdot\boldsymbol{m})\,\boldsymbol{n}$]

▪ Commutator

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

$$\left[\hat{O}, \hat{P}\right] = \hat{O}\,\hat{P} - \hat{P}\,\hat{O}. \tag{119}$$

- 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

$$\begin{aligned}\left[\hat{O}, \hat{P}+\hat{Q}\right] &= \left[\hat{O}, \hat{P}\right] + \left[\hat{O}, \hat{Q}\right],\\ \left[\hat{O}+\hat{P}, \hat{Q}\right] &= \left[\hat{O}, \hat{Q}\right] + \left[\hat{P}, \hat{Q}\right].\end{aligned} \tag{120}$$

Exc 13

Prove Eq. (120).

- Product rules

$$\left[\hat{O}, \hat{P}\,\hat{Q}\right] = \left[\hat{O}, \hat{P}\right]\hat{Q} + \hat{P}\left[\hat{O}, \hat{Q}\right],$$
$$\left[\hat{O}\,\hat{P}, \hat{Q}\right] = \left[\hat{O}, \hat{Q}\right]\hat{P} + \hat{O}\left[\hat{P}, \hat{Q}\right]. \tag{122}$$

Exc 14 Prove Eq. (122).

- Jacobi identity (as a replacement of associative law)

$$\left[\hat{O}, \left[\hat{P}, \hat{Q}\right]\right] + \left[\hat{P}, \left[\hat{Q}, \hat{O}\right]\right] + \left[\hat{Q}, \left[\hat{O}, \hat{P}\right]\right] = 0,$$
$$\left[\left[\hat{O}, \hat{P}\right], \hat{Q}\right] + \left[\left[\hat{P}, \hat{Q}\right], \hat{O}\right] + \left[\left[\hat{Q}, \hat{O}\right], \hat{P}\right] = 0. \tag{124}$$

Example: Commutators of Pauli operators

$$\left[\hat{\sigma}^x, \hat{\sigma}^y\right] = 2\,i\,\hat{\sigma}^z,$$
$$\left[\hat{\sigma}^y, \hat{\sigma}^z\right] = 2\,i\,\hat{\sigma}^x,$$
$$\left[\hat{\sigma}^z, \hat{\sigma}^x\right] = 2\,i\,\hat{\sigma}^y. \tag{125}$$

Or more compactly as

$$\boxed{\left[\hat{\sigma}^a, \hat{\sigma}^b\right] = 2\,i\,\epsilon^{abc}\,\hat{\sigma}^c,} \tag{126}$$

for $a, b, c = 1, 2, 3$ (stand for x, y, z). This can be considered as the defining algebraic properties of *single-qubit operators* (Pauli matrices). Or even more compactly using the **cross product** of vectors

$$\boxed{\hat{\boldsymbol{\sigma}} \times \hat{\boldsymbol{\sigma}} = 2\,i\,\hat{\boldsymbol{\sigma}}.} \tag{127}$$

■ Operator Function

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

$$\hat{O}^n = \hat{O}\,\hat{O} \ldots (n\text{ times}) \ldots \hat{O}. \tag{128}$$

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

$$f(x) = \sum_n c_n\, x^n, \tag{129}$$

the corresponding operator function is defined as

$$\boxed{f(\hat{O}) = \sum_n c_n\, \hat{O}^n,} \tag{130}$$

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

$$e^{x} = 1 + x + \frac{x^2}{2!} + \ldots = \sum_{n=0}^{\infty} \frac{1}{n!}\, x^n, \tag{131}$$

the exponential of an operator is defined as

$$e^{\hat{O}} = \mathbb{1} + \hat{O} + \frac{\hat{O}^2}{2!} + \ldots = \sum_{n=0}^{\infty} \frac{1}{n!}\, \hat{O}^n, \tag{132}$$

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

Example: exponentiating a Pauli matrix

Exc 15

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 4

Use the definition Eq. (132) 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

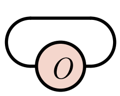
$$\mathrm{Tr}\ \hat{O} = \sum_i \langle i|\,\hat{O}\,|i\rangle. \tag{137}$$

The result is a scalar.

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

$$\mathrm{Tr}\begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} = O_{11} + O_{22} + \ldots = \sum_i O_{ii}. \tag{138}$$

- Tensor network representation (tracing = closing the legs)



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

$$\mathrm{Tr}\left(\alpha\,\hat{O} + \beta\,\hat{P}\right) = a\,\mathrm{Tr}\ \hat{O} + \beta\,\mathrm{Tr}\ \hat{P}. \tag{139}$$

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

$$\mathrm{Tr}\left(\hat{O}\,\hat{P}\right) = \mathrm{Tr}\left(\hat{P}\,\hat{O}\right),$$
$$\mathrm{Tr}\left(\hat{O}\,\hat{P}\,\hat{Q}\right) = \mathrm{Tr}\left(\hat{P}\,\hat{Q}\,\hat{O}\right) = \mathrm{Tr}\left(\hat{Q}\,\hat{O}\,\hat{P}\right), \tag{140}$$
$$\ldots$$

Exc 16 Prove Eq. (140).

Example: trace of Pauli operators

Pauli operators are *traceless*.

$$\mathrm{Tr}\,\hat{\sigma}^x = \mathrm{Tr}\,\hat{\sigma}^y = \mathrm{Tr}\,\hat{\sigma}^z = 0. \tag{143}$$

This is true for a Pauli operator along any direction

$$\boxed{\mathrm{Tr}\,\boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}} = 0.} \tag{144}$$

■ Projection Operators

■ Projectors

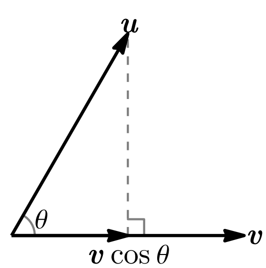
State projector: the projection operator onto a state $|v\rangle$

$$\boxed{\hat{\mathcal{P}}_v = |v\rangle\,\langle v|.} \tag{145}$$

Such that for any state $|u\rangle$, applying the projection operator $\hat{\mathcal{P}}_v$, the result is the projection of $|u\rangle$ along $|v\rangle$

$$\hat{\mathcal{P}}_v\,|u\rangle = |v\rangle\,\langle v|u\rangle. \tag{146}$$

Example: analog in the *real* vector space



$\boldsymbol{u}$ and $\boldsymbol{v}$ are two unit vectors, the projection of $\boldsymbol{u}$ on $\boldsymbol{v}$ is given by

$$\boldsymbol{v}\cos\theta = \boldsymbol{v}\,(\boldsymbol{v}\cdot\boldsymbol{u}). \tag{147}$$

Basis projector: the projection operator onto a basis state $|i\rangle$

$$\boxed{\hat{\mathcal{P}}_i = |i\rangle\,\langle i|.} \tag{148}$$

- Basis projectors satisfies the following properties

$$\begin{aligned} &\hat{\mathcal{P}}_i^2 = \hat{\mathcal{P}}_i, \\ &\hat{\mathcal{P}}_i \hat{\mathcal{P}}_j = 0 \quad \text{if } i \neq j. \end{aligned} \tag{149}$$

Or more compactly written as

$$\boxed{\hat{\mathcal{P}}_i \hat{\mathcal{P}}_j = \delta_{ij} \hat{\mathcal{P}}_i.} \tag{150}$$

Exc 17 Verify Eq. (149), following the definition Eq. (148).

- Given the one-hot representation of orthonormal basis

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \ |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \ \ldots. \tag{153}$$

Matrix representations of the corresponding basis projectors are

$$\hat{\mathcal{P}}_1 \doteq \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & \ddots \end{pmatrix}, \ \hat{\mathcal{P}}_2 \doteq \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 0 & \\ & & & \ddots \end{pmatrix}, \ \ldots. \tag{154}$$

Subspace projector: the projection operator onto a subspace. Suppose a subspace $\mathcal{H}_1$ is spanned by a set of orthonormal basis $\mathcal{B}_1 \subseteq \mathcal{B}$, its projector is

$$\boxed{\hat{\mathcal{P}}_{\mathcal{H}_1} = \sum_{|i\rangle \in \mathcal{B}_1} |i\rangle \langle i|.} \tag{155}$$

- Dimension of the subspace $\mathcal{H}_1$ is given by the trace of its projector (as it counts the number of basis states in $\mathcal{B}_1$)

$$\operatorname{Tr} \hat{\mathcal{P}}_{\mathcal{H}_1} = \dim \mathcal{H}_1. \tag{156}$$

- **Completeness relation**: *full* Hilbert space projector ≡ **identity operator**

$$\boxed{\hat{\mathcal{P}}_{\mathcal{H}} = \sum_{|i\rangle \in \mathcal{B}} |i\rangle \langle i| = \mathbb{1}.} \tag{157}$$

Recall Eq. (97) that $\mathbb{1} = \sum_i |i\rangle \langle i|$. Hilbert space dimension is given by

$$\dim \mathcal{H} = \operatorname{Tr} \hat{\mathcal{P}}_{\mathcal{H}} = \operatorname{Tr} \mathbb{1}. \tag{158}$$

HW 5

Consider a Hilbert space $\mathcal{H}$ spanned by three vectors
$|x\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|y\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, $|z\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.
Let $\mathcal{H}_{\parallel} = \text{span}\{|x\rangle, |y\rangle\}$ and $\mathcal{H}_{\perp} = \text{span}\{|z\rangle\}$ be complementary subspaces.
(i) Construct the subspace projectors $\hat{\mathcal{P}}_{\mathcal{H}_{\parallel}}$ and $\hat{\mathcal{P}}_{\mathcal{H}_{\perp}}$ and represent them as 3×3 matrices (in the $\{|x\rangle, |y\rangle, |z\rangle\}$ basis).
(ii) For any $|v\rangle \in \mathcal{H}$, show that $|v_{\parallel}\rangle = \hat{\mathcal{P}}_{\mathcal{H}_{\parallel}} |v\rangle$ and $|v_{\perp}\rangle = \hat{\mathcal{P}}_{\mathcal{H}_{\perp}} |v\rangle$ give the subspace decomposition of $|v\rangle$ such that $|v\rangle = |v_{\parallel}\rangle + |v_{\perp}\rangle$ with $|v_{\parallel}\rangle \in \mathcal{H}_{\parallel}$ and $|v_{\perp}\rangle \in \mathcal{H}_{\perp}$.

■ Quantum State Collapse*

What happens when we observe a quantum system?

Observing a quantum system can be viewed as a **hypothesis testing**.

- Given the **prior knowledge** that a quantum system is described by a state $|v\rangle$.
- An observer comes with an objective to test the **hypothesis** that "the quantum system is in a target state $|u\rangle$".
  - For this purpose, two projection operators are defined

$$\begin{aligned}\hat{\mathcal{P}}_u &= |u\rangle\langle u|, \text{ (projector to the state } |u\rangle) \\ \hat{\mathcal{P}}_{\overline{u}} &= \mathbb{1} - \hat{\mathcal{P}}_u. \text{ (projector to the complement subspace)}\end{aligned} \tag{159}$$

- Quantum mechanics predicts that the observation will *accept* the hypothesis with the **probability**

$$\boxed{p(u \mid v) = \langle v|\hat{\mathcal{P}}_u|v\rangle = |\langle u|v\rangle|^2,} \tag{160}$$

and *reject* the hypothesis with the (complement) probability

$$p(\overline{u} \mid v) = \langle v|\hat{\mathcal{P}}_{\overline{u}}|v\rangle = 1 - |\langle u|v\rangle|^2. \tag{161}$$

- After observation, if the hypothesis is *accepted* (the state $|u\rangle$ is observed), we must update our knowledge about the quantum system to the **posterior knowledge** described by the state $|u\rangle$. In this sense, the original quantum state $|v\rangle$ *collapses* to

$$\boxed{|v\rangle \to |u\rangle = \frac{\hat{\mathcal{P}}_u|v\rangle}{\sqrt{p(u \mid v)}} = \frac{\hat{\mathcal{P}}_u|v\rangle}{\sqrt{\langle v|\hat{\mathcal{P}}_u|v\rangle}}.} \tag{162}$$

- However, if the hypothesis is *rejected* (the state $|u\rangle$ is not observed), we must also update our posterior knowledge by collapsing to

$$|v\rangle \to \frac{\hat{\mathcal{P}}_{\overline{u}}|v\rangle}{\sqrt{p(\overline{u} \mid v)}} = \frac{\hat{\mathcal{P}}_{\overline{u}}|v\rangle}{\sqrt{\langle v|\hat{\mathcal{P}}_{\overline{u}}|v\rangle}}. \tag{163}$$

Exc 18 Verify Eq. (160), Eq. (161) and Eq. (162).

Summary: the **collapse** of any *prior* state $|v\rangle$ to the *target* state $|u\rangle$ is described by the state **projection operator** $\hat{\mathcal{P}}_u$ (associated with the *target* state).

- As an observable, it gives the probability $p(u \mid v)$ for the state collapse to happen.
- As an operator, it implements the state collapse $|v\rangle \to |u\rangle$ (Note: this is not a linear operation, as $|v\rangle$ appears on both the numerator and the denominator).

Example: Observing a qubit

Given the prior knowledge that a qubit is in the state

$$|\psi\rangle \doteq \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}. \tag{167}$$

The probability $p(0 \mid \psi)$ to observe the qubit in the state $|0\rangle$

$$|0\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow \hat{\mathcal{P}}_0 = |0\rangle\langle 0| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{168}$$

is given by

$$\begin{aligned} p(0 \mid \psi) &= \langle\psi|\,\hat{\mathcal{P}}_0\,|\psi\rangle \\ &= \begin{pmatrix} \psi_0^* & \psi_1^* \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} \\ &= \psi_0^*\,\psi_0 = |\psi_0|^2. \end{aligned} \tag{169}$$

If $|0\rangle$ state is indeed observed, the quantum state should collapse to

$$\begin{aligned} \frac{\hat{\mathcal{P}}_0\,|\psi\rangle}{\sqrt{p(0 \mid \psi)}} &\doteq \frac{1}{\sqrt{|\psi_0|^2}}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} \\ &= \frac{\psi_0}{|\psi_0|}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix} \doteq |0\rangle. \end{aligned} \tag{170}$$

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	$\mathcal{B} = \{\lvert i\rangle\}$	$\mathcal{B}^* = \{\langle i\rvert\}$
state	$\lvert v\rangle = \sum_i v_i \lvert i\rangle$	$\langle v\rvert = \sum_i v_i^* \langle i\rvert$
vector	$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix}$	$\begin{pmatrix} v_1^* & v_2^* & \cdots \end{pmatrix}$
component	$v_i = \langle i\vert v\rangle$	$v_i^* = \langle v\vert i\rangle$
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	$\lvert w\rangle = \hat{O} \lvert v\rangle$	$\langle w\rvert = \langle v\rvert \hat{O}^\dagger$

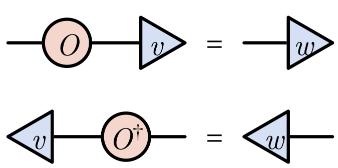
- Just like the *bra* $\langle v\rvert$ is the **dual** of the *ket* $\lvert u\rangle$, the **Hermitian conjugate** operator $\hat{O}^\dagger$ is the **dual** of the original operator $\hat{O}$, such that
  - if the operator $\hat{O}$ takes $\lvert v\rangle$ to $\lvert w\rangle$:

$$\begin{aligned} \hat{O} : \mathcal{H} &\to \mathcal{H} \\ \lvert v\rangle &\mapsto \lvert w\rangle = \hat{O} \lvert v\rangle \end{aligned} \tag{172}$$

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

$$\begin{aligned} \hat{O}^\dagger : \mathcal{H}^* &\to \mathcal{H}^* \\ \langle v\rvert &\mapsto \langle w\rvert = \langle v\rvert \hat{O}^\dagger \end{aligned} \tag{173}$$

- Tensor network representation



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

$$\hat{O} = \sum_{ij} \lvert i\rangle O_{ij} \langle j\rvert, \tag{174}$$

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

$$\boxed{\hat{O}^\dagger = \sum_{ij} \lvert i\rangle O_{ji}^* \langle j\rvert.} \tag{175}$$

Exc 19 Verify that Eq. (175) is consistent with the definition Eq. (173).

- 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.

$$\begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}^{\dagger} = \begin{pmatrix} O_{11}^{*} & O_{21}^{*} & \cdots \\ O_{12}^{*} & O_{22}^{*} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}. \tag{180}$$

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

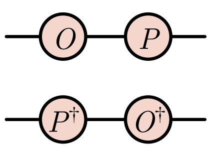
$$(\hat{O}^{\dagger})^{\dagger} = \hat{O}. \tag{181}$$

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

$$\left(\alpha\,\hat{O} + \beta\,\hat{P}\right)^{\dagger} = \alpha^{*}\,\hat{O}^{\dagger} + \beta^{*}\,\hat{P}^{\dagger}. \tag{182}$$

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

$$\boxed{\left(\hat{O}\,\hat{P}\right)^{\dagger} = \hat{P}^{\dagger}\,\hat{O}^{\dagger}.} \tag{183}$$



Exc 20 Prove the property Eq. (183).

■ 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.
- 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

$$\hat{O} = \hat{O}^\dagger, \tag{186}$$

or in terms of matrix elements,

$$O_{ij} = O_{ji}^*. \tag{187}$$

- Given a complex number z, real part: $\text{Re}\, z = (z + z^*)/2$, imaginary part: $\text{Im}\, z = (z - z^*)/(2\,i)$. Similarity, given a generally non-Hermitian operator $\hat{P}$

$$\text{Re}\,\hat{P} = \frac{1}{2}\left(\hat{P} + \hat{P}^\dagger\right),\ \text{Im}\,\hat{P} = \frac{1}{2\,i}\left(\hat{P} - \hat{P}^\dagger\right). \tag{188}$$

  - Both $\text{Re}\,\hat{P}$ and $\text{Im}\,\hat{P}$ are Hermitian operators.

Eigenvalues and Eigenvectors (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

$$\hat{O}\,|O_k\rangle = O_k\,|O_k\rangle,\ \ (k = 1, 2, \ldots) \tag{189}$$

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

- Eq. (189) is called the **eigen equation** of an operator $\hat{O}$.
  - The eigenvalues can be found by solving the algebraic (polynomial) equation for $O \in \mathbb{R}$

$$\det\left(\hat{O} - O\,\mathbb{1}\right) = 0. \tag{190}$$

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

$$\left(\hat{O} - O_k\,\mathbb{1}\right)|O_k\rangle = 0. \tag{191}$$

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

```
Eigensystem[{{1, -1}, {1, 1}}]
{{1 + i, 1 - i}, {{i, 1}, {-i, 1}}}
```

Degeneracy: an eigenvalue O_k of an operator $\hat{O}$ is called g_k-fold *degenerated*, if there are exactly g_k linearly independent eigenvectors corresponding to the same eigenvalue

$$\hat{O}\,|O_k, m\rangle = O_k\,|O_k, m\rangle,\ (m = 1, 2, \ldots, g_k). \tag{192}$$

- Since any linear combination of the degenerated eigenvectors

$$\sum_{m=1}^{g_k} \alpha_m\,|O_k, m\rangle,\ \left(\text{with } \alpha_k \in \mathbb{C}\right) \tag{193}$$

is still an eigenvector of the same eigenvalue O_k, thus the **degenerated eigenvectors** forms a **degenerated subspace** $\mathcal{H}_{O=O_k}$ (the subspace of all eigenvectors of the same eigenvalue O_k)

$$\mathcal{H}_{O=O_k} = \text{span}\{|O_k,m\rangle : m = 1, 2, \ldots, g_k\}. \tag{194}$$

- **Eigen projector**: projection operator to the degenerated subspace associated with an eigenvalue O_k

$$\boxed{\hat{\mathcal{P}}_{O=O_k} = \sum_{m=1}^{g_k} |O_k,m\rangle\langle O_k,m|.} \tag{195}$$

▪ Eigenvalues and Eigenvectors (Hermitian Operator)

What is special about Hermitian operators?

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

$$\hat{O}|O_k\rangle = O_k|O_k\rangle, \; (k = 1, 2, \ldots). \tag{196}$$

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

$$\hat{O} = \hat{O}^\dagger \Rightarrow O_k \in \mathbb{R}. \tag{197}$$

- **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)

$$O_k \neq O_l \Rightarrow \langle O_k|O_l\rangle = 0. \tag{198}$$

  - 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 21 | Prove Eq. (197) and Eq. (198).

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 $\hat{O}$.

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

$$\hat{O} = \sum_k |O_k\rangle\, O_k\, \langle O_k|. \tag{205}$$

- Note: unlike a generic matrix representation $\hat{O} = \sum_{ij} |i\rangle\, O_{ij}\, \langle j|$, in the spectral decomposition Eq. (205), the summation only run through the eigenbasis once.
- In the eigenbasis, the Hermitian operator is represented as a **diagonal matrix**.

$$\hat{O} \simeq \begin{pmatrix} O_1 & & \\ & O_2 & \\ & & \ddots \end{pmatrix}. \tag{206}$$

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.)

- More generally, when there are **degeneracies**, Eq. (205) should be written to

$$\begin{aligned}\hat{O} &= \sum_k \sum_{m=1}^{g_k} |O_k, m\rangle\, O_k\, \langle O_k, m| \\ &= \sum_k O_k\, \hat{\mathcal{P}}_{O=O_k},\end{aligned} \tag{207}$$

where the eigen projector $\hat{\mathcal{P}}_{O=O_k}$ was defined in Eq. (195).

- The fact that all eigenvectors of $\hat{O}$ form a complete set of orthonormal basis can be rephrases as the following properties of eigen projectors
  - Orthonormality

$$\hat{\mathcal{P}}_{O=O_k}\, \hat{\mathcal{P}}_{O=O_l} = \delta_{kl}\, \hat{\mathcal{P}}_{O=O_k}. \tag{208}$$

Meaning that $\hat{\mathcal{P}}^2_{O=O_k} = \hat{\mathcal{P}}_{O=O_k}$ and $\hat{\mathcal{P}}_{O=O_k}\, \hat{\mathcal{P}}_{O=O_l} = 0$ if $k \neq l$ (i.e. $O_k \neq O_l$).

  - Completeness

$$\sum_k \hat{\mathcal{P}}_{O=O_k} = \hat{\mathcal{P}}_{\mathcal{H}} \equiv \mathbb{1}. \tag{209}$$

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	$\lvert + \rangle$	$\lvert - \rangle$	$\lvert i \rangle$	$\lvert \bar{i} \rangle$	$\lvert 0 \rangle$	$\lvert 1 \rangle$
(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	$\lvert + \rangle \langle + \rvert$	$\lvert - \rangle \langle - \rvert$	$\lvert i \rangle \langle i \rvert$	$\lvert \bar{i} \rangle \langle \bar{i} \rvert$	$\lvert 0 \rangle \langle 0 \rvert$	$\lvert 1 \rangle \langle 1 \rvert$
(matrix)	$\frac{1}{2}\begin{pmatrix}1&1\\1&1\end{pmatrix}$	$\frac{1}{2}\begin{pmatrix}1&-1\\-1&1\end{pmatrix}$	$\frac{1}{2}\begin{pmatrix}1&-i\\i&1\end{pmatrix}$	$\frac{1}{2}\begin{pmatrix}1&i\\-i&1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&0\end{pmatrix}$	$\begin{pmatrix}0&0\\0&1\end{pmatrix}$

Spectral decompositions:

- Pauli-x

$$\hat{\sigma}^x = \hat{\mathcal{P}}_{\sigma^x=+1} - \hat{\mathcal{P}}_{\sigma^x=-1}, \tag{211}$$

with projection operators

$$\begin{aligned}\hat{\mathcal{P}}_{\sigma^x=+1} &= \lvert + \rangle \langle + \rvert = \frac{\mathbb{1} + \hat{\sigma}^x}{2},\\ \hat{\mathcal{P}}_{\sigma^x=-1} &= \lvert - \rangle \langle - \rvert = \frac{\mathbb{1} - \hat{\sigma}^x}{2}.\end{aligned} \tag{212}$$

- Pauli-y

$$\hat{\sigma}^y = \hat{\mathcal{P}}_{\sigma^y=+1} - \hat{\mathcal{P}}_{\sigma^y=-1}, \tag{213}$$

with projection operators

$$\begin{aligned}\hat{\mathcal{P}}_{\sigma^y=+1} &= \lvert i \rangle \langle i \rvert = \frac{\mathbb{1} + \hat{\sigma}^y}{2},\\ \hat{\mathcal{P}}_{\sigma^y=-1} &= \lvert \bar{i} \rangle \langle \bar{i} \rvert = \frac{\mathbb{1} - \hat{\sigma}^y}{2}.\end{aligned} \tag{214}$$

- Pauli-z

$$\hat{\sigma}^z = \hat{\mathcal{P}}_{\sigma^z=+1} - \hat{\mathcal{P}}_{\sigma^z=-1}, \tag{215}$$

with projection operators

$$\begin{aligned}\hat{\mathcal{P}}_{\sigma^z=+1} &= \lvert 0 \rangle \langle 0 \rvert = \frac{\mathbb{1} + \hat{\sigma}^z}{2},\\ \hat{\mathcal{P}}_{\sigma^z=-1} &= \lvert 1 \rangle \langle 1 \rvert = \frac{\mathbb{1} - \hat{\sigma}^z}{2}.\end{aligned} \tag{216}$$

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

$$\boxed{\boldsymbol{n} \cdot \hat{\boldsymbol{\sigma}} = \hat{\mathcal{P}}_{\boldsymbol{n}\cdot\boldsymbol{\sigma}=+1} - \hat{\mathcal{P}}_{\boldsymbol{n}\cdot\boldsymbol{\sigma}=-1},} \tag{217}$$

with the projection operators

$$\hat{\mathcal{P}}_{\boldsymbol{n}\cdot\boldsymbol{\sigma}=\pm 1} = |\boldsymbol{n}\cdot\boldsymbol{\sigma}=\pm 1\rangle\langle\boldsymbol{n}\cdot\boldsymbol{\sigma}=\pm 1| = \frac{\mathbb{1} \pm \boldsymbol{n}\cdot\hat{\boldsymbol{\sigma}}}{2}. \tag{218}$$

Exc 22

Prove Eq. (217) and Eq. (218).

HW 6

Assuming $\hat{O}$ is a Hermitian operator, use the spectral decomposition Eq. (207) and the properties of projection operators to show that
(i) The operator power can be expanded as $\hat{O}^n = \sum_k O_k^n \hat{\mathcal{P}}_{O=O_k}$.
(ii) More generally, the operator function $f(\hat{O})$ defined in Eq. (130) can be expanded as $f(\hat{O}) = \sum_k f(O_k)\hat{\mathcal{P}}_{O=O_k}$.

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 $|O_k, m\rangle$ $(m = 1, 2, \ldots, g_k)$,

$$\hat{O} = \sum_k O_k \hat{\mathcal{P}}_{O=O_k}, \tag{226}$$

where the eigen projector is

$$\hat{\mathcal{P}}_{O=O_k} = \sum_{m=1}^{g_k} |O_k, m\rangle\langle O_k, m|. \tag{227}$$

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 $\mathcal{H}_k$ of the corresponding measurement outcome O_k. The state collapse is implemented by the *eigen projector* $\hat{\mathcal{P}}_{\mathcal{H}_k}$.

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 $p(O_k \mid \psi) = \langle\psi| \hat{\mathcal{P}}_{O=O_k} |\psi\rangle$,
(ii) if O_k is observed, the state will **collapse** to $\hat{\mathcal{P}}_{O=O_k} |\psi\rangle \big/ \sqrt{p(O_k \mid \psi)}$.

In quantum measurement, there is no way to tell for certain which outcome will be observed. There is only a conditional probability $p(O_k \mid \psi)$ that we can compute.

- **Non-degenerated case**: Suppose O_k has *no* degeneracy,

$$\hat{\mathcal{P}}_{O=O_k} = |O_k\rangle \langle O_k|. \tag{228}$$

  - The *probability* to observe O_k is given by the squared overlap between the prior state $|\psi\rangle$ and the eigenstate $|O_k\rangle$

$$p(O_k \mid \psi) = |\langle O_k|\psi\rangle|^2. \tag{229}$$

  - After the measurement, if O_k is observed, the system collapses to the posterior state $|O_k\rangle$

$$|\psi\rangle \xrightarrow{\text{measure } O, \text{ observe } O_k} |O_k\rangle. \tag{230}$$

These results are consistent with our previous discussions in Eq. (160) and Eq. (162) about quantum state collapse.

- **Degenerated case** (generic): With degeneracy, the eigen projector is

$$\hat{\mathcal{P}}_{O=O_k} = \sum_{m=1}^{g_k} |O_k, m\rangle \langle O_k, m|. \tag{231}$$

  - The *probability* to observe O_k is given by the squared overlap between the prior state $|\psi\rangle$ and all eigenstates $|O_k, m\rangle$ in the degenerate subspace

$$\boxed{p(O_k \mid \psi) = \sum_{m=1}^{g_k} |\langle O_k, m|\psi\rangle|^2.} \tag{232}$$

  - After the measurement, if O_k is observed, the system collapses to the posterior state, given by a linear superposition of $|O_k, m\rangle$

$$\boxed{|\psi\rangle \xrightarrow{\text{measure } O, \text{ observe } O_k} \sum_{m=1}^{g_k} \alpha_m |O_k, m\rangle,} \tag{233}$$

  where the coefficients α_m are given by

$$\alpha_m = \frac{\langle O_k, m|\psi\rangle}{\sqrt{p(O_k \mid \psi)}}. \tag{234}$$

Exc 23 Derive Eq. (232) and Eq. (233) from Eq. (195).

HW 7

> 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

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

$$\begin{aligned}\langle O\rangle &:= \sum_k O_k\, p(O_k\,|\,\psi) \\ &= \sum_k O_k \langle\psi|\,\hat{\mathcal{P}}_{O=O_k}\,|\psi\rangle.\end{aligned} \tag{238}$$

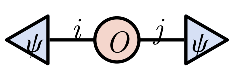
Given $\hat{O} = \sum_k O_k \hat{\mathcal{P}}_{O=O_k}$, we conclude

$$\boxed{\langle O\rangle = \langle\psi|\,\hat{O}\,|\psi\rangle.} \tag{239}$$

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

$$\langle O\rangle = (\,\psi_1^* \;\; \psi_2^* \;\; \cdots\,)\begin{pmatrix} O_{11} & O_{12} & \cdots \\ O_{21} & O_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix}\psi_1 \\ \psi_2 \\ \vdots\end{pmatrix}. \tag{240}$$

- Tensor network representation

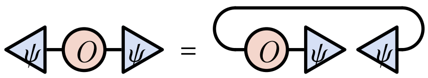


$$\langle O\rangle = \sum_{ij} \psi_i^*\, O_{ij}\, \psi_j.$$

Alternatively, the expectation value can also be written as a trace of the product of the observable operator $\hat{O}$ and the state projector $\hat{\mathcal{P}}_\psi = |\psi\rangle\langle\psi|$ [defined in Eq. (145)]

$$\boxed{\langle O\rangle = \mathrm{Tr}\; \hat{O}\,\hat{\mathcal{P}}_\psi.} \tag{241}$$

- The equivalence between Eq. (239) and Eq. (241) is self-evident from the tensor network diagrams



- 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 8

> 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 $\boldsymbol{n}$.]

Sequential Measurements

Commuting Operators

Commuting operators share common eigenbasis, and the converse is also true.

- **Commuting operators**: Two operators $\hat{A}$ and $\hat{B}$ **commute**, if $\hat{A}\,\hat{B} = \hat{B}\,\hat{A}$ (operators can commute through each other), i.e.

$$\left[\hat{A},\, \hat{B}\right] = 0. \tag{242}$$

(Here 0 denotes the *zero operator*, a matrix whose elements are all zeros.)

- **Common eigenbasis**: Two operators $\hat{A}$ and $\hat{B}$ share a *common* eigenbasis, if there exist a complete set of basis $\mathcal{B} = \{|A_k, B_k\rangle : k = 1, 2, \ldots, \dim\mathcal{H}\}$ such that both operators are *diagonal* in the basis $\mathcal{B}$, i.e.

$$\begin{aligned} \hat{A}\,|A_k,B_k\rangle &= A_k\,|A_k,B_k\rangle, \\ \hat{B}\,|A_k,B_k\rangle &= B_k\,|A_k,B_k\rangle. \end{aligned} \tag{243}$$

Idea: commuting operators can *pass through* each other as if they were *numbers*. If $\hat{A}$ and $\hat{B}$ share a common eigenbasis, when acting on their common eigenvectors, they behave like numbers (by their eigenvalues),

$$\hat{A}\,\hat{B}\,|A_k,B_k\rangle = A_k\,B_k\,|A_k,B_k\rangle = B_k\,A_k\,|A_k,B_k\rangle = \hat{B}\,\hat{A}\,|A_k,B_k\rangle. \tag{244}$$

Any state $|v\rangle = \sum_k \alpha_k\,|A_k,B_k\rangle$ is just a linear superposition of the basis states, so the behavior of $\hat{A}\,\hat{B}\,|v\rangle = \hat{B}\,\hat{A}\,|v\rangle$ is generic for all states, thus the equality can be promoted from the state level to the operator level $\hat{A}\,\hat{B} = \hat{B}\,\hat{A}$, i.e. the two operators commute.

Example: Finding common eigenbasis of commuting operators. Consider two Hermitian operators

$$\hat{A} \simeq \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \; \hat{B} \simeq \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}. \tag{245}$$

```
A = {{0, 0, 0, 1}, {0, 0, 1, 0}, {0, 1, 0, 0}, {1, 0, 0, 0}};
B = {{0, -i, 0, 0}, {i, 0, 0, 0}, {0, 0, 0, i}, {0, 0, -i, 0}};
A // MatrixForm
B // MatrixForm
```

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

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

It can be checked that $\hat{A}$ and $\hat{B}$ commute (by showing that $\left[\hat{A}, \hat{B}\right] = 0$)

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

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

They must share a set of common eigenbasis. How to find that? - Strategy: using a random algorithm.

- Construct a random operator $\hat{H} = a\,\hat{A} + b\,\hat{B}$ by combining $\hat{A}$ and $\hat{B}$ with random numbers a and b.

```
(H = 0.2 A + 0.5 B) // MatrixForm
```

$$\begin{pmatrix} 0. & 0. - 0.5\,i & 0. & 0.2 \\ 0. + 0.5\,i & 0. & 0.2 & 0. \\ 0. & 0.2 & 0. & 0. + 0.5\,i \\ 0.2 & 0. & 0. - 0.5\,i & 0. \end{pmatrix}$$

- Find the eigenbasis of $\hat{H}$

```
{vals, vecs} = Chop@Eigensystem[H]
```

```
{{0.7, -0.7, 0.3, -0.3},
 {{-0.5, 0. - 0.5 i, 0. - 0.5 i, -0.5}, {-0.5, 0. + 0.5 i, 0. - 0.5 i, 0.5},
  {-0.5, 0. - 0.5 i, 0. + 0.5 i, 0.5}, {-0.5, 0. + 0.5 i, 0. + 0.5 i, -0.5}}}
```

$$|1\rangle = \frac{1}{2}\begin{pmatrix} -1 \\ -i \\ -i \\ -1 \end{pmatrix},\ |2\rangle = \frac{1}{2}\begin{pmatrix} -1 \\ +i \\ -i \\ +1 \end{pmatrix},\ |3\rangle = \frac{1}{2}\begin{pmatrix} -1 \\ -i \\ +i \\ +1 \end{pmatrix},\ |4\rangle = \frac{1}{2}\begin{pmatrix} -1 \\ +i \\ +i \\ -1 \end{pmatrix} \tag{246}$$

- With probability 1, the eigenbasis of $\hat{H}$ is the common eigenbasis of $\hat{A}$ and $\hat{B}$, such that both operators are diagonal in this basis.

```
Chop[vecs.A.ConjugateTranspose[vecs]] // MatrixForm
Chop[vecs.B.ConjugateTranspose[vecs]] // MatrixForm
```

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

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

We might rename the eigenvectors by their eigenvalues under both $\hat{A}$ and $\hat{B}$,

$$|1\rangle \to |+1,-1\rangle,\ |2\rangle \to |-1,+1\rangle,\ |3\rangle \to |-1,-1\rangle,\ |4\rangle \to |+1,+1\rangle; \tag{247}$$

such that the eigen equations can be written in the standard form Eq. (243)

$$\begin{aligned} \hat{A}\,|A_k,B_k\rangle &= A_k\,|A_k,B_k\rangle, \\ \hat{B}\,|A_k,B_k\rangle &= B_k\,|A_k,B_k\rangle; \end{aligned} \tag{248}$$

with the eigenvalues arranged as

$$\begin{aligned} (A_1, A_2, A_3, A_4) &= (+1, -1, -1, +1), \\ (B_1, B_2, B_3, B_4) &= (-1, +1, -1, +1). \end{aligned} \tag{249}$$

▪ Compatible Observables

Suppose A and B are two *observables* and we perform the following **sequential measurements** on a single quantum system:

1. measure A,

2. measure B,

3. measure A.

We say that A and B are **compatible observables**, iff the result of **3** is always *certain* to be the same as the result of **1**.

In general, this will not be the case.

- In step **1**, we measure A and suppose that we obtain the outcome A_1 (as one eigenvalue of $\hat{A}$), the system has collapse to the state $|A_1\rangle$.
- In step **2**, we measure B and suppose that we obtain the outcome B_1 (as one eigenvalue of $\hat{B}$), the system will collapse to the state $|B_1\rangle$. (This will happen with probability $|\langle B_1|A_1\rangle|^2$).
- In step **3**, we measure A again. There is no guarantee that the previous outcome A_1 will appear again. Instead we may obtain a different outcome A_2 with probability $|\langle A_2|B_1\rangle|^2$ in general.
- In order to obtain A_1 again with probability 1, we must require

  $$|\langle A_1|B_1\rangle|^2 = 1, \tag{250}$$

  i.e. $|A_1\rangle$ and $|B_1\rangle$ labels the identical state. Since $|A_1\rangle$ is an eigenstate of $\hat{A}$ with eigenvalue A_1 and $|B_1\rangle$ is an eigenstate of $\hat{B}$ with eigenvalue B_1, the state must be a common eigenstate $|A_1,B_1\rangle$ of both $\hat{A}$ and $\hat{B}$, s.t.

  $$\begin{aligned}\hat{A}\,|A_1,B_1\rangle &= A_1\,|A_1,B_1\rangle,\\ \hat{B}\,|A_1,B_1\rangle &= B_1\,|A_1,B_1\rangle.\end{aligned} \tag{251}$$

- For this scenario to always happen regardless the choice of (A_1, B_1), $\hat{A}$ and $\hat{B}$ share a set of common eigenbasis $|A_k,B_k\rangle$ $(k = 1, 2, \ldots, \dim\mathcal{H})$.

Conclusion: Given two *observables* A and B, described by Hermitian operators $\hat{A}$ and $\hat{B}$, then following statements are equivalent

- A and B are *compatible observables*;
- $\hat{A}$ and $\hat{B}$ share *common eigenbasis*;
- $\hat{A}$ and $\hat{B}$ are *commuting operators*: $\left[\hat{A}, \hat{B}\right] = 0$.

Repeated Measurements

Statistics of Measurements

Repeated measurements: Given a state $|\psi\rangle$ and an observable O, perform the following repeatedly:

1. prepare a quantum system in the state $|\psi\rangle$ (e.g. by measuring $\hat{\mathcal{P}}_\psi = |\psi\rangle\langle\psi|$ and post-select);
2. measure O on the state $|\psi\rangle$ (the outcome O_k will be obtained with probability $p(O_k\,|\,\psi) = \langle\psi|\,O_k\,|\psi\rangle$)
3. discard the quantum system (or reset the state).

This will collect an ensemble of measurement outcomes

$$\left\{O_k : p(O_k\,|\,\psi) = |\langle O_k|\psi\rangle|^2\right\}. \tag{252}$$

With this ensemble, we can define the following statistics

- **Mean** (expectation value):

$$\langle O\rangle = \sum_k O_k\, p(O_k \mid \psi) = \langle\psi|\,\hat{O}\,|\psi\rangle. \tag{253}$$

- **Variance** (2nd moment):

$$\operatorname{var} O = \sum_k (O_k - \langle O\rangle)^2\, p(O_k \mid \psi) = \langle\psi|\left(\hat{O} - \langle O\rangle\, \mathbb{1}\right)^2 |\psi\rangle. \tag{254}$$

  Introduce the observable ΔO (the deviation of O from its expectation value)

$$\Delta O = O - \langle O\rangle\, \mathbb{1}, \tag{255}$$

  The variance can be written as $\operatorname{var} O = \left\langle(\Delta O)^2\right\rangle$.

- **Standard deviation**: characterizes the **uncertainty** of the measurement of O

$$\operatorname{std} O = (\operatorname{var} O)^{1/2} = \left\langle(\Delta O)^2\right\rangle^{1/2}. \tag{256}$$

▪ Uncertainty Relation

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

$$\boxed{(\operatorname{std} A)\,(\operatorname{std} B) \geq \frac{1}{2}\,|\langle[A, B]\rangle|.} \tag{257}$$

- 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 ($[A, B] = 0$), $(\operatorname{std} A)\,(\operatorname{std} B) \geq 0$, it is possible to have $\operatorname{std} A = \operatorname{std} B = 0$ 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 $\operatorname{std} A = \operatorname{std} B = 0$ simultaneously, i.e. A and B can not be jointly measured with certainty.

Proof of the uncertainty relation:

Suppose $\hat{A}$ and $\hat{B}$ are Hermitian operators. Let $|\phi\rangle = \left(\hat{A} + i\,x\,\hat{B}\right)|\psi\rangle$. For any choice of $x \in \mathbb{R}$,

$$\langle\psi|\left(\hat{A} - i\,x\,\hat{B}\right)\left(\hat{A} + i\,x\,\hat{B}\right)|\psi\rangle = \langle\phi \mid \phi\rangle \geq 0. \tag{258}$$

On the other hand,

$$\begin{aligned} &\langle\psi|\left(\hat{A} - i\,x\,\hat{B}\right)\left(\hat{A} + i\,x\,\hat{B}\right)|\psi\rangle \\ &= \langle\psi|\,\hat{A}^2 + i\,x\left[\hat{A}, \hat{B}\right] + x^2\,\hat{B}^2\,|\psi\rangle \\ &= \left\langle B^2\right\rangle x^2 + i\,\langle[A, B]\rangle\,x + \left\langle A^2\right\rangle \geq 0. \end{aligned} \tag{259}$$

The quadratic equation $\langle B^2 \rangle x^2 + i \langle [A, B] \rangle x + \langle A^2 \rangle = 0$ has no (or only one) real root, implying that its discriminant Δ must be negative (or zero), i.e.

$$\Delta = (i \langle [A, B] \rangle)^2 - 4 \langle B^2 \rangle \langle A^2 \rangle \leq 0. \tag{260}$$

Therefore for any A, B on any state $|\psi\rangle$,

$$\langle A^2 \rangle^{1/2} \langle B^2 \rangle^{1/2} \geq \frac{1}{2} |\langle [A, B] \rangle|. \tag{261}$$

The uncertainty relation Eq. (257) can be shown by replacing $A \to \Delta A$ and $B \to \Delta B$.

HW 9

Suppose A and B are Hermitian operators.
(i) Show that $\langle A^2 \rangle$, $\langle B^2 \rangle$ and $i \langle [A, B] \rangle$ are real.
(ii) Show that $[\Delta A, \Delta B] = [A, B]$.

Dynamics

Unitary Operators

Basis Transformation

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

$$\begin{aligned} \mathcal{B} &= \{|i\rangle : i = 1, 2, \ldots, \dim \mathcal{H}\}, \\ \mathcal{B}' &= \{|i\rangle' : i = 1, 2, \ldots, \dim \mathcal{H}\}. \end{aligned} \tag{262}$$

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

$$v_i = \langle i| |v\rangle, \ \ v'_i = \langle i|' |v\rangle. \tag{263}$$

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

$$O_{ij} = \langle i| \hat{O} |j\rangle, \ \ O'_{ij} = \langle i|' \hat{O} |j\rangle'. \tag{264}$$

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

$$\boxed{U_{ij} = \langle i|' |j\rangle.} \tag{265}$$

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

$$\begin{aligned} v'_i &= \sum_j U_{ij} v_j, \\ O'_{ij} &= \sum_{kl} U_{ik} O_{kl} U^*_{jl}. \end{aligned} \tag{266}$$

Exc 24 Using Eq. (265) to prove that Eq. (266) is compatible with Eq. (263) and Eq. (264).

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

$$\hat{U} = \sum_i |i\rangle \langle i|'. \tag{269}$$

Exc 25 Check that the matrix element of $\hat{U}$ in Eq. (269) is indeed given by Eq. (265), when represented in either the basis $\mathcal{B}$ or $\mathcal{B}'$.

$\hat{U}$ in Eq. (269) is an example of the **unitary operator**.

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

$$\hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = \mathbb{1}. \tag{272}$$

Exc 26 Check that Eq. (269) satisfies the defining property Eq. (272) for unitary operator.

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

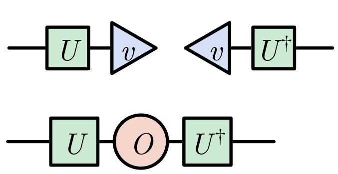
$$\hat{U}^{-1} = \hat{U}^\dagger. \tag{274}$$

  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. (266) can be written as

$$\begin{aligned} &\text{for ket state}: \quad |v\rangle \to \hat{U}\,|v\rangle, \\ &\text{for bra state}: \quad \langle v| \to \langle v|\,\hat{U}^\dagger, \\ &\text{for operator}: \quad \hat{O} \to \hat{U}\,\hat{O}\,\hat{U}^\dagger. \end{aligned} \tag{275}$$



- 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*.)

$$\langle O \rangle = \langle \psi | \, \hat{O} \, | \psi \rangle \to \langle \psi | \, \hat{U}^\dagger \, \hat{U} \, \hat{O} \, \hat{U}^\dagger \, \hat{U} \, | \psi \rangle = \langle \psi | \, \mathbb{1} \, \hat{O} \, \mathbb{1} \, | \psi \rangle = \langle O \rangle. \tag{276}$$

■ 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*.

$$\begin{aligned} \hat{O} &= \sum_k |O_k\rangle \, O_k \, \langle O_k|, \\ \hat{U} &= \sum_k |k\rangle \, \langle O_k|, \end{aligned} \tag{277}$$

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

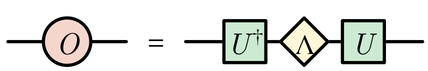
$$\hat{\Lambda} = \hat{U} \, \hat{O} \, \hat{U}^\dagger = \sum_k |k\rangle \, O_k \, \langle k| \doteq \begin{pmatrix} O_1 & & \\ & O_2 & \\ & & \ddots \end{pmatrix} \tag{278}$$

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

- Every *Hermitian* matrix can be written as

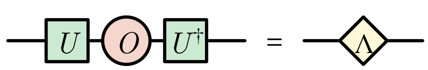
$$\hat{O} = \hat{U}^\dagger \, \hat{\Lambda} \, \hat{U}, \tag{279}$$

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,

$$\hat{U} \, \hat{O} \, \hat{U}^\dagger = \hat{\Lambda}. \tag{280}$$



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 $\hat{\sigma}^x$)

$$\hat{U}_{\mathsf{H}} = \begin{pmatrix} \langle + | \\ \langle - | \end{pmatrix} \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{281}$$

- 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 $\hat{\sigma}^z$

$$\hat{U}_{\mathsf{H}}\,\hat{\sigma}^x\,\hat{U}_{\mathsf{H}}^\dagger \simeq \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \simeq \hat{\sigma}^z. \tag{282}$$

▪ Hermitian Generators

If **Hermitian operators** are generalization of **real numbers**, then **unitary operators** are generalization of **phase factors**. ($z \in \mathbb{C}$ and $|z| = 1$)

$$z^*\,z = z\,z^* = |z|^2 = 1. \tag{283}$$

- For complex numbers, a phase factor can be written as $z = e^{i\,\theta}$, where $\theta \in \mathbb{R}$ is a *real* phase angle.
- Similar ideas apply to unitary operators: every **unitary operator** can be **generated** by a **Hermitian operator** $\hat{\Theta}$ in the form of

$$\boxed{\hat{U} = e^{i\,\hat{\Theta}}.} \tag{284}$$

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

$$\hat{\Theta} = \sum_k \Theta_k\,\hat{\mathcal{P}}_{\Theta=\Theta_k} \tag{285}$$

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

- either by operator Taylor expansion Eq. (132)

$$e^{i\,\hat{\Theta}} = \mathbb{1} + i\,\hat{\Theta} + \frac{\left(i\,\hat{\Theta}\right)^2}{2!} + \frac{\left(i\,\hat{\Theta}\right)^3}{3!} + \ldots. \tag{286}$$

- or by spectral decomposition (HW 6)

$$e^{i\,\hat{\Theta}} = \sum_k e^{i\,\Theta_k}\,\hat{\mathcal{P}}_{\Theta=\Theta_k} \tag{287}$$

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

Exc 27 Use Eq. (287) 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 15).

$$\hat{U}(\theta) = e^{i\,\theta\,\hat{\sigma}^y} \simeq \begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix}. \tag{289}$$

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

$$\hat{U}(\theta)\,|0\rangle \simeq \begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = \begin{pmatrix}\cos\theta\\ -\sin\theta\end{pmatrix}. \tag{290}$$

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

$$\hat{U}(\Delta\theta) = \hat{U}(0) + \hat{U}'(0)\,\Delta\theta + \ldots = \mathbb{1} + \hat{U}'(0)\,\Delta\theta + \ldots, \tag{291}$$

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**

$$\hat{U}(\Delta\theta) = \mathbb{1} + i\,\Delta\theta\,\hat{G} + \ldots. \tag{292}$$

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

$$\begin{aligned} &U(\Delta\theta)^\dagger\,U(\Delta\theta) \\ &= \left(\mathbb{1} - i\,\Delta\theta\,\hat{G}^\dagger + \ldots\right)\left(\mathbb{1} + i\,\Delta\theta\,\hat{G} + \ldots\right) \\ &= \mathbb{1} + i\,\Delta\theta\left(\hat{G} - \hat{G}^\dagger\right) + \ldots = \mathbb{1}. \end{aligned} \tag{293}$$

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

$$\hat{U}(N\,\Delta\theta) = \hat{U}(\Delta\theta)^N = \left(\mathbb{1} + i\,\Delta\theta\,\hat{G}\right)^N. \tag{294}$$

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

$$\ln \hat{U}(N\,\Delta\theta) = N \ln\left(\mathbb{1} + i\,\Delta\theta\,\hat{G}\right) = i\,N\,\Delta\theta\,\hat{G}, \tag{295}$$

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

$$\boxed{\hat{U}(\theta) = e^{i\,\theta\,\hat{G}}.} \tag{296}$$

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 $\Rightarrow$ **remains** in **different** states (towards both future and past).
- start out in the **same** state $\Rightarrow$ 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.

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle, \tag{297}$$

$|\psi(0)\rangle$ 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*:

$$\langle\phi(0)\mid\psi(0)\rangle = 0 \Rightarrow \langle\phi(t)\mid\psi(t)\rangle = \langle\phi(0)|\,\hat{U}(t)^\dagger\,\hat{U}(t)\,|\psi(0)\rangle = 0. \tag{298}$$

- *Identical* states remain the *identical*:

$$\langle\psi(0)\mid\psi(0)\rangle = 1 \Rightarrow \langle\psi(t)\mid\psi(t)\rangle = \langle\psi(0)|\,\hat{U}(t)^\dagger\,\hat{U}(t)\,|\psi(0)\rangle = 1. \tag{299}$$

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. (298) and Eq. (299) implies

$$\langle i|\,\hat{U}(t)^\dagger\,\hat{U}(t)\,|j\rangle = \delta_{ij} \Rightarrow \hat{U}(t)^\dagger\,\hat{U}(t) = \mathbb{1}. \tag{300}$$

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**,

$$\hat{H} = i\,\hat{U}'(0) = i\,\partial_t\,\hat{U}(t)\,|_{t=0}\,. \tag{301}$$

For small Δt, *infinitesimal* evolution is given by

$$\hat{U}(\Delta t) = \mathbb{1} - i\,\hat{H}\,\Delta t + \ldots, \tag{302}$$

therefore the state evolves as

$$|\psi(\Delta t)\rangle = \hat{U}(\Delta t)\,|\psi(0)\rangle = |\psi(0)\rangle - i\,\Delta t\,\hat{H}\,|\psi(0)\rangle, \tag{303}$$

meaning that

$$i\,\partial_t|\psi(0)\rangle = i\,\frac{|\psi(\Delta t)\rangle - |\psi(0)\rangle}{\Delta t} = \hat{H}\,|\psi(0)\rangle. \tag{304}$$

There is nothing special about $t = 0$. Eq. (304) should hold at any time.

$$i\,\partial_t|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle. \tag{305}$$

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?

$$\hbar = \frac{h}{2\pi} = 1.0545718\,(13) \times 10^{-34}\ \text{J s}. \tag{306}$$

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. (305):

$$i\,\hbar\,\partial_t |\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle. \tag{307}$$

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**.

$$\boxed{i\,\hbar\,\partial_t |\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle.} \tag{308}$$

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

$$\boxed{\hat{H}\,|E_k\rangle = E_k\,|E_k\rangle.} \tag{309}$$

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*,

$$|E_k(t)\rangle = e^{-\frac{i}{\hbar} E_k t}\,|E_k\rangle. \tag{310}$$

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

Exc 28 Verify that Eq. (310) is a solution of Eq. (308):

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,

$$\begin{aligned}|\psi(t)\rangle &= \sum_i e^{-\frac{i}{\hbar} E_i t} |E_i\rangle \langle E_i \mid \psi(0)\rangle \\ &= e^{-\frac{i}{\hbar} \hat{H} t} |\psi(0)\rangle.\end{aligned} \tag{313}$$

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

$$\boxed{\hat{U}(t) = e^{-\frac{i}{\hbar} \hat{H} t}.} \tag{314}$$

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

$$\hat{U}(t) = \mathcal{T} \exp\left(-\frac{i}{\hbar} \int_0^t \hat{H}(t')\, d t'\right). \tag{315}$$

▫ 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

$$\begin{aligned}\hat{H} &= h_0\, \mathbb{1} + h_x\, \hat{\sigma}^x + h_y\, \hat{\sigma}^y + h_z\, \hat{\sigma}^z \\ &= h_0\, \mathbb{1} + \boldsymbol{h} \cdot \hat{\boldsymbol{\sigma}},\end{aligned} \tag{316}$$

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)

$$\begin{aligned}\hat{U}(t) &= e^{-i \hat{H} t} \\ &= e^{-i h_0 t}\left(\cos(|\boldsymbol{h}|\, t)\, \mathbb{1} - i \sin(|\boldsymbol{h}|\, t)\, \tilde{\boldsymbol{h}} \cdot \hat{\boldsymbol{\sigma}}\right),\end{aligned} \tag{317}$$

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

Exc 29 Derive Eq. (317) from Eq. (316).

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

$$\begin{aligned}|\psi(t)\rangle &= \hat{U}(t)\, |\psi(0)\rangle \\ &= e^{-i h_0 t}\left(\cos(|\boldsymbol{h}|\, t)\, \mathbb{1} - i \sin(|\boldsymbol{h}|\, t)\, \tilde{\boldsymbol{h}} \cdot \hat{\boldsymbol{\sigma}}\right) |\psi(0)\rangle.\end{aligned} \tag{319}$$

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

$$\begin{aligned}\langle \boldsymbol{\sigma} \rangle_t &= \langle \psi(t)|\, \hat{\boldsymbol{\sigma}}\, |\psi(t)\rangle \\ &= \cos(2\, |\boldsymbol{h}|\, t)\, \langle \boldsymbol{\sigma} \rangle_0 + \sin(2\, |\boldsymbol{h}|\, t)\, \tilde{\boldsymbol{h}} \times \langle \boldsymbol{\sigma} \rangle_0 + (1 - \cos(2\, |\boldsymbol{h}|\, t))\, \tilde{\boldsymbol{h}}\left(\tilde{\boldsymbol{h}} \cdot \langle \boldsymbol{\sigma} \rangle_0\right).\end{aligned} \tag{320}$$

which also evolves with time.

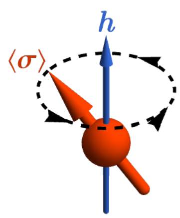
Exc 30 Derive Eq. (320) from Eq. (319).
Hint: Eq. (117) can make life much more easier.

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

$$\langle\boldsymbol{\sigma}\rangle_t = (\sin\theta_0 \cos(\varphi_0 + 2\,h_z\,t),\ \sin\theta_0 \sin(\varphi_0 + 2\,h_z\,t), \cos\theta_0), \tag{326}$$

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).

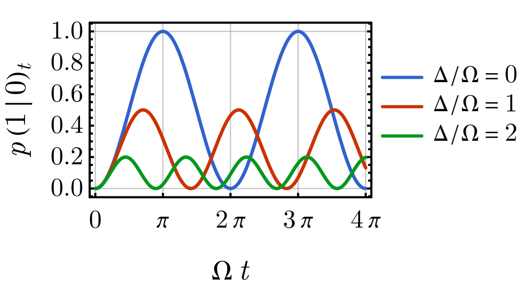
Rabi oscillation: a qubit initially prepared in state $|0\rangle$, evolved under the Hamiltonian

$$\hat{H} = \Omega\,\hat{\sigma}^x + \Delta\,\hat{\sigma}^z \simeq \begin{pmatrix} \Delta & \Omega \\ \Omega & -\Delta \end{pmatrix}, \tag{327}$$

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

$$p(1\,|\,0)_t = \langle\mathcal{P}_1\rangle_t = \frac{1 - \langle\sigma^z\rangle_t}{2} = \frac{\sin^2(\omega\,t/2)}{1 + (\Delta/\Omega)^2}, \tag{328}$$

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,

$$\langle O(t)\rangle = \langle\psi(t)|\, \hat{O}\, |\psi(t)\rangle. \tag{329}$$

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

$$\langle O(t)\rangle = \langle\psi|\, \hat{O}(t)\, |\psi\rangle. \tag{330}$$

The two pictures are consistent, if

$$|\psi(t)\rangle = \hat{U}(t)\, |\psi\rangle \Rightarrow \hat{O}(t) = \hat{U}(t)^\dagger\, \hat{O}\, \hat{U}(t), \tag{331}$$

such that Eq. (329) and Eq. (330) are consistent, as they both implies

$$\langle O(t)\rangle = \langle\psi|\, \hat{U}(t)^\dagger\, \hat{O}\, \hat{U}(t)\, |\psi\rangle. \tag{332}$$

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

$$\boxed{\hat{O}(t) = \hat{U}(t)^\dagger\, \hat{O}\, \hat{U}(t),} \tag{333}$$

described by the **Heisenberg equation**

$$\boxed{i\,\hbar\,\partial_t\, \hat{O}(t) = \left[\hat{O}(t),\, \hat{H}\right].} \tag{334}$$

Exc 31 Derive Eq. (334) from Eq. (333).

Correspondingly, its expectation value evolves as

$$i\,\hbar\,\partial_t \langle O(t)\rangle = \left\langle\left[\hat{O}(t),\, \hat{H}\right]\right\rangle. \tag{337}$$

If $\left[\hat{O},\, \hat{H}\right] = 0$, the *Heisenberg equation* Eq. (334) 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 10

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.