

1. Quantum mechanics essentials

1.1. States and wave functions

- A particle's position on the real line is given by a wave function $\psi(x, t) \rightarrow \mathbb{C}$.
- Probability of finding particle in (a, b) is

$$P(a, b) = \int_a^b |\psi(x, t)|^2 dx$$

- Time-evolution of wave function given by **Schrodinger equation**:

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x)\psi(x, t) = \hat{H}\psi(x, t)$$

where

$$\hat{H} = \hat{K} + \hat{V}$$

is the Hamiltonian operator.

- Schrodinger equation is **linear**, so any linear combination of solutions is another solution (**principle of superposition**).
- An inner product is defined on the space of solutions to the Schrodinger equation:

$$\langle \psi, \varphi \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) \varphi(x, t) dx$$

- **Hilbert space**: vector space with inner product satisfying $\langle \psi, a\varphi_1 + b\varphi_2 \rangle = a\langle \psi, \varphi_1 \rangle + b\langle \psi, \varphi_2 \rangle$ and $\langle \psi, \varphi \rangle = \langle \varphi, \psi \rangle^*$
- Write $|\psi\rangle$ (a **ket**) for vector in Hilbert space \mathcal{H} corresponding to wave function ψ .
- Write $\langle \varphi|$ (a **bra**) for **dual** vector in \mathcal{H}^* .
- **Dirac (bra-ket) notation**:

$$\langle \varphi | \psi \rangle := \langle \varphi, \psi \rangle = \int_{-\infty}^{\infty} \varphi^*(x, t) \psi(x, t) dx$$

- **Dual** of vector space V is set of linear functionals from V to \mathbb{C} :

$$V^* := \{ \Phi : V \rightarrow \mathbb{C} : \forall (a, b) \in \mathbb{C}^2, \forall (z, w) \in V^2, \quad \Phi(a\underline{z} + b\underline{w}) = a\Phi(\underline{z}) + b\Phi(\underline{w}) \}$$

We have $\dim(V^*) = \dim(V)$.

- If $V = \mathbb{C}^n$, can think of vectors in V as $n \times 1$ matrices and vectors in V^* as $1 \times n$ matrices.
- A quantum mechanical system is described by a ket $|\psi\rangle$ in Hilbert space \mathcal{H} . For all $|\psi\rangle, |\varphi\rangle \in \mathcal{H}$:
 - $\forall (a, b) \in \mathbb{C}^2, a|\psi\rangle + b|\varphi\rangle \in \mathcal{H}$
 - Inner product of $|\psi\rangle$ with $|\varphi\rangle$ is a complex number written as $\langle \psi | \varphi \rangle$. It is Hermitian: $\langle \psi | \varphi \rangle = \langle \varphi | \psi \rangle^*$.
 - Inner product is **sesquilinear** (linear in the second factor, anti-linear in the first). For $|\varphi\rangle = c_1|\varphi_1\rangle + c_2|\varphi_2\rangle$:

$$\langle \psi | \varphi \rangle = c_1 \langle \psi | \varphi_1 \rangle + c_2 \langle \psi | \varphi_2 \rangle$$

$$\langle \varphi | \psi \rangle = c_1^* \langle \varphi_1 | \psi \rangle + c_2^* \langle \varphi_2 | \psi \rangle$$

- $\langle \psi | \psi \rangle \geq 0$ and $\langle \psi | \psi \rangle = 0 \iff |\psi\rangle = 0$.
- States which differ by only a normalisation factor are physically equivalent:

$$\forall c \in \mathbb{C}^*, \quad |\psi\rangle \sim c|\psi\rangle$$

So we normally assume that a state $|\psi\rangle$ has norm 1: $\| |\psi\rangle \| = 1$.

- Note that the state labelled zero, $|0\rangle$, is not equal to the zero state (the 0 vector).
- If \hat{A} is linear operator then $\hat{A}(a|\psi\rangle + b|\varphi\rangle) = a(\hat{A}|\psi\rangle) + b(\hat{A}|\varphi\rangle)$
- Products and combinations of linear operators are also linear operators.
- **Adjoint (Hermitian conjugate)** of \hat{A} , \hat{A}^\dagger is defined by

$$\langle \psi | (\hat{A}^\dagger | \varphi \rangle) = (\langle \varphi | (\hat{A} | \psi \rangle))^*$$

- \hat{A} is **self-adjoint (Hermitian)** if $\hat{H}^\dagger = \hat{H}$. Self-adjoint operators correspond to **observables** (measurable quantities) since they have real eigenvalues. Similarly, a **hermitian matrix** H satisfies $H^\dagger = (H^T)^* = H$.
- \hat{U} is **unitary** if $\hat{U}^\dagger \hat{U} = \hat{I}$. Unitary operators describe time-evolution in quantum mechanics. Similarly, a unitary matrix U satisfies $U^\dagger U = U U^\dagger = I$.
- If we have $\langle n | m \rangle = \delta_{nm}$, the basis is orthonormal.
- **Qubit system:** Hilbert space $\mathcal{H} = \text{span}(|0\rangle, |1\rangle)$. Any $|\psi\rangle \in \mathcal{H}$ can be written as $a_0|0\rangle + a_1|1\rangle$. If $|\varphi\rangle = b_0|0\rangle + b_1|1\rangle$,

$$\begin{aligned} \langle \varphi | \psi \rangle &= (b_0^* \langle 0| + b_1^* \langle 1|)(a_0|0\rangle + a_1|1\rangle) \\ &= b_0^* a_0 \langle 0|0\rangle + b_1^* a_1 \langle 1|1\rangle + b_0^* a_1 \langle 0|1\rangle + b_1^* a_0 \langle 1|0\rangle = b_0^* a_0 + b_1^* a_1 \\ &= [b_0^* \ b_1^*] \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} \end{aligned}$$

If $|0\rangle, |1\rangle$ is an energy eigenbasis, then $\hat{H}|0\rangle = E_0|0\rangle$ and $\hat{H}|1\rangle = E_1|1\rangle$ where E_0, E_1 are eigenvalues.

$\mathbb{P}(\text{measuring } E_0) = a_0^2 = |\langle 0 | \psi \rangle|^2$, $\mathbb{P}(\text{measuring } E_1) = a_1^2 = |\langle 1 | \psi \rangle|^2$. If $a_0^2 + a_1^2 = 1$, then $\langle \psi | \psi \rangle = 1$ so ψ is normalised. The expected energy measurement is $\langle E \rangle = E_0 |a_0|^2 + E_1 |a_1|^2$.

- **Matrix form** of operator \hat{A} :

$$A_{nm} = \langle n | \hat{A} | m \rangle$$

For \hat{A}^\dagger , $\langle n | \hat{A}^\dagger | m \rangle = \langle m | \hat{A} | n \rangle^*$.

- **Change of basis:** $B = S^{-1} A S$.
- **Schrodinger equation in bracket notation:**

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

If \hat{H} independent of t , then $|\psi(t)\rangle = e^{-\frac{i}{\hbar} \hat{H} t} |\psi(0)\rangle$.

- **Exponential of operator:**

$$\exp(\hat{A}) = \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!}$$

- If $\hat{A} = \text{diag}(a_1, \dots, a_n)$ is diagonal, then $\exp(\hat{A}) = \text{diag}(e^{a_1}, \dots, e^{a_n})$.
- If $J^2 = -I$ (I is identity matrix) then

$$\exp(Jt) = \cos(t)I + \sin(t)J$$

- \hat{A} **diagonalisable** if $\hat{A} = \hat{S}\hat{D}\hat{S}^{-1}$ where \hat{D} is diagonal and \hat{S} has columns corresponding to eigenvectors of \hat{A} .
- For \hat{A} diagonalisable,

$$\exp(\hat{A}) = \sum_{n=0}^{\infty} \frac{(\hat{S}\hat{D}\hat{S}^{-1})^n}{n!} = \hat{S} \left(\sum_{n=0}^{\infty} \frac{\hat{D}^n}{n!} \right) \hat{S}^{-1} = \hat{S} \exp(\hat{D}) \hat{S}^{-1}$$

- For an orthonormal basis $\{|n\rangle\}$, the identity operator is given by

$$I = \sum_n |n\rangle\langle n|$$

- **Spectral representation of operator:**

$$\hat{A} = \sum_n \lambda_n |n\rangle\langle n|$$

for orthonormal eigenvectors $\{|n\rangle\}$. We can view a function f acting on real numbers as acting on \hat{A} by

$$f(\hat{A}) = \sum_n f(\lambda_n) |n\rangle\langle n|$$

1.2. Pure states and mixed states

- **Pure state:** linear combination of states $|\psi\rangle = |\psi_1\rangle + \dots + |\psi_n\rangle$. Probability of being in this state is 1.
- For a **density matrix** describing a **pure state** $\hat{\rho}_\psi = |\psi\rangle\langle\psi|$,

$$\begin{aligned} \text{tr}(\hat{\rho}_\psi) &= \sum_n \langle n|\hat{\rho}|n\rangle = \sum_n \langle n|\psi\rangle\langle\psi|n\rangle \\ &= \sum_n \langle\psi|n\rangle\langle n|\psi\rangle = \langle\psi| \left(\sum_n |n\rangle\langle n| \right) |\psi\rangle = \langle\psi|\psi\rangle = 1 \end{aligned}$$

Also $\text{tr}(\hat{\rho}_\psi^2) = 1$.

- $\langle E \rangle_\psi = \langle\psi|\hat{H}|\psi\rangle = \sum_n \langle\psi|\hat{H}|n\rangle\langle n|\psi\rangle$
 $= \sum_n \langle n|\psi\rangle\langle\psi|\hat{H}|n\rangle = \sum_n \langle n|\hat{\rho}_\psi|\hat{H}|n\rangle = \text{tr}(\hat{\rho}_\psi \hat{H})$

- **Mixed state:** probability p_i for each state $|\psi_i\rangle$. $\hat{\rho}_i = |\psi_i\rangle\langle\psi_i|$ and

$$\hat{\rho} = \sum_i p_i \hat{\rho}_i$$

For observable \hat{A} expressed in matrix form with basis as the states $|\psi_i\rangle$, then $\langle \hat{A} \rangle = \text{tr}(\hat{\rho}\hat{A})$. For mixed state, we still have $\text{tr}(\hat{\rho}) = 1$ but $\text{tr}(\hat{\rho}^2) = \sum_i p_i^2 \leq 1$ with equality only when some $p_i = 1$ (i.e. a pure state). It conveys how “mixed” the state is.

- **Example:** for ensemble $\{(\frac{3}{4}, |0\rangle), (\frac{1}{4}, |1\rangle)\}$,

$$\hat{\rho} = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| = \begin{bmatrix} 3/4 & 0 \\ 0 & 1/4 \end{bmatrix}$$

This ensemble is **not** unique:

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

gives an equivalent density matrix:

$$\begin{aligned} \hat{\rho}_1 &= \left(\sqrt{\frac{3}{4}}|0\rangle + \sqrt{\frac{1}{4}}|1\rangle \right) \left(\sqrt{\frac{3}{4}}\langle 0| + \sqrt{\frac{1}{4}}\langle 1| \right) \\ &= \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| + \dots, \hat{\rho}_2 = \dots, \frac{1}{2}\hat{\rho}_1 + \frac{1}{2}\hat{\rho}_2 = \begin{bmatrix} 3/4 & 0 \\ 0 & 1/4 \end{bmatrix} \end{aligned}$$

- **Definition: trace distance** between two density matrices:

$$D(\hat{\rho}_1, \hat{\rho}_2) = \frac{1}{2} \text{tr}|\hat{\rho}_1 - \hat{\rho}_2| = \sum_i |\lambda_i|$$

where $|\hat{A}| = \sqrt{\hat{A}^\dagger \hat{A}}$ and λ_i are the eigenvalues of $\hat{\rho}_1 - \hat{\rho}_2$.