

# 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  $\psi$ .
- 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  $\psi$  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

- For  $\hat{\rho}_\psi = |\psi\rangle\langle\psi|$ ,

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