1. Quantum mechanics essentials

1.1. States and wave functions

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

$$P(a,b) = \int_a^b |\psi(x,t)|^2 \, \mathrm{d}x$$

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

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

  where

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

  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:

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

- **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**:

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

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

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

  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 opearator 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

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

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

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

If $|0\rangle, |1\rangle$ is an energy eigenbasis, then $\widehat{H}|0\rangle = E_0|0\rangle$ and $\widehat{H}|1\rangle = E_1|1\rangle$ 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 $E_0\ |a_0|^2 + E_1\ |a_1|^2$.