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

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

- $\hat{A}$ 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 $\langle E\rangle = E_0\ |a_0|^2 + E_1\ |a_1|^2$.

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

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

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

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

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

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

- **Exponential of operator**:

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

- If $\hat{A} = \operatorname{diag}(a_1, ..., a_n)$ is diagonal, then $\exp\left(\hat{A}\right) = \operatorname{diag}(e^{a_1}, ..., e^{a_n})$.
- 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,

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

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

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

1.2. Pure states and mixed states

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

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

  Also $\operatorname{tr}\left(\hat{\rho}_\psi^2\right) = 1$.
- $$\begin{aligned}\langle E\rangle_\psi &= \left\langle\psi|\hat{H}|I|\psi\right\rangle = \sum_n \left\langle\psi|\hat{H}|n\right\rangle\langle n|\psi\rangle \\ &= \sum_n \langle n|\psi\rangle\left\langle\psi|\hat{H}|n\right\rangle = \sum_n \left\langle n|\hat{\rho}_\psi|\hat{H}|n\right\rangle = \operatorname{tr}\left(\hat{\rho}_\psi\hat{H}\right)\end{aligned}$$
- **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 $\langle\hat{A}\rangle = \operatorname{tr}\left(\hat{\rho}\hat{A}\right)$. For mixed state, we still have $\operatorname{tr}(\hat{\rho}) = 1$ but $\operatorname{tr}(\hat{\rho}^2) = \sum_i p_i^2 \leq 1$ with equality only when some $p_i = 1$ (i.e. a pure state). It conveys how "mixed" the state is.

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

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

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:

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

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

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

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

2. Bipartite systems

2.1. Tensor products

- **Tensor product** $|\varphi\rangle \otimes |\psi\rangle$ in $H_1 \otimes H_2$ satisfies:
  - **Scalar multiplication**: $c(|\varphi\rangle \otimes |\psi\rangle) = (c|\varphi\rangle) \otimes |\psi\rangle = |\varphi\rangle \otimes (c|\psi\rangle)$
  - **Linearity**:
    - $a|\psi\rangle \otimes |\varphi_1\rangle + b|\psi\rangle \otimes |\varphi_2\rangle = |\psi\rangle \otimes (a|\varphi_1\rangle + b|\varphi_2\rangle)$
    - $a|\psi_1\rangle \otimes |\varphi\rangle + b|\psi_2\rangle \otimes |\varphi\rangle = (a|\psi_1\rangle + b|\psi_2\rangle) \otimes |\varphi\rangle$
- Inner products of H_1 and H_2 induce an inner product on $H_1 \otimes H_2$: for $|\psi_1\rangle, |\psi_2\rangle \in H_1$, $|\varphi_1\rangle, |\varphi_2\rangle \in H_2$,

$$(\langle\psi_1| \otimes \langle\varphi_1|)(|\psi_2\rangle \otimes |\varphi_2\rangle) = \langle\psi_1|\psi_2\rangle\langle\varphi_1|\varphi_2\rangle$$

- For a bases $\{|i\rangle\}$ for H_1 and $\{|j\rangle\}$ for H_2, $\{|i\rangle \otimes |j\rangle\}$ is basis for $H_1 \otimes H_2$: for $|\psi\rangle \in H_1$, $|\varphi\rangle \in H_2$,

$$|\psi\rangle \otimes |\varphi\rangle = \left(\sum_i a_i|i\rangle\right) \otimes \left(\sum_j b_j|j\rangle\right) = \sum_{i,j} a_i b_j |i\rangle \otimes |j\rangle$$

- The most general vector $|\psi\rangle \in H_1 \otimes H_2$ is

$$|\psi\rangle = \sum_{i,j} c_{i,j} |i\rangle \otimes |j\rangle$$

Generally, this cannot be written as a tensor product $|\psi\rangle \otimes |\varphi\rangle$. If it can be, it is a **separable** state. If not, it is **entangled** (e.g. a linear combination of separable states is generally entangled).

- If $\{|i\rangle\}$, $\{|j\rangle\}$ orthonormal then the inner product in $H_1 \otimes H_2$ is given by

$$\begin{aligned} \langle \varphi | \psi \rangle &= \left(\sum_{i,j} d_{i,j}^* \langle i| \otimes \langle j| \right) \left(\sum_{m,n} c_{m,m} |m\rangle \otimes |n\rangle \right) \\ &= \sum_{i,j,m,n} d_{i,j}^* c_{m,n} \langle i|m\rangle \langle j|n\rangle = \sum_{i,j} c_{i,j}^* d_{i,j} \end{aligned}$$