# 1. Quantum mechanics essentials

- 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

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

Wave function is normalised so that  $P(-\infty, +\infty; t) = 1$ .

• 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  $\widehat{H}=\widehat{K}+\widehat{V}$  is the Hamiltonian operator,  $\widehat{K}$  is kinetic energy operator,  $\widehat{V}$  is potential energy 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**: (complex) vector space with Hermitian inner product that is also a complete metric space with metric induced by the inner product:
  - $\langle \psi, a\varphi_1 + b\varphi_2 \rangle = a \langle \psi, \varphi_1 \rangle + b \langle \psi, \varphi_2 \rangle$
  - $\langle \psi, \varphi \rangle = \langle \varphi, \psi \rangle^*$
- Dirac notation:
  - 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  $\mathcal{H}^*$ .
  - bra-ket:

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

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

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

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  $|\varphi\rangle = c_1|\varphi_1\rangle + c_2|\varphi_2\rangle$ :

$$\begin{split} \langle \psi | \varphi \rangle &= c_1 \langle \psi | \varphi_1 \rangle + c_2 \langle \psi | \varphi_2 \rangle \\ \langle \varphi | \psi \rangle &= c_1^* \langle \varphi_1 | \psi \rangle + c_2^* \langle \varphi_2 | \psi \rangle \end{split}$$

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

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

For this reason, pure quantum mechanical states are called **rays** in the Hilbert space, and we normally assume that a state  $|\psi\rangle$  has norm 1:  $||\psi\rangle|| = 1$ .

- Physical state condition:  $\langle \psi | \psi \rangle \ge 0$  and  $\langle \psi | \psi \rangle = 0 \iff | \psi \rangle = 0$ .
- 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

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

- $\widehat{A}$  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  $H^{\dagger} = (H^T)^* = H$ .
- $\hat{U}$  is **unitary** if  $\hat{U}^{\dagger}\hat{U} = \hat{I}$ . Unitary operators describe time-evolution in quantum mechanics. Similarly, a unitary matrix U satisfies  $U^{\dagger}U = UU^{\dagger} = I$ .
- Commutator of operators  $\hat{A}$  and  $\hat{B}$ :

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

• Anti-commutator:

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

• Expectation value of observable  $\hat{A}$  on state  $|\psi\rangle$ :

$$\langle A \rangle_{\psi} := \langle \psi | \hat{A} | \psi \rangle$$

Interpreted as average outcome of many measurements of  $\hat{A}$  on same state  $|\psi\rangle$ .

- 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  $|\varphi\rangle = b_0|0\rangle + b_1|1\rangle$ ,

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

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.

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

• 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:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \widehat{H}|\psi(t)\rangle \Longrightarrow |\psi(t)\rangle = \widehat{U}_t|\psi(0)\rangle$$

where  $\hat{U}_t$  is unitary operator. If  $\hat{H}$  independent of t, then  $\hat{U}_t = \exp(-\frac{i}{\hbar}t\hat{H})$ .

• Exponential of operator:

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

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

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

# 2. Measurement and uncertainty

- For Hilbert space of finite dimension N, operator  $\widehat{M}$  has N eigenvalues (counting multiplicities). Eigenvalues of operator  $\widehat{M}$  to possible values of the measurable quantity it represents.
- Spectrum of  $\widehat{H}$ :

$$\operatorname{Spec} \left( \widehat{H} \right) \coloneqq \left\{ \lambda \in \mathbb{C} : \widehat{H} - \lambda \widehat{I} \text{ non invertible} \right\}$$

For finite-dimensional Hilbert space, this is equal to the set of eigenvalues of  $\widehat{H}$ .

- For self-adjoint operator  $\widehat{H}$ , eigenstates  $|n\rangle$  corresponding to different eigenvalues  $\lambda_n$  are orthogonal. If eigenvalue is degenerate (multiplicity greater than one) then for each eigenspace (vector space spanned by the eigenvectors) with dimension greater than one, we can choose an orthogonal basis of eigenstates (e.g. with Gram-Schmidt).
- Only eigenvalue of identity operator is 1 with degeneracy N, so for any orthonormal basis of  $\mathcal{H}$ :

$$\hat{I} = \sum_n |n\rangle\langle n|$$

- $\hat{A}$  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,

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

• Spectral representation of operator:

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

for orthonomal eigenvectors  $\{|n\rangle\}$  and eigenvalues  $\lambda_n$ . When measurement is made on state

$$|\psi\rangle = \sum_n c_n |n\rangle$$

the result is  $\lambda_n$  with probability  $p_n = |\langle n|\psi\rangle|^2 = |c_n|^2$ . If result is  $\lambda_n$ , measuring again immediately after the measurement will yield  $\lambda_n$ , so the state is no longer  $|\psi\rangle$  but  $|n\rangle$ . This **collapse of the wavefunction** cannot be represented by a unitary operation, and is not reversible.

• Can describe measurement process as set of projection operators  $\hat{P}_n = |n\rangle\langle n|$ , then  $p_n = \left\langle \psi | \hat{P}_n | \psi \right\rangle$  and resulting state  $\frac{1}{\sqrt{p_n}} \hat{P}_n | \psi \rangle$  which is equal to  $|n\rangle$  up to an irrelevant overall phase.  $\hat{P}_n^\dagger = \hat{P}_n$  and  $\hat{P}_n^2 = \hat{P}_n$ . If the spectrum of  $\hat{A}$  is degenerate, we can define

$$\hat{\boldsymbol{P}}_{\lambda}\coloneqq\sum_{n:\lambda_n=\lambda}|n\rangle\langle n|$$

then we still have  $p_{\lambda} = \langle \psi | \hat{P}_{\lambda} | \psi \rangle$  and resulting state is  $1/\sqrt{p_{\lambda}} \hat{P}_{\lambda} | \psi \rangle$ .

- $\hat{A}$  and  $\hat{B}$  are compatible if  $[\hat{A}, \hat{B}] = 0$ .
- A state can only have definite values for observables A and B if it is a simultaneous eigenstate of both  $\hat{A}$  and  $\hat{B}$ .
- There always exist simultaneous eigenstates for compatible operators.
- If  $\hat{A}$  and  $\hat{B}$  are not compatible, measuring A then B then A again will not necessarily give the same result for the two measurements of A.
- We can view a function f acting on real numbers as acting on  $\hat{A}$  by

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

- A **pure state** is definite, i.e. the state of the system is completely known, and the only uncertainties are due to the uncertain nature of quantum mechanics. This is classical uncertainty rather than quantum uncertainty.
- The **density matrix** of a pure state  $|\psi\rangle$  is

$$\hat{\rho} := |\psi\rangle\langle\psi|$$

• There is a bijective correspondence between density matrices and the associated pure states:

$$\begin{split} \widehat{M}|\psi\rangle &= \lambda|\psi\rangle &\quad \longleftrightarrow \quad \widehat{M}\widehat{\rho} = \lambda\widehat{\rho} \\ |\psi\rangle &\rightarrow \widehat{U}|\psi\rangle &\quad \longleftrightarrow \quad \widehat{\rho} \rightarrow \widehat{U}\widehat{\rho}\widehat{U}^\dagger \end{split}$$

i.e. transforming a state  $|\psi\rangle$  by unitary operator  $\hat{U}$  is equivalent to transforming the density matrix  $\hat{\rho}$  to  $\hat{U}\hat{\rho}\hat{U}^{\dagger}$ .

• For orthonormal basis states  $|n\rangle$ , trace of  $\hat{A}$  is

$$\operatorname{tr}\left(\hat{A}\right) = \sum_{n} \left\langle n|\hat{A}|n\right\rangle$$

Cyclicity of trace:

$$tr(ABC) = tr(BCA) = tr(CAB)$$

• For a density matrix describing a pure state  $\hat{\rho} = |\psi\rangle\langle\psi|$ ,

$$\begin{split} \operatorname{tr}(\hat{\rho}) &= \sum_{n} \langle n | \hat{\rho} | n \rangle = \sum_{n} \langle n | \psi \rangle \langle \psi | n \rangle \\ &= \sum_{n} \langle \psi | n \rangle \langle n | \psi \rangle = \langle \psi | \left( \sum_{n} | n \rangle \langle n | \right) | \psi \rangle = \left\langle \psi | \hat{I} | \psi \right\rangle = \langle \psi | \psi \rangle = 1 \end{split}$$

Also  $\operatorname{tr}(\hat{\rho}^2) = 1$  since  $\hat{\rho}$  is a projector and hence  $\hat{\rho}^2 = \hat{\rho}$ .

- A **mixed state** is one where the state of the system is not known. It is an ensemble of pure states each with an associated probability of the system being in that state:  $\{(p_i, |i\rangle)\}$ , where the  $|i\rangle$  are normalised (not necessarily orthogonal).
- **Density matrix** of a **mixed state** is lienar combination of density matrices for each pure state weighted by probability:

$$\hat{\rho} \coloneqq \sum_i p_i |i\rangle\langle i|$$

Can generalise definition to include possibility of ensembles containing mixed states:  $\hat{\rho} = \sum_i p_i \hat{\rho}_i$  where  $\hat{\rho}_i$  are mixed and/or pure density matrices.

- **Note**: generally the ensemble that gives rise to a given density matrix for a mixed state is not unique.
- **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:

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

- For observable  $\hat{A}$  expressed in matrix form with basis as the states  $|\psi_i\rangle$ , then  $\langle \hat{A} \rangle = \operatorname{tr}(\hat{\rho} \hat{A})$ . 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).  $\operatorname{tr}(\hat{\rho}^2)$  conveys how "mixed" the state is.
- Example:

$$\begin{split} \left\langle E \right\rangle_{\psi} &= \left\langle \psi | \widehat{H} | I | \psi \right\rangle = \sum_{n} \left\langle \psi | \widehat{H} | n \right\rangle \langle n | \psi \rangle \\ &= \sum_{n} \langle n | \psi \rangle \left\langle \psi | \widehat{H} | n \right\rangle = \sum_{n} \left\langle n | \widehat{\rho}_{\psi} | \widehat{H} | n \right\rangle = \mathrm{tr} \left( \widehat{\rho}_{\psi} \widehat{H} \right) \end{split}$$

- Mixed states can only give a pure state when there is one pure state with probability 1.
- **Definition**:  $\hat{\rho}$  is a **density operator** on a Hilbert space if
  - Normalised:  $tr(\hat{\rho}) = 1$
  - Hermitian:  $\hat{\rho}^{\dagger} = \hat{\rho}$
  - Semi-positive-definite: for every state  $|\psi\rangle$ ,  $\langle\psi|\hat{\rho}|\psi\rangle \geq 0$  (can be = 0 when  $|\psi\rangle \neq 0$ ).
- All density matrices are density operators.
- After taking a measurement of a pure or mixed state:
  - The measurement is  $\lambda$  with probability  $p_{\lambda} = \operatorname{tr}(\hat{P}_{\lambda}\hat{\rho}\hat{P}_{\lambda}) = \operatorname{tr}(\hat{P}_{\lambda}\hat{\rho})$ .
  - Density matrix after measuring value of  $\lambda$  is

$$\hat{\rho} \to \frac{1}{p_{\lambda}} \hat{P}_{\lambda} \hat{\rho} \hat{P}_{\lambda} = \frac{1}{\operatorname{tr}(\hat{P}_{\lambda} \hat{\rho} \hat{P}_{\lambda})} = \hat{P}_{\lambda} \hat{\rho} \hat{P}_{\lambda}$$

• **Theorem**: let  $\hat{\rho}$  be a density operator on a Hilbert space, then  $\hat{\rho}$  corresponds to a pure state iff  $\operatorname{tr}(\hat{\rho}^2) = 1$ .

# 3. Qubits and the Bloch sphere

### 3.1. Qubits

- **Definition**: a **qubit** is a state in a two-dimensional Hilbert space. Usually the **computational basis**  $\{|0\rangle, |1\rangle\}$  is used to denote the basis for such a Hilbert space.
- A general pure state in a qubit system is of the form

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\varphi}\sin\left(\frac{\theta}{2}\right)|1\rangle, \quad 0 \le \theta \le \pi, 0 \le \varphi < 2\pi$$

This state is normalised:  $|\cos(\frac{\theta}{2})|^2 + |e^{i\varphi}\sin(\frac{\theta}{2})|^2 = 1$ . This gives a bijection between pure qubit states and points on  $S^2$ , called the **Bloch sphere**.

• Any point on the Bloch sphere can be labelled by its position vector:

$$m{r} = egin{bmatrix} x \\ y \\ z \end{bmatrix}, \quad x = \sin(\theta)\cos(\varphi), y = \sin(\theta)\sin(\varphi), z = \cos(\theta)$$

• There are six special states on the Bloch sphere:

$$\begin{split} |+\rangle &\coloneqq \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \leftrightarrow \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} : \quad \boldsymbol{r} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad (\theta,\varphi) = (\pi/2,0) \\ |-\rangle &\coloneqq \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \leftrightarrow \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} : \quad \boldsymbol{r} = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix}, \quad (\theta,\varphi) = (\pi/2,\pi) \\ |L\rangle &\coloneqq \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle) \leftrightarrow \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} : \quad \boldsymbol{r} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad (\theta,\varphi) = (\pi/2,\pi/2) \\ |R\rangle &\coloneqq \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle) \leftrightarrow \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} : \quad \boldsymbol{r} = \begin{bmatrix} 0 \\ -1 \\ 0 \end{bmatrix}, \quad (\theta,\varphi) = (\pi/2,3\pi/2) \\ |0\rangle \leftrightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix} : \quad \boldsymbol{r} = \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}, \quad (\theta,\varphi) = (0,\cdot) \\ |1\rangle \leftrightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix} : \quad \boldsymbol{r} = \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}, \quad (\theta,\varphi) = (\pi,\cdot) \end{split}$$

### 3.2. Inside the Bloch sphere

• Definition: Pauli  $\sigma$ -matrices are

$$\sigma_1 \coloneqq \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 \coloneqq \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 \coloneqq \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

• Density matrix for  $|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\varphi}\sin\left(\frac{\theta}{2}\right)|1\rangle$  is given by

$$\begin{split} \hat{\rho} &= |\psi\rangle\langle\psi| \to \rho = \begin{bmatrix} \cos\left(\frac{\theta}{2}\right) \\ e^{i\varphi}\sin\left(\frac{\theta}{2}\right) \end{bmatrix} \begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & e^{-i\varphi}\sin\left(\frac{\theta}{2}\right) \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} 1 + \cos(\theta) & e^{-i\varphi}\sin(\theta) \\ e^{i\varphi}\sin(\theta) & 1 - \cos(\theta) \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 + z & x - iy \\ x + iy & 1 - z \end{bmatrix} \\ &= \frac{1}{2} (I_2 + r \cdot \sigma) \end{split}$$

where  $\mathbf{r} \cdot \mathbf{\sigma} = r_1 \sigma_1 + r_2 \sigma_2 + r_3 \sigma_3 = x \sigma_1 + y \sigma_2 + z \sigma_3$ .

- Density matrix for pure state is linear in the Bloch vector  $\mathbf{r}$ , so mixed states have Bloch vector given by linear combination of Bloch vectors of states in the ensemble.
- For mixed state  $\{(p_i, \rho_i) : i \in [m]\}$  where  $\rho_i$  are pure state density matrices defined by Bloch vectors  $\mathbf{r}_i$ , density matrix for mixed state is

$$\rho = \sum_{i=1}^m p_i \rho_i = \sum_{i=1}^m p_i \frac{1}{2} (I_2 + \boldsymbol{r}_i \cdot \boldsymbol{\sigma}) = \frac{1}{2} (I_2 + \boldsymbol{r} \cdot \boldsymbol{\sigma})$$

where  $\mathbf{r} = \sum_{i=1}^{m} p_i r_i$ . Now

$$\begin{split} |\boldsymbol{r}|^2 &= |\sum_{i=1}^m p_i \boldsymbol{r}_i|^2 = \sum_{(i,j) \in [m]^2} p_i p_j \boldsymbol{r}_i \cdot \boldsymbol{r}_j \\ &\leq \sum_{(i,j) \in [m]^2} p_i p_j \; |\boldsymbol{r}_i|^2 \; |\boldsymbol{r}_j|^2 = \sum_{(i,j) \in [m]^2} p_i p_j = \sum_{i=1}^m p_i \sum_{j=1}^m p_j = 1 \end{split}$$

by Cauchy-Schwartz inequality. Equality holds iff all  $r_i$  are collinear, hence iff it is a pure state. So strictly mixed states are defined by a Bloch vector r with |r| < 1.

• For any density matrix  $\rho$ ,

$$\operatorname{tr}(\rho^2) = \frac{1}{2}(1+|{m r}|^2)$$

### 3.3. Time evolution of a qubit

- Unitary transformations of a qubit correspond to rotations of points on/in the Bloch sphere about the origin, representing the fact that unitary transformations cannot transform pure states to mixed states
- $\operatorname{tr}(\rho^2) = \frac{1}{2}(1+|r|^2)$  is invariant under unitary transformations. It measures how mixed a state is:  $\operatorname{tr}(\rho^2) = 1$  for pure states,  $\operatorname{tr}(\rho^2) = \frac{1}{2}$  for the most mixed state (corresponds to the origin, r = 0,  $\rho = \frac{1}{2}I$ ).
- Measurements are not unitary transformations but projection operators, and can transform any state to a pure state.

### • Example:

• For  $r_1, r_2$  distinct points on the Bloch sphere, density matrix corresponding to mixed state  $\{(p, r_1), (1-p, r_2)\}$  is

$$\rho = p \rho_1 + (1-p) \rho_2 = \frac{1}{2} (I + \boldsymbol{r} \cdot \boldsymbol{\sigma}), \quad \boldsymbol{r} = p \boldsymbol{r_1} + (1-p) \boldsymbol{r_2}$$

- Geometrically, r lies in line between  $r_1$  and  $r_2$  inside the Bloch sphere (since  $p \in [0,1]$ ).
- Mixing states can never produce a state further from the origin than the furthest initial state.
- There are an infinite number of ways of writing a mixed state as an ensemble of two pure states: any line passing through the point represented by the mixed states intersects with the Bloch sphere twice the intersection points give the pure states in the ensemble.
- Most mixed state, with  $\rho = \frac{1}{2}I_2$ , corresponds to ensemble of antipodal points, each with probability  $\frac{1}{2}$ .
- Definition: trace distance between two density matrices:

$$D(\hat{\rho}_1,\hat{\rho}_2) = \frac{1}{2}\operatorname{tr}|\hat{\rho}_1 - \hat{\rho}_2| = \frac{1}{4}\operatorname{tr}|(\boldsymbol{r_1} - \boldsymbol{r_2}) \cdot \boldsymbol{\sigma}| = \frac{1}{2}\;|\boldsymbol{r_1} - \boldsymbol{r_2}| = \sum_i |\lambda_i|$$

where  $|\hat{A}| = \sqrt{\hat{A}^{\dagger}\hat{A}}$  and  $\lambda_i$  are the eigenvalues of  $\hat{\rho}_1 - \hat{\rho}_2$  (equal to sum of eigenvalues assuming that  $\hat{\rho}_1 - \hat{\rho}_2$  is Hermitian).

• Trace distance defines a **metric** on set of density matrices:

- Non-negative:  $D(\hat{\rho}_1, \hat{\rho}_2) \geq 0$ .
- Separates points:  $D(\hat{\rho}_1, \hat{\rho}_2) = 0 \iff \hat{\rho}_1 = \hat{\rho}_2$ .
- Symmetric:  $D(\hat{\rho}_1, \hat{\rho}_2) = D(\hat{\rho}_2, \hat{\rho}_2)$ .
- Triangle inequality:  $D(\hat{\rho}_1,\hat{\rho}_3) \leq D(\hat{\rho}_1,\hat{\rho}_2) + D(\hat{\rho}_2,\hat{\rho}_3)$

#### 3.4. Pauli matrices

- Definition: Levi-Cevita tensor  $\varepsilon_{ijk}$  satisfies:
  - $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312}$ .
  - $\bullet \quad \varepsilon_{321}=\varepsilon_{132}=\varepsilon_{213}.$
  - $\varepsilon_{ijk} = 0$  otherwise for  $\{i, j, k\} \subseteq \{1, 2, 3\}$ .
- Properties of Pauli matrices:
  - Hermitian:  $\sigma_i^{\dagger} = \sigma_i$ .
  - Traceless:  $tr(\sigma_i) = 0$ .
  - $\bullet \quad \left[\sigma_i,\sigma_j\right] = \sigma_i\sigma_j \sigma_j\sigma_i = 2i\varepsilon_{ijk}\sigma_k.$
  - $\bullet \ \left\{\sigma_i,\sigma_j\right\} = \sigma_i \sigma_j + \sigma_j \sigma_i = 2 \delta_{ij} I_2.$
  - $\sigma_i \sigma_j = \delta_{ij} I_2 + i \varepsilon_{ijk} \sigma_k$ .
  - Form a basis for vector space of  $2 \times 2$  Hermitian traceless matrices.
- The operators

$$\begin{split} X &= \frac{1}{2}(I_2 - \sigma_1) = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \\ Y &= \frac{1}{2}(I_2 - \sigma_2) = \frac{1}{2} \begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix} \\ Z &= \frac{1}{2}(I_2 - \sigma_3) = \frac{1}{2} \begin{bmatrix} 0 & 0 \\ 0 & 2 \end{bmatrix} \end{split}$$

have their eigenvectors as the six special Bloch states, with eigenvalues 0 or 1:

$$X|+\rangle = 0|+\rangle, \quad X|-\rangle = 1|-\rangle,$$
  
 $Y|L\rangle = 0|L\rangle, \quad Y|R\rangle = 1|R\rangle,$   
 $Z|0\rangle = 0|0\rangle, \quad Z|1\rangle = 1|1\rangle$ 

• The exponentials of Pauli matrices are unitary matrices:  $\forall \alpha \in \mathbb{R}$ ,

$$\begin{split} &\exp(i\alpha\sigma_1) = \begin{bmatrix} \cos(\alpha) & i\sin(\alpha) \\ i\sin(\alpha) & \cos(\alpha) \end{bmatrix} = \cos(\alpha)I_2 + i\sin(\alpha)\sigma_1, \\ &\exp(i\alpha\sigma_2) = \begin{bmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{bmatrix} = \cos(\alpha)I_2 + i\sin(\alpha)\sigma_2, \\ &\exp(i\alpha\sigma_3) = \begin{bmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{bmatrix} = \cos(\alpha)I_2 + i\sin(\alpha)\sigma_3 \end{split}$$

• For  $\alpha \in \mathbb{R}$ ,  $n \in \mathbb{R}^3$ ,  $|n|^2 = 1$ ,

$$U_{\alpha}(\boldsymbol{n})\coloneqq \exp(i\alpha\boldsymbol{n}\cdot\boldsymbol{\sigma}) = \cos(\alpha)I_2 + i\sin(\alpha)\boldsymbol{n}\cdot\boldsymbol{\sigma}$$

is unitary transformation so is time evolution operator. If density mmatrix  $\rho = \frac{1}{2}(I_2 + r \cdot \sigma)$  evolves with time according to this operator, then

$$\rho \rightarrow U_{\alpha}(\boldsymbol{n}) \rho U_{\alpha}(\boldsymbol{n})^{\dagger} = \frac{1}{2} (I_2 + (R_{\alpha}(\boldsymbol{n})\boldsymbol{r}) \cdot \boldsymbol{\sigma})$$

where  $R_{\alpha}(n)$  is  $3 \times 3$  orthogonal matrix corresponding to rotation of angle  $2\alpha$  about axis in the direction of n.

# 4. Bipartite systems

### 4.1. 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 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  $|\psi\rangle\in H_1$ ,  $|\varphi\rangle\in H_2$ ,

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

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

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

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

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