Quantum Information
Lecture 1

Main Ref: Nielsen & Chuang. Ch. 2.

A Review of Quantum Mechanics:

Postulate 1:

Associated to every isolated quantum mechanical system is a complex vector space equipped with a positive-definite inner product. This vector space is known as a Hilbert space. Depending on the system the dimension of this space may be finite or infinite. The physical state of the system is completely described by a unit vector in this space. This vector is called the state vector.

Comment:

1. Suppose we have a system A whose physical state is ψ. Then we denote its state vector by $|\psi\rangle \in \mathcal{H}_A$. $|\;\rangle \to$ Ket / vector.

2. If $\alpha, \beta \in \mathbb{C}$ and $|\varphi\rangle, |\psi\rangle \in \mathcal{H}_A$, then $\alpha|\varphi\rangle + \beta|\psi\rangle \in \mathcal{H}_A$.

Examples:

1. **Free particle in 1D:** State with definite momentum and energy:

$$\psi_p(x,t) = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}(Et - px)} , \quad E = \frac{p^2}{2m}$$

Physical states are wave-packets: $\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} a(p)\, e^{-\frac{i}{\hbar}\frac{p^2}{2m}} e^{\frac{i}{\hbar}px}\, dp$

such that $(\psi,\psi) = \int dx\, \psi^*(x,t)\psi(x,t) < \infty$

Hilbert space is infinite dimensional

2. **Simple Harmonic Oscillator (1-D):** Energies: $E_n = (n+\frac{1}{2})\hbar\omega$, $n \in 0, 1, 2, \ldots$

$|n\rangle \to$ Energy eigenkets. Infinite dimensional. $\psi_n(x) = \langle x|n\rangle = H_n(x)\, e^{-x^2/2a}$

↳ Hermite func.

3. **Spin of an electron:** 2-dimensional vector space spanned by eigenkets of $S_z = \frac{\hbar}{2}\sigma_z$:

$S_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle$ ~ spin up state

$S_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle$ ~ spin down state.

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

S_z conventional choice. S_x, S_y also equally valid choices.

Def$\underline{\text{n}}$:

A qubit (short for quantum bit) is any quantum system with a two-dimensional Hilbert space $\mathcal{H} \cong \mathbb{C}^2$. We denote Pauli matrices $\sigma_X, \sigma_Y, \& \sigma_Z$ by X, Y, Z:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and choose the eigenbasis of Z as the computational basis: $\{|0\rangle, |1\rangle\}$

$$Z|0\rangle = |0\rangle \qquad |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

$$Z|1\rangle = -|1\rangle$$

or $$Z|x\rangle = (-1)^x |x\rangle, \quad x \in \{0, 1\}.$$

Note that $X|x\rangle = |x \oplus 1\rangle$ where $\oplus$ denotes mod 2 addition.

The eigenkets of X are $|X \pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$

The eigenkets of Y are $|Y \pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm i|1\rangle)$

Comments: 1. For QI applications we usually require $\mathrm{Dim}(\mathcal{H})$ to be finite and $\underbrace{\mathcal{H} = \mathbb{C}^{\otimes N}}$ so that $\mathrm{Dim}(\mathcal{H}) = 2^N$.

Tensor products of N qubits.

2. **Hilbert spaces vs. Projective Hilbert Spaces:** Two vectors $|\psi\rangle$ & $|\varphi\rangle \in \mathcal{H}$ st $|\psi\rangle = \lambda |\varphi\rangle$ for some $\lambda \in \mathbb{C} - \{0\}$, represent the same physical states. Thus space of physical states $\mathcal{H}/\sim$ where $\sim$ is the equivalence relationship $|\psi\rangle \sim |\varphi\rangle$. $\mathcal{H}/\sim$ is a projective Hilbert space. It is not a vector space. For most part we avoid using projective Hilbert spaces. For a qubit $\mathbb{C}^2/\sim \;\cong\; \mathbb{C}\mathbb{P}^1$.

Some linear algebra:

1. **Basis:** If $d = \mathrm{Dim}(\mathcal{H})$, $\exists$ a linearly dependent set of vectors $\{|\psi_i\rangle \mid i = 1, 2, \ldots d\}$ st $|\varphi\rangle = \sum_{i=1}^{d} c_i |\psi_i\rangle \;\; \forall\; |\varphi\rangle \in \mathcal{H}$ with some $\{c_i \in \mathbb{C}\}$. The set $\{|\psi_i\rangle\}$ forms a basis of $\mathcal{H}$.

2. **Positive-definite Inner Product:** Since $\mathcal{H}$ is a Hilbert space $\exists$ an inner product

$$\langle \,|\, \rangle : \mathcal{H} \times \mathcal{H} \longrightarrow \mathbb{C}$$

$$\langle \,|\, \rangle : |\psi\rangle \times |\varphi\rangle \longmapsto \langle \psi|\varphi\rangle \in \mathbb{C}$$

s.t. i) $\langle \psi|\varphi\rangle = \langle \varphi|\psi\rangle^*$

ii) $\langle \psi| \left(\alpha|\varphi_1\rangle + \beta|\varphi_2\rangle\right) = \alpha \langle \psi|\varphi_1\rangle + \beta \langle \psi|\varphi_2\rangle$

iii) $\langle \psi|\psi\rangle \geq 0$. $\langle \psi|\psi\rangle = 0$ iff $|\psi\rangle = 0$.

Easy to see that if $|x\rangle = \alpha|\varphi_1\rangle + \beta|\varphi_2\rangle$ then $\langle x|\psi\rangle = \alpha^*\langle\varphi_1|\psi\rangle + \beta^*\langle\varphi_2|\psi\rangle$.

3. Since $|\psi\rangle \sim \lambda|\psi\rangle$, we may normalize our basis. A basis $\{|\psi_i\rangle \mid i = 1,2,\dots d\}$ that satisfies $\langle\psi_i|\psi_j\rangle = \delta_{ij}$ is known as an orthonormal basis.

4. Dual Vector Space $\mathcal{H}^*$: Consider all linear maps $\mathcal{H} \longrightarrow \mathbb{C}$. It is a vector space $\mathcal{H}^*$ of dim d and it is isomorphic to $\mathcal{H}$. $\mathcal{H}^* \cong \mathcal{H}$. Thus we identify the map $\langle\varphi| \in \mathcal{H}^*$ to the ket $|\varphi\rangle \in \mathcal{H}$ s.t. $\langle\varphi| : \mathcal{H} \to \mathbb{C}$, $\langle\varphi| : |\psi\rangle \longmapsto \langle\varphi|\psi\rangle$.

$\langle\varphi|$ is called a bra and $\langle\varphi|\psi\rangle$ is a bracket.

Example: $|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}$, $|1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ $\Rightarrow$ $\langle 0| = (1, 0)$, $\langle 1| = (0, 1)$.

$$\langle i|j\rangle = \delta_{ij}$$

Exercises:

1. Prove the Cauchy-Schwartz inequality: If $|\psi\rangle$ & $|\varphi\rangle$ are two kets in $\mathcal{H}$ (not necessarily normalized) show that $$|\langle\psi|\varphi\rangle| \leq |\psi||\varphi|$$
where $|\psi|^2 = \langle\psi|\psi\rangle$ & $|\varphi|^2 = \langle\varphi|\varphi\rangle$.

Hint: Evaluate $\langle\xi|\xi\rangle$ where $|\xi\rangle = |\psi\rangle - c|\varphi\rangle$ where $c = \langle\varphi|\psi\rangle/\langle\varphi|\varphi\rangle$.

2. For two kets $|\psi\rangle$ & $|\varphi\rangle$, prove the triangle inequality:

$$|\psi+\varphi| \leq |\psi| + |\varphi|$$

where $|\psi+\varphi|^2 = (\langle\psi| + \langle\varphi|)(|\psi\rangle + |\varphi\rangle)$

Linear Maps or Operators:

A linear map $\mathcal{O} : \mathcal{H} \to \mathcal{H}$ satisfies

$$\mathcal{O}(\alpha|\psi\rangle) = \alpha(\mathcal{O}|\psi\rangle) \quad \forall\ |\psi\rangle \in \mathcal{H} \text{ and } \forall\ \alpha \in \mathbb{C}.$$

$$\mathcal{O}(|\psi\rangle + |\varphi\rangle) = (\mathcal{O}|\psi\rangle) + (\mathcal{O}|\varphi\rangle) \quad \forall\ |\psi\rangle, |\varphi\rangle \in \mathcal{H}$$

Hermitian conjugation:

1. For every linear map $\mathcal{O}$ $\exists$ another map $\mathcal{O}^\dagger$, called the Hermitian conjugate of $\mathcal{O}$ st:

$$\langle\psi|(\mathcal{O}|\varphi\rangle) = \langle\varphi|(\mathcal{O}^\dagger|\psi\rangle) \quad \forall\ |\varphi\rangle, |\psi\rangle \in \mathcal{H}.$$

2. An operator or a linear map is called Hermitian or self-adjoint if

$$\langle\psi|(\mathcal{O}|\phi\rangle) = \langle\psi|(\mathcal{O}^\dagger|\phi\rangle) \quad \forall\ |\phi\rangle \ \&\ |\psi\rangle \in \mathcal{H}.$$

Thus we can write $\mathcal{O} = \mathcal{O}^\dagger$.

Exercise: Let $|A\psi\rangle \equiv A|\psi\rangle$. Then show that $\langle\psi|(A|\phi\rangle) = \langle A^\dagger\psi|\phi\rangle$.

Comments:

1. When there is no room for confusion we write $\langle\psi|(\hat{O}|\varphi\rangle) = \langle\psi|\hat{O}|\varphi\rangle$.

2. Since $\langle\psi|(\hat{O}|\varphi\rangle) = \langle\hat{O}^{\dagger}\psi|\varphi\rangle$ we can write $\hat{O}|\varphi\rangle \Rightarrow \langle\varphi|\hat{O}^{\dagger}$.

3. Let $\hat{A}^{\dagger} = \hat{A}$, then if $\exists$ a vector $|\psi\rangle$ st. $\hat{A}|\psi\rangle = \alpha|\psi\rangle$ then $|\psi\rangle$ is an eigenvector belonging to the eigenvalue α. $\hat{A}^{\dagger} = \hat{A} \Rightarrow \alpha = \alpha^*$, α is real.

Proof: Let $\hat{A}^{\dagger} = \hat{A}$ and $\exists\ |\alpha\rangle$ st $\hat{A}|\alpha\rangle = \alpha|\alpha\rangle$

Then we can write $\langle\alpha|\hat{A}|\alpha\rangle = \alpha\langle\alpha|\alpha\rangle$ —— (1)

Now $\hat{A}|\alpha\rangle = \alpha|\alpha\rangle \Rightarrow \langle\alpha|\hat{A}^{\dagger} = \alpha^*\langle\alpha|$

$\Rightarrow \langle\alpha|\hat{A}^{\dagger}|\alpha\rangle = \alpha^*\langle\alpha|\alpha\rangle$

But $\hat{A} = \hat{A}^{\dagger}$ and so $\langle\alpha|\hat{A}|\alpha\rangle = \alpha^*\langle\alpha|\alpha\rangle$ —— (2)

(1) + (2) $\Rightarrow$ $\alpha = \alpha^*$.

Comments:

1. Hermitian operators play a central role in quantum mechanics. The complete set

of eigenvectors form a basis for the Hilbert space (Theorem).

2. If α is an eigenvalue of a Hermitian operator s.t. the equation $H|\psi\rangle = \alpha|\psi\rangle$ has more than one linearly independent solutions $|\psi\rangle$, then α is known as a degenerate eigenvalues. If $|\psi_i\rangle$ $i = 1, \dots, d_\alpha$ is the complete set of linearly independent eigenvectors, then there exists a procedure, known as the Gram-Schmidt orthogonalization process s.t. the set $|\psi_i\rangle$ yields an orthonormal set $|\tilde{\psi}_i\rangle$: $\langle \tilde{\psi}_i | \tilde{\psi}_j \rangle = \delta_{ij}$.

Projection Operators:

Projection operators are operators which project down to a subspace of the Hilbert space. Thus for a Hermitian operator

$$\hat{A}|\alpha_i\rangle = \alpha_i|\alpha_i\rangle$$

{ where the index i covers both degenerate and non-degenerate eigenvalues }

For any arbitrary state $|\varphi\rangle = \sum_i \varphi_i |\alpha_i\rangle$

We define P_i to a projection operator if $P_i|\varphi\rangle = \varphi_i|\alpha_i\rangle$.

We can write $P_i = |\alpha_i\rangle\langle\alpha_i|$. Note that

i) $P_i^2 = P_i$

ii) $P_i P_j = \delta_{ij} P_i$

Spectral Decomposition Theorem:

We have claimed (without proof) that the set of eigenvectors $\{|\alpha_i\rangle\}$ of a Hermitian operator form an orthonormal basis:

$$\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$$

and $$|\varphi\rangle = \sum_i \varphi_i |\alpha_i\rangle \quad \forall\, |\varphi\rangle \in \mathcal{H}.$$

It then follows that $A = \sum_i \alpha_i P_i$

$$\boxed{A = \sum_i \alpha_i |\alpha_i\rangle\langle\alpha_i|}$$

The spectral decomposition theorem

A very useful corollary of this theorem is that if $\exists$ an operator B st

$$[A, B] = 0$$

Then $B = \sum_i \beta_i |\alpha_i\rangle\langle\alpha_i|$. In particular the identity operator $\mathbb{1}$ can be expressed as $\boxed{\mathbb{1} = \sum_i |\alpha_i\rangle\langle\alpha_i|}$

Decomposition of identity

Comments:

1. Given an Operator O we can always express it in a given basis as a matrix $O_{ij} := \langle\alpha_i|O|\alpha_j\rangle$.

2. Suppose $\{|\alpha_i\rangle\}$ is an orthonormal basis. Let us define a set of new vectors $|\tilde{\gamma}_i\rangle$ st:

$$|\tilde{\gamma}_j\rangle = \sum_i U_{ij} |\alpha_i\rangle$$

If we require the new set $\{|\tilde{\gamma}_i\rangle\}$ to an orthonormal basis:

$$\langle\tilde{\gamma}_i|\tilde{\gamma}_j\rangle = \delta_{ij}$$

$$\text{LHS} = \sum_{l,k} \langle\alpha_l| U^*_{li} U_{kj} |\alpha_k\rangle$$

$$= \sum_{l,k} \delta_{lk} U^*_{li} U_{kj}$$

$$= \sum_k U^*_{ki} U_{kj}$$

$$= \sum_k U^\dagger_{ik} U_{kj}$$

$$\Rightarrow \quad \sum_k U^\dagger_{ik} U_{kj} = \delta_{ij}$$

U_{ij} is a unitary matrix. $U_{ij} := \langle \alpha_i | \tilde{\gamma}_j \rangle$

Postulate 2 :

A measurement is described by an observable A, a Hermitian operator on the Hilbert space of the system. The observable A has a spectral resolution:

$$A = \sum_i |\alpha_i\rangle\langle\alpha_i| \, \alpha_i$$

where $|\alpha_i\rangle\langle\alpha_i|$ is the projection operator that projects onto the subspace of $\mathcal{H}$ labelled by the (real) eigenvalue α_i. Upon measuring the state $|\psi\rangle$ the probability of obtaining the result α_i is

$$p(i) = \langle \psi | P_i | \psi \rangle .$$

Given that the outcome α_i has occurred, the state of the quantum system immediately afterwards is:

$$\frac{P_i |\psi\rangle}{\sqrt{p(i)}} .$$

An Example: Consider a qubit in the state $|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$ st

$$|\alpha|^2 + |\beta|^2 = 1 \iff \langle \varphi | \varphi \rangle = 1.$$

Then the Z observable is $Z = |0\rangle\langle 0| - |1\rangle\langle 1|$.

$X = |0\rangle\langle 1| + |1\rangle\langle 0|$

$Y = -i|0\rangle\langle 1| + i|1\rangle\langle 0|$

If we measure Z while the state of the system is $|\varphi\rangle$ then

$$p(0) = \langle \varphi | 0 \rangle\langle 0 | \varphi \rangle = |\alpha|^2$$

$$p(1) = \langle \varphi | 1 \rangle\langle 1 | \varphi \rangle = |\beta|^2$$

The conditional states right after observation are:

$$|0\rangle\langle 0| : \quad \frac{|0\rangle\langle 0|\varphi\rangle}{\sqrt{|\alpha|^2}} = \frac{|0\rangle\, \alpha}{\sqrt{|\alpha|^2}} = |0\rangle \quad \text{[up to a phase]}$$

$$|1\rangle\langle 1| : \quad \frac{|1\rangle\langle 1|\varphi\rangle}{\sqrt{|\beta|^2}} = |1\rangle \quad \text{[up to a phase].}$$

Unitary Operators: An operator U is called a unitary operator if it satisfies

$$U^\dagger U = U U^\dagger = \mathbb{1}$$

$$\Rightarrow \quad U^\dagger = U^{-1}.$$

Comment:

1. A unitary transformation U acting on a state $|\psi\rangle$ preserves all the information contained in that state: $|\varphi\rangle = U|\psi\rangle$. $|\psi\rangle = U^{-1}|\varphi\rangle$.

2. Unitary operators preserve the norm of a state $\Rightarrow$ Unitary transformations preserve probability. $|\varphi\rangle = U|\psi\rangle \Rightarrow \langle\varphi|\varphi\rangle = \langle\psi|U^\dagger U|\psi\rangle = \langle\psi|\psi\rangle$.

3. Physical transformation of an informationally isolated system is affected by the action of unitary operators on the Hilbert space.

Example: The rotation of a spin $\frac{1}{2}$ system by an angle θ around a axis $\hat{n}$ is given by the action of the following unitary operator on the Hilbert space $\mathbb{C}^2$:

$$U_{\hat{n}}(\theta) = \exp\left[\frac{i}{\hbar}\,\theta\,\hat{n}\cdot\bar{\sigma}/2\right]$$

4. Given an observable $\hat{A}^\dagger = \hat{A}$, one can construct a family of unitary operators:

$$U_\alpha = \exp[i\alpha\hat{A}], \qquad \alpha \in \mathbb{R}.$$

Exercise: Show that $U_\alpha^\dagger = U_\alpha^{-1} = U_{(-\alpha)}$.

Postulate 3:

The time evolution of an isolated quantum mechanical system is governed by a unitary operator $U(t-t') = \exp\left[-\frac{i}{\hbar}H(t-t')\right]$, where H is known as the Hamiltonian operator.

$$|\psi(t)\rangle = U(t-t')|\psi(t')\rangle$$

Note that $U(0) = \mathbb{1}$ and $U(t)$ satisfies:

$$\frac{dU(t)}{dt} = -\frac{i}{\hbar} H U(t)$$

The Schrödinger Equation

For any state $|\psi(0)\rangle$ this then implies $\boxed{i\hbar\frac{d|\psi(t)\rangle}{dt} = H|\psi(t)\rangle.}$

Stationary states:

The energy eigenstates of the Hamiltonian operator are called stationary states. This is because, despite having time dependence, their energy does not change.

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

Then $|\psi_n(t)\rangle = U(t)|\psi_n\rangle = e^{-\frac{i}{\hbar}E_n t}|\psi_n\rangle.$

The time evolution of any state $|\varphi(t)\rangle$ is given by stationary states:

Suppose: $$|\varphi(0)\rangle = \sum_n \varphi_n |\psi_n\rangle$$

Then $\varphi_n = \langle\psi_n|\varphi(0)\rangle$

and
$$|\varphi(t)\rangle = U(t)|\varphi(0)\rangle = \sum_n \underbrace{\varphi_n\, e^{-\frac{i}{\hbar}E_n t}}_{\varphi_n(t)} |\psi_n\rangle$$

Postulate 4

The state space of a composite physical system is the tensor product of the state spaces of the component physical systems. If the systems are labelled by numbers 1 through n and the i-th system has been prepared in the state $|\psi_i\rangle$ then joint state of the system is $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle$

Example: Consider a composite system made out of two qubits. Then a canonical basis is given by $|00\rangle = |0\rangle \otimes |0\rangle$, $|01\rangle = |0\rangle \otimes |1\rangle$ $|10\rangle = |1\rangle \otimes |0\rangle$, $|11\rangle = |1\rangle \otimes |1\rangle$.

The Density Operator / The Density Matrix:

Suppose we have probabilistic distribution of quantum states: The distinct (but not necessarily orthogonal) normalized states $|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_n\rangle$ occur with probabilities $p_1, p_2, \ldots, p_n$, respectively.

Under these circumstances the expectation value of an observable A will be given by:

$$\langle A \rangle = p_1 \langle \psi_1 | \hat{A} | \psi_1 \rangle + p_2 \langle \psi_2 | \hat{A} | \psi_2 \rangle + \cdots$$

$$\cdots + p_n \langle \psi_n | \hat{A} | \psi_n \rangle$$

$$= \sum_{i=1}^{n} p_i \langle \psi_i | \hat{A} | \psi_i \rangle$$

$$= \sum_{i=1}^{n} p_i \langle \psi_i | \varphi_i \rangle \qquad [\, |\varphi_i\rangle := \hat{A} |\psi_i\rangle \,]$$

$$= \sum_{i=1}^{n} p_i \, \mathrm{Tr} \, |\varphi_i\rangle\langle \psi_i| \qquad [\, \mathrm{Tr} \, |\varphi\rangle\langle x| = \langle x | \varphi \rangle \,]$$

$$= \mathrm{Tr} \left[\sum_{i=1}^{n} p_i \, \hat{A} |\psi_i\rangle\langle \psi_i| \right]$$

$$= \mathrm{Tr} \left[\hat{A} \sum_{i=1}^{n} p_i |\psi_i\rangle\langle \psi_i| \right]$$

$$= \mathrm{Tr} [A \rho]$$

where $\rho = \sum_{i=1}^{n} p_i |\psi_i\rangle\langle \psi_i|$ is the density operator / matrix that describes the statistical ensemble that is the state of the system.

Example: Suppose there is a black box which spits out the states $|0\rangle$ or $|1\rangle$ with probabilities p or $(1-p)$. Then the physical state of the system is described by the density operator:

$$\rho = p\,|0\rangle\langle 0| + (1-p)\,|1\rangle\langle 1|.$$

Exercise: Show that for $0<p<1$ there does not exist a 'pure' state

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

that can mimic the state ρ of the system.

Properties of Density Operators:

1. Suppose A is an observable then its average for a system in state ρ is given by $\langle A\rangle = \mathrm{Tr}[\rho A]$.

2. The probability of obtaining a_i is $\mathrm{Tr}[P_i\rho]$.

3. Conservation of probability $\Rightarrow$ $\mathrm{Tr}\,\rho = 1$.

4. For a pure state $\exists$ a state $|\psi\rangle$ s.t. $\rho = |\psi\rangle\langle\psi|$.
For pure states $\rho^2 = \rho$.

5. A non-pure state is called a mixed state. For mixed states
$\mathrm{Tr}\,\rho^2 < 1$.

6. The unitary time evolution of a density operator is given by

$$\rho(t) = U(t)\,\rho_0\,U^\dagger(t)$$

$$\Rightarrow \quad \boxed{\frac{d\rho(t)}{dt} = \frac{1}{i\hbar}[H, \rho(t)]}$$ Von-Neumann equation.

Examples: 1. The state $\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$ is called the maximally mixed state. It is the state that gives us the least information about a quantum system. The maximally mixed state has the same form in every ortho-normal basis

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

$$= \frac{1}{2}|x+\rangle\langle x+| + \frac{1}{2}|x+\rangle\langle x+|$$

2. The Gibbs state: Consider a quantum system with Hamiltonian H immersed in a heat bath at temperature T. Then according to quantum statistical mechanics the state of the system is given by the density matrix:

$$\rho = \frac{e^{-\beta H}}{Z} = \frac{\sum_n |E_n\rangle\langle E_n| \, e^{-\beta E_n}}{Z}, \quad \beta = \frac{1}{k_B T}$$

where $Z = \mathrm{Tr}\, e^{-\beta H}$ is the partition function.

Non. Unitary Evolution:

In the real world quantum systems are often neither isolated nor are they time-independent. So the time evolution of a quantum system may result in interaction which may result in loss/gain of information, and/or change of energy. This may result in loss of coherence. Even a pure quantum state may unitarily evolve in a way such that on a coarse-grained level the state may look thermal.

A general quantum evolution map then should have the following properties:

1. It must be trace-preserving. $\rho \to \sigma(\rho)$ then $\mathrm{Tr}\,\rho = \mathrm{Tr}\,\sigma$.

2. It must be completely positive. I.e. The eigenvalues of the density operators must remain positive. A positive map may not be completely positive. E.g. If ρ_1 is density matrix ρ_1^T is also a valid density matrix. But the map $\rho_1 \otimes \rho_2 \to \rho_1^T \otimes \rho_2$ results in negative eigenvalues and so it is not a CPTP map.

Krause Operator Representation of CPTP maps:

Every quantum map can be represented by a set of operators known as Kraus operators: $\{A_K\}$

So $\rho \to \sigma(\rho)$ can be written as:

$$\sigma(\rho) = \sum_K A_K \rho A_K^\dagger$$

Since $\mathrm{Tr}\,\sigma = \mathrm{Tr}\,\rho = 1 \Rightarrow \sum_K A_K^\dagger A_K = 1.$

An Example: Bit flip

Suppose we have a noisy quantum channel. If we want to send the state $|0\rangle$ or $|1\rangle$, the probability of the qubit passing through unchanged in p. And let the probability that $|0\rangle$ flips to $|1\rangle$ and vice-versa be $(1-p)$. This not represented by a unitary operator but with the two Kraus operators:

$$A_0 = \sqrt{p}\,\mathbb{I} \quad \& \quad A_1 = \sqrt{1-p}\,X.$$