Lecture 19: Dynamics of Open Quantum Systems (I)

- In a "closed" quantum system the state evolves according to a unitary transformation

$$\hat{\rho}(t) = \hat{U}(t)\,\hat{\rho}(0)\,\hat{U}^\dagger(t)$$

and since $\hat{U}(t)$ is generated by a Hamiltonian

$$\frac{\partial \hat{U}(t)}{\partial t} = -\frac{i}{\hbar}\hat{H}(t)\,\hat{U}(t)$$

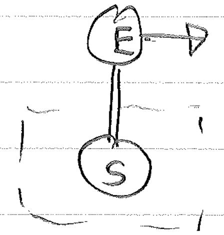
The state evolution is described by a Schrödinger equation

$$\frac{\partial \hat{\rho}(t)}{\partial t} = -\frac{i}{\hbar}\left[\hat{H}(t), \hat{\rho}(t)\right]$$

- In an "open" quatum system we want to track the dynamics of a "system" of interest without following the "environment". In fact, the whole point of calling certain degrees of freedom the environment is that the are uncontrolled and perhaps do complex to follow in detail. The point of this lecture is to develop the formalism to describe the evolution of the marginal state of the system given some overall evolution of the joint system + environment

$$\hat{\rho}_S(t) = \mathrm{Tr}_E\left(\hat{U}_{SE}(t)\,\hat{\rho}_{SE}(0)\,\hat{U}^\dagger_{SE}(t)\right)$$

An important special case is where initially the system and environment are uncorrelated. For the momentum we take the environment to be a pure state, like the vacuum, though the discussion below easily generalizes to mixed states, e.g., thermal reservoir.



$$\hat{\rho}_{SE}(0) = \hat{\rho}_S(0) \otimes \underset{\uparrow}{|0\rangle_E}\langle 0|$$

"fiducial state"

Then $\hat{\rho}_S(t) = \mathrm{Tr}_E\left(\hat{U}_{SE}(t)\; \hat{\rho}_S(0) \otimes |0\rangle_E\langle 0|\; \hat{U}^{\dagger}_{SE}(t)\right)$

Let $\{|\mu\rangle_E\}$ be an orthonormal basis for E

$$\Rightarrow \hat{\rho}_S(t) = \sum_\mu \underbrace{\langle \mu_E|\hat{U}_{SE}|0_E\rangle}_{\text{Partial matrix element } = \hat{M}_\mu(t)}\; \hat{\rho}_S(0)\; \langle 0_E|\hat{U}^{\dagger}|\mu_E\rangle$$

$$\Rightarrow \boxed{\hat{\rho}_S(t) = \sum_\mu \hat{M}_\mu(t)\; \hat{\rho}_S(0)\; \hat{M}^{\dagger}_\mu(t)}$$

This is known as the Kraus representation of the map on the density operator

$$\hat{\rho}_S(t) = \underset{\Uparrow}{\hat{\mathcal{A}}(t)}\left[\hat{\rho}_S(0)\right]$$

"Superoperator"

The operators $\hat{M}_\mu(t)$ are known as "<u>Kraus operators</u>"

To better understand the nature of this map consider the case that the initial state of the system is pure

$$\hat{\rho}_S(0) = |\psi_S(0)\rangle\langle\psi_S(0)|$$

The according to the map

$$\hat{\rho}_S(t) = \sum_\mu \hat{M}_\mu(t)|\psi_S(0)\rangle\langle\psi_S(0)|\hat{M}_\mu^\dagger(t)$$

Now $\hat{M}_\mu(t)|\psi_S(0)\rangle = \sqrt{p_\mu(t)}\,|\psi_\mu(t)\rangle$

where $p_\mu(t) \equiv \| \hat{M}_\mu(t)|\psi_S(0)\rangle\|^2$

$$= \langle\psi_S(0)|\hat{M}_\mu^\dagger(t)\hat{M}_\mu(t)|\psi_S(0)\rangle$$

And $\langle\psi_\mu|\psi_\mu\rangle = 1$

Thus $\boxed{\hat{\rho}_S(t) = \sum_\mu p_\mu(t)\,|\psi_\mu(t)\rangle\langle\psi_\mu(t)|}$

Therefore, in general the map takes a <u>pure state</u> to a <u>mixed state</u>. This is because the system becomes entangled with the environment throught the interation

$$|\Psi_{SE}(t)\rangle = \hat{U}_{SE}(t)\,|\psi_S(0)\rangle\otimes|0_E\rangle$$

$$= \sum_\mu \hat{M}_\mu(t)|\psi_S(0)\rangle \otimes |\mu\rangle_E$$

$$= \sum_\mu \sqrt{p_\mu(t)}\,|\psi_\mu(t)\rangle\otimes|\mu_E\rangle \quad \text{(Schmidt)}$$

Properties of the map

- Linear $\mathcal{A}[a\hat{\rho}_a + b\hat{\rho}_b] = a\,\mathcal{A}[\hat{\rho}_a] + b\,\mathcal{A}[\hat{\rho}_b]$

- Maps density operators to density operators
  - Hermitian $\hat{\rho}_S^{\dagger}(t) = \left(\sum_{\mu}' M_{\mu}(t)\,\hat{\rho}_S(0)\,\hat{M}_{\mu}^{\dagger}(t)\right)^{\dagger}$
  $$= \hat{\rho}_S(t)$$
  - Positive $\hat{\rho}_S(t) \geq 0$ (positive eigenvalues)

- Trace Preserving $\mathrm{Tr}_S(\hat{\rho}_S(t)) = \mathrm{Tr}_S\left(\sum_{\mu}' \hat{M}_{\mu}(t)\,\hat{\rho}_S(0)\,\hat{M}_{\mu}^{\dagger}(t)\right)$

$$= \mathrm{Tr}_S\left[\left(\sum_{\mu}' \hat{M}_{\mu}^{\dagger} M_{\mu}\right)\hat{\rho}_S\right] = \mathrm{Tr}_S\left[\langle 0_E|U_{SE}^{\dagger}\underbrace{\sum_{\mu}|\mu\rangle\langle\mu|}_{\mathbb{1}}\hat{U}_{SE}|0_E\rangle\,\hat{\rho}_S(0)\right]$$

$$= \mathrm{Tr}_S\left[\langle 0_{SE}|\hat{\mathbb{1}}_{SE}|0_{SE}\rangle\,\hat{\rho}_S(0)\right] = \mathrm{Tr}_S(\hat{\mathbb{1}}_S\hat{\rho}_S(0)) = \mathrm{Tr}_S(\hat{\rho}_S(0)) \checkmark$$

Uniqueness of Kraus decomposition

We have seen that given $\hat{\rho}_S(0) = |\psi_S(0)\rangle\langle\psi_S(0)|$

$$\hat{\rho}_S(t) = \sum_{\mu}' \hat{M}_{\mu}|\psi_S(0)\rangle\langle\psi_S(0)|\hat{M}_{\mu}^{\dagger}$$

$$= \sum_{\mu}' \sqrt{p_{\mu}}\,|\psi_{\mu}\rangle\langle\psi_{\mu}|$$

Recall that the ensemble decomposition is not unique. Let $|\tilde{\psi}_{\mu}\rangle = \hat{M}_{\mu}|\psi_{\mu}\rangle$

$$\hat{\rho}_S(t) = \sum_{\mu}' |\tilde{\psi}_{\mu}\rangle\langle\tilde{\psi}_{\mu}| = \sum_{\nu}' |\tilde{\phi}_{\nu}\rangle\langle\tilde{\phi}_{\nu}|$$

$$= \sum_{\mu} \hat{M}_{\mu}|\psi_S(0)\rangle\langle\psi_S(0)|\hat{M}_{\mu}^{\dagger} = \sum_{\nu} \hat{N}_{\nu}|\psi_S(0)\rangle\langle\psi_S(0)|\hat{N}_{\nu}^{\dagger}$$

iff
$$|\tilde{\Phi}_\nu\rangle = \sum_\nu \mathcal{U}_{\nu\mu} |\tilde{\Psi}_\mu\rangle$$

matrix with orthogonal rows & columns

$$\Rightarrow \hat{N}_\nu |\Psi_s(0)\rangle = \sum_\nu \mathcal{U}_{\nu\mu} \hat{M}_\mu |\Psi_s(0)\rangle$$

$\Rightarrow$ New Kraus operators (same map)

$$\boxed{\hat{N}_\nu = \sum_\nu \mathcal{U}_{\nu\mu} \hat{M}_\mu}$$

Thus, there are different sets of Kraus operators that correspond to same map. We will discuss the meaning of this soon.

Complete Posidivity

The map we have defined is said to be completely positive. This means that if there are other subsystems around and the map acts as

$$\mathcal{A}_{S_A} \otimes \hat{\mathbb{1}}_{S_B} \quad \text{on System B}$$

Then the extension is positive for all maps.

Every complete positive (CP) - map has a Kraus representation, derivable from the overall unitary evolution above.