CS191 – Fall 2014 Lecture 14: Open quantum systems: quantum process formulation

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I. TWO MISSING PIECES

Before we start on the bulk of this lecture, we need to cover two concepts that haven't been covered so far. The first is the concept of the entropy of a quantum state, which is defined as:

$$S(\rho) = -\mathrm{tr}\left(\rho\log\rho\right) \tag{1}$$

This expression is most easily evaluated by diagonalizing ρ , in which case $S(\rho) = -\sum_i \lambda_i \log \lambda_i$, where λ_i are the eigenvalues of ρ .¹ The entropy is a measure of how mixed a state is, or how much classical uncertainty it contains.

Another measure of how mixed a state is, which is actually an approximation of the inverse of the entropy is the *purity*, which is defined as:

$$P(\rho) = \operatorname{tr}\left(\rho^2\right) \tag{2}$$

Exercise: What are the entropy and purity of a pure state, $S(|\psi\rangle\langle\psi|)$ and $P(|\psi\rangle\langle\psi|)$? What are the entropy and purity of the completely mixed state in d dimensions, $S(\frac{I_d}{d})$ and $P(\frac{I_d}{d})$?

Note that as the mixedness or uncertainty in the state increases, the entropy increases and the purity decreases.

II. OPEN QUANTUM SYSTEMS AND NOISE

So far in this course you've mainly seen what ideal quantum operations looks like. For example, a state transformation is a unitary map $|\psi\rangle \rightarrow U|\psi\rangle$, and a projective measurement is the following map: $|\psi\rangle \rightarrow \frac{P_i|\psi\rangle}{\sqrt{P_i}}$. But in reality when we perform a quantum operation (*e.g.*, rotation, measurement, coupling) there will inevitably be errors due to noise in the experimental apparatus. Some examples of errors that are commonly encountered in quantum information processing are:

- 1. Uncertainty in the implemented rotation angle.
- 2. Control pulses with electronic noise.
- 3. Noise from nearby "junk", which are usually uncontrollable degrees of freedom that couple to qubits.

In this lecture and the next four we will discuss how to model these nonidealities and how to deal with them and do quantum information tasks reliably in their presence.

A. An example

Let's start with an example. Suppose we have a qubit that starts in the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, and we want to perform a σ_z rotation on it. To do so we turn on a Hamiltonian in the form

$$H = \frac{\omega}{2}\sigma_z.$$

Then ideally,

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle = \frac{1}{\sqrt{2}}(e^{-i\frac{\omega}{2}t}|0\rangle + e^{i\frac{\omega}{2}t}|1\rangle).$$

¹ We define $0 \log 0 = 0$.

This affects a rotation around the Z axis, and if we apply it for $t = \frac{\pi}{\omega}$, we get a Z-gate. That is,

$$\left|\psi(\frac{\pi}{\omega})\right\rangle = \frac{1}{\sqrt{2}}(-|0\rangle + |1\rangle) \equiv \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle),$$

where the last equivalence is due to the unimportance of the global phase of a quantum state.

But now, what if ω is not exactly known? Suppose we have some uncertainty in our calibration and all we can says is that $\omega \sim \mathcal{N}(\omega_0, \sigma^2)$. That is, ω is Gaussian distributed around some nominal value with some variance σ^2 . Then after a time t all we can say is that we have some distribution over Z rotations. We must average over this uncertainty to get an estimate of the actual state. Note that this is exactly what we do in classical physics also, we average over unknowns to get the state. Let's see what we get when we compute this average.

Anytime we average over quantum states, we should use the density matrix formalism. The state at time t, for a given value of ω is

$$\begin{split} \rho_{\omega}(t) &= |\psi_{\omega}(t)\rangle\langle\psi_{\omega}(t)| = \frac{1}{2} \Big[e^{-i\frac{\omega}{2}t} |0\rangle\langle0|e^{i\frac{\omega}{2}t} + e^{-i\frac{\omega}{2}t}|0\rangle\langle1|e^{-i\frac{\omega}{2}t} + e^{i\frac{\omega}{2}t}|1\rangle\langle0|e^{i\frac{\omega}{2}t} + e^{i\frac{\omega}{2}t}|1\rangle\langle1|e^{i\frac{\omega}{2}t} \Big] \\ &= \left(\begin{array}{cc} \frac{1}{2}e^{-i\omega t}\\ \frac{1}{2}e^{i\omega t} & \frac{1}{2} \end{array}\right) \end{split}$$

So then, when we average over the rotation parameters, the average state is:

$$\begin{split} \rho(t) &= \int_{\Omega} P(\omega)\rho_{\omega}(t)d\omega \\ &= \left(\begin{array}{c} \frac{1}{2}\int_{\Omega}P(\omega)d\omega & \frac{1}{2}\int_{\Omega}P(\omega)e^{-i\omega t}d\omega \\ \frac{1}{2}\int_{\Omega}P(\omega)e^{i\omega t}d\omega & \frac{1}{2}\int_{\Omega}P(\omega)d\omega \end{array} \right) \\ &= \left(\begin{array}{c} \frac{1}{2} & \frac{1}{2}\int_{\Omega}P(\omega)e^{-i\omega t}d\omega \\ \frac{1}{2}\int_{\Omega}P(\omega)e^{i\omega t}d\omega & \frac{1}{2} \end{array} \right), \end{split}$$

where Ω is the support of the probability distribution for ω (the whole real line for the normal distribution above). We see that the off-diagonal elements are complex conjugates of each other, so let's look at one of them:

$$\int_{\Omega} P(\omega) e^{-i\omega t} d\omega = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{-\frac{(\omega-\omega_0)^2}{2\sigma^2}} e^{-i\omega t} d\omega = e^{-\frac{(t\sigma)^2}{2} - i\omega_0 t}.$$
(3)

Therefore, the average density matrix is:

$$\rho(t) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2}e^{-\frac{(t\sigma)^2}{2} - i\omega_0 t} \\ \frac{1}{2}e^{-\frac{(t\sigma)^2}{2} + i\omega_0 t} & \frac{1}{2} \end{pmatrix}.$$
(4)

Exercise: Perform the generalized Gaussian integral required to get the last equality in Eq. (3). This is one of the most useful integrals in physics and it's usually obtained by completing the square in the exponent.

There are several things to note about the state in Eq. (4):

- 1. tr $(\rho^2) < 1$ for all t > 0. That means the state becomes mixed as a result of the uncertain rotation.
- 2. The off-diagonal elements oscillate at frequency ω_0 , but also decay exponentially with time and increasing uncertainty (σ^2).
- 3. As $t \to \infty$ or $\sigma \to \infty$,

$$\rho \to \frac{1}{2} \left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right),$$

So if we have too much uncertainty about the rotation angle or apply the Hamiltonian for too long, we just get the completely mixed state.

Exercise: Compute the purity and entropy of the state in Eq. (4) as a function of t and σ .



FIG. 1: A system embedded in a larger environment. Most coupling between a quantum system and its environment will result in decoherence of the system.

This example shows how uncertainty in the operations one performs can result in an increase in entropy or mixedness of the state. This is also true if there is noise (*e.g.*, if ω is a time-dependent random process). In this example, the uncertainty led to a decay of the off-diagonal element of the density matrix, which contains information about the phase of the state (in the computational basis). Consequently, this process is called *dephasing*. In general, external influences and uncertainty can lead to more general transformations of the state, and we collectively refer to the wide class of phenomena that cause the state of a quantum system to evolve nondeterministically and/or to increase in entropy as *decoherence*.

B. The operator sum decomposition

All decoherence arises from a coupling of the system we are interested in to an *environment* that is (at least partially) uncontrolled and unobserved. See figure 1. For instance, in the example above, the uncertainty in ω could be due to us not knowing the precise parameters that dictate the physics that determine this rotation frequency. As a result, we refer to the dynamics of a system under such couplings to external environments as *open system dynamics*. In fact, this perspective gives us a general way to model open system dynamics and decohernce processes mathematically. Suppose we begin with the system and environment in a product state at an initial time:

$$\varrho(0) = \rho_0^S \otimes \left| \phi^E \right\rangle \left\langle \phi^E \right|,\tag{5}$$

where ρ_0^S is the (possibly mixed) initial state of the system and $|\phi^E\rangle\langle\phi^E|$ is the pure initial state of the environment. We can always assume the environment is in a pure state initially since if it is not we can expand our definition of the environment until it is. Then, at some late time t, the joint state of the system and environment is:

$$\varrho(t) = U_{SE}\varrho(0)U_{SE}^{\dagger},\tag{6}$$

where $U_S E$ is a unitary evolution that captures the evolution of the system, the environment, and any coupling between them. Then the reduced state of the system at t is given by tracing out the environment from the above state, *i.e.*, $\rho^{S}(t) = \operatorname{tr}_{E}(\varrho(t))$. We can formally write down what this resulting state is as so:

$$\rho^{S}(t) = \operatorname{tr}_{E} \left[U_{SE} \rho_{0}^{S} \otimes |\phi^{E}\rangle \langle \phi^{E} | U_{SE}^{\dagger} \right] \\
= \sum_{k=1}^{K} \langle a_{k}^{E} | U_{SE} \rho_{0}^{S} \otimes |\phi^{E}\rangle \langle \phi^{E} | U_{SE}^{\dagger} | a_{k}^{E} \rangle \\
= \sum_{k=1}^{K} A_{k} \rho_{0}^{S} A_{k}^{\dagger},$$
(7)

where $|e_k^E\rangle$ for $1 \le k \le K$ is a complete set of orthonormal states (a basis) in the environment Hilbert space, and $A_k \equiv \langle a_k^E | U_{SE} | \phi^E \rangle$, which is an operator acting on the system Hilbert space only.

Example 1 [From Nielsen & Chuang, p.361] Consider an example where the system and environment are single qubits, and the environment starts off in the state $|0^E\rangle$. Then suppose the interaction between them after some time t, is described by the unitary

$$U_{SE} = \frac{\sigma_x}{\sqrt{2}} \otimes I + \frac{\sigma_y}{\sqrt{2}} \otimes \sigma_x.$$
(8)

Then the reduced state of the system at this time is given by Eq. (7), with

$$A_{0} = \langle 0^{E} | U_{SE} | 0^{E} \rangle = \frac{\sigma_{x}}{\sqrt{2}} \times \langle 0 | I | 0 \rangle + \frac{\sigma_{y}}{\sqrt{2}} \times \langle 0 | \sigma_{x} | 0 \rangle = \frac{\sigma_{x}}{\sqrt{2}}$$
$$A_{1} = \langle 1^{E} | U_{SE} | 0^{E} \rangle = \frac{\sigma_{x}}{\sqrt{2}} \times \langle 1 | I | 0 \rangle + \frac{\sigma_{y}}{\sqrt{2}} \times \langle 1 | \sigma_{x} | 0 \rangle = \frac{\sigma_{y}}{\sqrt{2}}$$

Explicitly,

$$\rho^S = \frac{1}{2} \sigma_x \rho_0^S \sigma_x + \frac{1}{2} \sigma_y \rho_0^S \sigma_y \tag{9}$$

Notice that Eq. (7) is a representation of the system density matrix at a fixed time t. It is a map of the density matrix from t = 0 to some future time.

Definiton: The map $\mathcal{E}: \rho_0 \to \rho$, with representation

$$\rho = \mathcal{E}(\rho_0) = \sum_{k=1}^{K} A_k \rho_0 A_k^{\dagger} \tag{10}$$

is referred to as an operator sum decomposition (OSR), or a Kraus representation, or a quantum process. The operators $\{A_k\}_{k=1}^{K}$ are referred to as Kraus operators. The only condition on A_k comes from the fact that we usually want the output of the map to be a trace 1 density matrix ². Therefore,

$$1 = \operatorname{tr}(\rho) = \operatorname{tr}\left(\sum_{k} A_{k}\rho_{0}A_{k}^{\dagger}\right) = \operatorname{tr}\left(\sum_{k} A_{k}^{\dagger}A_{k}\rho_{0}\right),$$

where we have used the cyclic property of trace (tr(AB) = tr(BA)) to get the last equality. Since this relationship has to hold for all ρ_0 , this means

$$\sum_{k} A_{k}^{\dagger} A_{k} = I$$

Apart from this condition, the Kraus operators are arbitrary.

We defined the OSR from a physical picture of a system coupling to an environment. However, one can also derive it from purely mathematical considerations. Suppose we require that a general map $\mathcal{E}: \rho_0 \to \rho$ satisfy the following conditions:

 $^{^{2}}$ There are some special cases where the quantum process does change the trace, but we will not encounter these in this course, and so we restrict ourselves to *trace-preserving* maps, where we specify that the output state has trace 1.



FIG. 2: The conceptual idea behind quantum processes/CPTP maps. Just as the unitary in the joint space of system and environment provides a map from initial state to final state (at some given time, t), the quantum process provides the map between an initial reduced system state and a final reduced system state (at some given time, t).

- 1. \mathcal{E} is linear, *i.e.*, $\mathcal{E}(\sum_{i} p_i \rho_i) = \sum_{i} p_i \mathcal{E}(\rho_i)$.
- 2. \mathcal{E} preserves hermiticity and trace.
- 3. \mathcal{E} preserves positivity, and is in fact, completely positive. The first part of this condition means that ρ is positive if ρ_0 is. The completely positive conditions means:

$$\left[\mathcal{I}_A \otimes \mathcal{E}_B\right](\rho_0^{AB}) = \rho^{AB} > 0. \tag{11}$$

Physically this condition means that if \mathcal{E} is applied to one subsystem (subsystem B) while nothing is done to another system (the \mathcal{I}_A is the identity map on subsystem A), then the resulting density matrix on the combined system, ρ^{AB} , is positive, if the initial density matrix, ρ_0^{AB} is positive. This has to be true regardless of the dimension of subsystem A.

I note that these conditions are very reasonable for a physical process, and any map that satisfies these conditions is called at *completely positive, trace preserving* (CPTP) map. It turns out that any map that satisfies these conditions also has a representation as Eq. (10).

So we see that we arrive at Eq. (10) from a physical perspective as well as a mathematical one. Almost every valid quantum process has an OSR representation, and we will see some examples below.

C. The OSR and POVMs

Notice the similarity between how we derived Eq. (7) and our definition of generalized measurements and POVMs. This is not coincidence, because we can in fact get a nice interpretation of open system dynamics by thinking in terms of generalized measurements. Conversely, we can think about generalized measurement as a special case of open system dynamics.

We saw that POVMs are implemented by coupling the main system to an ancilla and projectively measuring the ancilla, see figure 3. This is similar to what happens in open system dynamics, when a system is coupled to an environment. However, there is a crucial difference: for POVMs we assume that we have access to the ancilla and perform projective measurements on it. For open system dynamics, we do not assume any access to the environment. However, any open system dynamics (and any decoherence process) can be thought of as a coupling to an ancilla/environment after which *someone else* performs a projective measurement of the ancilla and does not tell you the result (but does tell you the basis they measured in ³). Therefore, we should average over all generalized measurements that could have been affected on the system to get an expression for the evolved state:

$$\rho = \sum_{k} p_k \rho_k,\tag{12}$$

where ρ_k is the post-measurement state after the result corresponding to measurement operator M_k was seen. However, we do not know which results occurred, and so we average over all results according to their probabilities,

³ This might seem fishy that you require knowledge of the basis, but not the result. Actually, the following argument also works if you don't know the basis, as we shall see in the next subsection.



FIG. 3: A general implementation of a POVM. The system is coupled to an ancilla which is then measured projectively.

 p_k . Remember from the lecture on generalized measurements that the post-measurement state corresponding to measurement operator M_k is

$$\rho_k = \frac{M_k \rho_0 M_k^{\dagger}}{p_k} \tag{13}$$

Substituting this into Eq. (12) we get

$$\rho = \sum_{k} M_k \rho_0 M_k^{\dagger},\tag{14}$$

which is an OSR. Therefore, we see that any open system dynamics can be interpreted as coupling to another system (call it ancilla or environment) that is measured projectively, but then the results of the measurement are averaged over.

D. Unitary freedom in Kraus operators

The Kraus operators that appear in the OSR for a quantum process, *i.e.*, the A_k in Eq. (10), are not unique. That is, $\sum_{k=1}^{K} A_k \rho A_k^{\dagger}$ could represent exactly the same process as $\sum_{k=1}^{K} B_k \rho B_k^{\dagger}$ if the two sets of Kraus operators are related by a unitary matrix. That is,

$$B_i = \sum_{j=1}^K u_{ij} A_j,$$

where u_{ij} are elements of a unitary matrix. To see the equivalence between the two representations, we write

$$\sum_{k=1}^{K} B_k \rho B_k^{\dagger} = \sum_{k=1}^{K} \left(\sum_{j=1}^{K} u_{kj} A_j \right) \rho \left(\sum_{i=1}^{K} u_{ik}^* A_i^{\dagger} \right)$$
$$= \sum_{kij} u_{ik}^* u_{kj} A_j \rho A_i^{\dagger}$$
$$= \sum_{ij} \delta_{ij} A_j \rho A_i^{\dagger} = \sum_{j=1}^{K} A_j \rho A_j^{\dagger}.$$

Here we have used the fact the u_{ij} are elements from a unitary matrix, and therefore $\sum_k u_{ik}^* u_{kj} = \delta_{ij}$.

From a physical perspective, we can trace the meaning of this unitary freedom back to the derivation of the OSR in the steps preceding Eq. (7). In this derivation, we took the trace over the environment in the basis $|a_k^E\rangle$. However, there is nothing that distinguishes this basis from another basis on the environment space (*e.g.*, for a qubit, $\{|0\rangle, |1\rangle\}$ or $\{|+\rangle, |-\rangle\}$ could be used as a basis). Two bases are related to each other by a unitary transform and this is exactly how different Kraus operators for the same quantum process are related to each other.

Example 2 To illustrate the non-uniqueness of the Kraus operators for a given quantum process, let us return to setup considered in example 1. Instead of measuring the environment qubit in the $|0^E\rangle$, $|1^E\rangle$ basis, let us see what happens if we measure it in the $|+^E\rangle$, $|-^E\rangle$ basis.

$$A_{+} = \left\langle +^{E} \left| U_{SE} \right| 0^{E} \right\rangle = \frac{\sigma_{x}}{\sqrt{2}} \times \left\langle + |I|0\rangle + \frac{\sigma_{y}}{\sqrt{2}} \times \left\langle + |\sigma_{x}|0\rangle \right| = \frac{1}{2}\sigma_{x} + \frac{1}{2}\sigma_{y}$$
$$A_{-} = \left\langle -^{E} \left| U_{SE} \right| 0^{E} \right\rangle = \frac{\sigma_{x}}{\sqrt{2}} \times \left\langle - |I|0\rangle + \frac{\sigma_{y}}{\sqrt{2}} \times \left\langle - |\sigma_{x}|0\rangle \right| = \frac{1}{2}\sigma_{x} - \frac{1}{2}\sigma_{y}$$

Therefore the Kraus operators are different as expected. However, note that the quantum process (*i.e.*, the map from input states to output states) is the same, since

$$\rho^{S} = \mathcal{E}(\rho_{0}^{S}) = \frac{1}{4}(\sigma_{x} + \sigma_{y})\rho_{0}^{S}(\sigma_{x} + \sigma_{y}) + \frac{1}{4}(\sigma_{x} - \sigma_{y})\rho_{0}^{S}(\sigma_{x} - \sigma_{y}) = \frac{1}{2}\sigma_{x}\rho_{0}^{S}\sigma_{x} + \frac{1}{2}\sigma_{y}\rho_{0}^{S}\sigma_{y},$$
(15)

is the same as Eq. (9).

III. EXAMPLES

Now we will see some examples of quantum processes. All these examples are one qubit maps since these are most relevant to quantum computing, but it should be kept in mind that the general formalism we went through in the previous sections applies more generally to any quantum system. Chapter 8.3 of Nielsen and Chuang has very nice geometric interpretations of each of these examples that you should definitely look at.

A. Dephasing or the phase-flip process

The phase-flip process has the OSR

$$\mathcal{E}(\rho_0) = p\rho_0 + (1-p)\sigma_z\rho_0\sigma_z,\tag{16}$$

for some $0 \le p \le 1$. This process represents scrambling of the phase of a qubit in the computational basis. Recall that the example we went through in section II A was one physical instance of this process.

Exercise: Show that after evolution by the uncertain Hamiltonian from section II A with $\omega \sim \mathcal{N}(0, \sigma^2)$, for a fixed time T, the resulting map on an arbitrary initial density matrix ρ_0 is given by Eq. (16), with

$$p = \frac{1 + e^{-\frac{(T\sigma)^2}{2}}}{2} \tag{17}$$

B. Bit-flip process

The bit-flip process has the OSR

$$\mathcal{E}(\rho_0) = p\rho_0 + (1-p)\sigma_x\rho_0\sigma_x,\tag{18}$$

for some $0 \le p \le 1$. This process represents scrambling of the amplitude of a qubit in the computational basis.

C. Depolarizing process

The depolarizing process has the OSR

$$\mathcal{E}(\rho_0) = \left(1 - \frac{3p}{4}\right)\rho_0 + \frac{p}{4}\left(\sigma_x\rho_0\sigma_x + \sigma_y\rho_0\sigma_y + \sigma_z\rho_0\sigma_z\right),\tag{19}$$

for some $0 \le p \le 1$. This process represents scrambling of both the phase and amplitude of a qubit simultaneously. It can also be written in an alternate form, that is not an OSR, but is sometimes more useful:

$$\mathcal{E}(\rho_0) = p \frac{I}{2} + (1-p)\rho_0.$$
(20)

You saw this form in some of the problems in homework 4.

D. Amplitude damping process

The amplitude damping process has the OSR

$$\mathcal{E}(\rho_0) = A_0 \rho_0 A_0^{\dagger} + A_1 \rho_0 A_1^{\dagger}, \tag{21}$$

with

$$A_0 = \begin{pmatrix} 1 & 0\\ 0 & \sqrt{1-p} \end{pmatrix} \tag{22}$$

$$A_1 = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix} \tag{23}$$

for some $0 \le p \le 1$. This process represents the relaxation of a qubit from the excited state to the ground state (e.g., due to spontaneous emission). The parameter p represents the probability of this relaxation per unit time.

Exercise: Show that the amplitude damping channel leaves the ground state, $\rho_0 = |0\rangle\langle 0|$, unchanged.

IV. REFERENCES AND FURTHER READING

- 1. Chapters 8.1, 8.2 & 8.3 of Nielsen & Chuang.
- 2. Chapters 5.4, 6.1 of Benenti, Casati, & Strini, Volume 2.