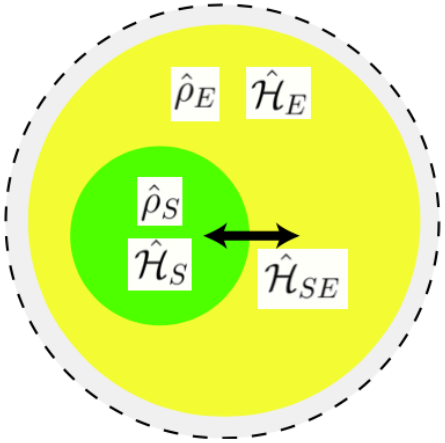
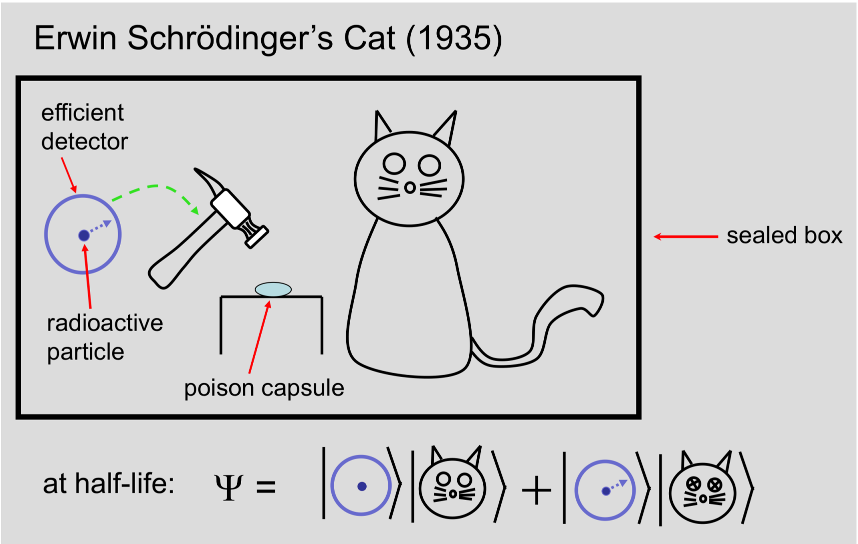
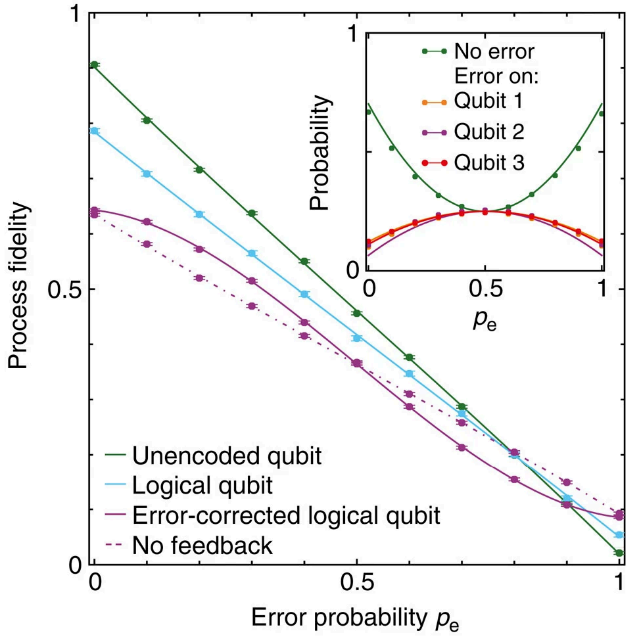
Open quantum systems

Topics for today:

- Welcome
- Overview of course syllabus and schedule
- Density matrix refresher
- Time evolution of open quantum systems
- Kraus operators
- Lindblad equation
- Distance measures







J. Cramer et al., *Nature Comm* (2015)

Density matrix refresher

In quantum mechanics time evolution is a unitary process. A quantum state evolves as:

$$|\psi\rangle \rightarrow |\psi'\rangle = U|\psi\rangle$$

This means any quantum time evolution or process can be undone:

$$U^\dagger|\psi'\rangle = U^\dagger U|\psi\rangle = |\psi\rangle$$

However, in this class we will instead spend almost all of our time considering "open quantum systems," where we have incomplete knowledge about the state, process, or access/control over only part of the full system.

Density matrix refresher

We can describe a quantum state we have imperfect knowledge about using a density matrix, which captures the probabilities of it occupying a set of pure states:

$$\hat{\rho} = \sum_i P_i |\psi_i\rangle\langle\psi_i|$$

For a pure state:

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

Question for the class:

What is the physical meaning of the diagonal matrix elements $\hat{\rho}_{ii}$ of the density matrix mean?

What about the off-diagonal elements $\hat{\rho}_{ij}$?

Density matrix refresher

Question for the class:

Consider these two density matrices for a single qubit:

$$\hat{\rho}_A = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

$$\hat{\rho}_B = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

What is probability to find the qubit in $|0\rangle$ for each density matrix?

What states do these density matrices describe?

Density matrices

A few important properties of density matrices:

$$\hat{\rho} = \hat{\rho}^\dagger \quad \text{(Hermitian, from definition)}$$

$$\mathrm{Tr}[\hat{\rho}] = 1 \quad \text{(Conservation of probability)}$$

$$\langle j | \hat{\rho}^2 | i \rangle \leq \langle j | \hat{\rho} | i \rangle$$

(Equality only for pure state.)

For an arbitrary operator:

$$\langle \hat{O} \rangle = \mathrm{Tr}[\hat{\rho}\hat{O}] = \mathrm{Tr}[\hat{O}\hat{\rho}]$$

Time evolution of open quantum systems

The unitary time evolution of a density matrix is given by:

$$\frac{d\hat{\rho}}{dt} = \frac{i}{\hbar}[\hat{\rho}, \hat{H}]$$

(Can be derived by plugging $\hat{\rho}$ into Schrodinger equation.)

The solution of this equation is:

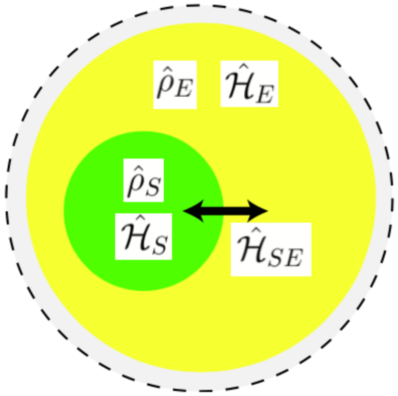
$$\hat{\rho}(t) = U(t)\hat{\rho}(t_0)U^{\dagger}(t)$$

Where U is the unitary time evolution operator.

At first glance we have not gained anything by adding in the density matrix formalism, as this is still unitary.

Time evolution of open quantum systems

But we now consider a composite system composed of our quantum system of interest *S*, and the surrounding environment *E*:



$$\hat{H} = \hat{H}_S + \hat{H}_E + \hat{H}_{SE}$$

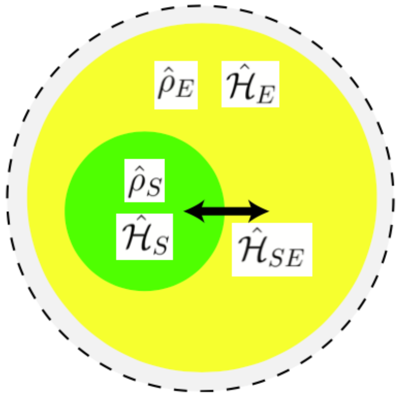
We assume that at time t_0, *S* and *E* are in separable states:

$$\hat{\rho}_{SE}(t_0) = \hat{\rho}_S(t_0) \otimes \hat{\rho}_E(t_0)$$

<u>Question for the class:</u>

What are some simple examples of such a composite system like this?

Time evolution of open quantum systems



$$\hat{H} = \hat{H}_S + \hat{H}_E + \hat{H}_{SE}$$

After time *t*, *S* and *E* will become entangled due to $\hat{H}_{SE}$.
The time evolution is described by:

$$\hat{\rho}_{SE}(t) = U\hat{\rho}_{SE}(t_0)U^\dagger$$

We can't measure the environment, only the system, so we are interested in the state of the system alone:

$$\hat{\rho}_S(t) = \mathrm{Tr}_E[U\hat{\rho}_{SE}(t_0)U^\dagger] = \mathrm{Tr}_E[U\hat{\rho}_S(t_0) \otimes \hat{\rho}_E(t_0)U^\dagger]$$

Define superoperator $\mathscr{E}$: $\hat{\rho}_S(t) = \mathscr{E}[\hat{\rho}_S(t_0)]$

Time evolution of open quantum systems

We define a basis of environment states $|E_j\rangle$:

$$\hat{\rho}_S(t) = \mathrm{Tr}_E[U\hat{\rho}_S(t_0) \otimes \hat{\rho}_E(t_0)U^\dagger]$$

$$\hat{\rho}_S(t) = \sum_j \langle E_j | U\hat{\rho}_S(t_0) \otimes \hat{\rho}_E(t_0)U^\dagger | E_j\rangle$$

Assume the initial states of both the environment and system are pure states:

$$\hat{\rho}_S(t_0) = |S_0\rangle\langle S_0|,\ \hat{\rho}_E(t_0) = |E_0\rangle\langle E_0|$$

$$\hat{\rho}_S(t) = \sum_j \langle E_j | U | S_0\rangle\langle S_0| \otimes |E_0\rangle\langle E_0| U^\dagger | E_j\rangle$$

$$\hat{\rho}_S(t) = \sum_j \langle E_j | U | S_0\rangle |E_0\rangle \otimes \langle S_0| \langle E_0| U^\dagger | E_j\rangle$$

$$\hat{\rho}_S(t) = \sum_j \langle E_j | U | S_0\rangle |E_0\rangle \otimes \langle S_0| \langle E_0| U^\dagger | E_j\rangle$$

Time evolution of open quantum systems

$$\hat{\rho}_S(t) = \sum_j \langle E_j | U | E_0 \rangle | S_0 \rangle \otimes \langle S_0 | \langle E_0 | U^\dagger | E_j \rangle$$

We can now define a new operator $\hat{A}_j$:

$$\hat{A}_j | S_0 \rangle = \sum_j \langle E_j | U | E_0 \rangle | S_0 \rangle$$

Plug this in to find:

$$\hat{\rho}_S(t) = \sum_j \hat{A}_j | S_0 \rangle \langle S_0 | \hat{A}_j^\dagger$$

Recall that $\hat{\rho}_S(t_0) = | S_0 \rangle \langle S_0 |$, so:

$$\boxed{\hat{\rho}_S(t) = \mathscr{E}[\hat{\rho}_S(t_0)] = \sum_j \hat{A}_j \hat{\rho}_S(t_0) \hat{A}_j^\dagger}$$

Time evolution of open quantum systems

We have arrived at the general result that a quantum process acts on a density matrix as:

$$\hat{\rho} \to \hat{\rho}' = \mathscr{E}[\hat{\rho}] = \sum_j \hat{A}_j \hat{\rho} \hat{A}_j^\dagger$$

The operators $\hat{A}_j$ are called Kraus operators. They need not be unitary, so the evolution of the density matrix can also be non-unitary. The act of tracing over the environment has resulted in non-unitary system evolution.

The Kraus operators satisfy a normalization condition:

$$\sum_j \hat{A}_j^\dagger \hat{A}_j = \hat{I}$$

Kraus operators

Before we continue to consider time evolution, it is useful to define the Kraus operators for some common quantum processes:

A bit flip with probability *p* is described by

$$\hat{\rho} \rightarrow \hat{\rho}' = \mathscr{E}[\hat{\rho}] = (1-p)\hat{\rho} + p\hat{X}\hat{\rho}\hat{X}$$

The Kraus operators are therefore:

$$\hat{A}_0 = \sqrt{1-p}\hat{I},\ \hat{A}_x = \sqrt{p}\hat{X}$$

<u>**Question for the class:**</u>

What about a phase flip?

Kraus operators

A phase flip with probability p is described by

$$\hat{\rho} \to \hat{\rho}' = \mathscr{E}[\hat{\rho}] = (1-p)\hat{\rho} + p\hat{Z}\hat{\rho}\hat{Z}$$

The Kraus operators are therefore:

$$\hat{A}_0 = \sqrt{1-p}\,\hat{I},\ \hat{A}_z = \sqrt{p}\hat{Z}$$

Kraus operators

A combined bit and phase flip with probability *p* is described by

$$\hat{\rho} \to \hat{\rho}' = \mathscr{E}[\hat{\rho}] = (1-p)\hat{\rho} + p\hat{X}\hat{Z}\hat{\rho}(\hat{X}\hat{Z})^{\dagger}$$

The Kraus operators are therefore:

$$\hat{A}_0 = \sqrt{1-p}\hat{I},\ \hat{A}_{xz} = \sqrt{p}\hat{X}\hat{Z}$$

Since $\hat{X}\hat{Z} = -i\hat{Y}$, we rewrite all this as:

$$\hat{\rho} \to \hat{\rho}' = = (1-p)\hat{\rho} + p(-i\hat{Y})\hat{\rho}(i\hat{Y}) = (1-p)\hat{\rho} + p\hat{Y}\hat{\rho}\hat{Y}$$

The Kraus operators are therefore also:

$$\hat{A}_0 = \sqrt{1-p}\hat{I},\ \hat{A}_y = \sqrt{p}\hat{Y}$$

Kraus operators

The depolarizing channel for a single qubit is the quantum process where an $\hat{X}$, $\hat{Y}$, or $\hat{Z}$ operation all occur with equal probability:

$$\hat{\rho} \to \hat{\rho}' = (1-p)\hat{\rho} + \frac{p}{3}\hat{X}\hat{\rho}\hat{X} + \frac{p}{3}\hat{Y}\hat{\rho}\hat{Y} + \frac{p}{3}\hat{Z}\hat{\rho}\hat{Z}$$

$$\hat{A}_0 = \sqrt{1-p}\,\hat{I},\ \hat{A}_1 = \sqrt{p/3}\,\hat{X},\ \hat{A}_2 = \sqrt{p/3}\,\hat{Y},\ \hat{A}_3 = \sqrt{p/3}\,\hat{Z}$$

It is not hard to show that for any $\hat{\rho}$:

$$\frac{\hat{I}}{2} = \frac{\hat{\rho} + \hat{X}\hat{\rho}\hat{X} + \hat{Y}\hat{\rho}\hat{Y} + \hat{Z}\hat{\rho}\hat{Z}}{4}$$

$$\hat{X}\hat{\rho}\hat{X} + \hat{Y}\hat{\rho}\hat{Y} + \hat{Z}\hat{\rho}\hat{Z} = 2\hat{I} - \hat{\rho}$$

The depolarizing channel can therefore be written as

$$\hat{\rho} \to \hat{\rho}' = (1 - \frac{4p}{3})\hat{\rho} + \frac{4p}{3}\frac{\hat{I}}{2}$$

Hence the name depolarizing channel, as with probability 4*p*/3 the initial qubit state $\hat{\rho}$ is depolarized and is replaced by the completely mixed state $\hat{I}/2$.

Time evolution of open quantum systems

Armed with our new-found knowledge of Kraus operators, we can return to the time evolution of an open quantum system. We consider the infinitesimal time evolution

$$\mathscr{E}[\hat{\rho}] = \hat{\rho}(t + \delta t) = \sum_j \hat{A}_j \hat{\rho} \hat{A}_j^\dagger$$

We assume one of the Kraus operators is dominant and is given by:

$$\hat{A}_0 = \hat{I} + \hat{L}_0 \delta t$$

And the other operators are

$$\hat{A}_j = \hat{L}_j \sqrt{\delta t},\ j \neq 0$$

Time evolution of open quantum systems

$\hat{A}_0 = \hat{I} + \hat{L}_0\delta t$, so we have

$$\hat{A}_0\hat{\rho}\hat{A}_0^\dagger = \hat{\rho} + (\hat{L}_0\hat{\rho} + \hat{\rho}\hat{L}_0^\dagger)\delta t + \mathcal{O}(\delta t)^2$$

And $\hat{A}_j = \hat{L}_j\sqrt{\delta t}$ so:

$$\hat{A}_j\hat{\rho}\hat{A}_j^\dagger = \hat{L}_j\hat{\rho}\hat{L}_j^\dagger\delta t$$

To lowest order in δt we therefore have:

$$\hat{\rho}(t+\delta t) = \sum_j \hat{A}_j\hat{\rho}\hat{A}_j^\dagger = \hat{\rho} + \left(\hat{L}_0\hat{\rho} + \hat{\rho}\hat{L}_0^\dagger + \sum_{j\neq 0}\hat{L}_j\hat{\rho}\hat{L}_j^\dagger\right)\delta t$$

Time evolution of open quantum systems

$$\hat{\rho}(t+\delta t) = \sum_j \hat{A}_j \hat{\rho} \hat{A}_j^\dagger = \hat{\rho} + \left(\hat{L}_0 \hat{\rho} + \hat{\rho} \hat{L}_0^\dagger + \sum_{j \neq 0} \hat{L}_j \hat{\rho} \hat{L}_j^\dagger \right) \delta t$$

This implies the differential equation:

$$\frac{d\hat{\rho}}{dt} = \hat{L}_0 \hat{\rho} + \hat{\rho} \hat{L}_0^\dagger + \sum_{j \neq 0} \hat{L}_j \hat{\rho} \hat{L}_j^\dagger$$

In order to recover the Hamiltonian component of the dynamics we put $\hat{L}_0 = -i\hat{H}/\hbar + \hat{L}_0'$ to give:

$$\frac{d\hat{\rho}}{dt} = \frac{i}{\hbar}[\hat{\rho}, \hat{H}] + \hat{L}_0' \hat{\rho} + \hat{\rho} \hat{L}_0'^\dagger + \sum_{j \neq 0} \hat{L}_j \hat{\rho} \hat{L}_j^\dagger$$

Time evolution of open quantum systems

Conservation of probability requires $\mathrm{Tr}[\hat{\rho}] = 1$, so we require $\mathrm{Tr}[d\hat{\rho}/dt] = 0$. This results in the condition:

$$\hat{L}_0' = -\frac{1}{2}\sum_j \hat{L}_J^\dagger \hat{L}_J$$

Plugging this in yields

$$\boxed{\frac{d\hat{\rho}}{dt} = \frac{i}{\hbar}[\hat{\rho}, \hat{H}] + \sum_{j\neq 0} \hat{L}_j \hat{\rho} \hat{L}_j^\dagger - \frac{1}{2}\hat{L}_j^\dagger \hat{L}_j \hat{\rho} - \frac{1}{2}\hat{\rho}\hat{L}_j^\dagger \hat{L}_j}$$

This is called the Lindblad form of the master equation, with the operator $\hat{L}$ called the Lindblad or "jump" operator. It is widely used to describe open quantum systems, and we will use specific forms of it throughout the course.

Distance measures

Due to interactions with the environment, errors in applied control fields, or imperfect state preparation and readout, a quantum system will almost never end up in exactly the state desired. It is therefore important to quantify how close the state $\hat{\rho}$ is to a desired state $\hat{\rho}_o$.

There is no universal answer to this question, as it depends on what $\hat{\rho}$ will be used for. Nevertheless, it is useful to define figures of merit to quantify and compare quantum processes.

Distance measures

The most common measure you are likely to encounter is the trace overlap or fidelity:

$$F(\hat{\rho}, \hat{\rho}_o) = \mathrm{Tr}\left[\sqrt{\sqrt{\hat{\rho}}\hat{\rho}_o\sqrt{\hat{\rho}}}\right]$$

$$F(\hat{\rho}_o, \hat{\rho}_o) = 1,\ F(\hat{\rho}, \hat{\rho}_o) = F(\hat{\rho}_o, \hat{\rho})$$

The square of the fidelity is also used:

$$F_{sq}(\hat{\rho}, \hat{\rho}_o) = \left(\mathrm{Tr}\left[\sqrt{\sqrt{\hat{\rho}}\hat{\rho}_o\sqrt{\hat{\rho}}}\right]\right)^2$$

$F_{sq}(\hat{\rho}, \hat{\rho}_o)$ corresponds to the probability of observing $\hat{\rho}$, but $F(\hat{\rho}, \hat{\rho}_o)$ is used more commonly.

Distance measures

Another useful distance measure is the trace distance

$$D(\hat{\rho}, \hat{\rho}_o) = \frac{1}{2}\mathrm{Tr}\left[\sqrt{(\hat{\rho} - \hat{\rho}_o)^\dagger(\hat{\rho} - \hat{\rho}_o)}\right]$$

Note that $D(\hat{\rho}_o, \hat{\rho}_o) = 0$, and $1 - D(\hat{\rho}, \hat{\rho}_o)$ gives a measure of the similarity between the states that can be compared to the fidelity.

The trace distance is an alternative to fidelity that is sensitive to phase errors that may not be picked up by fidelity.