Physics 581: Lecture 7
Introduction to Open Quantum Systems

Quantum mechanics, in its fundamental description, is governed by unitary evolution. Such evolution is deterministic and reversible. The same is true in classical physics. Hamiltonian evolution is reversible and deterministic. We know, however, that many phenomena in physics are not reversible and often not deterministic. How irreversibility and randomness emerge as "effective" descriptions is a fundamental problem in physics, be it in the classical or quantum theory. It becomes, however, particularly poignant in the quantum theory as it is tied to fundamental questions of dissipation (energy relaxation), decoherence (the decay of quantum coherence), and measurement (the emergence of a classical outcome), and more broadly, the emergence of the classical description of phenomena from a fundamentally quantum world.

Last semester, we treated the effect of dissipation and decoherence in a phenomenological manner, by adding an imaginary part to the Hamiltonian. For the next few lectures, we will develop the theory from first principles, and thus develop a much deeper understanding of the problem of decoherence.

We have seen two very different kinds of dynamics in the evolution of a two-level atom coupled to the quantized electromagnetic field:

- Spontaneous emission: Atoms in free space, initially prepared to the excited state, with field in the vacuum

$$|\psi(0)\rangle = |e\rangle_A \otimes |0\rangle_F$$

At a later time, the probability to find an excited atom

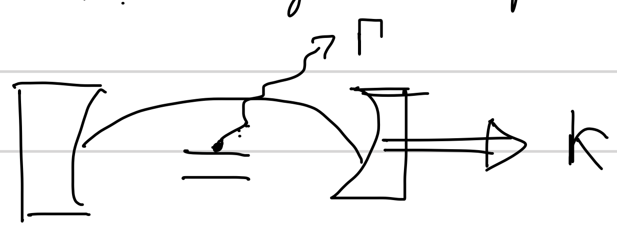
$$P_e(t) = e^{-\Gamma t} \qquad \Gamma = \frac{4}{3}\frac{|\vec{d}_{eg}|^2}{\hbar}\left(\frac{\omega_{eg}}{c}\right)^3 \quad \left(\text{Einstein-A coeff}\right)$$

• <u>Jaynes-Cummings Model</u>: Atom in a <u>perfect cavity</u> (infinite finesse) initially prepared in the excited state with field in the vacuum:

$$|\psi(0)\rangle = |e\rangle \otimes |0\rangle$$

At a later time: $P_e(t) = \cos^2(gt)$, $g = \sqrt{\frac{2\pi\hbar\omega}{V}}\,\frac{|d_{eg}|}{\hbar}$

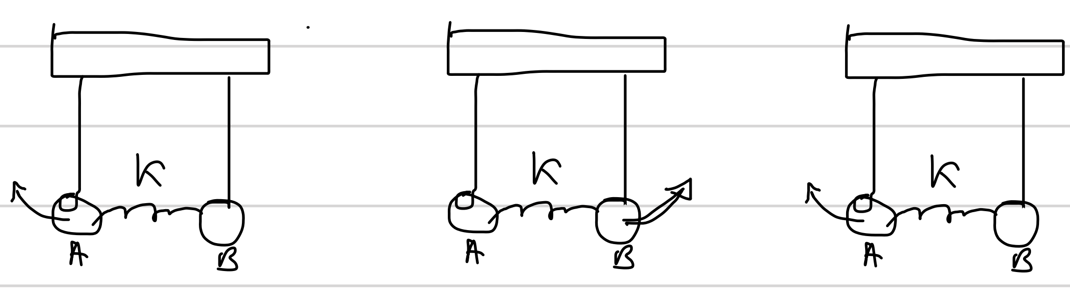
These represent two extremes of reversible and irreversible behavior. In a certain sense, the irreversible behavior is more generic; it is characteristic of what is typically observed in the laboratory. For example, the J-C model is an idealization. Rabi flopping between $|e\rangle\otimes|0\rangle$ and $|g\rangle\otimes|1\rangle$. Eventually, the photon will be spontaneously emitted and leave out the side of the cavity, or absorbed/transmitted through one of the mirrors:



The J-C model only holds approximately when $g \gg \kappa, \Gamma$. This is usually called the "strong coupling regime." Whereas the ideal JC model applies to a <u>closed quantum system</u>, the real world is not. The atom is coupled to other modes of field which is radiates into (spontaneous emission) and the cavity mirrors couple the mode inside to the propagating fields outside (as well as to the material degrees of freedom inside the mirror wall itself).

To understand the emergence of irreversible behavior, consider a simple classical picture.

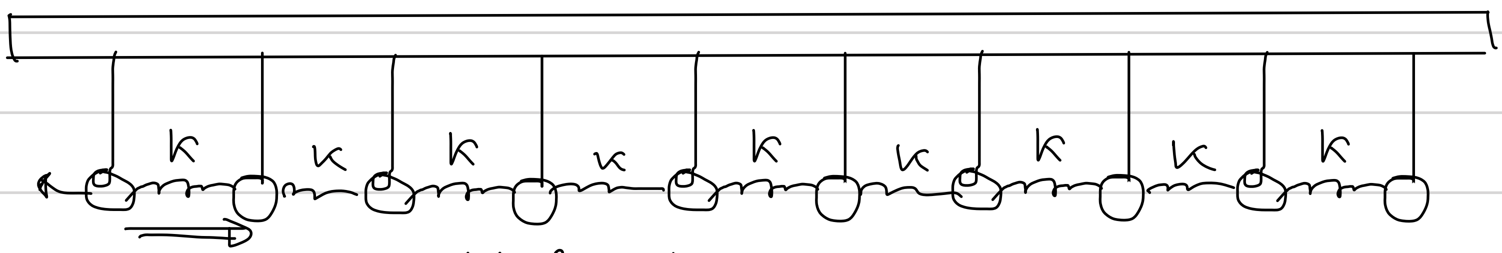
2 Coupled Pendula:



$t=0$ $\quad$ $t=\frac{\pi}{\kappa}$ $\quad$ $t=\frac{2\pi}{\kappa}$

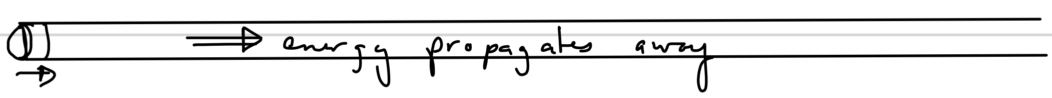
Energy periodically exchanged between A and B

Many coupled pendula:



energy propagated for a long time

Continuum limit: Elastic rod



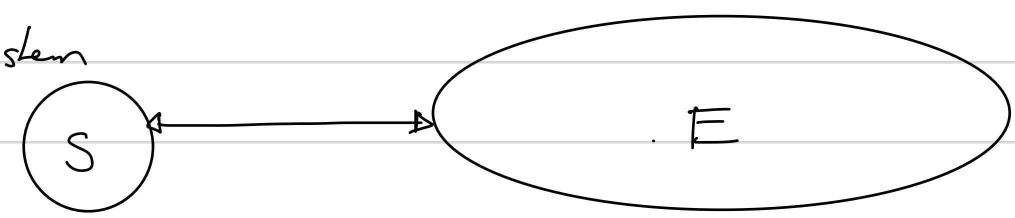
$\Rightarrow$ Uncountable infinite # of normal modes

$\Rightarrow$ Recurrence time $\rightarrow \infty$

$\Rightarrow$ Effectively irreversible.

In dealing with an "open system" we typically divide the degrees of freedom of the "system" from the "enviroment." Sometimes we call the enviroment a "reservoir," or "bath" a term used in thermodynamics when a system is put in thermal equilibrium with a typically liquid bath/reservoir at some temperature.

System



Environment

- many (approaching continuum) degrees of freedom

- few degrees of freedom

In the classically context, we use this description to study how the system comes to thermal equilibrium. In particular excitations flow to and from the envirmment, but because the reservoir is so large, its state rapidly comes back into equilibrium much faster than energy energy flow. Thus information about the correlations are quickly lost, and the dynamics become effectively irreversible. We are ultimately interested in the quantum description. The system reservoir interaction not only has the effect of dissipation, as in classical physics, but also a damping of quantum coherence – decoherence. This is our main focus.

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

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

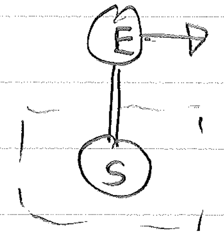
The state evolution is described by a Schrödinger equation

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

- 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 to 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.



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

"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

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

"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 through the interaction

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

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

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

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 <u>not unique</u>. 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 Positivity

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.