1 Overview

Until now, our discussion has primarily been about closed quantum systems, which evolve unitarily. Specifically, we considered single and multiple component systems, such as atoms and photons, but we kept every part, and never threw anything away.

However, in real systems, we often want to be able to disregard certain microscopic dynamics, or do not have access to certain parts of a system. For example, we may want to cool an atom, but will not keep track of the microscopic state of the cooling laser beam after it has interacted with the atom. Or an atom may interact with the vacuum, emitting a photon which we do not track.

The study of such topics is the subject of open quantum system dynamics. Open systems are also studied classically, of course, and one starting point for comparison is the Einstein rate equations for a two-level atom coupled to a black-body electromagnetic field,

\[ \frac{dN_g}{dt} = A_{eg}N_e + u(\omega_{eg}) \left( B_{ge}N_e - B_{ge}N_g \right) \]
\[ \frac{dN_e}{dt} = -A_{eg}N_e + u(\omega_{eg}) \left( B_{ge}N_g - B_{eg}N_e \right), \]

where \( A_{eg} \) is the spontaneous emission rate, \( B_{ge} \) and \( B_{eg} \) are stimulated emission rates, and \( u(\omega_{eg}) \) is the field energy density at atomic frequency \( \omega_{eg} \), for levels denoted by \( |e\rangle \) and \( |g\rangle \).

Is there a straightforward quantum analogue of this? We might be tempted to simply add a damping term to the Schrödinger equation, like

\[ i\hbar \partial_t |\psi\rangle = H |\psi\rangle - i\Gamma |\psi\rangle, \]

but this is not physically allowed by QM! (note: wait for lecture #20)

How, then, can we construct a fully QM description of open system dynamics? The key concept is that we must properly account for noise:
From classical thermodynamics, we know that any time there is energy transfer from a system to the environment, there is entropy exchanged back from the environment to the system. This is a simple illustration of the very basic fluctuation–dissipation principle: there can be no relaxation without con-commitment noise! To study quantum open system, we must model the appropriate quantum noise contribution which goes along with relaxation.

2 Summary of approach

We now build a mathematical model for quantum open system dynamics, based on four basic ideas:

1. Density matrix evolution
   Instead of pure states (e.g., $|\psi\rangle$), we describe the system state using a density matrix $\rho$. The equation of motion for $\rho$ is
   $$\dot{\rho} = \mathcal{L}[\rho],$$
   where $\mathcal{L}$ is known as the Liouvillian operator. For example, for Hamiltonian evolution, we have:
   $$i\hbar \partial_t |\psi\rangle = H|\psi\rangle$$
   which, for $\rho = |\psi\rangle \langle \psi|$ gives
   $$\partial_t \rho = |\dot{\psi}\rangle \langle \psi| + |\psi\rangle \langle \dot{\psi}|$$
   $$= -\frac{i}{\hbar} H|\psi\rangle \langle \psi| + |\psi\rangle \langle \psi| \frac{i}{\hbar} H$$
   $$= -\frac{i}{\hbar} [H, \rho].$$
   This is unitary evolution, but in general, the differential equation for $\rho$ can describe non-unitary evolution. Such differential equations are known as “master equations”.

2. Partial trace
   We are interested in the state of the system alone, and want to disregard the state of the environment. If $\rho_{\text{total}}$ is the state of the whole system + environment, then the state of the system alone is
   $$\rho_{\text{sys}} = \text{Tr}_{\text{env}} \left[ \rho_{\text{total}} \right]$$
   $$= \sum_{\text{env}} \langle \text{env}|\rho_{\text{total}}|\text{env} \rangle.$$  

3. Assumptions about the environment
   The environment is also known as a “bath” or a “reservoir” (cf API). We model it as being an ensemble of oscillators, of a variety of frequencies, which are weakly coupled to the system. It has several important properties:
   - Large and unchanging – Born approximation
   - Short correlation time $\tau_c$ – Markov approximation

4. Two (very different) timescales
   There are two important timescales in this model:
\begin{itemize}
  \item $T_{\text{relax}}$: A slow evolution of the system
  \item $\tau_c$: The fast fluctuations of the environment
\end{itemize}

We will build equations of motion which have a timescale $\Delta t$, chosen such that $\tau_c \ll \Delta t \ll T_{\text{relax}}$.

Our goal is to construct a model dynamical equation of motion for $\rho_{\text{sys}}$ of the form

$$\frac{\Delta \rho_{\text{sys}}}{\Delta t} = M \rho_{\text{sys}},$$

where $M$ is time independent. This is known as a “coarse grained” evolution equation. In the coming lectures, we will study $M$ for a variety of scenarios, including interactions where the system + environment are atom + light, light + light, and atom + motion, for example. Today, we will construct a master equation for the atom + vacuum using two different approaches.

## 3 Beamsplitter model

The physical intuition behind the master equation can be captured with a simple example, which builds on previous lectures. Consider a single photon state $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ (for simplicity, let the coefficients be real-valued) entering a beamsplitter of angle $\theta$:

A vacuum state $|0\rangle$ is input to the other port, whose output we discard. Let us consider the photon as being our system, and the other (initially vacuum) mode as being our environment. What is the quantum state of the undiscounted output? Naively, we might argue that a single photon is discarded into the environment with probability $p_1 = \beta^2 \sin^2 \theta$, so that we might expect the output to be $|0\rangle$ with probability $p_1$, and $|\psi\rangle$ with probability $1 - p_1$. However, that (semi-)classical argument is incorrect.

The output state $|\phi\rangle$ of the system + environment is

$$|\phi\rangle = e^{i \theta a^\dagger b + b^\dagger a} \left[ |\psi\rangle \otimes |0\rangle \right]$$

$$= \alpha |00\rangle + \beta \left[ \cos \theta |10\rangle + \sin \theta |01\rangle \right]$$

$$= \left[ \alpha |0\rangle + \beta \cos \theta |1\rangle \right] \otimes |0\rangle + \left[ \beta \sin \theta |0\rangle \right] \otimes |1\rangle.$$  \hfill \(12\)

Thus, the correct result is that the output is $|\psi_0\rangle = (\alpha |0\rangle + \beta \cos \theta |1\rangle) / \sqrt{\alpha^2 + \beta^2 \cos^2 \theta}$, with probability $1 - p_1$, and $|\psi_1\rangle = |0\rangle$ with probability $p_1$. 

3
These states can conveniently be written as density matrices. The input state is
\[ \rho_{\text{in}} = |\psi\rangle \langle \psi| = \begin{bmatrix} \alpha^2 & \alpha \beta \\ \alpha \beta & \beta^2 \end{bmatrix}, \] (15)
and the output state is
\[ \rho_{\text{out}} = p_1 |\psi_1\rangle \langle \psi_1| + p_0 |\psi_0\rangle \langle \psi_0| = \begin{bmatrix} \alpha^2 + \beta^2 \sin^2 \theta & \alpha \beta \cos \theta \\ \alpha \beta \cos \theta & \beta^2 \cos^2 \theta \end{bmatrix}. \] (16)

Note that \( \rho_{\text{out}} \) cannot be written as \( |\chi\rangle \langle \chi| \) for any pure state \( |\chi\rangle \), because it is not pure (it is a statistical mixture).

Now imagine that we send the single photon state through \textit{many} beamsplitters in a sequence, each with some small tap angle \( \theta = \sqrt{\Gamma \Delta t}/2 \):

We make two assumptions: the environment modes always begin in the vacuum \( |0\rangle \) (this is the Born approximation), and the environment is completely different and uncorrelated between scattering events (this is the Markov approximation).

This allows us to write a coarse-grained differential equation for the photon state
\[ \frac{\Delta \rho}{\Delta t} \approx \begin{bmatrix} \dot{\rho}_{00} & \dot{\rho}_{01} \\ \dot{\rho}_{10} & \dot{\rho}_{11} \end{bmatrix} = -\Gamma \begin{bmatrix} -\beta^2 & \alpha \beta/2 \\ \alpha \beta/2 & \beta^2 \end{bmatrix}. \] (18)

Expressed as differential equations for each of the independent matrix elements, we get (using Eq.(15) for \( \rho(t = 0) \))
\[ \frac{d}{dt} \rho_{00} = +\Gamma \rho_{11} \] (19)
\[ \frac{d}{dt} \rho_{10} = -\Gamma \rho_{11} \] (20)
for the diagonal elements. These describe the evolutions of the probabilities of finding the photon in the \( |0\rangle \) and \( |1\rangle \) states, and are analogous to the Einstein rate equations. And for the off-diagonal elements we get
\[ \frac{d}{dt} \rho_{01} = -\frac{\Gamma}{2} \rho_{01} \] (21)
\[ \frac{d}{dt} \rho_{10} = -\frac{\Gamma}{2} \rho_{10} \] (22)
which show the decay of the quantum coherence of the state.

The form of these differential equations, which are master equations, is very general, and almost exactly the same result is obtained for a two-level atom interacting with the vacuum. In that situation, the solution differs essentially only in that the coherences evolve as

\[ \frac{d}{dt} \rho_{01} = -\left( i\Delta + \frac{\Gamma}{2} \right) \rho_{01}, \]  

(23)

where \( \Delta \) is a frequency shift of the system known as the "Lamb shift," which is due to virtual excitations to higher atomic levels. In the atomic master equation, \( \Gamma \) is the spontaneous emission rate, given by Fermi’s golden rule

\[ \Gamma = \frac{2\pi}{\hbar} \sum_{\kappa \epsilon} |\langle g; \kappa \epsilon | V | e; 0 \rangle|^2 \delta(\hbar \omega - \hbar \omega_{\kappa \epsilon}), \]  

(24)

as derived in API.

4 Full derivation \textendash walk-through

We now turn to a full derivation of the general master equation. Following the notation used in API, Chapter 4, let \( A \) denote the system, and \( R \) the environment (known as the reservoir in API). The full Hamiltonian is

\[ H = H_A + H_R + V, \]  

(25)

where \( V \) is the system-reservoir interaction potential. In the interaction picture defined by \( H_A \) and \( H_R \), the equation of motion for the full system + reservoir density matrix is

\[ i\hbar \dot{\rho} = [V, \rho]. \]  

(26)

Integrating this once gives

\[ i\hbar \rho(t) = \int_0^t [V(t'), \rho(t')] dt'. \]  

(27)

Substituting this back into Eq.(26) gives

\[ \dot{\rho} = -\frac{1}{\hbar^2} \int_0^t [V(t), [V(t'), \rho(t')]] dt'. \]  

(28)

If we assume that the system and reservoir are initially uncorrelated, and make the approximation that the reservoir stays unchanged (the Born approximation), then

\[ \rho(t) \approx \rho_A(t) \otimes \rho_R(0) = \rho_A(t) \otimes \rho_R \]  

(29)

This gives us our starting point for a general master equation:

\[ \dot{\rho}_A = -\frac{1}{\hbar^2} \text{Tr}_R \int_0^t [V(t), [V(t'), \rho_A(t') \otimes \rho_R]] dt'. \]  

(30)

An example is helpful in seeing how this equation works. Generally, we will take system + reservoir interactions of the form \( V = -AR \), where \( A \) acts only on the system, and \( R \) acts only on the reservoir. Specifically, let the
system be a two-level atom, and the environment be a single electromagnetic mode initially in the vacuum state $|0\rangle$. The atom interacts with the usual dipole interaction,

$$V = -\Gamma(b|g\rangle\langle e| + b|e\rangle\langle g|),$$  \hspace{1cm} (31)

which is conveniently written using Pauli raising and lowering operators

$$\sigma_{\pm} = \frac{\sigma_x \pm i\sigma_y}{2}$$  \hspace{1cm} (32)

where

$$\sigma_- = |g\rangle\langle e| \quad \text{and} \quad \sigma_+ = |e\rangle\langle g|.$$  \hspace{1cm} (33)

Insert this now into Eq.(30), but disregard the integral over time (this lets us see what the essential dynamics are, at the expense of not obtaining the correct specific rates). The relevant commutators are

$$[V, \rho_A \otimes |0\rangle\langle 0|] = (\sigma_- \rho_A) \otimes |1\rangle\langle 0| - (\rho_A \sigma_+) \otimes |0\rangle\langle 1|$$  \hspace{1cm} (34)

and

$$[V, [V, \rho_A \otimes |0\rangle\langle 0|]] = (\sigma_+ \sigma_- \rho_A) \otimes |0\rangle\langle 0| - 2(\sigma_- \rho_A \sigma_+) \otimes |1\rangle\langle 1| + (\rho_A \sigma_+ \sigma_-) |0\rangle\langle 0| + \text{other},$$  \hspace{1cm} (35)

where the “other” terms are not diagonal in the electromagnetic mode states, and thus disappear in the partial trace over the reservoir. We find, finally:

$$\dot{\rho}_A = -\Gamma \left[ \sigma_+ \sigma_- \rho_A - 2\sigma_- \rho_A \sigma_+ + \rho_A \sigma_+ \sigma_- \right].$$  \hspace{1cm} (36)

This is the master equation for a two-level atom dipole coupled to a single electromagnetic mode initially in the vacuum state. It is written in a form known as the “Lindblad” form, which is very common. In atomic physics, you will often see master equations like this.

Using the definitions for $\sigma_{\pm}$, if we express $\rho_A$ as

$$\rho_A = \begin{bmatrix} a & b \\ c & d \end{bmatrix},$$  \hspace{1cm} (37)

then we find

$$\dot{\rho}_A = -\Gamma \begin{bmatrix} 2a & b \\ c & -2a \end{bmatrix},$$  \hspace{1cm} (38)

which is identical to the master equation we constructed for the beamsplitter example, Eq.(18), up to a relabeling of $|g\rangle$ and $|e\rangle$.

As shown by this example, the physical picture behind the master equation is not so complicated, even though the mathematics (used in all its glory) can be overwhelming. The real challenge is precise computation of the relaxation rates, such as $\Gamma$, and this is comprehensively covered in chapter 4 of API. The book also gives detailed physical arguments as to why the above approximations are physically valid in important scenarios. The following four slides summarize highlights of the API derivation of the full, and general, master equation.
**B—DERIVATION OF THE MASTER EQUATION FOR A SMALL SYSTEM $A$ INTERACTING WITH A RESERVOIR $R$**

1. **Equation Describing the Evolution of the Small System in the Interaction Representation**

Let

$$ H = H_A + H_R + V $$

be the Hamiltonian of the global system $A + R$: $H_A$ is the Hamiltonian of $A$, $H_R$ is the Hamiltonian of $R$, and $V$ is the interaction between $A$ and $R$.

which becomes, in the interaction representation with respect to $H_A + H_R$:

$$ \frac{\mathrm{d}}{\mathrm{d}t} \tilde{\rho}(t) = \frac{1}{i \hbar} [\tilde{V}(t), \tilde{\rho}(t)] $$  \hspace{1cm} (B.3)

Integrating Equation (B.3) between $t$ and $t + \Delta t$ yields

$$ \tilde{\rho}(t + \Delta t) = \tilde{\rho}(t) + \frac{1}{i \hbar} \int_t^{t + \Delta t} \mathrm{d}t' [\tilde{V}(t'), \tilde{\rho}(t')] $$  \hspace{1cm} (B.5)

By taking the trace with respect to $R$ of Equation (B.6), we obtain

$$ \Delta \tilde{\rho}(t) = \frac{1}{i \hbar} \int_t^{t + \Delta t} \mathrm{d}t' \text{Tr}_R[\tilde{V}(t'), \tilde{\rho}(t)] + $$

$$ + \left( \frac{1}{i \hbar} \right)^2 \int_t^{t + \Delta t} \mathrm{d}t' \int_t^{t''} \mathrm{d}t'' \text{Tr}_R[\tilde{V}(t'), [\tilde{V}(t''), \tilde{\rho}(t'')]] $$  \hspace{1cm} (B.9)

Up to this point, no approximation has been introduced and Equation (B.9) is exact. Before going further and introducing some approximations, we must now describe the assumptions concerning the reservoir.
Let the system-reservoir interaction be:
\[ \tilde{V}(t) = -\tilde{A}(t)\tilde{R}(t) \]  \hfill (B.17)

A physically important quantity arises:
\[ g(t', t'') = \text{Tr}[\sigma_R \tilde{R}(t') \tilde{R}(t'')] \]  \hfill (B.21)

As long as \( \tau_c \ll \Delta t \ll T_{\text{relax}} \) then:
\[ \tilde{\rho}(t) = \tilde{\sigma}(t) \otimes \sigma_R. \]  \hfill (B.28)

\[
\frac{\Delta \tilde{\sigma}}{\Delta t} = -\frac{1}{\hbar^2} \frac{1}{\Delta t} \int_t^{t+\Delta t} dt' \int_t^{t'} dt'' \text{Tr}_R [\tilde{V}(t'), [\tilde{V}(t''), \tilde{\sigma}(t) \otimes \sigma_R]].
\]  \hfill (B.30)

Substituting (B.17) gives:
\[
\frac{\Delta \tilde{\sigma}}{\Delta t} = -\frac{1}{\hbar^2} \int_0^\infty d\tau \frac{1}{\Delta t} \int_t^{t+\Delta t} dt' \times \\
\times \{ g(\tau)[\tilde{A}(t') \tilde{A}(t' - \tau) \tilde{\sigma}(t) - \tilde{A}(t' - \tau) \tilde{\sigma}(t) \tilde{A}(t') ] + \\
+ g(-\tau)[\tilde{\sigma}(t) \tilde{A}(t' - \tau) \tilde{A}(t') - \tilde{A}(t') \tilde{\sigma}(t) \tilde{A}(t' - \tau)] \}. \]  \hfill (B.33)

To go further and carry out the integration over \( t' \), we now project the operator Equation (B.33) over a basis of states.
Master equation in energy-state basis:

Let \( |a\rangle \) be the eigenstates of \( H_A \), having eigenvalues \( E_a \):

\[
H_A |a\rangle = E_a |a\rangle.
\]

Equation (B.33) becomes, in the orthonormal basis \( \{ |a\rangle \} \)

\[
\frac{\Delta \tilde{\sigma}_{ab}}{\Delta t} = \sum_{cd} \gamma_{abcd}(t) \tilde{\sigma}_{cd}(t)
\]

Back to lab frame:

\[
\sigma_{ab}(t) = e^{-i\omega_{ab}t} \tilde{\sigma}_{ab}(t)
\]

\[
\frac{d}{dt} \sigma_{ab}(t) = -i\omega_{ab} \sigma_{ab}(t) + \sum_{c,d}^{(sec)} \mathcal{H}_{abcd} \sigma_{cd}(t).
\]

Linear diff. eq.

Remaining steps: matrix elements

1. Populations

\[
\mathcal{R}_{aacc} = \Gamma_{c \rightarrow a}
\]

\[
\Gamma_{c \rightarrow a} = \frac{2\pi}{\hbar} \sum_{\mu} p_{\mu} \sum_{\nu} |\langle \nu, a | V | \mu, c \rangle|^2 \delta(E_{\mu} + E_c - E_{\nu} - E_a).
\]

The physical interpretation of \( \Gamma_{c \rightarrow a} \) is very clear. \( \Gamma_{c \rightarrow a} \) is the probability per unit time for the system \( \mathcal{A} \) to make a transition from level \( c \) to level \( a \) as a result of its coupling with \( \mathcal{R} \). Indeed, such a transition corresponds, for the global system \( \mathcal{A} + \mathcal{R} \), to a transition \( |\mu, c\rangle \rightarrow |\nu, a\rangle \) (Figure 2). Equation (C.5) gives the rate for this transition (in agreement with the Fermi golden rule), averaged over all the possible initial states \( \mu \) of the reservoir (weighted by \( p_{\mu} \)) and summed over all the final states \( \nu \) of the reservoir, with the delta function expressing the conservation of energy for the global system \( \mathcal{A} + \mathcal{R} \).
2. Off-diagonal elements

\[
\frac{d}{dt} \sigma_{ab} = -i \omega_{ab} \sigma_{ab} + \mathcal{R}_{abab} \sigma_{ab}. \tag{C.11}
\]

\[
\mathcal{R}_{abab} = -\Gamma_{ab} - i \Delta_{ab} \tag{C.13}
\]

\[
\mathcal{R}_{abab} = -\frac{1}{\hbar^2} \int_0^\infty d\tau \left\{ g(\tau) \left[ \sum_n |A_{an}|^2 e^{i\omega_{an}\tau} - A_{aa} A_{bb} \right] + g(-\tau) \left[ \sum_n |A_{bn}|^2 e^{-i\omega_{bn}\tau} - A_{aa} A_{bb} \right] \right\}. \tag{C.12}
\]

\[
\Delta_a = \frac{1}{\hbar} \mathcal{R} \sum_\mu p_\mu \sum_\nu \sum_n \frac{|\langle \nu, n | V | \mu, a \rangle|^2}{E_\mu + E_a - E_\nu - E_n} \tag{C.15}
\]

\[
\Gamma_{ab} = \Gamma_{ab}^{\text{nonad.}} + \Gamma_{ab}^{\text{ad.}} \tag{C.16}
\]

\[
\Gamma_{ab}^{\text{nonad.}} = \frac{1}{2} \left( \sum_{n \neq a} \Gamma_{a \to n} + \sum_{n \neq b} \Gamma_{b \to n} \right) \tag{C.17}
\]

\[
\Gamma_{ab}^{\text{ad.}} = \frac{2\pi}{\hbar} \sum_\mu p_\mu \sum_\nu \delta(E_\mu - E_\nu) \times \left( \frac{1}{2} |\langle \nu, a | V | \mu, a \rangle|^2 + \frac{1}{2} |\langle \mu, b | V | \nu, b \rangle|^2 - \right.
\]

\[- \text{Re} \langle \nu, a | V | \mu, a \rangle \langle \nu, b | V | \mu, b \rangle \right). \tag{C.18}
\]

Dominant physics: dephasing (no energy change)