Lecture 7 – Open quantum systems

Up until now, apart from in our discussion of linear response, quantum mechanics has only entered indirectly, for example through calculations of transition rates via the golden rule. We have explored various ways of following the dynamics of classical probabilities with varying degree of microscopic detail. In particular we have seen how, in the Langevin equation, the effect of an environment can be included via noise, whose properties are constrained by fluctuation-dissipation relations. We then further showed how, if we don't want just individual trajectories, master equations describe the evolution of probability distribution functions. We have also discussed how entropy is in a sense a measure of information (or lack thereof) about degrees of freedom in our system. Depending on what degrees of freedom we were looking at ($\rho(\bar{r}_1, \bar{p}_1, \ldots, \bar{r}_N \bar{p}_N)$, $f(\bar{r}, \bar{p})$ or $n(\bar{r})$) we got different entropies, but the conceptual framework was always the same. We now want to generalize these things to quantum systems. When we do this, two main things will happen: our probability densities become a density matrix $f \to S$, and then we need an equation describing the time evolution of S, a quantum master equation. We will in particular explore a form called the Lindblad equation (after Göran Lindblad who is a retired professor at KTH).

A closed quantum system

To start, define a closed quantum system as a system that can be described by a Hamiltonian $\hat{H}$ and therefore has unitary time evolution with time evolution operator $\hat{U}(t,t_0)$.

The density matrix evolves according to

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

($\hat{H}$ could depend on t, but let's for simplicity just think of time-independent Hamiltonians).

Sometimes this is written in the form (Liouville-von Neumann equation)

$$\frac{d}{dt}\hat{\rho} = \mathcal{L}[\hat{\rho}] \qquad \text{or} \qquad \frac{d}{dt}\hat{\rho} = \hat{\mathcal{L}}\hat{\rho}$$

where $\hat{\mathcal{L}}$ is the Liouville operator (or more accurately the Liouville super-operator, since it maps an operator to an operator).

It is defined as

$$\mathcal{L} : \hat{\rho} \mapsto -i[\hat{H},\hat{\rho}]$$

Formally, one could then write

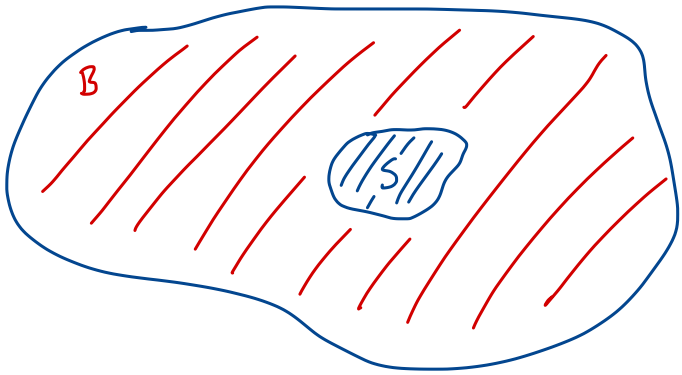
$$\hat{\rho}(t) = e^{\hat{\mathcal{L}}t}\rho(0)$$

The structure of the time dynamics is such that $\mathcal{L}$ is linear in $\hat{\rho}$ and subsequent time translations do not depend on the detailed history but only on the state at a given time, e.g. $\rho(t_1+t_2) = e^{\hat{\mathcal{L}}t_2}e^{\hat{\mathcal{L}}t_1}\rho(0)$.

Open system and reduced density matrix

In order to have a closed system, we need to have its degrees of freedom completely isolated from any outside degrees of freedom. We can of course always achieve this by including larger and larger parts in our system, but the full dynamics quickly

become very complicated and impossible to treat exactly. Instead we need to focus on the relevant degrees of freedom, very much as we have been doing in this course. For example in the Brownian motion example we only included the coordinates of the Brownian particle but the surrounding liquid was just an environment that induced some noise. Here we can achieve the same by taking a closed system and separating it into two parts: A subsystem, which we will simply refer to as the system (S), and the rest, which we call the environment or sometimes bath (B).



The Hilbert space of the full system is then a tensor product of the Hilbert spaces of the system and bath, i.e.,

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$$

The total Hamiltonian will describe the dynamics of the environment, the system, and interaction between the system and environment:

$$\hat{H} = \hat{H}_S \otimes \mathbb{1}_B + \mathbb{1}_S \otimes \hat{H}_B + \hat{H}_I$$

Again, any or all of these could in principle depend on time.

A state of the system could be describe by a wave function $|\psi\rangle \in \mathcal{H}$, or more appropriately for our purposes a density matrix $\hat{\rho}$.

Now, generally the degrees of freedom of the environment will not be accessible to us, and we are only interested in observables $\hat{A}_S$ that only act in the system. We therefore also only need the density matrix ρ_S describing the state of the system. This is the reduced density matrix obtained by tracing out the environment degrees of freedom from the full density matrix $\hat{\rho}$. This was covered in advanced quantum mechanics, but let's remind ourselves of how this works

Reduced density matrix

Let's assume $\{|n\rangle\}$ is a basis for $\mathcal{H}_S$ and $\{|\mu\rangle\}$ a basis for $\mathcal{H}_B$. (i.e., we use latin indices for the system and greek for the environment).

Then

$$\text{span}(\{|n\rangle\}) = \mathcal{H}_S$$

$$\text{span}(\{|\nu\rangle\}) = \mathcal{H}_B$$

$$\text{span}\{|n\rangle \otimes |\nu\rangle\}) = \mathcal{H}.$$

Often we simply write $|n\rangle \otimes |\nu\rangle \equiv |n\nu\rangle$

The full density matrix is then, in this basis,

$$\hat{\rho} = \sum_{\substack{n,m \\ \nu,\mu}} \rho_{n\nu;m\mu} \, |n\nu\rangle\langle m\mu|$$

with $\rho_{n\nu;m\mu} = \langle n\nu|\hat{\rho}|m\mu\rangle$.

We define the density matrix of the system as

$$\hat{\rho}_S = \text{tr}_B(\hat{\rho}) = \sum_{\lambda} \langle\lambda|\hat{\rho}|\lambda\rangle = \sum_{\lambda} \sum_{\substack{n,m \\ \nu,\mu}} \rho_{n\nu;m\mu} \, |n\rangle \otimes \underbrace{\langle\lambda|\nu\rangle}_{\delta_{\lambda\nu}} \langle m| \otimes \underbrace{\langle\mu|\lambda\rangle}_{\delta_{\mu\lambda}}$$

$$= \sum_{\mu} \sum_{n,m} \rho_{n\mu;m\mu} \, |n\rangle\langle m|.$$

This is meaningful, since if $\hat{A}_S$ is an observable for the system only, it means that it is of the form $\hat{A}_S = \hat{A} \otimes \mathbb{1}_B$. The expected value of this observable in the state $\hat{\rho}$ is

$$\langle \hat{A}_S \rangle = \mathrm{tr}\left(\hat{A}_S \hat{\rho} \right)$$

where the trace is here over the basis of full Hilbert space. That is

$$\langle \hat{A}_S \rangle = \sum_{n,\nu} \langle n\nu | \hat{A} \otimes \mathbb{1}_B \cdot \hat{\rho} | n\nu \rangle$$

$$= \sum_{n\nu} \langle n\nu | \hat{A} \otimes \mathbb{1}_B \sum_{\substack{m,l \\ \mu,\lambda}} \rho_{m\mu;l\lambda} | m\mu \rangle \underbrace{\langle l\lambda | n\nu \rangle}_{\delta_{ln}\delta_{\lambda\nu}}$$

$$= \sum_{n\nu} \sum_{m\mu} \rho_{m\mu,n\nu} \langle n | \hat{A} | m \rangle \underbrace{\langle \nu | \mu \rangle}_{\delta_{\mu\nu}}$$

where we used that $\langle n\nu | \hat{A} \otimes \hat{B} | m\mu \rangle = \langle n | \hat{A} | m \rangle \langle \nu | \hat{B} | \mu \rangle$. Continuing,

$$= \sum_{n,m} A_{nm} \underbrace{\sum_{\mu} \rho_{m\mu;n\mu}}_{= (\rho_S)_{mn}} = \sum_{n,m} A_{nm} (\rho_S)_{mn} = \sum_{n,m} \langle n | \hat{A} | m \rangle \langle m | \hat{\rho}_S | n \rangle$$

$$= \sum_{n} \langle n | \hat{A} \hat{\rho}_S | n \rangle = \mathrm{Tr}_S\left(\hat{A} \hat{\rho}_S \right)$$

We can in principle write down the time evolution of $\hat{\rho}_S(t)$. Namely, since if $\hat{U}(t,t_0)$ is the time evolution operator for the whole system, generated by the full Hamiltonian $\hat{H}$, then

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

and therefore

$$\hat{\rho}_S(t) = \mathrm{tr}_B\left(\hat{U}(t,t_0)\, \hat{\rho}_0\, \hat{U}^{-1}(t,t_0) \right)$$

or

$$\frac{d}{dt} \hat{\rho}_S = -i\, \mathrm{tr}_B\left([\hat{H}, \hat{\rho}(t)] \right)$$

This equation is generally to complicated to be useful, as the right hand side requires knowledge of the full density matrix $\hat{\rho}(t)$. How do we deal with this? One way would be to make some assumptions about the interaction between the environment and the system, $\hat{H}_I$, for example that it is small in some sense and that the enviroment is so big that it's state is not affected by this interaction. This amounts essentially to a kind of markov approximation about the environment-system interaction. This calculation, which is a little bit tendious, eventually leads to a quantum master equation of the form

$$\frac{d}{dt}\hat{\rho}_s = \mathcal{L}\hat{\rho}_s$$

with $\mathcal{L}$ a super-operator that generalizes the Liouville super-operator. Instead of going through the microscopic derivation, let us motivate the form $\mathcal{L}$ takes with some analogies with what we did for the Langevin equation and a bit of hand waving.

The Schrödinger-Langevin equation

Let us imagine we can take into account the effects of the enviroment through damping terms and noise, as in the Langevin equation. That is, we write a Schrödinger-Langevin equation

$$i\frac{d}{dt}|\psi(t)\rangle = \left(\hat{H} - i\hat{w} + i\eta(t)\hat{V}\right)|\psi(t)\rangle$$

Here $\hat{w}^\dagger = \hat{w}$ is a hermitian operator, and therefore $(i\hat{w})^\dagger = -i\hat{w}$ is anti-hermitian. The reason we can take $\hat{w}$ hermitian is that if it had a anti-hermitian part we could always include that in the hermitian Hamiltonian. $\hat{V}$ is a generic operator at this point, characterizing

the noise. $\eta(t)$ is a normal function we take to be gaussian white noise

$$\langle\langle \eta(t) \rangle\rangle \quad , \quad \langle\langle \eta(t)\eta^*(t') \rangle\rangle = \delta(t-t')$$

where $\langle\langle\ \rangle\rangle$ means average over the noise distribution. Note that we allow for the possibility that $\eta(t)$ is complex.

Remember that the Langevin equation was not a well defined differential equation. We could fix that by introducing stochastic calculus. There is no such firm mathematical ground for us to tread in this case, but we don't need to worry. We will only use it to motivate the form of the Lindblad equation, which can be obtained by other more mathematically rigourous ways.

Anyway, we proceed similar to before and integrate over a short time interval to obtain

$$i\left(|\psi(t+\delta t)\rangle - |\psi(t)\rangle\right) = \left[\hat{H}\,\delta t - i\hat{w}\,\delta t + i\int_t^{t+\delta t} \eta(t')\,dt'\,\hat{v}\right]|\psi(t)\rangle$$

$$|\psi(t+\delta t)\rangle = \left[(1 - i\hat{H}\,\delta t - \hat{w}\,\delta t) + \int_t^{t+\delta t} \eta(t')\,dt'\,\hat{V}\right]|\psi(t)\rangle$$

From this we have

$$\begin{aligned}\langle\psi(t+\delta t)|\psi(t+\delta t)\rangle = {} & \langle\psi(t)|(1+i\hat{H}\,\delta t - \hat{w}\,\delta t)(1 - i\hat{H}\,\delta t - \hat{w}\,\delta t)|\psi(t)\rangle \\ & + \langle\psi(t)|(1 + i\hat{H}\,\delta t - \hat{w}\,\delta t)\int_t^{t+\delta t} \eta(t')\,dt'\,\hat{v}\,|\psi(t)\rangle \\ & + \langle\psi(t)|\hat{v}^+\int_t^{t+\delta t} \eta(t')\,dt'\,(1 - i\hat{H}\,\delta t - \hat{w}\,\delta t)|\psi(t)\rangle \\ & + \langle\psi(t)|\hat{v}^+\int_t^{t+\delta t} dt' \int_t^{t+\delta t} dt''\ \eta^*(t')\eta(t'')\,\hat{v}\,|\psi(t)\rangle\end{aligned}$$

Now, take the average $\langle\langle\ \rangle\rangle$. The terms with only one integral give zero, and we obtain

$$\begin{aligned}\langle\psi(t+\delta t)|\psi(t+\delta t)\rangle = {} & \langle\psi(t)|\psi(t)\rangle - 2\langle\psi(t)|\hat{w}|\psi(t)\rangle\,\delta t \\ & + \langle\psi(t)|\hat{v}^+\hat{v}|\psi(t)\rangle\,\delta t\end{aligned}$$

So, in order for the norm of the wave function to be conserved on average, and for every $|\psi(t)\rangle$, we require

$$\hat{\omega} = \frac{1}{2}\hat{v}^+\hat{v}$$

The damping and the noise are therefore closely linked, just as the fluctuation and dissipation in the classical case. The Schrödinger-Langevin equation therefore takes the form:

$$\boxed{i\frac{d}{dt}|\psi(t)\rangle = \left[\hat{H} - \frac{i}{2}\hat{v}^+\hat{v} + i\eta(t)\hat{v}\right]|\psi(t)\rangle}$$

This means that formally we have a time evolution operator

$$\hat{U}(t,0) = \exp\left\{-i\left(\hat{H} - \frac{i}{2}\hat{v}^+\hat{v}\right)t + i\hat{v}\int_0^t \eta(t')dt'\right\}$$

Writing $\hat{\rho}(t) = \hat{U}(t,0)\rho_0\hat{U}^+(t,0)$, or $\hat{\rho}(t+dt) = \hat{U}(t+dt,t)\hat{\rho}(t)\hat{U}^+(t+dt,t)$

we get

$$\hat{\rho}(t+dt) = \left[1 - i\left(\hat{H} - \frac{i}{2}\hat{v}^+\hat{v}\right)dt + i\int_t^{t+dt}\eta(t')dt'\hat{v}\right]\rho(t)\left[1 + i\left[\hat{H} + \frac{i}{2}\hat{v}^+\hat{v}\right)dt - i\hat{v}^+\int_t^{t+dt}\eta^*(t'')dt''\right]$$

averaging over $\langle\langle\ \rangle\rangle$ the noise

$$= \hat{\rho}(t) + \left[-i(\hat{H}\hat{\rho} - \hat{\rho}\hat{H}) - \frac{1}{2}\hat{v}^+\hat{v}\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{v}^+\hat{v} + \hat{v}\hat{\rho}\hat{v}^+\right]dt$$

Taking the limit $dt \to 0$

$$\frac{d}{dt}\hat{\rho} = -i[\hat{H},\hat{\rho}] - \frac{1}{2}\hat{v}^+\hat{v}\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{v}^+\hat{v} + \hat{v}\hat{\rho}\hat{v}$$

This is what we get if there is only one noise term $\hat{v}$. Since everything we did is linear, we can generalize this to include a set $\{\hat{v}_\alpha\}$ of noise terms. We then get

$$\boxed{\frac{d}{dt}\hat{\rho} = -i[\hat{H},\hat{\rho}] + \sum_\alpha\left(\hat{v}_\alpha\hat{\rho}\hat{v}_\alpha^+ - \frac{1}{2}\hat{v}_\alpha^+\hat{v}_\alpha\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{v}_\alpha^+\hat{v}_\alpha\right)}$$

The Lindblad equation

Note that this equation is of the form

$$\frac{d}{dt}\rho_s(t) = \mathcal{L}\rho_s$$

with the super-operator $\mathcal{L}$ satisfying that it is linear and conserves the essential properties of ρ, namely unit trace and positive definite. It can be shown that the most general map that satisfies this, and has the structure above, takes the form of the Lindblad equation.

Note that the Lindblad equation is often written in the form

$$\frac{d}{dt}\hat{\rho} = -i[\hat{H}, \hat{\rho}] + \sum_\alpha \mathcal{D}[\hat{V}_\alpha]\hat{\rho}$$

where the dissipator $\mathcal{D}[\hat{V}_\alpha]$ is defined by

$$\begin{aligned}\mathcal{D}[\hat{V}_\alpha]\hat{\rho} &= \hat{V}_\alpha \hat{\rho} \hat{V}_\alpha^+ - \frac{1}{2}\hat{V}_\alpha^+ \hat{V}_\alpha \hat{\rho} - \frac{1}{2}\hat{\rho}\hat{V}_\alpha^+ \hat{V}_\alpha \\ &= \hat{V}_\alpha \hat{\rho} \hat{V}_\alpha^+ - \frac{1}{2}\{\hat{V}_\alpha^+ \hat{V}_\alpha, \hat{\rho}\}.\end{aligned}$$

To understand what the dissipator does we can set $H = 0$ and take only one $\hat{V}_\alpha = \hat{V}$. Then

$$\frac{d\hat{\rho}}{dt} = \mathcal{D}[\hat{V}]\hat{\rho}$$

This has a stationary state $\hat{\rho}_{ss}$ defined by $\hat{V}\rho_{ss} = 0$ since in that case $\mathcal{D}[\hat{V}]\hat{\rho}_{ss} = 0 = \frac{d\hat{\rho}_{ss}}{dt}$. Note if $\hat{V}\rho_{ss} = 0$ then $\rho_{ss}\hat{V}^+ = 0$

That is, the stationary state is annihilated by $\hat{V}$. A given dissipator thus acts to drive $\hat{\rho}$ towards that state.