

Lecture 9 - Quantum master equations

①

In earlier lecture we obtained the Lindblad equation phenomenologically. This can also be obtained formally as the most general expression for the generator of a quantum dynamical semigroup that is a map of a density matrix to a density matrix with the appropriate conditions (this is essentially what Lindblad did). Here, instead we want to study a microscopic derivation of a quantum master equation that with a set of (physical) approximations, results in a Lindblad type equation. The derivation is best done in the interaction picture, so we begin with a quick review of the different pictures in quantum mechanics.

Time evolution of density matrices and the pictures of Q.M.

Denote with $\rho(t)$ the density matrix of a system, which can be either pure or mixed.

The time evolution of $\rho(t)$ is governed by the quantum version of the Liouville equation, the von Neumann eq.

$$\frac{\partial \rho}{\partial t} = -L\rho = \frac{-i}{\hbar} [H, \rho] \quad (\text{put } \hbar=1)$$

This follows from the Schrödinger equation, if we write

$$\rho = \sum_{n,m} \langle n | \rho | m \rangle |n\rangle \langle m|$$

so $i\partial_t \rho = \sum_{n,m} \langle n | (i\partial_t \rho) | m \rangle |n\rangle \langle m| + \langle n | \rho | i\partial_t | m \rangle$

Now $i\partial_t |n\rangle = H |n\rangle$ so

$$i\partial_t g = \sum_{n,m} g_{nm} (H|n\rangle\langle m| - |n\rangle\langle m|H) \\ = Hg - gH = [H, g]$$

In the Schrödinger picture all the time dependence is in the states

$$i\partial_t |n\rangle = H|n\rangle \Rightarrow |n(t)\rangle = u(t)|n\rangle$$

where if H independent of time $u(t) = e^{-iHt}$

Then

$$g(t) = \sum_{n,m} g_{nm} |n(t)\rangle\langle m(t)| = u(t)g u^{-1}(t)$$

In the Heisenberg picture the states are time independent, but the operators have a time dependence

$$A(t) = u^{-1}(t) A u(t)$$

while the states and g are time independent.

These pictures are equivalent, since they give the same expectation value of all observables

$$\langle A \rangle(t) = \text{Tr}(g(t) A) = \text{Tr}(u(t)g u^{-1}(t) A)$$

$$= \text{Tr}(g u^{-1}(t) A u(t)) = \text{Tr}(g A(t))$$

\uparrow cyclic invariance of trace

$$\text{Tr}(ABC) = \text{Tr}(BCA) = \text{Tr}(CAB)$$

The third option is the interaction picture. Here we assume we have a Hamiltonian

$$H = H_0 + V$$

To be explicit, say $|\psi_s(t)\rangle$ is the state in the Schrödinger picture. Then

$$i\partial_t |\psi_s(t)\rangle = H |\psi_s(t)\rangle$$

(2)

(3)

Define the state in the interaction picture as

$$|\psi_I(t)\rangle = e^{iH_0 t} |\psi_s(t)\rangle = U_o(t) |\psi_s(t)\rangle$$

Then

$$\begin{aligned} i\partial_t |\psi_I(t)\rangle &= e^{iH_0 t} (H - H_0) |\psi_s(t)\rangle \\ &= e^{iH_0 t} V e^{-iH_0 t} e^{iH_0 t} |\psi_s(t)\rangle = V_I(t) |\psi_I(t)\rangle \end{aligned}$$

and therefore

$$i\partial_t S_I = [V_I(t), S_I(t)]$$

Now, for everything to be consistent, we also need

$$\begin{aligned} \langle \psi_s(t) | A_s | \psi_s(t)\rangle &= \langle \psi_I(t) | A_I(t) | \psi_I(t)\rangle = \\ &= \langle \psi_s(t) | e^{-iH_0 t} A_I(t) e^{iH_0 t} | \psi_s(t)\rangle \end{aligned}$$

or

$$A_I(t) = e^{iH_0 t} A_s e^{-iH_0 t}$$

and therefore

$$i\partial_t A_I(t) = [A_I(t), H_0]$$

The Redfield equation

(the rest of this lecture follows closely section 3.3 in Breuer & Petruccione)

We now turn to the derivation, starting from the system-bath Hamiltonian of the last lecture

$$\hat{H} = \hat{H}_S \otimes \mathbb{1}_B + \mathbb{1}_S \otimes \hat{H}_B + \hat{H}_I = \hat{H}_0 + \hat{H}_I$$

We denote with $\hat{\rho}(t)$ the state of the total system. In the interaction picture

$$i\partial_t \hat{\rho}(t) = [\hat{H}_I(t), \hat{\rho}(t)]$$

where I am not explicitly writing the subscript I on $\hat{\rho}$ for simplicity of notation. We can integrate the equation of motion to obtain

$$\hat{\rho}(t) = \hat{\rho}(0) - i \int_0^t [\hat{H}_I(t'), \hat{\rho}(t')] dt'$$

Using this expression for $\hat{\rho}(t)$ on the right hand side of the equation of motion:

$$i\partial_t \hat{\rho} = [\hat{H}_I(t), \hat{\rho}(0)] - i \int_0^t dt' [\hat{H}_I(t), [\hat{H}_I(t'), \hat{\rho}(t')]]$$

We are only really interested in the dynamics of the reduced density matrix of the system. We obtain this by tracing over the bath. Assuming that $\text{tr}_B [\hat{H}_I(t), \hat{\rho}(0)] = 0$, and using $\hat{\rho}_S = \text{tr}_B \hat{\rho}$, we get

$$\partial_t \hat{\rho}_S = - \int_0^t dt' \text{tr}_B [\hat{H}_I(t), [\hat{H}_I(t'), \hat{\rho}(t')]].$$

The assumption that $\text{tr}_B [\hat{H}_I(t), \hat{\rho}(0)] = 0$ can be relaxed. Including it just amounts to adding terms to the system Hamiltonian.

This integro-differential equation still contains the full density matrix $\hat{\rho}(t)$ on the right hand side. If the bath is much larger than the system, and they are only weakly coupled, the state of the bath is not much affected by the system. We can then write for the density matrix inside the integral

$$\hat{\rho}(t') \approx \hat{\rho}_S(t) \otimes \hat{\rho}_B$$

Note that it is not the case that the total state of the system and bath is a product state at all times. The interaction definitely entangles the system and bath. But as the state of the bath quickly relaxes back to $\hat{\rho}_B$ this entanglement effectively gets lost to the environment (this is a bit vague, I know). Maybe one way to think about this approximation is as a weak coupling limit: since the right hand side is already second order in \hat{H}_I we can replace $\hat{\rho}(t)$ in the integral with the $\hat{\rho}(t)$ one would obtain if $\hat{H}_I = 0$. Then, since \hat{H}_0 does not couple bath and system $\hat{\rho}(t) = \hat{\rho}_S(t) \otimes \hat{\rho}_B(t)$, where $\hat{\rho}_S(t)$ and $\hat{\rho}_B(t)$ are the interaction picture density matrix of system and bath generated by \hat{H}_S and \hat{H}_B . We then make the further assumption that $\hat{\rho}_B(t) = \hat{\rho}_B$ is stationary.

We have now, having made the above approximation, often called the Born approximation,

$$\partial_t \hat{\rho}_S = - \int_0^t dt' \text{tr}_B \left\{ [\hat{H}_I(t), [\hat{H}_I(t'), \hat{\rho}_S(t') \otimes \hat{\rho}_B]] \right\}$$

The right hand side is now a functional of $\hat{\rho}_S$, but it

still depends on the whole history up to the point t , since it depends on $\hat{g}_s(t')$ with t' integrated from 0 to t . To get a master equation we make the Markov approximation, replacing $\hat{g}_s(t')$ with $\hat{g}_s(t)$ in the integral, resulting in the Redfield equation:

$$\partial_t \hat{g}_s(t) = - \int_0^t dt' \text{tr}_B \left\{ [\hat{H}_I(t), [\hat{H}_I(t'), \hat{g}_s(t) \otimes \hat{g}_B]] \right\}$$

The Markov approximation is justified by the weak coupling limit. The above expression depends on $\hat{g}_s(t')$ and a kind of correlation function of the bath through the $\hat{H}_I(t)$, $\hat{H}_I(t')$, \hat{g}_B and tr_B terms. The time scale τ_B for bath correlation functions to decay to zero is very short compared with typical relaxation time scales of the system $\tau_s \gg \tau_B$. Therefore, where the integrand is nonzero the system density matrix $\hat{g}_s(t')$ doesn't vary very much, and therefore we can simply make the replacement $\hat{g}_s(t') \rightarrow \hat{g}_s(t)$. The Redfield equation is local in time, but not quite a Markovian master equation, as it depends on the choice of the initial time. Using again that the bath correlation function decays very quickly, we can make the change of integration variables

$$t' \rightarrow t - t'$$

$$\partial_t \hat{g}_s(t) = \int_t^\infty dt' \text{tr}_B \left\{ [\hat{H}_I(t), [\hat{H}_I(t-t'), \hat{g}_s(t) \otimes \hat{g}_B]] \right\}$$

The lower limit t is now actually the time elapsed since the

initial time in the past. Once this is larger than the bath time scale τ_B the integrand has decay to zero and we can take the integration limit to infinity

$$\partial_t \hat{\rho}_S = - \int_0^\infty dt' \text{tr}_B \left\{ [\hat{H}_I(t), [\hat{H}_I(t-t'), \hat{\rho}_S(t) \otimes \hat{\rho}_B]] \right\}$$

In this limit we obtain a quantum master equation (in the Born-Markov approximation).

The Lindblad form

The quantum master equation we just derived can be cast in the Lindblad form with a few more manipulations.

We first write the interaction Hamiltonian, in the Schrödinger picture, as

$$\hat{H}_I = \sum_\alpha \hat{A}_\alpha \otimes \hat{B}_\alpha$$

where \hat{A}_α acts only on the system degrees of freedom and \hat{B}_α on the bath degrees of freedom. Such an expansion can always be made with an appropriate choice of basis for the system and bath (convince yourself of this!) We then expand \hat{A}_α in a basis of eigenoperators of the system Hamiltonian \hat{H}_S

$$\hat{A}_\alpha = \sum_\omega \hat{A}_\alpha(\omega)$$

That this is possible can be shown as follows: Denote with $|\varepsilon\rangle$ the eigenstates of \hat{H}_S with eigenvalue ε , i.e., $\hat{H}_S |\varepsilon\rangle = \varepsilon |\varepsilon\rangle$. The projector onto the subspace with energy ε is then

$$\hat{\Pi}(\varepsilon) = |\varepsilon\rangle \langle \varepsilon|$$

Here we are assuming π is non-degenerate, but this is easily extended to degenerate π by just summing over additional quantum numbers. Given this, we have

$$\mathbb{1} = \sum_{\varepsilon} \hat{\pi}(\varepsilon)$$

We then have

$$\hat{A}_{\alpha} = \mathbb{1} \hat{A}_{\alpha} \mathbb{1} = \sum_{\varepsilon, \varepsilon'} \hat{\pi}(\varepsilon) \hat{A}_{\alpha} \hat{\pi}(\varepsilon')$$

we now write the sum over $\omega = \varepsilon - \varepsilon'$ and ε , so that

$$\hat{A}_{\alpha} = \sum_{\omega} \sum_{\varepsilon' - \varepsilon = \omega} \hat{\pi}(\varepsilon) \hat{A}_{\alpha} \hat{\pi}(\varepsilon') \equiv \sum_{\omega} \hat{A}_{\alpha}(\omega)$$

where in the inner sum we sum over all $\varepsilon, \varepsilon'$ such that their difference is $\omega = \varepsilon' - \varepsilon$. Direct calculation now gives

$$\begin{aligned} [\hat{H}_S, \hat{A}_{\alpha}(\omega)] &= \sum_{\varepsilon' - \varepsilon = \omega} [\hat{H}_S, \hat{\pi}(\varepsilon) \hat{A}_{\alpha} \hat{\pi}(\varepsilon')] = \sum_{\varepsilon' - \varepsilon = \omega} (\varepsilon - \varepsilon') \hat{\pi}(\varepsilon) \hat{A}_{\alpha} \hat{\pi}(\varepsilon') \\ &= -\omega \hat{A}_{\alpha}(\omega) \end{aligned}$$

where we used that $\hat{H}_S \hat{\pi}(\varepsilon) = \varepsilon \hat{\pi}(\varepsilon)$ and $\hat{\pi}(\varepsilon') \hat{H}_S = \varepsilon' \hat{\pi}(\varepsilon')$

The operators $\hat{A}_{\alpha}(\omega)$ satisfy

$$[\hat{H}_S, \hat{A}_{\alpha}(\omega)] = -\omega \hat{A}_{\alpha}(\omega)$$

and, by hermitian conjugation-

$$[\hat{H}_S, \hat{A}_{\alpha}^+(\omega)] = +\omega \hat{A}_{\alpha}^+(\omega)$$

Furthermore, using $[\hat{A}, \hat{B}\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{A}\hat{C} = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$,

we have

$$[\hat{H}_S, \hat{A}_{\alpha}^+(\omega) \hat{A}_{\beta}^-(\omega)] = \hat{A}_{\alpha}^+(\omega) (-\omega) \hat{A}_{\beta}^-(\omega) + \omega \hat{A}_{\alpha}^+(\omega) \hat{A}_{\beta}^-(\omega) = 0$$

and

$$\hat{A}_{\alpha}^+(\omega) = \hat{A}_{\alpha}(-\omega)$$

With these definitions we have

$$\hat{H}_I = \sum_{\alpha, \omega} \hat{A}_\alpha(\omega) \otimes \hat{B}_\alpha$$

This operator takes a simple form in the interaction picture:

$$\begin{aligned}\hat{H}_I(t) &= e^{i\hat{H}_0 t} \hat{H}_I e^{-i\hat{H}_0 t} \\ &= \sum_{\alpha, \omega} e^{i\hat{H}_S t} \hat{A}_\alpha(\omega) e^{-i\hat{H}_S t} e^{+i\hat{H}_B t} \hat{B}_\alpha e^{-i\hat{H}_B t}\end{aligned}$$

Now

$$e^{i\hat{H}_S t} \hat{A}_\alpha(\omega) e^{-i\hat{H}_S t} = e^{-i\omega t} \hat{A}_\alpha(\omega) e^{+i\hat{H}_S t} e^{-i\hat{H}_S t} = e^{-i\omega t} \hat{A}_\alpha(\omega)$$

Therefore,

$$\hat{H}_I(t) = \sum_{\alpha, \omega} e^{-i\omega t} \hat{A}_\alpha(\omega) \otimes \hat{B}_\alpha(t) = \sum_{\alpha, \omega} e^{+i\omega t} \hat{A}_\alpha^+(\omega) \otimes \hat{B}_\alpha^+(t)$$

$$\text{with the bath operators } \hat{B}_\alpha(t) = e^{+i\hat{H}_B t} \hat{B}_\alpha e^{-i\hat{H}_B t}$$

Using these expression in the master equation, we obtain (exercise!)

$$\partial_t \hat{g}_S = \sum_{\omega_1, \omega'} \sum_{\alpha, \beta} e^{i(\omega' - \omega)t} T_{\alpha\beta}(\omega) (\hat{A}_\beta(\omega) \hat{g}_S(t) \hat{A}_\alpha^+(\omega) - \hat{A}_\alpha^+(\omega') \hat{A}_\beta(\omega) \hat{g}_S(t)) + h.c.$$

with h.c. the hermitian conjugate and

$$T_{\alpha\beta}(\omega) \equiv \int_0^\infty ds e^{i\omega s} \langle \hat{B}_\alpha^+(t) \hat{B}_\beta(t-s) \rangle$$

is the (one-sided) Fourier transform of the bath correlation functions

$$\langle \hat{B}_\alpha^+(t) \hat{B}_\beta(t-s) \rangle = \text{tr}_B (\hat{B}_\alpha^+(t) \hat{B}_\beta(t-s) \hat{g}_B)$$

Since we are assuming \hat{g}_B is stationary, the bath correlation function

is also stationary, and

$$\langle \hat{B}_\alpha^+(t) \hat{B}_\beta(t-s) \rangle = \langle \hat{B}_\alpha^+(s) \hat{B}_\beta(0) \rangle$$

is independent of time t . As discussed above, the bath correlation functions decay rapidly with a time scale T_B which we assume to be the smallest time scale in the problem. It is worth noting that we require a large bath for this to hold.

We now make our last approximation. The sum over ω and ω' contains terms with $\omega \neq \omega'$ with $(\omega - \omega')$ of the order of typical level spacing in the system Hamiltonian \hat{H}_S . The inverse of this gives the time scale for the intrinsic system dynamics $\tau_S \sim \frac{1}{|\omega - \omega'|}$. If this time scale is much shorter than the relaxation time τ_R of the open system, then $e^{i(\omega-\omega')t}$ is a highly oscillating function over the relevant time scales. $(\omega - \omega' \tau_R \gg 1)$ or $\tau_R \gg \tau_S$. In this case the sum over ω will average to zero all terms except the terms with $\omega = \omega'$. Keeping only these terms is referred to as the rotating wave approximation.

This gives

$$\partial_t \hat{g}_S = \sum_{\omega} \sum_{\alpha, \beta} T_{\alpha\beta}(\omega) (\hat{A}_\beta(\omega) \hat{g}_S(t) \hat{A}_\alpha^+(\omega) - \hat{A}_\alpha^+(\omega') \hat{A}_\beta(\omega) \hat{g}_S(t)) + \text{h.c.}$$

Finally we write

$$T_{\alpha\beta}(\omega) = \frac{1}{2} \gamma_{\alpha\beta}(\omega) + i S_{\alpha\beta}(\omega)$$

with

$$S_{\alpha\beta}(\omega) = \frac{1}{2i} (T_{\alpha\beta}(\omega) - T_{\beta\alpha}^*(\omega))$$

$$\gamma_{\alpha\beta}(\omega) = T_{\alpha\beta}(\omega) + T_{\beta\alpha}^*(\omega)$$

$S_{\alpha\beta}$ is a hermitian matrix and $\gamma_{\alpha\beta}$ is positive.

We have (I'll skip writing (ω) and (t) simplifying in the intermediate steps).

$$\partial_t \hat{\rho}_S = \sum_{\omega} \sum_{\alpha, \beta} T_{\alpha\beta} \hat{A}_{\beta} \hat{\rho}_S \hat{A}_{\alpha}^+ + T_{\alpha\beta}^* \hat{A}_{\alpha} \hat{\rho}_S \hat{A}_{\beta}^+ - T_{\alpha\beta} \hat{A}_{\alpha}^+ \hat{A}_{\beta} \hat{\rho}_S - T_{\alpha\beta}^* \hat{\rho}_S \hat{A}_{\beta}^+ \hat{A}_{\alpha}$$

$$= \sum_{\omega} \sum_{\alpha, \beta} (T_{\alpha\beta} + T_{\beta\alpha}^*) \hat{A}_{\beta} \hat{\rho}_S \hat{A}_{\alpha}^+ - T_{\alpha\beta} \hat{A}_{\alpha}^+ \hat{A}_{\beta} \hat{\rho}_S - T_{\beta\alpha}^* \hat{\rho}_S \hat{A}_{\alpha}^+ \hat{A}_{\beta}$$

where in the conjugated terms we have take $\alpha \leftrightarrow \beta$.

$$= \sum_{\omega} \sum_{\alpha, \beta} \gamma_{\alpha\beta} \hat{A}_{\beta} \hat{\rho}_S \hat{A}_{\alpha}^+ - (\frac{1}{2} \gamma_{\alpha\beta} + i S_{\alpha\beta}) \hat{A}_{\alpha}^+ \hat{A}_{\beta} \hat{\rho}_S - (\frac{1}{2} \gamma_{\alpha\beta} - i S_{\alpha\beta}) \hat{\rho}_S \hat{A}_{\alpha}^+ \hat{A}_{\beta}$$

$$= \sum_{\omega} \sum_{\alpha, \beta} -i [S_{\alpha\beta} \hat{A}_{\alpha}^+ \hat{A}_{\beta}, \hat{\rho}_S] + \gamma_{\alpha\beta} (\hat{A}_{\beta} \hat{\rho}_S \hat{A}_{\alpha}^+ - \frac{1}{2} \hat{A}_{\alpha}^+ \hat{A}_{\beta} \hat{\rho}_S - \frac{1}{2} \hat{\rho}_S \hat{A}_{\alpha}^+ \hat{A}_{\beta})$$

That is

$$\partial_t \hat{\rho}_S(t) = -i [\hat{H}_L, \hat{\rho}_S(t)] + D[\rho_S(t)]$$

where

$$\hat{H}_L = \sum_{\omega} \sum_{\alpha, \beta} S_{\alpha\beta}(\omega) \hat{A}_{\alpha}^+(\omega) \hat{A}_{\beta}(\omega)$$

and the dissipator

$$D[\rho_S(t)] = \sum_{\omega} \sum_{\alpha, \beta} \gamma_{\alpha\beta}(\omega) \left(\hat{A}_{\beta}(\omega) \hat{\rho}_S \hat{A}_{\alpha}^+(\omega) - \frac{1}{2} \{ \hat{A}_{\alpha}^+(\omega) \hat{A}_{\beta}(\omega), \hat{\rho}_S \} \right)$$

This is already in Lindblad form, but do get to the diagonal form we had in the lecture on the Lindblad equation we just need to diagonalize $\gamma_{\alpha\beta}(\omega)$, that is, we write

$$\gamma_{\alpha\beta}(\omega) = \sum_{\mu} U_{\alpha\mu} \gamma_{\mu} (U^+)^{\mu}_{\beta}$$

We then define

$$\hat{L}_{\mu} = \sum_{\omega} \sum_{\alpha} U_{\alpha\mu} \sqrt{\gamma_{\mu}} \cdot \hat{A}_{\alpha}(\omega)$$

With this definition the dissipator becomes

$$D[\hat{\rho}_S] = \sum_{\mu} (\hat{L}_{\mu}^+ \hat{\rho}_S \hat{L}_{\mu} - \frac{1}{2} \{ \hat{L}_{\mu}^+ \hat{L}_{\mu}, \hat{\rho}_S \})$$

The term \hat{H}_{ls} is often called the Lamb-shift Hamiltonian as it leads to a renormalization of energy levels similar to the case of the Lamb shift. That it has this effect can be seen from the fact that

$$[\hat{H}_s, \hat{H}_{ls}] = \sum_{\omega} \sum_{\alpha, \beta} S_{\alpha \beta}(\omega) [\hat{H}_s, \hat{A}_{\alpha}^{\dagger}(\omega) \hat{A}_{\beta}(\omega)] = 0$$