PHYS 610: Recent Developments in Quantum Mechanics and Quantum Information (Spring 2009)

Notes: Master Equation

1 Master Equation

A main and obvious advantage of the density-operator formalism is that it provides a method for handling *nonunitary* evolution of the quantum state. This generally occurs in the treatment of *open* quantum systems: quantum systems coupled to external systems that we do not directly track.[1]

We will now study the evolution of a quantum system, described by Hamiltonian H_{S}, interacting with a reservoir, described by Hamiltonian H_{R}. We will assume the system–reservoir interaction, described by H_{SR}, to be weak, causing slow evolution on the uncoupled time scales of the system and reservoir separately. The evolution of the *total* system is unitary, given by

$$\partial_t \rho_{\text{SR}} = -\frac{i}{\hbar}[H, \rho_{\text{SR}}], \tag{1}$$

where ρ_{SR} is the combined state of the system and reservoir, and the total Hamiltonian is

$$H = H_{\text{S}} + H_{\text{R}} + H_{\text{SR}}. \tag{2}$$

Our goal is to derive an equation of motion for the state of the system alone, given by a partial trace over the reservoir degrees of freedom:

$$\rho := \text{Tr}_{\text{R}}[\rho_{\text{SR}}]. \tag{3}$$

Note that so long as we are interested in operators that act solely on the system's Hilbert space, this reduced density operator is sufficient to compute any appropriate expectation values.

We will derive the master equation with a number of approximations and idealizations, mostly related to the reservoir having many degrees of freedom. The approximations here typically work extremely well in quantum optics, though not necessarily in other areas such as condensed-matter physics where, for example, the weak-coupling idealization may break down. Examples of reservoirs include the quantum electromagnetic field (in a vacuum or thermal state), or the internal degrees of freedom of a composite object.

1.1 Interaction Representation

The first step is to switch to the interaction representation, in effect hiding the fast dynamics of the uncoupled system and reservoir, and focusing on the slow dynamics induced by H_{SR}. We do this via the transformations

$$\begin{aligned}\tilde{\rho}_{\text{SR}}(t) &= e^{i(H_{\text{S}}+H_{\text{R}})t/\hbar}\rho_{\text{SR}}(t)e^{-i(H_{\text{S}}+H_{\text{R}})t/\hbar}\\ \tilde{H}_{\text{SR}}(t) &= e^{i(H_{\text{S}}+H_{\text{R}})t/\hbar}H_{\text{SR}}e^{-i(H_{\text{S}}+H_{\text{R}})t/\hbar},\end{aligned} \tag{4}$$

so that the formerly time-independent interaction becomes explicitly time-dependent. The equation of motion then becomes

$$\partial_t \tilde{\rho}_{\text{SR}}(t) = -\frac{i}{\hbar}[\tilde{H}_{\text{SR}}(t), \tilde{\rho}_{\text{SR}}(t)]. \tag{5}$$

[1]For further reading, see William H. Louisell, *Quantum Statistical Properties of Radiation* (Wiley, 1973), Chapter 6; Claude Cohen–Tannoudji, Jacques Dupont-Roc, and Gilbert Grynberg, *Atom–Photon Interactions: Basic Processes and Applications* (Wiley, 1992), Chapter IV; and Howard Carmichael, *An Open Systems Approach to Quantum Optics* (Springer, 1993), Chapter 1.

Integrating this from t to $t + \Delta t$,

$$\tilde{\rho}_{\rm SR}(t + \Delta t) = \tilde{\rho}_{\rm SR}(t) - \frac{i}{\hbar} \int_t^{t+\Delta t} dt' \, [\tilde{H}_{\rm SR}(t'), \tilde{\rho}_{\rm SR}(t')]. \tag{6}$$

Iterating this equation by using it as an expression for $\tilde{\rho}_{\rm SR}(t')$,

$$\tilde{\rho}_{\rm SR}(t + \Delta t) - \tilde{\rho}_{\rm SR}(t) = -\frac{i}{\hbar} \int_t^{t+\Delta t} dt' \, [\tilde{H}_{\rm SR}(t'), \tilde{\rho}_{\rm SR}(t)] - \frac{1}{\hbar^2} \int_t^{t+\Delta t} dt' \int_t^{t'} dt'' \, [\tilde{H}_{\rm SR}(t'), [\tilde{H}_{\rm SR}(t''), \tilde{\rho}_{\rm SR}(t'')]]. \tag{7}$$

Now in taking the trace over the reservoir. In doing so, we will assume that the first term on the right-hand side vanishes. More specifically, we assume

$$\mathrm{Tr}_{\rm R}[\tilde{H}_{\rm SR}(t')\tilde{\rho}_{\rm SR}(t)] = 0. \tag{8}$$

This follows by assuming that the total system–reservoir state always approximately factorizes

$$\tilde{\rho}_{\rm SR}(t) \approx \tilde{\rho}(t) \otimes \tilde{\rho}_{\rm R}, \tag{9}$$

where $\tilde{\rho}_{\rm R}$ is the *stationary* state of the reservoir. This amounts to assuming that the reservoir is large and complex, and weak coupling of the system to the reservoir, so that the perturbation to the reservoir by the system is small. In this case, the time interval $\Delta t \gg \tau_{\rm c}$, where $\tau_{\rm c}$ is the correlation time of the reservoir—the time for reservoir and system–reservoir correlations to decay away. This also amounts to a **coarse-graining approximation**, which means that we are smoothing out any fast dynamics on time scales of the order of $\tau_{\rm c}$ or shorter. Thus, any correlations that have arisen in past time intervals have decayed away. Of course, *new* correlations arise due to the coupling in the present time interval, which will give rise to nonunitary terms in the evolution equation for the reduced state. Then the assumption (8) amounts to

$$\mathrm{Tr}_{\rm R}[\tilde{H}_{\rm SR}(t')\tilde{\rho}_{\rm R}] = 0. \tag{10}$$

This assumption means essentially that there is no dc component to the system–reservoir coupling—that is, the system–reservoir coupling consists of *fluctuations* about a zero mean. This can always be arranged by absorbing any nonzero mean into the system Hamiltonian.

1.2 Born–Markov Approximation

Since the first term vanishes under the partial trace, with the trace Eq. (7) becomes

$$\Delta\tilde{\rho}(t) \approx -\frac{1}{\hbar^2} \int_t^{t+\Delta t} dt' \int_t^{t'} dt'' \, \mathrm{Tr}_{\rm R}[\tilde{H}_{\rm SR}(t'), [\tilde{H}_{\rm SR}(t''), \tilde{\rho}_{\rm SR}(t'')]], \tag{11}$$

with $\Delta\tilde{\rho}(t) := \tilde{\rho}(t + \Delta t) - \tilde{\rho}(t)$. Now we will make the **Born–Markov approximation** by setting

$$\tilde{\rho}_{\rm SR}(t'') \approx \tilde{\rho}(t) \otimes \tilde{\rho}_{\rm R}. \tag{12}$$

In fact there is a pair of approximations at work here. The **Born approximation** amounts to assuming the factorization in (9), which we have justified in terms of a large, complex reservoir with a short coherence time. The **Markov approximation** amounts to setting $\rho(t'')$ to $\rho(t)$ in (12), which will result in an evolution equation that only depends on $\rho(t)$, and not the past history of the density operator. We can justify this approximation by noting that Δt is small and $H_{\rm SR}$ induces a weak perturbation, so that $\rho(t'') = \rho(t) + O(\Delta t)$. Then this amounts to a lowest-order expansion in Δt of the right-hand side of Eq. (11), which is appropriate in view of the limit $\Delta t \longrightarrow 0$ to obtain a differential equation (though in a coarse-grained sense, since strictly speaking we always require $\Delta t \gg \tau_{\rm c}$).

Next we change integration variables by setting

$$\tau := t' - t'', \tag{13}$$

so that the integration becomes

$$\begin{aligned}\int_t^{t+\Delta t} dt' \int_t^{t'} dt'' &= \int_0^{\Delta t} d\tau \int_{t+\tau}^{t+\Delta t} dt' \\ &\approx \int_0^{\infty} d\tau \int_t^{t+\Delta t} dt'.\end{aligned} \tag{14}$$

In writing down the final, approximate form for the integrals, we have used the fact that the integrand involves an expectation value of the interaction Hamiltonian taken at times that differ by τ, as we will explore further shortly. That is, the integrand involves reservoir correlation functions, which decay away on the time scale τ_c.

1.3 Interaction

Now we make a reasonably general assumption regarding the interaction Hamiltonian; namely, that it can be written as a sum of products over system and reservoir operators:

$$H_{\text{SR}} = \hbar S_\alpha R_\alpha. \tag{15}$$

(Recall that repeated indices imply summation.) The interpretation here is that if S_α is a Hermitian operator, then it represents an observable that is being effectively (or actually) monitored via coupling to the environment. For example, a position measurement is represented by an interaction of the form $H_{\text{SR}} = xR$. Alternately, the operators need not be Hermitian. For example, an interaction of the form $H_{\text{SR}} = SR^\dagger + S^\dagger R$ represents the exchange of quanta (e.g., of energy) between the system and reservoir, and would thus represent dissipation or loss of energy to the reservoir. Such interactions occur in spontaneous emission and cavity decay.

With the interaction of the form (15) and the change of integration in Eqs. (14), the change (11) in the quantum state becomes

$$\begin{aligned}\Delta\tilde{\rho}(t) \approx -\int_0^\infty d\tau \int_t^{t+\Delta t} dt' \bigg\{ &\Big[\tilde{S}_\alpha(t')\tilde{S}_\beta(t'-\tau)\tilde{\rho}(t) - \tilde{S}_\beta(t'-\tau)\tilde{\rho}(t)\tilde{S}_\alpha(t')\Big] G_{\alpha\beta}(\tau) \\ &+ \Big[\tilde{\rho}(t)\tilde{S}_\beta(t'-\tau)\tilde{S}_\alpha(t') - \tilde{S}_\alpha(t')\tilde{\rho}(t)\tilde{S}_\beta(t'-\tau)\Big] G_{\beta\alpha}(-\tau)\bigg\},\end{aligned} \tag{16}$$

where we have defined the reservoir correlation functions

$$G_{\alpha\beta}(\tau) := \mathrm{Tr}_{\text{R}}\Big[\tilde{R}_\alpha(t')\tilde{R}_\beta(t'-\tau)\Big] = \Big\langle \tilde{R}_\alpha(t')\tilde{R}_\beta(t'-\tau)\Big\rangle_{\text{R}} = \Big\langle \tilde{R}_\alpha(\tau)\tilde{R}_\beta(0)\Big\rangle_{\text{R}}, \tag{17}$$

which depend only on the time difference because the reservoir is in a stationary state. Now we make the further assumption

$$\tilde{S}_\alpha(t) = e^{iH_{\text{S}}t/\hbar} S_\alpha e^{-iH_{\text{S}}t/\hbar} = e^{i\omega_\alpha t} \tag{18}$$

about the interaction-picture system operators. This is not necessarily a restrictive assumption, since multiple frequencies for a given system operator may be separated in the sum in (15). Then Eq. (16) becomes

$$\begin{aligned}\Delta\tilde{\rho}(t) \approx -\int_0^\infty d\tau \int_t^{t+\Delta t} dt' \bigg\{ &\Big[S_\alpha S_\beta\tilde{\rho}(t) - S_\beta\tilde{\rho}(t)S_\alpha\Big] G_{\alpha\beta}(\tau) \\ &+ \Big[\tilde{\rho}(t)S_\beta S_\alpha - S_\alpha\tilde{\rho}(t)S_\beta\Big] G_{\beta\alpha}(-\tau)\bigg\} e^{i\omega_\alpha t'} e^{i\omega_\beta(t'-\tau)}.\end{aligned} \tag{19}$$

Now defining

$$
\begin{aligned}
I(\omega_\alpha + \omega_\beta) &:= \int_t^{t+\Delta t} dt'\, e^{i(\omega_\alpha+\omega_\beta)t'} \\
w_{\alpha\beta}^{+} &:= \int_0^\infty d\tau\, e^{-i\omega_\beta\tau} G_{\alpha\beta}(\tau) \\
w_{\beta\alpha}^{-} &:= \int_0^\infty d\tau\, e^{-i\omega_\beta\tau} G_{\beta\alpha}(-\tau),
\end{aligned}
\tag{20}
$$

we can write

$$
\Delta\tilde{\rho}(t) \approx -\bigg\{ \Big[S_\alpha S_\beta \tilde{\rho}(t) - S_\beta \tilde{\rho}(t) S_\alpha \Big] w_{\alpha\beta}^{+} + \Big[\tilde{\rho}(t) S_\beta S_\alpha - S_\alpha \tilde{\rho}(t) S_\beta \Big] w_{\beta\alpha}^{-} \bigg\} I(\omega_\alpha + \omega_\beta). \tag{21}
$$

Under the assumption of fast (uncoupled) system and reservoir dynamics,

$$
\Delta t \gg (\omega_\alpha + \omega_\beta)^{-1}, \tag{22}
$$

the integral $I(\omega_\alpha + \omega_\beta)$ averages to zero unless $\omega_\alpha + \omega_\beta = 0$. Thus we may replace the integral with a Kronecker delta,

$$
I(\omega_\alpha + \omega_\beta) = \Delta t\, \delta(\omega_\alpha, -\omega_\beta). \tag{23}
$$

Now formally taking the limit of small Δt,

$$
\partial_t \tilde{\rho}(t) \approx \frac{\Delta\tilde{\rho}(t)}{\Delta t} = -\delta(\omega_\alpha, -\omega_\beta) \bigg\{ \Big[S_\alpha S_\beta \tilde{\rho}(t) - S_\beta \tilde{\rho}(t) S_\alpha \Big] w_{\alpha\beta}^{+} + \Big[\tilde{\rho}(t) S_\beta S_\alpha - S_\alpha \tilde{\rho}(t) S_\beta \Big] w_{\beta\alpha}^{-} \bigg\}, \tag{24}
$$

where again we must keep in mind that this differential equation is coarse-grained in the sense of not representing dynamics on time scales as short as τ_c or $(\omega_\alpha + \omega_\beta)^{-1}$ for different frequencies. Now transforming out of the interaction representation, using the assumption (18) and $\omega_\alpha = -\omega_\beta$,

$$
\partial_t \rho(t) = -\frac{i}{\hbar}[H_\mathrm{S}, \rho(t)] - \delta(\omega_\alpha, -\omega_\beta) \bigg\{ \Big[S_\alpha S_\beta \rho(t) - S_\beta \rho(t) S_\alpha \Big] w_{\alpha\beta}^{+} + \Big[\rho(t) S_\beta S_\alpha - S_\alpha \rho(t) S_\beta \Big] w_{\beta\alpha}^{-} \bigg\}. \tag{25}
$$

Now we use the fact that H_SR is Hermitian, so terms of the form SR in (15) that are not Hermitian must be accompanied by their adjoint terms $S^\dagger R^\dagger$. Clearly, terms where $S_\alpha = S_\beta^\dagger$ satisfy $\delta(\omega_\alpha, -\omega_\beta) = 1$, so we can explicitly combine these pairs of terms to write the master equation in terms of only a single sum:

$$
\partial_t \rho(t) = -\frac{i}{\hbar}[H_\mathrm{S}, \rho(t)] + \sum_\alpha \bigg\{ \Big[S_\alpha \rho(t) S_\alpha^\dagger - S_\alpha^\dagger S_\alpha \rho(t) \Big] w_\alpha^{+} + \Big[S_\alpha \rho(t) S_\alpha^\dagger - \rho(t) S_\alpha^\dagger S_\alpha \Big] w_\alpha^{-} \bigg\}. \tag{26}
$$

Of course, terms of the same form carry through when S_α is Hermitian. In the expression above we have also defined the reduced integrals

$$
\begin{aligned}
w_\alpha^{+} &:= \int_0^\infty d\tau\, e^{-i\omega_\alpha\tau} \Big\langle \tilde{R}_\alpha^\dagger(\tau) \tilde{R}_\alpha(0) \Big\rangle_\mathrm{R} \\
w_\alpha^{-} &:= \int_0^\infty d\tau\, e^{i\omega_\alpha\tau} \Big\langle \tilde{R}_\alpha^\dagger(0) \tilde{R}_\alpha(\tau) \Big\rangle_\mathrm{R} = [w_\alpha^{+}]^*.
\end{aligned}
\tag{27}
$$

Note that other cross-terms could in principle occur in Eq. (25) that satisfy $\omega_\alpha = -\omega_\beta$, which we appear to be missing here. However, if we end up with terms like $S_1 \rho S_2^\dagger$, this can always be absorbed into terms of the form $(S_1 + S_2)\rho(S_1 + S_2)^\dagger$, representing interferences in the couplings represented by $S_{1,2}$. The cross terms are weighted by a cross-correlation function between R_1 and R_2, representing the cross terms of the coherece. In the absence of cross coherence, only terms of the form $S_1 \rho S_1^\dagger$ and $S_2 \rho S_2^\dagger$ should appear. Weighted combinations of these terms with $(S_1 + S_2)\rho(S_1 + S_2)^\dagger$ terms can account for any degree of coherence.

Now separating out the real and imaginary parts of the integrals (27) in (26),

$$\partial_t \rho(t) = -\frac{i}{\hbar}[H_{\rm S}, \rho(t)] + \sum_\alpha k_\alpha \left\{ S_\alpha \rho(t) S_\alpha^\dagger - \frac{1}{2}\Big[S_\alpha^\dagger S_\alpha \rho(t) + \rho(t) S_\alpha^\dagger S_\alpha\Big] \right\} - i{\rm Im}[w_\alpha^+]\Big[S_\alpha^\dagger S_\alpha, \rho(t)\Big]. \tag{28}$$

where

$$k_\alpha := 2{\rm Re}[w_\alpha^+]. \tag{29}$$

Since the last term has the form of Hamiltonian evolution, we may drop it, assuming it is accounted for by $H_{\rm S}$ (or arranging the definition of the system such that it does). Now separating out the real and imaginary parts of the integrals,

$$\partial_t \rho(t) = -\frac{i}{\hbar}[H_{\rm S}, \rho(t)] + \sum_\alpha k_\alpha \left\{ S_\alpha \rho(t) S_\alpha^\dagger - \frac{1}{2}\Big[S_\alpha^\dagger S_\alpha \rho(t) + \rho(t) S_\alpha^\dagger S_\alpha\Big] \right\}.$$

(Born–Markov master equation) (30)

We have thus arrived at the general **Lindblad form** of the master equation in the Born–Markov approximation. Again, the system operators S_α represent the coupling channel of the system to the reservoir, and thus the channel by which the system may be observed. Thus, for example, if $S_\alpha \longrightarrow x$, then we have the master equation for a position measurement, whereas if $S_\alpha \longrightarrow a$, where a is the annihilation operator for the harmonic oscillator, then we have the master equation for energy loss (and thus damping) of a quantum harmonic oscillator.