Open quantum systems – lecture 3

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1.3.2 Explicit example

To make the microscopic derivation explicit, we consider a model system that is simple enough to be readily followed and close to what one considers in standard quantum mechanics lectures but nevertheless general enough to capture a wide range of scenarios: A universe made of harmonic oscillators

$$H = H_S + H_I + H_B\,, \qquad H_S = \Omega a^\dagger a\,, \qquad H_B = \sum_k \omega_k b_k^\dagger b_k\,,$$
$$H_I = (a + a^\dagger)\sum_k (h_k b_k + h_k^* b_k^\dagger)\,, \tag{1.1}$$

where $\Omega > 0$ is the system frequency, $\omega_k > 0$ are the reservoir frequencies, and h_k are bare emission amplitudes. The operators a and b_k annihilate a photon from the system (which could be a cavity) or the bath (which could be the surrounding) in mode k, respectively. It should be noted that the above Hamiltonian is only valid for small h_k (which is the case we are interested in), so it should not be naively used for strong couplings.

Interaction picture transformation

The full von-Neumann equation $\dot\rho = -\mathrm{i}[H_S + H_I + H_B, \rho]$ does not directly allow for a perturbative treatment, such that we transform to the interaction picture with respect to $H_S + H_B$ (denoted by bold symbols)

$$\boldsymbol{\rho}(t) = e^{+\mathrm{i}(H_S+H_B)t}\rho(t)e^{-\mathrm{i}(H_S+H_B)t}\,, \qquad \boldsymbol{H_I}(t) = e^{+\mathrm{i}(H_S+H_B)t}H_I e^{-\mathrm{i}(H_S+H_B)t}\,, \tag{1.2}$$

which recasts the von-Neumann equation into

$$\dot{\boldsymbol{\rho}} = -\mathrm{i}\left[\boldsymbol{H_I}(t), \boldsymbol{\rho}(t)\right]\,, \qquad \boldsymbol{H_I}(t) = (ae^{-\mathrm{i}\Omega t} + a^\dagger e^{+\mathrm{i}\Omega t})\sum_k (h_k b_k e^{-\mathrm{i}\omega_k t} + h_k^* b_k^\dagger e^{+\mathrm{i}\omega_k t}) \tag{1.3}$$

such that the r.h.s. is now small and admits a perturbative treatment. To get it, we integrate the above equation with initial condition $\boldsymbol{\rho}(0) = \rho(0) = \rho_0$ and insert the result $\boldsymbol{\rho} = \rho_0 - \mathrm{i}\int_0^t [\boldsymbol{H_I}(t'), \boldsymbol{\rho}(t')]\,dt'$ back into the r.h.s.

$$\boldsymbol{\rho}(t) = -\mathrm{i}\left[\boldsymbol{H_I}(t), \rho_0\right] - \int_0^t \left[\boldsymbol{H_I}(t), [\boldsymbol{H_I}(t'), \boldsymbol{\rho}(t')]\right] dt'\,. \tag{1.4}$$

Performing the partial trace over the reservoir then yields

$$\boldsymbol{\rho_S}(t) = -\mathrm{i}\mathrm{Tr}_\mathrm{B}\left\{[\boldsymbol{H_I}(t), \rho_0]\right\} - \int_0^t \mathrm{Tr}_\mathrm{B}\left\{[\boldsymbol{H_I}(t), [\boldsymbol{H_I}(t'), \boldsymbol{\rho}(t')]]\right\} dt'\,, \tag{1.5}$$

which is still exact, but unfortunately not closed, since the r.h.s. still contains the full universe density matrix $\boldsymbol{\rho}$.

Born approximation

Closure is achieved by applying the Born approximation

$$\boldsymbol{\rho}(t) = \boldsymbol{\rho_S}(t) \otimes \bar\rho_B + \mathcal{O}\{h_k\}\,, \qquad \bar\rho_B = \frac{e^{-\beta H_B}}{Z_B} \tag{1.6}$$

for all times, where β is the inverse temperature of the bath (we use $k_B = 1$). For systems with particle exchange, other suitable choices for the bath density matrix could be $\bar{\rho}_B = \frac{e^{-\beta(H_B - \mu N_B)}}{Z_B}$, with bath particle number operator N_B and chemical potential μ. Since our interaction Hamiltonian is linear in the b_k operators, we have $\mathrm{Tr_B}\left\{[\boldsymbol{H_I}(t), \rho_0]\right\} = 0$ (after suitable transformations of both H_S and H_I, this case can always be achieved), which eventually leads to the **Non-Markovian master equation**

$$\dot{\boldsymbol{\rho_S}} = -\int_0^t \mathrm{Tr_B}\left\{[\boldsymbol{H_I}(t), [\boldsymbol{H_I}(t'), \boldsymbol{\rho_S}(t') \otimes \bar{\rho}_B]]\right\} dt' + \mathcal{O}\{h_k^3\}\,, \tag{1.7}$$

which is a closed, integro-differential equation for $\boldsymbol{\rho_S}$ that preserves trace and hermiticity (but not positivity). Making the above explicit for our example, it reads

$$\begin{aligned}
\dot{\boldsymbol{\rho_S}} &= -\int_0^t \left[\left(ae^{-\mathrm{i}\Omega t} + a^\dagger e^{+\mathrm{i}\Omega t}\right), \left(ae^{-\mathrm{i}\Omega t'} + a^\dagger e^{+\mathrm{i}\Omega t'}\right)\boldsymbol{\rho_S}(t')\right] C(t-t') + \mathrm{h.c.} \\
&= -\int_0^t \left[\left(ae^{-\mathrm{i}\Omega t} + a^\dagger e^{+\mathrm{i}\Omega t}\right), \left(ae^{-\mathrm{i}\Omega (t-\tau)} + a^\dagger e^{+\mathrm{i}\Omega (t-\tau)}\right)\boldsymbol{\rho_S}(t-\tau)\right] C(\tau) + \mathrm{h.c.}\,, \\
C(\tau) &= \sum_k |h_k|^2 \left(e^{-\mathrm{i}\omega_k \tau}(1 + n_B(\omega_k)) + e^{+\mathrm{i}\omega_k \tau} n_B(\omega_k)\right)\,,
\end{aligned} \tag{1.8}$$

where $n_B(\omega_k) = [e^{\beta\omega_k} - 1]^{-1}$ is the Bose distribution and $C(\tau)$ is the **reservoir correlation function**. We perform the limit to a continuous reservoir by introducing the **spectral coupling density** or **spectral function** of the reservoir

$$\Gamma(\omega) = 2\pi \sum_k |h_k|^2 \delta(\omega - \omega_k)\,, \tag{1.9}$$

which contains information on the system-reservoir coupling strength (h_k) and the reservoir frequency spacing (ω_k). As $\omega_k > 0$, it follows that $\Gamma(\omega)$ vanishes at negative frequencies. For comparison, the spectral density of the reservoir alone would be given by $\mathcal{D}(\omega) = 2\pi \sum_k \delta(\omega - \omega_k)$. Noting that we can analytically continue the spectral function as an odd function via $\tilde{\Gamma}(\omega > 0) = \Gamma(\omega)$ and $\tilde{\Gamma}(\omega < 0) = -\Gamma(|\omega|)$, this trick together with $n_B(-\omega) = -[1 + n_B(+\omega)]$ allows us to write the correlation function as a Fourier transform

$$C(\tau) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \tilde{\Gamma}(\omega)[1 + n_B(\omega)] e^{-\mathrm{i}\omega\tau} d\omega \equiv \frac{1}{2\pi}\int_{-\infty}^{+\infty} \gamma(\omega) e^{-\mathrm{i}\omega\tau} d\omega \tag{1.10}$$

of the analytically continued spectral function and the Bose distribution, combined in the function $\gamma(\omega)$. We will use the analytic continuation of the spectral function without notice below, i.e., we drop the $\tilde{\Gamma}(\omega) \to \Gamma(\omega)$.

Markov approximation

For typical reservoirs with a dense spectrum (i.e., a continuous spectral function $\Gamma(\omega)$), the Fourier transform $\gamma(\omega)$ of the correlation function is approximately flat over large frequency scales (for $\omega \to \pm\infty$ however it will decay to zero as $\Gamma(\omega)$ enforces this). For the correlation function this means that for such scenarios, it is a rapidly decaying function of τ. We may therefore perform the Markov approximation by two steps

$$\boldsymbol{\rho_S}(t-\tau) \to \boldsymbol{\rho_S}(t)\,, \qquad \int_0^t [\ldots] d\tau \to \int_0^\infty [\ldots] d\tau\,, \tag{1.11}$$

which are both justified in the limit where the correlation function $C(\tau)$ decays rapidly. The result of this procedure is the **Redfield-II** master equation, which for our example reads

$$\dot{\boldsymbol{\rho}}_{\boldsymbol{S}} = -\int_0^\infty \left[\left(ae^{-\mathrm{i}\Omega t} + a^\dagger e^{+\mathrm{i}\Omega t}\right), \left(ae^{-\mathrm{i}\Omega(t-\tau)} + a^\dagger e^{+\mathrm{i}\Omega(t-\tau)}\right)\boldsymbol{\rho}_{\boldsymbol{S}}(t)\right] C(\tau) + \mathrm{h.c.}\,. \tag{1.12}$$

It preserves trace and hermiticity, but not positivity. It is much simpler to solve than the non-Markovian master equation as it is time local. When we transform it back to the Schrödinger picture, we even obtain a time-independent equation. However, it is not yet of Lindblad form.

Secular approximation

Expanding the terms in (1.12), we see that some terms oscillate with $e^{\pm\mathrm{i}2\Omega t}$, whereas other terms do not oscillate in t. If we formally integrate the equation over long timescales, the oscillatory terms will average out (assuming that everything else does not compensate this oscillation). Therefore, the secular approximation just drops these terms, and results in an equation where annihilation operators can only be combined with creation operators

$$\dot{\boldsymbol{\rho}}_{\boldsymbol{S}} = -\int_0^\infty \left[a, a^\dagger\boldsymbol{\rho}_{\boldsymbol{S}}(t)\right] e^{-\mathrm{i}\Omega\tau} C(\tau)d\tau - \int_0^\infty \left[a^\dagger, a\boldsymbol{\rho}_{\boldsymbol{S}}(t)\right] e^{+\mathrm{i}\Omega\tau} C(\tau)d\tau + \mathrm{h.c.}\,. \tag{1.13}$$

This equation preserves trace, hermiticity, and positivity. It is actually of Lindblad form, which can be seen after some rewritings: First, we insert the Fourier transform (1.10) of the correlation function. Second, we perform the $d\tau$ integrals by using the **Sokhotskij-Plemelj theorem**

$$\frac{1}{2\pi}\int_0^\infty e^{\pm\mathrm{i}\omega\tau}d\tau = \frac{1}{2}\delta(\omega) \pm \frac{\mathrm{i}}{2\pi}\mathcal{P}\frac{1}{\omega}\,, \tag{1.14}$$

where $\mathcal{P}$ denotes the Cauchy principal value. Third, we collect the terms with principal value integrals and with δ functions, performing the $d\omega$ integrations on the latter. This yields

$$\begin{aligned}\dot{\boldsymbol{\rho}}_{\boldsymbol{S}} = {}& \gamma(+\Omega)\left[a\boldsymbol{\rho}_{\boldsymbol{S}}a^\dagger - \frac{1}{2}\left\{a^\dagger a, \boldsymbol{\rho}_{\boldsymbol{S}}\right\}\right] \\ & + \gamma(-\Omega)\left[a^\dagger\boldsymbol{\rho}_{\boldsymbol{S}}a - \frac{1}{2}\left\{aa^\dagger, \boldsymbol{\rho}_{\boldsymbol{S}}\right\}\right] \\ & - \frac{\mathrm{i}}{2\pi}\mathcal{P}\int\frac{\gamma(\omega)}{\Omega-\omega}d\omega\left[a^\dagger a, \boldsymbol{\rho}_{\boldsymbol{S}}\right] + \frac{\mathrm{i}}{2\pi}\mathcal{P}\int\frac{\gamma(\omega)}{\omega+\Omega}d\omega\left[aa^\dagger, \boldsymbol{\rho}_{\boldsymbol{S}}\right]\,.\end{aligned} \tag{1.15}$$

Transforming back to the Schrödinger picture eventually yields – after combining the commutator terms and using the symmetry relations of $\gamma(\omega)$ – the form

$$\begin{aligned}\dot{\rho}_S = {}& -\mathrm{i}\left[(\Omega+\Delta\Omega)a^\dagger a, \rho_S\right] \\ & + \Gamma(\Omega)[1+n_B(\Omega)]\left[a\rho_S a^\dagger - \frac{1}{2}\left\{a^\dagger a, \rho_S\right\}\right] \\ & + \Gamma(\Omega)n_B(\Omega)\left[a^\dagger\rho_S a - \frac{1}{2}\left\{aa^\dagger, \rho_S\right\}\right]\,. \\ \Delta\Omega = {}& \frac{1}{\pi}\mathcal{P}\int\frac{\gamma(\omega)\omega}{\Omega^2-\omega^2}d\omega\,,\end{aligned} \tag{1.16}$$

where the Lindblad form is explicit, but we also note a small correction to the system Hamiltonian – often called **Lamb shift**.