3.4 Microscopic derivation of the Born-Markov master equation

Here, we provide an heuristic derivation of the dynamics of an open quantum system in interaction with its surrounding environment. The following scheme summarises the approach:

$$\begin{array}{ccc} \hat\rho & \xrightarrow[\hat{\mathcal{U}}_t]{\text{unitary evolution}} & \hat\rho(t)=\hat{\mathcal{U}}_t\hat\rho\hat{\mathcal{U}}_t^\dagger \\ \mathrm{Tr}^{(\mathrm{E})}[\,\cdot\,]\big\downarrow & & \big\downarrow\mathrm{Tr}^{(\mathrm{E})}[\,\cdot\,] \\ \hat\rho_{\mathrm{S}} & \xrightarrow[\text{reduced evolution}]{\mathcal{T}_t} & \hat\rho_{\mathrm{S}}(t)=\mathrm{Tr}^{(\mathrm{E})}\left[\hat{\mathcal{U}}_t\hat\rho\hat{\mathcal{U}}_t^\dagger\right]. \end{array} \tag{3.37}$$

In particular, we will derive the generator of the dynamics under the Born-Markov approximations. We assume to have a system in interaction with its surrounding environment. The total Hamiltonian reads

$$\hat H=\hat H_0+\hat H_{\mathrm{int}}, \tag{3.38}$$

where $\hat H_0=\hat H_{\mathrm{S}}+\hat H_{\mathrm{E}}$ contains the free Hamiltonian of the system $\hat H_{\mathrm{S}}$ and that of the environment $\hat H_{\mathrm{E}}$, while $\hat H_{\mathrm{int}}$ describes the interaction among the two. The total state, in the interaction picture, evolves as

$$\hat\rho^{(\mathrm{I})}(t)=e^{i\hat H_0t/\hbar}\hat\rho(t)e^{-i\hat H_0t/\hbar}, \tag{3.39}$$

where $\hat\rho(t)$ is the total state evolved with respect to $\hat H$ starting from the initial state $\hat\rho(0)$, i.e.

$$\hat\rho(t)=e^{-i\hat Ht/\hbar}\hat\rho(0)e^{i\hat Ht/\hbar}. \tag{3.40}$$

The evolution of $\hat\rho^{(\mathrm{I})}(t)$ is described by the following dynamical equation

$$\frac{\mathrm{d}\hat\rho^{(\mathrm{I})}(t)}{\mathrm{d}t}=-\frac{i}{\hbar}\left[\hat H^{(\mathrm{I})}_{\mathrm{int}}(t),\hat\rho^{(\mathrm{I})}(t)\right], \tag{3.41}$$

where $\hat H^{(\mathrm{I})}_{\mathrm{int}}(t)=e^{i\hat H_0t/\hbar}\hat H_{\mathrm{int}}e^{-i\hat H_0t/\hbar}$. Now, by integrating Eq. (3.41) in time from 0 to t, one obtains the formal solution

$$\hat\rho^{(\mathrm{I})}(t)=\hat\rho(0)-\frac{i}{\hbar}\int_0^t\mathrm{d}s\,\left[\hat H^{(\mathrm{I})}_{\mathrm{int}}(s),\hat\rho^{(\mathrm{I})}(s)\right]. \tag{3.42}$$

By inserting the latter expression back in Eq. (3.41) and tracing over the degrees of freedom of the environment, we find

$$\frac{\mathrm{d}\hat\rho^{(\mathrm{I})}_{\mathrm{S}}(t)}{\mathrm{d}t}=-\frac{i}{\hbar}\,\mathrm{Tr}^{(\mathrm{E})}\left[\left[\hat H^{(\mathrm{I})}_{\mathrm{int}}(t),\hat\rho(0)\right]\right]-\frac{1}{\hbar^2}\int_0^t\mathrm{d}s\;\mathrm{Tr}^{(\mathrm{E})}\left[\left[\hat H^{(\mathrm{I})}_{\mathrm{int}}(t),\left[\hat H^{(\mathrm{I})}_{\mathrm{int}}(s),\hat\rho^{(\mathrm{I})}(s)\right]\right]\right]. \tag{3.43}$$

This is an integro-differential equation, which is not time local since the last term contains the total state $\hat\rho^{(\mathrm{I})}(s)$ evaluated at time s. This allows to have memory effects in the dynamics: the evolution of the reduced state at time t depends on the (total) state at all times s between 0 and t. Without loss of generality, we assume that $-\frac{i}{\hbar}\,\mathrm{Tr}^{(\mathrm{E})}\left[\left[\hat H^{(\mathrm{I})}_{\mathrm{int}}(t),\hat\rho(0)\right]\right]=0$, and that the initial state is separable, i.e.

$$\hat\rho(0)=\hat\rho_{\mathrm{S}}(0)\otimes\hat\rho_{\mathrm{E}}(0). \tag{3.44}$$

Since the initial state in the interaction and in the Schrödinger picture are the same, the same relation holds also for $\hat\rho^{(\mathrm{I})}(0)$. In the following we apply two important approximations.

3.4.1 Born approximation

The Born approximation assumes that the correlations between the system and the environment are negligible, and that the environment is not influenced by the dynamics of the system. Thus, one can approximate the total state as

$$\hat{\rho}^{(\mathrm{I})}(s) \simeq \hat{\rho}_{\mathrm{S}}^{(\mathrm{I})}(s) \otimes \hat{\rho}_{\mathrm{E}}, \tag{3.45}$$

for all times $s \geq 0$, where $\hat{\rho}_{\mathrm{E}}$ is the initial state of the environment. Now, by assuming that the interaction Hamiltonian has a bilinear form, i.e. $\hat{H}_{\mathrm{int}} = \sum_\alpha \hat{S}_\alpha \otimes \hat{E}_\alpha$, one has that its time evolved version reads

$$\hat{H}_{\mathrm{int}}^{(\mathrm{I})}(t) = \sum_\alpha \hat{S}_\alpha^{(\mathrm{I})}(t) \otimes \hat{E}_\alpha^{(\mathrm{I})}(t), \tag{3.46}$$

where

$$\hat{S}_\alpha^{(\mathrm{I})}(t) = e^{i\hat{H}_{\mathrm{S}}t/\hbar}\hat{S}_\alpha e^{-i\hat{H}_{\mathrm{S}}t/\hbar}, \quad \text{and} \quad \hat{E}_\alpha^{(\mathrm{I})}(t) \quad = e^{i\hat{H}_{\mathrm{E}}t/\hbar}\hat{E}_\alpha e^{-i\hat{H}_{\mathrm{E}}t/\hbar}, \tag{3.47}$$

evolve respectively with respect to $\hat{H}_{\mathrm{S}}$ and $\hat{H}_{\mathrm{E}}$. By putting together Eq. (3.45) and Eq. (3.46), we have that the trace of the double commutator in Eq. (3.43) reads

$$\mathrm{Tr}^{(\mathrm{E})}\left[\left[\sum_\alpha \hat{S}_\alpha^{(\mathrm{I})}(t) \otimes \hat{E}_\alpha^{(\mathrm{I})}(t), \left[\sum_\beta \hat{S}_\beta^{(\mathrm{I})}(s) \otimes \hat{E}_\beta^{(\mathrm{I})}(s), \hat{\rho}_{\mathrm{S}}^{(\mathrm{I})}(s) \otimes \hat{\rho}_{\mathrm{E}}\right]\right]\right]. \tag{3.48}$$

By exploiting the linearity and the cyclicity of the trace, the latter expression becomes

$$\sum_{\alpha\beta}\left(C_{\alpha\beta}(t,s)\left[\hat{S}_\alpha^{(\mathrm{I})}(t), \hat{S}_\beta^{(\mathrm{I})}(s)\hat{\rho}_{\mathrm{S}}^{(\mathrm{I})}(s)\right] + C_{\beta\alpha}(s,t)\left[\hat{\rho}_{\mathrm{S}}^{(\mathrm{I})}(s)\hat{S}_\beta^{(\mathrm{I})}(s), \hat{S}_\alpha^{(\mathrm{I})}(t)\right]\right), \tag{3.49}$$

where we defined the two-time correlation functions for the environment

$$C_{\alpha\beta}(t,s) = \mathrm{Tr}^{(\mathrm{E})}\left[\hat{E}_\alpha^{(\mathrm{I})}(t)\hat{E}_\beta^{(\mathrm{I})}(s)\hat{\rho}_{\mathrm{E}}\right]. \tag{3.50}$$

Under the assumption that $\hat{\rho}_{\mathrm{E}}$ is a stationary state with respect to the evolution due to $\hat{H}_{\mathrm{E}}$, i.e. $\left[\hat{H}_{\mathrm{E}}, \hat{\rho}_{\mathrm{E}}\right] = 0$, then $C_{\alpha\beta}(t,s)$ can be expressed as

$$C_{\alpha\beta}(t,s) = \mathrm{Tr}^{(\mathrm{E})}\left[\hat{E}_\alpha^{(\mathrm{I})}(t-s)\hat{E}_\beta^{(\mathrm{I})}\hat{\rho}_{\mathrm{E}}\right], \tag{3.51}$$

thus $C_{\alpha\beta}(t,s) = C_{\alpha\beta}(t-s)$. Correspondingly, Eq. (3.43) becomes

$$\frac{\mathrm{d}\hat{\rho}_{\mathrm{S}}^{(\mathrm{I})}(t)}{\mathrm{d}t} = -\frac{1}{\hbar^2}\int_0^t \mathrm{d}s \sum_{\alpha\beta}\left(C_{\alpha\beta}(t-s)\left[\hat{S}_\alpha^{(\mathrm{I})}(t), \hat{S}_\beta^{(\mathrm{I})}(s)\hat{\rho}_{\mathrm{S}}^{(\mathrm{I})}(s)\right] + C_{\beta\alpha}(s-t)\left[\hat{\rho}_{\mathrm{S}}^{(\mathrm{I})}(s)\hat{S}_\beta^{(\mathrm{I})}(s), \hat{S}_\alpha^{(\mathrm{I})}(t)\right]\right), \tag{3.52}$$

which is the result of the Born approximation.

3.4.2 Markov approximation

Typically, the two-time correlation function $C_{\alpha\beta}(t-s)$ is characterized by a correlation time τ_{corr}, which describes the timescale for which the state at time s influences that at the time $t \geq s$. The Markov approximation assumes that such a correlation time τ_{corr} is much smaller than the system's dynamical timescale τ_{S} characterising the dynamics of the system, i.e. under such a scale the state of the system does not change noticeably. Thus, one assumes that *i)* for any time s such that $t-s$ is smaller than $\tau_{\rm S}$, one can approximate $\hat\rho_{\rm S}^{(\rm I)}(s) \simeq \hat\rho_{\rm S}^{(\rm I)}(t)$, and that *ii)* for any time s such that $t-s \geq \tau_{\rm corr}$, the two-time correlation function is negligibly small, i.e. $C_{\alpha\beta}(t-s) \simeq 0$. The application of the approximation *i)* to Eq. (3.52) leads to the so-called Redfield equation, which is a time-local equation for $\hat\rho_{\rm S}^{(\rm I)}(t)$ and it reads

$$\frac{\mathrm{d}\hat\rho_{\rm S}^{(\rm I)}(t)}{\mathrm{d}t} = -\sum_\alpha \left(\left[\hat S_\alpha^{(\rm I)}(t), \hat B_\alpha^{(\rm I)}(t)\hat\rho_{\rm S}^{(\rm I)}(t)\right] + \left[\hat\rho_{\rm S}^{(\rm I)}(t)\hat C_\alpha^{(\rm I)}(t), \hat S_\alpha^{(\rm I)}(t)\right]\right), \tag{3.53}$$

where we defined

$$\hat B_\alpha^{(\rm I)}(t) = \sum_\beta \int_0^t \frac{\mathrm{d}s}{\hbar^2} C_{\alpha\beta}(t-s)\hat S_\beta^{(\rm I)}(s), \quad \text{and} \quad \hat C_\alpha^{(\rm I)}(t) = \sum_\beta \int_0^t \frac{\mathrm{d}s}{\hbar^2} C_{\beta\alpha}(s-t)\hat S_\beta^{(\rm I)}(s). \tag{3.54}$$

The application of *ii)* allows instead to extend the limits of the time integral: $\int_0^t \mathrm{d}s \to \int_{-\infty}^t \mathrm{d}s$ as the integrand is suppressed by $C_{\alpha\beta}(t-s)$ for any $t-s \geq \tau_{\rm corr}$. With a change of integration variable reading $s \to \tau = t-s$, one finds

$$\hat B_\alpha^{(\rm I)}(t) = \frac{1}{\hbar^2}\sum_\beta \int_0^{+\infty} \mathrm{d}\tau\, C_{\alpha\beta}(\tau) S_\beta^{(\rm I)}(t-\tau), \quad \text{and} \quad \hat C_\alpha^{(\rm I)}(t) = \frac{1}{\hbar^2}\sum_\beta \int_0^{+\infty} \mathrm{d}\tau\, C_{\beta\alpha}(-\tau) S_\beta^{(\rm I)}(t-\tau). \tag{3.55}$$

Now, we move back to the Schrödinger picture. By exploiting that

$$\hat\rho_{\rm S}^{(\rm I)}(t) = e^{i\hat H_{\rm S}t/\hbar}\hat\rho_{\rm S}(t)e^{-i\hat H_{\rm S}t/\hbar}, \tag{3.56}$$

we find that

$$\frac{\mathrm{d}\hat\rho_{\rm S}(t)}{\mathrm{d}t} = -\frac{i}{\hbar}\left[\hat H_{\rm S}, \hat\rho_{\rm S}(t)\right] + e^{-i\hat H_{\rm S}t/\hbar}\left(\frac{\mathrm{d}\hat\rho_{\rm S}^{(\rm I)}(t)}{\mathrm{d}t}\right)e^{i\hat H_{\rm S}t/\hbar}. \tag{3.57}$$

The last contribution contains terms as

$$e^{-i\hat H_{\rm S}t/\hbar}\hat S_\alpha^{(\rm I)}(t)\hat S_\beta^{(\rm I)}(t-\tau)\hat\rho_{\rm S}^{(\rm I)}(t)e^{i\hat H_{\rm S}t/\hbar} = \hat S_\alpha \hat S_\beta(-\tau)\hat\rho_{\rm S}(t), \tag{3.58}$$

where we employed Eq. (3.47). Accordingly, one obtains

$$\frac{\mathrm{d}\hat\rho_{\rm S}(t)}{\mathrm{d}t} = -\frac{i}{\hbar}\left[\hat H_{\rm S}, \hat\rho_{\rm S}(t)\right] - \sum_\alpha \left(\left[\hat S_\alpha, \hat B_\alpha \hat\rho_{\rm S}(t)\right] + \left[\hat\rho_{\rm S}(t)\hat C_\alpha, \hat S_\alpha\right]\right), \tag{3.59}$$

where $\hat B_\alpha$ and $\hat C_\alpha$ can be obtained from Eq. (3.55) by setting $t=0$.

Assuming that the time correlations are proportional to a Dirac delta, i.e. $C_{\alpha\beta}(t) = C_{\alpha\beta}\delta(t)$, one finds

$$\frac{\mathrm{d}\hat\rho_{\rm S}(t)}{\mathrm{d}t} = -\frac{i}{\hbar}\left[\hat H_{\rm S}, \hat\rho_{\rm S}(t)\right] - \frac{1}{\hbar^2}\sum_{\alpha\beta}\left(C_{\alpha\beta}\left[\hat S_\alpha, \hat S_\beta \hat\rho_{\rm S}(t)\right] + C_{\beta\alpha}\left[\hat\rho_{\rm S}(t)\hat S_\beta, \hat S_\alpha\right]\right). \tag{3.60}$$

By inverting the indexes α and β in the second term, one obtains

$$\frac{\mathrm{d}\hat\rho_{\rm S}(t)}{\mathrm{d}t} = -\frac{i}{\hbar}\left[\hat H_{\rm S}, \hat\rho_{\rm S}(t)\right] + \frac{2}{\hbar^2}\sum_{\alpha\beta} C_{\alpha\beta}\left(\hat S_\beta\hat\rho_{\rm S}\hat S_\alpha - \frac{1}{2}\left\{\hat\rho_{\rm S}, \hat S_\alpha\hat S_\beta\right\}\right), \tag{3.61}$$

which can be seen as the non-diagonal version of Eq. (3.22).