Reduced Dynamics in Born Markov Approximation

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A completely generic Hamiltonian in system + bath form is used to derive the Lindblad master equation for the reduced density operator of the system.

Start with a completely generic Hamiltonian, in which we only assume that the system-bath interaction may be written as a summation of terms that are tensor products of operators acting on the system Hilbert space and operators acting on the bath Hilbert space. We write these terms with a generic index α.

$$H = H_S + H_B + \sum_\alpha S_\alpha B_\alpha. \tag{1}$$

Assume that the system Hamiltonian H_S consists only of discrete energy levels, $\hbar\omega_n$, indexed by integers n, and that this is the definition of H_S. That is, any continuous degrees of freedom of the complete system are taken to form part of H_B. We can write S_α in terms of operators that turn out to have simpler time-dependence below. Let $\Pi(E)$ be projection operator that projects to the subspace of system Hilbert space in which states have energy E. Note that this may be only one state for some E. Then we can write,

$$S_\alpha = \sum_\omega A_\alpha^-(\omega) + \sum_\omega A_\alpha^+(\omega), \quad \omega \geq 0, \tag{2}$$

$$\text{where, } A_\alpha^-(\omega) \equiv \sum_{E'-E=\omega} \Pi(E) S_\alpha \Pi(E'), \tag{3}$$

$$\Rightarrow A_\alpha^+(\omega) = \sum_{E-E'=\omega} \Pi(E) S_\alpha^\dagger \Pi(E'). \tag{4}$$

In these equations ω is discrete and the last equation, follows from hermitian conjugate of the middle one and re-labelling the E, E'.

Born Approximation: The separation between energy levels of H_S is much larger than the interaction energy, $\hbar(\omega_n - \omega_m) \gg |\sum_\alpha S_\alpha B_\alpha|$ for all $\omega_n > \omega_m$.

Bath Memory: The timescale over which the bath correlation functions decay is much shorter than the timescale over which the system evolves in the interaction picture.

Neglect Bath Perturbation: the state of the total system specified as the density matrix, $\varrho(t) = \rho(t)R$, where $\rho(t)$ is the density operator for the system, and R is that for the bath degrees of freedom. We assume that the bath remains unperturbed. We arrange for the operators S_α to have the property that at time $t = 0$, $\mathrm{Tr}\left[S_\alpha B_\alpha \varrho(0)\right] = 0$.

Interaction picture: with the Hamiltonian $H_0 = H_S + H_B$, and use I to indicate the interaction picture. In this picture

$$e^{iH_0 t/\hbar} S_\alpha B_\alpha e^{-iH_0 t/\hbar} = \sum_\omega A_\alpha(\omega) e^{-i\omega t} B_{I\alpha}(t) + A_\alpha^\dagger(\omega) e^{i\omega t} B_{I\alpha}(t),$$

and the density operator obeys the equation,

$$\frac{d}{dt}\varrho_I(t) = -\frac{i}{\hbar}\sum_\alpha \left[S_{I\alpha}(t) B_{I\alpha}(t), \varrho I(t)\right].$$

Formally integrate this equation once,

$$\frac{d}{dt}\varrho_I(t) = \varrho_I(0) - \frac{i}{\hbar}\sum_\alpha \int_0^t dt' \left[S_{I\alpha}(t') B_{I\alpha}(t'), \varrho_I(t')\right].$$

Substitute it back into the dynamical equation, and take the trace over bath, and recall that we constructed the interaction Hamiltonian to have the property, $\mathrm{Tr}\left[S_\alpha B_\alpha \varrho(0)\right]=0$,

$$\frac{d}{dt}\rho_I(t) \;=\; -\frac{1}{\hbar^2}\sum_{\alpha,\beta}\int_0^t dt'\mathrm{Tr}_B\left[S_{I\alpha}(t)B_{I\alpha}(t),\left[S_{I\beta}(t')B_{I\beta}(t'),\rho_I(t')R\right]\right].$$

Coarse-graining: Integrate this equation over a time interval of size t_c, such that $t_c \gg |\omega_m-\omega_n|^{-1}$ for all $|\omega_m-\omega_n|>0$,

$$\begin{aligned}&\frac{1}{t_c}\left[\rho_I\left(t+\frac{t_c}{2}\right)-\rho_I\left(t-\frac{t_c}{2}\right)\right]\\ =\;& -\frac{1}{\hbar^2}\sum_{\alpha,\beta}\frac{1}{t_c}\int_{t-t_c/2}^{t+t_c/2}dt'\int_0^{t'}d\tau\mathrm{Tr}_B\left[S_{I\alpha}(t')B_{I\alpha}(t'),\left[S_{I\beta}(t'-\tau)B_{I\beta}(t'-\tau),\rho_I(t'-\tau)R\right]\right].\end{aligned}$$

Ignore second order terms in the left hand side: $\rho_I(t)$ does not change over t_c appreciably so that the left hand side becomes $\approx d\rho_I/dt$.

Now substitute (2) in the right hand side.

$$\begin{aligned}&-\frac{1}{\hbar^2}\sum_{\alpha,\beta}\sum_{\omega,\omega'}\sum_{\sigma\sigma'=\pm}\Bigg(\frac{1}{t_c}\int_{t-t_c/2}^{t+t_c/2}dt'\int_0^{t'}dt''\\ &\mathrm{Tr}_B\left[A_\alpha^\sigma(\omega)e^{i\sigma\omega t'}B_{I\alpha}(t'),\left[A_\beta^{\sigma'}(\omega')e^{i\sigma'\omega'(t'-\tau)}B_{I\beta}(t'-\tau),\rho_I(t'-\tau)R\right]\right]\Bigg).\end{aligned}$$

Introduce the variable $\tau=t'-t''$ and expand this expression out into individual terms explicitly,

$$\begin{aligned}&-\frac{1}{\hbar^2}\sum_{\alpha,\beta}\sum_{\omega,\omega'}\sum_{\sigma\sigma'=\pm}\frac{1}{t_c}\int_{t-t_c/2}^{t+t_c/2}dt'e^{i(\sigma\omega+\sigma'\omega')t'}\int_0^{t'}d\tau e^{-i\sigma'\omega'\tau}\,(\\ &\quad A_\alpha^\sigma(\omega)A_\beta^{\sigma'}(\omega')\rho_I(t'-\tau)\;\;\mathrm{Tr}\left[B_{I\alpha}(t')B_{I\beta}(t'-\tau)R\right]\\ &-A_\alpha^\sigma(\omega)\rho_I(t'-\tau)A_\beta^{\sigma'}(\omega')\;\;\mathrm{Tr}\left[B_{I\alpha}(t')RB_{I\beta}(t'-\tau)\right]\\ &-A_\beta^{\sigma'}(\omega')\rho_I(t'-\tau)A_\alpha^\sigma(\omega)\;\;\mathrm{Tr}\left[B_{I\beta}(t'-\tau)RB_{I\alpha}(t')\right]\\ &+\rho_I(t'-\tau)A_\beta^{\sigma'}(\omega')A_\alpha^\sigma(\omega)\;\;\mathrm{Tr}\left[RB_{I\beta}(t'-\tau)B_{I\alpha}(t')\right]\,).\end{aligned}$$

Use the cyclic property of trace, since the trace is now applied to operators acting only over bath degrees of freedom,

$$\begin{aligned}&-\frac{1}{\hbar^2}\sum_{\alpha,\beta}\sum_{\omega,\omega'}\sum_{\sigma\sigma'=\pm}\frac{1}{t_c}\int_{t-t_c/2}^{t+t_c/2}dt'e^{i(\sigma\omega+\sigma'\omega')t'}\int_0^{t'}d\tau\;\;e^{-i\sigma'\omega'\tau}\,(\\ &A_\alpha^\sigma(\omega)A_\beta^{\sigma'}(\omega')\rho_I(t'-\tau)\;\;\mathrm{Tr}\left[B_{I\alpha}(t')B_{I\beta}(t'-\tau)R\right]+\rho_I(t'-\tau)A_\beta^{\sigma'}(\omega')A_\alpha^\sigma(\omega)\;\;\mathrm{Tr}\left[B_{I\beta}(t'-\tau)B_{I\alpha}(t')R\right]\\ &-A_\alpha^\sigma(\omega)\rho_I(t'-\tau)A_\beta^{\sigma'}(\omega')\;\;\mathrm{Tr}\left[B_{I\beta}(t'-\tau)B_{I\alpha}(t')R\right]-A_\beta^{\sigma'}(\omega')\rho_I(t'-\tau)A_\alpha^\sigma(\omega)\;\;\mathrm{Tr}\left[B_{I\alpha}(t')B_{I\beta}(t'-\tau)R\right]\,).\end{aligned}$$

Apply the **bath memory approximation**, $\rho_I(t'-\tau)\approx\rho_I(t')$, and stationarity of bath to define a *causal function,*

$$K_{\alpha\beta}(\tau)\;\equiv\;\frac{1}{\hbar^2}\mathrm{Tr}\left[B_{I\alpha}(t')B_{I\beta}(t'-\tau)R\right].$$

Now apply the assumption that the coarse graining time t_c is much shorter than the system dynamics ρ_I. The t' integral yields in this case,

$$\frac{1}{t_c}\int_{t-t_c/2}^{t+t_c/2}dt'e^{i(\sigma\omega+\sigma'\omega')t'}\;=\;\frac{\sin\left[(\sigma\omega+\sigma'\omega')\,\frac{t_c}{2}\right]}{(\sigma\omega+\sigma'\omega')t_c/2}e^{i(\sigma\omega+\sigma'\omega')t}.$$

By assumption of coarse-graining above, that t_c is much longer than any of the system energy separations. This yields the result

$$\frac{\sin\left[(\sigma\omega+\sigma'\omega')\,\frac{t_c}{2}\right]}{(\sigma\omega+\sigma'\omega')t_c/2}e^{i(\sigma\omega+\sigma'\omega')t} \;=\; \begin{cases}1 & \omega'=\omega,\ \sigma'=-\sigma\\ 0 & \text{otherwise}\end{cases}$$

Now apply the assumption that bath correlation time is much shorter than the time scale of t' so that the upper limit in the integral over τ can be set to ∞. The right hand side now becomes,

$$-\sum_{\alpha,\beta}\sum_{\omega}\sum_{\sigma=\pm}A^{\sigma}_{\alpha}(\omega)A^{-\sigma}_{\beta}(\omega)\rho_I(t)\int_0^{\infty}d\tau e^{i\sigma\omega\tau}K_{\alpha\beta}(\tau)+\rho_I(t)\sum_{\alpha,\beta}\sum_{\omega}\sum_{\sigma=\pm}A^{-\sigma}_{\beta}(\omega)A^{\sigma}_{\alpha}(\omega)\int_0^{\infty}d\tau e^{i\sigma\omega\tau}K_{\beta\alpha}(-\tau)$$
$$+\sum_{\alpha,\beta}\sum_{\omega}\sum_{\sigma=\pm}A^{\sigma}_{\alpha}(\omega)\rho_I(t)A^{-\sigma}_{\beta}(\omega)\int_0^{\infty}d\tau e^{i\sigma\omega\tau}K_{\beta\alpha}(-\tau)+\sum_{\alpha,\beta}\sum_{\omega}\sum_{\sigma=\pm}A^{-\sigma}_{\beta}(\omega)\rho_I(t)A^{\sigma}_{\alpha}(\omega)\int_0^{\infty}d\tau e^{i\sigma\omega\tau}K_{\alpha\beta}(\tau).$$

In the second term of the first line, and the first term of the second line, we re-label the by switching α and β, and sum over $-\sigma$ instead of σ. In the τ integrals of these two terms, we change the variable of integration to $-\tau$. This yields

$$-\sum_{\alpha,\beta}\sum_{\omega}\sum_{\sigma=\pm}\left[A^{\sigma}_{\alpha}(\omega)A^{-\sigma}_{\beta}(\omega)\rho_I(t)\int_0^{+\infty}d\tau e^{i\sigma\omega\tau}K_{\alpha\beta}(\tau)+\rho_I(t)A^{\sigma}_{\alpha}(\omega)A^{-\sigma}_{\beta}(\omega)\int_{-\infty}^{0}d\tau e^{i\sigma\omega\tau}K_{\alpha\beta}(\tau)\right]$$
$$+\sum_{\alpha,\beta}\sum_{\omega}\sum_{\sigma=\pm}\left[A^{-\sigma}_{\beta}(\omega)\rho_I(t)A^{\sigma}_{\alpha}(\omega)\int_{-\infty}^{0}d\tau e^{i\sigma\omega\tau}K_{\alpha\beta}(\tau)+A^{-\sigma}_{\beta}(\omega)\rho_I(t)A^{\sigma}_{\alpha}(\omega)\int_0^{+\infty}d\tau e^{i\sigma\omega\tau}K_{\alpha\beta}(\tau)\right].$$

We now define the Fourier spectrum

$$\Gamma_{\alpha\beta}(\omega) \;=\; \int_{-\infty}^{+\infty}e^{i\omega\tau}K_{\alpha\beta}(\tau).$$

In terms of this spectral function,

$$\int_0^{+\infty}d\tau e^{i\omega\tau}K_{\alpha\beta}(\tau) \;=\; \frac{1}{2}\Gamma_{\alpha\beta}(\omega)+i\text{p.v.}\int\frac{d\omega'}{2\pi}\frac{\Gamma_{\alpha\beta}(\omega')}{\omega-\omega'}$$
$$\int_{-\infty}^{0}d\tau e^{i\omega\tau}K_{\alpha\beta}(\tau) \;=\; \frac{1}{2}\Gamma_{\alpha\beta}(\omega)-i\text{p.v.}\int\frac{d\omega'}{2\pi}\frac{\Gamma_{\alpha\beta}(\omega')}{\omega-\omega'}.$$

Define the operator

$$\delta H_I \;=\; \sum_{\alpha,\beta}\sum_{\sigma=\pm}\sum_{\omega}A^{\sigma}_{\alpha}(\omega)A^{-\sigma}_{\beta}(\omega)\left(\text{p.v.}\int\frac{d\omega'}{2\pi}\frac{\hbar\Gamma_{\alpha\beta}(\omega')}{\omega-\omega'}\right).$$

Substituting this in the above, we obtain the **Lindblad Form,**

$$\frac{d}{dt}\rho_I(t) \;\approx\; -\frac{i}{\hbar}\left[\delta H_I,\rho_I(t)\right]+\sum_{\alpha,\beta}\sum_{\omega}\sum_{\sigma=\pm}\Gamma_{\alpha\beta}(\omega)\left[A^{-\sigma}_{\beta}(\omega)\rho_I(t)A^{\sigma}_{\alpha}(\omega)-\frac{1}{2}\left\{A^{\sigma}_{\alpha}(\omega)A^{-\sigma}_{\beta}(\omega),\rho_I(t)\right\}\right]. \tag{5}$$