Notes on the Born-Markov Master Equations

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1 Closed Systems Formalism

1.1 Setup

For all calculations, we use a unit system in which $\hbar = 1$. Consider a bipartite system consisting of subsystems A and B, each of which are possibly multipartite. We write the Hamiltonian of the entire system as

$$H_{AB} = H_0 + V_I \tag{1}$$

where $H_0 = (H_A + V_A) \otimes \mathcal{I}_B + \mathcal{I}_A \otimes (H_B + V_B)$ is the free Hamiltonian for systems A and B, and where V_I mediates the shared behavior between the systems. For now we will only consider the case in which the total Hamiltonian is time-independent, reserving the time-dependent case for a later analysis.

We assume that the systems A and B, when taken together, form a closed system. In this case, the state of the system evolves under standard von Neumann evolution:

$$\dot{\rho}_{AB}(t) = -i[H_{AB}, \rho_{AB}(t)] \tag{2}$$

Here, ρ_{AB} is the density operator describing the state of the closed system. It is expected that any such density operator must satisfy the following conditions:

1. Hermiticity: $\rho = \rho^\dagger$
2. Positivity: $\rho \geq 0$ (i.e., $\forall \lambda \in \text{Spec}(\rho),\ \lambda \geq 0$)
3. Normalization: $\text{Tr}\{\rho\} = 1$

These properties are required in order to ensure that the density operator gives rise to proper statistical distributions. The first condition ensures that the probabilities are real numbers, the second ensures that the probabilities are non-negative, and the final condition ensures that the probabilities sum to 1.

1.2 Interaction Picture

We will now switch from the Schrödinger picture to the interaction picture by introducing the invertible mapping

$$\widetilde{A}(t) = e^{iH_0 t} A e^{-iH_0 t} \tag{3}$$

where A is an arbitrary operator in the Schrödinger picture, and $\widetilde{A}(t)$ is the corresponding operator in the interaction picture. It is stressed that $\widetilde{A}(t)$ is usually time-dependent, even if A is time-independent. An example of them both being time-independent occurs when $[A, H_0] = 0$, in which case $\widetilde{A}(t) = A$. Further, note that $\widetilde{A}(0) = A$ is always true. In the interaction picture, the von Neumann equation is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\rho}_{AB}(t) = -i\Big[\widetilde{V}_I(t), \widetilde{\rho}_{AB}(t)\Big] \tag{4}$$

Switching from the Schrödinger picture to the interaction picture has the effect of removing the free Hamiltonians from the dynamics, allowing us to focus our attention on the interaction between systems A and B. Equation 4 may be formally integrated to give

$$\widetilde{\rho}_{AB}(t) = \widetilde{\rho}_{AB}(0) + (-i)\int_0^t \mathrm{d}t_1 \left[\widetilde{V}_I(t_1), \widetilde{\rho}_{AB}(t_1)\right] \tag{5}$$

Unfortunately, the right hand side of equation 5 still contains $\widetilde{\rho}_{AB}(t)$ at an intermediate time value, so it isn't particularly useful. However, we may substitute equation 5 into equation 4 to obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\rho}_{AB}(t) = (-i)\Big[\widetilde{V_I}(t), \widetilde{\rho}_{AB}(0)\Big] + (-i)^2\int_0^t \mathrm{d}t_1 \left[\widetilde{V_I}(t), \left[\widetilde{V}_I(t_1), \widetilde{\rho}_{AB}(t_1)\right]\right]. \tag{6}$$

This will serve as the starting point for our upcoming approximations.

2 Open Formalism from Closed Formalism

Our goal is to try to extract information regarding system A while ignoring system B. Physically, this may simply be because system B has too many degrees of freedom to be feasibly studied, such as the case of an atom coupled to a thermal reservoir. In order to quantify the known information regarding the subsystem A, we want to create a density operator ρ_A from the operator ρ_{AB}. The map $\rho_{AB} \mapsto \rho_A$ is given by the expression

$$\rho_A = \mathrm{Tr}_A\{\rho_{AB}\} \equiv \sum_\beta (\mathcal{I} \otimes \langle\beta|)\rho_{AB}(\mathcal{I} \otimes |\beta\rangle) \tag{7}$$

where $\{|\beta\rangle\}$ is an orthonormal basis of system B. This mapping is called the *partial trace*, taken with respect to system B. It can be shown that this mapping is the *unique* mapping that satisfies the three density operator conditions (for a nice proof of this statement, see Box 2.6 in Nielsen and Chuang, *Quantum Computation and Quantum Information*).

BRIEFLY DISCUSS THE PROPERTIES OF PARTIAL TRACE

1. $\mathrm{Tr}_A\{\mathrm{Tr}_B\{\rho_{AB}\}\} = \mathrm{Tr}_B\{\mathrm{Tr}_A\{\rho_{AB}\}\} = \mathrm{Tr}\{\rho_{AB}\}$

We will now apply the partial trace to the von Neumann evolution in the interaction picture in an attempt to derive the dynamics for $\widetilde{\rho}_A(t)$. It can be shown (see Appendix) that the order of applying partial trace and interaction picture is irrelevant, so that we can safely obtain the correct dynamics by first computing the interaction picture density operator and then applying the partial trace, instead of going the other direction. Applying partial trace, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}_B\{\widetilde{\rho}_{AB}(t)\} = (-i)\,\mathrm{Tr}_B\left\{\Big[\widetilde{V_I}(t), \widetilde{\rho}_{AB}(0)\Big]\right\} + (-i)^2\int_0^t \mathrm{d}t_1\,\mathrm{Tr}_B\left\{\Big[\widetilde{V_I}(t), \Big[\widetilde{V}_I(t_1), \widetilde{\rho}_{AB}(t_1)\Big]\Big]\right\}. \tag{8}$$

Everything to this point has been exact, and we are ready to begin making assumptions and approximations about the model.

3 Approximations

Before we move further, we make the assumption that the inter-system interaction V_I takes on a bilinear form

$$V_I = \sum_\alpha A_\alpha \otimes X_\alpha \tag{9}$$

Although we require that V_I be Hermitian, we do not necessarily require that A_α and X_α be Hermitian. We simply require that if $A_\alpha \otimes X_\alpha$ is in the summation, then there exists an index β such that $A_\beta^\dagger \otimes X_\beta^\dagger$ is also in the summation (for example, consider $V_I = \sigma^\dagger \otimes X + \sigma \otimes X^\dagger$, where σ and X are not necessarily Hermitian). With this setup, we write

$$V_I^\dagger = \sum_\beta A_\beta^\dagger \otimes X_\beta^\dagger = V_I \tag{10}$$

We will use equation 9 for $\widetilde{V}_I(t)$ and equation 10 for $\widetilde{V}_I(t_1)$. (We should explicitly compute the interaction picture versions of $\widetilde{V}_I$, but it should also be trivial.) Substituting these into equation 8, we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\operatorname{Tr}_B\{\widetilde{\rho}_{AB}(t)\} = (-i)\sum_\alpha \operatorname{Tr}_B\left\{\left[\widetilde{A}_\alpha(t)\otimes\widetilde{X}_\alpha(t), \widetilde{\rho}_{AB}(0)\right]\right\} \\ + (-i)^2\sum_{\alpha,\beta}\int_0^t \mathrm{d}t_1 \operatorname{Tr}_B\left\{\left[\widetilde{A}_\alpha(t)\otimes\widetilde{X}_\alpha(t), \left[\widetilde{A}_\beta^\dagger(t_1)\otimes\widetilde{X}_\beta^\dagger(t_1), \widetilde{\rho}_{AB}(t_1)\right]\right]\right\}\end{aligned} \tag{11}$$

3.1 Born Approximation

We assume that system B has many, many more degrees of freedom than system A, and we further assume that system B is initially in a Gibbs state ρ_B^G, so that the initial state of the system is $\rho_{AB}(0) = \rho_A(0)\otimes\rho_B^G$. During the course of the total evolution, system B will cause changes in system A, and system A will likewise cause changes in system B. However, because system B has so many degrees of freedom, system B will quickly relax to another Gibbs state, thus staying in a Gibbs state for all perceivable time (this is the typicality argument). Because we assume that the systems are weakly coupled, we may make the Born approximation

$$\rho_{AB}(t) = \rho_A(t)\otimes\rho_B(t) + \rho_{corr}(t) \approx \rho_A(t)\otimes\rho_B^G \tag{12}$$

Substituting 12 into 11 and expanding the Kronecker products and partial traces, we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\rho}_A(t) = (-i)\sum_\alpha\left[\widetilde{A}_\alpha(t), \widetilde{\rho}_A(t)\right]\langle\widetilde{X}_\alpha(t)\rangle_{\rho_B^G} \\ + (-i)^2\sum_{\alpha,\beta}\int_0^t \mathrm{d}t_1\left\{\left[\widetilde{A}_\alpha(t), \widetilde{A}_\beta^\dagger(t_1)\widetilde{\rho}_A(t_1)\right]G_{\alpha\beta}(t,t_1) - \left[\widetilde{A}_\alpha(t), \widetilde{\rho}_A(t_1)\widetilde{A}_\beta^\dagger(t_1)\right]G_{\alpha\beta}^*(t,t_1)\right\}\end{aligned} \tag{13}$$

where $G_{\alpha,\beta}(t,t_1) = \langle\widetilde{X}_\alpha(t)\widetilde{X}_\beta^\dagger(t_1)\rangle_{\rho_B^G} = \operatorname{Tr}\left\{\widetilde{X}_\alpha(t)\widetilde{X}_\beta^\dagger(t_1)\rho_B^G\right\}$. By redefining the zero-point energy of the bath, we can always set $\langle\widetilde{X}_\alpha(t)\rangle_{\rho_B^G} = 0$, so that the Redfield equation becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\rho}_A(t) = (-i)^2\sum_{\alpha,\beta}\int_0^t \mathrm{d}t_1\left\{\left[\widetilde{A}_\alpha(t), \widetilde{A}_\beta^\dagger(t_1)\widetilde{\rho}_A(t_1)\right]G_{\alpha\beta}(t,t_1) - \left[\widetilde{A}_\alpha(t), \widetilde{\rho}_A(t_1)\widetilde{A}_\beta^\dagger(t_1)\right]G_{\alpha\beta}^*(t,t_1)\right\} \tag{14}$$

3.2 Markov Approximation

We now introduce the Markov Approximation by writing

$$\widetilde{\rho}_A(t_1) = \widetilde{\rho}_A(t) + (t_1 - t)\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\rho}_A(t) + \ldots \approx \widetilde{\rho}_A(t). \tag{15}$$

This approximation is justified in the weak coupling limit because $\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\rho}_A(t)$ is second order in the coupling strength. Inserting this into equation 14 and factoring out the operators that are independent of t_1, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\rho}_A(t) = -\sum_{\alpha,\beta}\left[\widetilde{A}_\alpha(t), \widetilde{\Lambda}_{\alpha\beta}(t)\widetilde{\rho}_A(t) - \widetilde{\rho}_A(t)\widetilde{\Lambda}^\dagger_{\alpha\beta}(t)\right] \tag{16}$$

where

$$\widetilde{\Lambda}_{\alpha\beta}(t) = \int_o^t \mathrm{d}t_1\, \widetilde{A}^\dagger_\beta(t_1) G_{\alpha\beta}(t,t_1) \tag{17}$$

Equation 16 is called the *Redfield* equation.

4 Conversion to Schrödinger Picture

We will now convert equation 16 to the Schrödinger picture by using equation 3. Direct calculation yields the following conversions from the interaction picture to the Schrödinger picture:

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\rho}_A(t) = e^{iH_At}\left\{i[H_A,\rho_A(t)] + \frac{\mathrm{d}}{\mathrm{d}t}\rho_A(t)\right\} \tag{18}$$

$$\left[\widetilde{A}_\alpha(t), \widetilde{\Lambda}_{\alpha\beta}(t)\widetilde{\rho}_A(t)\right] = e^{iH_At}[A_\alpha, \Lambda_{\alpha\beta}(t)\rho_A(t)]e^{-iH_At} \tag{19}$$

$$\left[\widetilde{A}_\alpha(t), \widetilde{\rho}_A(t)\widetilde{\Lambda}^\dagger_{\alpha\beta}(t)\right] = e^{iH_At}\left[A_\alpha, \rho_A(t)\Lambda^\dagger_{\alpha\beta}(t)\right]e^{-iH_At} \tag{20}$$

where

$$\Lambda_{\alpha\beta}(t) = \int_o^t \mathrm{d}t_1\, e^{-iH_A(t-t_1)}A^\dagger_\beta e^{iH_A(t-t_1)}G_{\alpha\beta}(t,t_1) \tag{21}$$

Inserting these equations into equation 16, we obtain the dynamical equation in the Schrödinger picture:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_A(t) = -i[H_A,\rho_A(t)] - \sum_{\alpha,\beta}\left[A_\alpha, \Lambda_{\alpha\beta}(t)\rho_A(t) - \rho_A(t)\Lambda^\dagger_{\alpha\beta}(t)\right] \tag{22}$$

5 Symmetric Spin-Boson Model

We will consider the case of two qubits coupled to two baths. The total Hilbert space is $\mathcal{H} = \mathcal{H}^1 \otimes \mathcal{H}^2 \otimes \mathcal{H}^H \otimes \mathcal{H}^C$. Each qubit is coupled to a separate bath, and the qubits themselves are coupled together. The free Hamiltonian of the entire system may be written as

$$\begin{aligned} H_0 &= (H_1 \otimes \mathcal{I}_2 + \mathcal{I}_1 \otimes H_2 + V_{1,2}) \otimes (\mathcal{I}_H \otimes \mathcal{I}_C) + (\mathcal{I}_1 \otimes \mathcal{I}_2) \otimes [H_H \otimes \mathcal{I}_C + \mathcal{I}_H \otimes H_C] \\ &= (H_A + V_A) \otimes \mathcal{I}_B + \mathcal{I}_A \otimes H_B \end{aligned} \tag{23}$$

We keep the Hamiltonian for the qubits general, but we assume that the baths are composed of an infinite number of non-interacting quantum harmonic oscillators, so that the Hamiltonians of the baths may be written as

$$H_l = \sum_k \left[\left(\bigotimes_{i=1}^{k-1}\mathcal{I}_i\right) \otimes \left(\omega_l(k)a^\dagger_l(k)a_l(k)\right) \otimes \left(\bigotimes_{i=k+1}^{\infty}\mathcal{I}_i\right)\right],\ l = H, C \tag{24}$$

The coupling term is written as

$$V_I = (V_{1,H} \otimes \mathcal{I}_2) \otimes (Y_H \otimes \mathcal{I}_C) + (\mathcal{I}_1 \otimes V_{2,C}) \otimes (\mathcal{I}_H \otimes Y_C) \tag{25}$$

where

$$Y_l = \sum_k \left[\left(\bigotimes_{i=1}^{k-1}\mathcal{I}_i\right) \otimes \left(\epsilon_l(k)\left[a^\dagger_l(k) + a_l(k)\right]\right) \otimes \left(\bigotimes_{i=k+1}^{\infty}\mathcal{I}_i\right)\right],\ l = H, C \tag{26}$$

In terms of our previously defined operators, we have

$$\begin{aligned} A_1 &= V_{1,H} \otimes \mathcal{I}_2 \\ X_2 &= Y_H \otimes \mathcal{I}_C \\ A_2 &= \mathcal{I}_1 \otimes V_{2,C} \\ X_3 &= \mathcal{I}_H \otimes Y_C \end{aligned} \tag{27}$$

We may now calculate the bath correlation functions $G_{\alpha,\beta}(t_1, t_2)$. When $\alpha \neq \beta$, $G_{\alpha,\beta}(t_1, t_2) = 0$ because we defined $\langle \widetilde{X}_\alpha(t) \rangle_{\rho_l^G} = 0$. The remaining correlations are

$$\begin{aligned} G_{1,1}(t_1, t_2) &= \langle \widetilde{Y}_H(t_1) \widetilde{Y}_H(t_2) \rangle_{\rho_H^G} = G_H(t_1, t_2) = G_1(t_1, t_2) \\ G_{2,2}(t_1, t_2) &= \langle \widetilde{Y}_C(t_1) \widetilde{Y}_C()t_2) \rangle_{\rho_C^G} = G_C(t_1, t_2) = G_2(t_1, t_2) \end{aligned} \tag{28}$$

In order to calculate 28, we introduce the Drude-Lorentz model of the bath spectral density as

$$J_l(\omega) = \frac{2\lambda_l}{\pi} \frac{\omega \gamma_l}{\omega^2 + \gamma_l^2}, \; l = 1, 2 \tag{29}$$

where λ_l is the coupling strength between the l^{th} bath and the system, and γ_l is the relaxation rate of the l^{th} bath. With this spectral density, the bath correlation functions become

$$G_l(t_1, t_2) = 2\lambda_l \gamma_l \left[\cot\left(\frac{\beta_l \gamma_l}{2} \right) - i \right] e^{-\gamma_l \tau} + \sum_{n=1}^{\infty} \frac{4\lambda_l \gamma_l}{\beta_l} \frac{\nu_n}{\nu_n^2 - \gamma_l^2} e^{-\nu_n \tau} \tag{30}$$

where $\nu_n = \frac{2\pi}{\beta_l} n$ and $\tau = t_1 - t_2$. Equation 14 now becomes

$$\begin{aligned} \widetilde{\rho}_A(t + \mathrm{d}t) - \widetilde{\rho}_A(t) = (-i)^2 \sum_{\alpha=1}^{2} \int_t^{t+\mathrm{d}t} \mathrm{d}t_1 \int_t^{t_1} \mathrm{d}t_2 \Big\{ &\left[\widetilde{A}_\alpha(t_1) \widetilde{A}_\alpha^\dagger(t_2) \widetilde{\rho}_A(t) - \widetilde{A}_\alpha^\dagger(t_2) \widetilde{\rho}_A(t) \widetilde{A}_\alpha(t_1) \right] G_\alpha(t_1, t_2) \\ &+ \left[\widetilde{\rho}_A(t) \widetilde{A}_\alpha^\dagger(t_2) \widetilde{A}_\alpha(t_1) - \widetilde{A}_\alpha(t_1) \widetilde{\rho}_A(t) \widetilde{A}_\alpha^\dagger(t_2) \right] G_\alpha^*(t_1, t_2) \Big\} \end{aligned} \tag{31}$$

where $G_\alpha(t_1, t_2)$ as defined in equation 30.

The series in 30 is not easily done numerically. Because of the exponential decay, we can just compute the bulk of the series, and approximate the tail of the series as a delta function of τ. For now, we will only include one Matsubara term, so that we can approximate our series as

$$\begin{aligned} G_l(t_1, t_2) = G_l(\tau) = &2\lambda_l \gamma_l \left[\cot\left(\frac{\beta_l \gamma_l}{2} \right) - i \right] e^{-\gamma_l \tau} + \frac{4\lambda_l \gamma_l}{\beta_l} \frac{\nu_1}{\nu_1^2 - \gamma_l^2} e^{-\nu_1 \tau} \\ &+ \left[\frac{4\lambda_l}{\beta_l \gamma_l} - 2\lambda_l \cot\left(\frac{\beta_l \gamma_l}{2} \right) - \frac{8\lambda_l \gamma_l \beta_l}{(2\pi)^2 - (\beta_l \gamma_l)^2} \right] \delta(\tau) \end{aligned} \tag{32}$$