Open quantum systems – lecture 5

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1.5 Entropic balances

We saw that the thermal state is a steady state of the BMS master equation, i.e., that the system equilibrates with the reservoir. For a reservoir at low temperatures, this would essentially mean relaxation to the ground state, which reduces the entropy of the system.

1.5.1 Hermitian Lindblad operators

Let us consider the specific case of hermitian Lindblad operators (for simplicity consider just one $L = L^\dagger$, but this can be easily generalized)

$$\dot\rho = -\mathrm{i}\,[H,\rho] + L\rho L - \frac{1}{2}L^2\rho - \frac{1}{2}\rho L^2\,. \tag{1.1}$$

Then, the effect on the system entropy is

$$\begin{aligned}\frac{d}{dt}S(t) &= -\frac{d}{dt}\mathrm{Tr}\left\{\rho\ln\rho\right\} = -\mathrm{Tr}\left\{\dot\rho\ln\rho\right\} = -\mathrm{Tr}\left\{[L\rho L - \frac{1}{2}L^2\rho - \frac{1}{2}\rho L^2]\ln\rho\right\}\\ &= \mathrm{Tr}\left\{L^2\rho\ln\rho - L\rho L\ln\rho\right\}\,,\end{aligned} \tag{1.2}$$

where in the second equality we used that under the trace, terms like $\mathrm{Tr}\left\{\rho\frac{d}{dt}\ln\rho\right\} = 0$ vanish due to trace conservation, in the third equality we used that the contribution of the commutator with H vanishes, and in the second line we used the invariance of the trace under cyclic permutations. To further evaluate the change rate of the system entropy, we insert the spectral decomposition $\rho = \sum_m \lambda_m \left|m\right\rangle\!\left\langle m\right|$ with orthonormal $\langle m|n\rangle = \delta_{nm}$.

$$\begin{aligned}\frac{d}{dt}S(t) &= \sum_n \langle n|\,L^2\,|n\rangle\lambda_n\ln\lambda_n - \sum_{n,m}\langle n|\,L\,|m\rangle\langle m|\,L\,|n\rangle\lambda_m\ln\lambda_n\\ &= \sum_{n,m}\left|\langle n|\,L\,|m\rangle\right|^2\left[\lambda_n\ln\lambda_n - \lambda_m\ln\lambda_n\right] = \sum_{n,m}\left|\langle n|\,L\,|m\rangle\right|^2\lambda_n\ln\frac{\lambda_n}{\lambda_m}\\ &= \sum_{n,m}\left|\langle n|\,L\,|m\rangle\right|^2\lambda_n\ln\frac{\lambda_n\left|\langle n|\,L\,|m\rangle\right|^2}{\lambda_m\left|\langle n|\,L\,|m\rangle\right|^2} \ge 0\,.\end{aligned} \tag{1.3}$$

In the last line, we used the logarithmic sum inequality $\sum_{nm} a_{nm}\ln\frac{a_{nm}}{b_{nm}} \ge a\ln\frac{a}{b}$ with $a_{nm} = \left|\langle n|\,L\,|m\rangle\right|^2\lambda_n \ge 0$ and $b_{nm} = \left|\langle n|\,L\,|m\rangle\right|^2\lambda_m \ge 0$, such that $a = \sum_{nm} a_{nm} = \mathrm{Tr}\left\{L^2\rho\right\}$ and $b = \sum_{nm} b_{nm} = \mathrm{Tr}\left\{L^2\rho\right\} = a$.

This means that hermitian Lindblad operators always increase the entropy of the system (the same holds for anti-hermitian Lindblad operators with $L_\alpha^\dagger = -L_\alpha$). If additionally the Lindblad operators commute with the system Hamiltonian (energy-dephasing models), they do this without actually changing the system energy.

1.5.2 Thermodynamics

It is been shown by Lindblad [1] that the quantum relative entropy between two states ρ and σ

$$D(\rho,\sigma) = \mathrm{Tr}\left\{\rho\left[\ln\rho - \ln\sigma\right]\right\} \tag{1.4}$$

is always decreasing under the action of a completely positive trace-preserving (CPTP) map. Taking $\sigma = \bar\rho$ as the stationary state with $\mathcal{L}\bar\rho = 0$ and considering infinitesimal differences, we can show Spohn's inequality [2].

Def. 1 (Spohn's inequality)**.** *For any Lindblad equation $\dot\rho = \mathcal{L}\rho$ with time-dependent solution $\rho(t)$ and stationary state $\bar\rho$ obeying by $\mathcal{L}\bar\rho = 0$ one has*

$$-\mathrm{Tr}\left\{(\mathcal{L}\rho)\left[\ln\rho - \ln\bar\rho\right]\right\} \geq 0\,. \tag{1.5}$$

This is valid for any Lindblad master equation, independent on whether it is microscopically derived or just invented. In case of a thermalized system stationary state

$$\bar\rho = \frac{e^{-\beta(H_S-\mu N_S)}}{Z_S}\,, \tag{1.6}$$

we can read Spohn's inequality as

$$\frac{d}{dt}\left[-\mathrm{Tr}\left\{\rho\ln\rho\right\}\right] - \beta\mathrm{Tr}\left\{(\mathcal{L}\rho)(H_S-\mu N_S)\right\} \geq 0\,. \tag{1.7}$$

The first term is readily recognizable as the entropy of the system. For a reservoir in thermal equilibrium (which is what is assumed in the microscopic derivation), we can write (there is no volume change here)

$$d\left\langle H_B\right\rangle = \beta^{-1}dS_B + \mu d\left\langle N_B\right\rangle\,, \tag{1.8}$$

and dividing by dt and solving for $d\left\langle S_B\right\rangle/dt$ one gets

$$\frac{dS_B}{dt} = \beta\left[\frac{d\left\langle H_B\right\rangle}{dt} - \mu\frac{d\left\langle N_B\right\rangle}{dt}\right] \approx -\beta\left[\frac{d\left\langle H_S\right\rangle}{dt} - \mu\frac{d\left\langle N_S\right\rangle}{dt}\right]\,, \tag{1.9}$$

where we have assumed energy and particle conservation at the system-reservoir junction. The terms on the right just correspond to the second term in Spohn's inequality. Hence, it encodes the second law of thermodynamics

$$\frac{dS}{dt} - \beta[I_E(t) - \mu I_M(t)] = \frac{d}{dt}S(t) + \frac{d}{dt}S_{\mathrm{B}} \geq 0\,, \tag{1.10}$$

where $I_E(t) = \mathrm{Tr}\left\{\dot\rho H_S\right\}$ and $I_M(t) = \mathrm{Tr}\left\{\dot\rho N_S\right\}$ are the time-dependent energy and matter currents entering the system. The entropic change of the system is bounded by the heat entering the system from the reservoir.

1.6 Solution Methods

1.6.1 Brute-force calculation

To bring the master equation (e.g. Redfield or Lindblad) into a matrix-vector form, one first vectorizes the density matrix, e.g. by stacking rows

$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} \to \begin{pmatrix} \rho_{00} \\ \rho_{01} \\ \rho_{10} \\ \rho_{11} \end{pmatrix} = |\rho\rangle\rangle\,. \tag{1.11}$$

Other vectorizations are possible (e.g. by stacking columns). If we stack rows as above, one finds in general

$$A\rho B \to A \otimes B^{\mathrm{T}} \,|\rho\rangle\rangle \,, \tag{1.12}$$

where B^{T} denotes the transpose of B (not dagger!). A Lindblad form master equation

$$\dot{\rho} = -\mathrm{i}\,[H,\rho] + \sum_\alpha \left[L_\alpha \rho L_\alpha^\dagger - \frac{1}{2}\left\{ L_\alpha^\dagger L_\alpha, \rho \right\} \right] \,, \tag{1.13}$$

would then have the matrix representation of the Liouvillian

$$\mathcal{L} = \sum_\alpha L_\alpha \rho L_\alpha^* - \mathrm{i}\left(H - \frac{\mathrm{i}}{2}\sum_\alpha L_\alpha^\dagger L_\alpha \right) \otimes \mathbf{1} + \mathrm{i}\mathbf{1} \otimes \left(H + \frac{\mathrm{i}}{2}\sum_\alpha L_\alpha^\dagger L_\alpha \right)^{\mathrm{T}} \,. \tag{1.14}$$

The Liouvillian obtained in this way has dimension d^4 for a $d \times d$ density matrix, but it can be directly used to compute eigenvalues or the propagator $e^{\mathcal{L}t}$.

Bibliography

[1] Göran Lindblad. Completely positive maps and entropy inequalities. *Communications in Mathematical Physics*, 40:147, 1975.

[2] H. Spohn and J. L. Lebowitz. Irreversible thermodynamics for quantum systems weakly coupled to thermal reservoirs. *Advances in Chemical Physics*, 38:109, 1978.