Open quantum systems – lecture 11

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3.3 Symmetries in Full Counting Statistics

When for a multi-terminal system with junctions ν, counting of both particles (with counting field χ_ν) and energy (with counting field ξ_ν) is performed, we may often have the situation where the Liouvillian acquires block form

$$\mathcal{L} = \begin{pmatrix} \mathcal{L}_{\rm pop}(\boldsymbol{\chi}, \boldsymbol{\xi}) & \mathbf{0} \\ \mathbf{0} & \mathcal{L}_{\rm coh} \end{pmatrix} , \tag{3.1}$$

where the populations obey a generalized rate equation

$$\dot{P}_a = \sum_\nu \sum_b \gamma^\nu_{ab,ab} e^{+{\rm i}(N_a - N_b)\chi_\nu} e^{+{\rm i}(E_a - E_b)\xi_\nu} P_b - \sum_\nu \sum_b \gamma^\nu_{ba,ba} P_a \, , \tag{3.2}$$

which we can also write as $\boldsymbol{P} = W(\boldsymbol{\chi}, \boldsymbol{\xi})\boldsymbol{P}$ with generalized rate matrix $W(\boldsymbol{\chi}, \boldsymbol{\xi})$ including the counting fields. From the fact that the rates obey local detailed balance

$$\frac{\gamma^\nu_{ab,ab}}{\gamma^\nu_{ba,ba}} = e^{\beta_\nu [(E_b - E_a) - \mu_\nu (N_b - N_a)]} \tag{3.3}$$

one may conclude that the rate matrix obeys the symmetry

$$\mathcal{W}^T(-\boldsymbol{\chi} - {\rm i}\boldsymbol{A}, -\boldsymbol{\xi} - {\rm i}\boldsymbol{B}) = \mathcal{W}(\boldsymbol{\chi}, \boldsymbol{\xi}) \, , \tag{3.4}$$

with the affinities (the terminology arises from the observation that the stationary entropy production rate may be decomposed into a standard affinity-flux form $\sigma_{\rm i} = -\sum_\nu \beta_\nu (I_E^\nu - \mu_\nu I_M^\nu) = -\sum_\nu (B_\nu I_E^\nu + A_\nu I_M^\nu)$)

$$\boldsymbol{B} = (\beta_1, \ldots, \beta_N)^T \, , \qquad \boldsymbol{A} = -(\mu_1 \beta_1, \ldots, \mu_N \beta_N)^T \, , \tag{3.5}$$

where T denotes the transpose. This symmetry transfers to the long-term cumulant-generating function. The eigenvalues $\lambda_\alpha(\boldsymbol{\chi}, \boldsymbol{\xi})$ of the rate matrix solve the characteristic polynomial at all $\boldsymbol{\chi}$ and $\boldsymbol{\xi}$

$$|\mathcal{W}(\boldsymbol{\chi}, \boldsymbol{\xi}) - \lambda_\alpha(\boldsymbol{\chi}, \boldsymbol{\xi})| = 0 \, . \tag{3.6}$$

Evaluating this at shifted values we see that

$$\begin{aligned} &|\mathcal{W}(-\boldsymbol{\chi} - {\rm i}\boldsymbol{A}, -\boldsymbol{\xi} - {\rm i}\boldsymbol{B}) - \lambda_\alpha(-\boldsymbol{\chi} - {\rm i}\boldsymbol{A}, -\boldsymbol{\xi} - {\rm i}\boldsymbol{B}) \cdot \mathbf{1}| \\ &= \left|\mathcal{W}^T(-\boldsymbol{\chi} - {\rm i}\boldsymbol{A}, -\boldsymbol{\xi} - {\rm i}\boldsymbol{B}) - \lambda_\alpha(-\boldsymbol{\chi} - {\rm i}\boldsymbol{A}, -\boldsymbol{\xi} - {\rm i}\boldsymbol{B}) \cdot \mathbf{1}\right| \\ &= |\mathcal{W}(\boldsymbol{\chi}, \boldsymbol{\xi}) - \lambda_\alpha(-\boldsymbol{\chi} - {\rm i}\boldsymbol{A}, -\boldsymbol{\xi} - {\rm i}\boldsymbol{B}) \cdot \mathbf{1}| \, , \end{aligned} \tag{3.7}$$

where we have used that the eigenvalues do not change under transposition for an arbitrary quadratic matrix. Therefore, the eigenvalues and in particular the long-term cumulant-generating function inherit this symmetry

$$\lim_{t\to\infty} C(-\boldsymbol{\chi} - {\rm i}\boldsymbol{A}, -\boldsymbol{\xi} - {\rm i}\boldsymbol{B}, t) = \lim_{t\to\infty} C(\boldsymbol{\chi}, \boldsymbol{\xi}, t) \, . \tag{3.8}$$

Since the probability distribution $P_n(t)$ is given by a Fourier transform of the exponential of the cumulant-generating function, it follows that a symmetry relation of the form $C(-\chi - {\rm i}\alpha, t) =$

$C(+\chi, t)$ implies a fluctuation theorem of the form $P_{+n}(t)/P_{-n}(t) = e^{-n\alpha}$. Now, applying this to $2N$ dimensions, we conclude

$$\lim_{t\to\infty} \frac{P_{+\boldsymbol{\Delta N},+\boldsymbol{\Delta E}}(t)}{P_{-\boldsymbol{\Delta N},-\boldsymbol{\Delta E}}(t)} = e^{-(\boldsymbol{\Delta E}\cdot\boldsymbol{B}+\boldsymbol{\Delta N}\cdot\boldsymbol{A})} = e^{-\sum_\nu \beta_\nu[\Delta E_\nu - \mu_\nu \Delta N_\nu]} . \tag{3.9}$$

In the exponent, we recognize the integrated entropy change of the reservoirs, which in the long-term limit for a transport setup becomes the total entropy production, since the system contribution is negligible. Therefore, the interpretation of the above formula is as follows: Each trajectory with an exchange of $\boldsymbol{\Delta N}$ particles and an energy of $\boldsymbol{\Delta E}$ is associated with an entropy production of $\Delta_{\rm i} S = -\sum_\nu \beta_\nu \left[\Delta E_\nu - \mu_\nu \Delta N_\nu\right]$. Then, the fluctuation theorem corresponds to a stochastic formulation of the second law

Def. 1 (Crooks fluctuation theorem)**.** *A stochastic formulation of the second law is given by Crooks fluctuation theorem*

$$\frac{P_{+\Delta_{\rm i} S}}{P_{-\Delta_{\rm i} S}} = e^{+\Delta_{\rm i} S} , \tag{3.10}$$

where $\Delta_{\rm i} S$ is the total entropy production.

The Crooks relation [1] is more quantitative than the average statement of the second law discussed before. We just check here that the second law follows from it

$$\begin{aligned} \langle \Delta_{\rm i} S\rangle &= \sum_{\Delta_{\rm i} S} \Delta_{\rm i} S P_{\Delta_{\rm i} S} = \sum_{\Delta_{\rm i} S>0} \Delta_{\rm i} S \left[P_{+\Delta_{\rm i} S} - P_{-\Delta_{\rm i} S}\right] \\ &= \sum_{\Delta_{\rm i} S>0} \Delta_{\rm i} S P_{-\Delta_{\rm i} S} \underbrace{\left[\frac{P_{+\Delta_{\rm i} S}}{P_{-\Delta_{\rm i} S}} - 1\right]}_{\geq 0} \geq 0 . \end{aligned} \tag{3.11}$$

We note that Eq. (3.9) only holds at large times, since for finite times, the entropy change of the system has to be taken into account. In other words, the Crooks fluctuation theorem also holds at finite times when $\Delta_{\rm i} S$ denotes the full entropy production along a trajectory.

Chapter 4

Exact Results

4.1 A non-perturbative form for entropy production

A recent paper by M. Esposito nicely discusses general properties of entropy production that hold independent of the used master equation approaches [2]. We start from a setting where both system and interaction Hamiltonians are allowed to be time-dependent

$$H(t) = H_S(t) + \sum_\nu H_I^{(\nu)}(t) + \sum_\nu H_B^{(\nu)} . \tag{4.1}$$

Initially, we assume that the system and reservoirs are uncorrelated, and that the reservoirs are initially at thermal equilibrium states

$$\rho(0) = \rho_S(0) \bigotimes_\nu \bar{\rho}_\nu , \qquad \bar{\rho}_\nu = \frac{e^{-\beta_\nu (H_B^{(\nu)} - \mu_\nu N_B^{(\nu)})}}{Z_\nu} , \tag{4.2}$$

where Z_ν and $N_B^{(\nu)}$ denote partition function and reservoir particle number of reservoir ν, respectively. We will only assume this at the initial time, but not for $t > 0$. In fact, the treatment is so general that the reservoirs can be arbitrarily small, they can even consist of single qubits and they can move arbitrarily far away from any product state during the evolution. The only formal requirement is that they are initially represented as a thermal equilibrium state.

Since the evolution of the total universe is unitary, its total entropy is a constant of motion, yielding the relation

$$\Sigma(t) = -\mathrm{Tr}\left\{\rho(t) \ln \rho(t)\right\} = -\mathrm{Tr}\left\{\rho(0) \ln \rho(0)\right\} = -\mathrm{Tr_S}\left\{\rho_S(0) \ln \rho_S(0)\right\} - \sum_\nu \mathrm{Tr}_\nu \left\{\bar{\rho}_\nu \ln \bar{\rho}_\nu\right\} , \tag{4.3}$$

where we have used that for an initial product state it is additive in system and reservoir contributions. Now, we introduce the exact (i.e., without any master equation approximation) local reduced density matrices of system and reservoirs

$$\rho_S(t) = \mathrm{Tr}_{\{\nu\}}\left\{\rho(t)\right\} , \qquad \rho_\nu(t) = \mathrm{Tr}_{\mathrm{S},\nu' \neq \nu}\left\{\rho(t)\right\} , \tag{4.4}$$

and turn to the entropy of the system

$$S(t) = -\mathrm{Tr_S}\left\{\rho_S(t) \ln \rho_S(t)\right\} . \tag{4.5}$$

We see that its initial value is related to the full entropy of the universe via

$$S(0) = \Sigma(t) + \sum_\nu \mathrm{Tr}_\nu \left\{\bar\rho_\nu \ln \bar\rho_\nu\right\} . \tag{4.6}$$

Its change can therefore be written as

$$\begin{aligned}
\Delta S(t) &= S(t) - S(0)\\
&= -\mathrm{Tr}_{\mathrm{S}} \left\{\rho_S(t) \ln \rho_S(t)\right\} + \mathrm{Tr}\left\{\rho(t)\ln\rho(t)\right\} - \sum_\nu \mathrm{Tr}_\nu \left\{\bar\rho_\nu \ln \bar\rho_\nu\right\}\\
&= -\mathrm{Tr} \left\{\rho(t) \ln \rho_S(t)\right\} + \mathrm{Tr}\left\{\rho(t)\ln\rho(t)\right\} - \sum_\nu \mathrm{Tr}_\nu \left\{\bar\rho_\nu \ln \bar\rho_\nu\right\}\\
&= -\mathrm{Tr}\left\{\rho(t)\ln\left[\rho_S(t)\bigotimes_\nu \bar\rho_\nu\right]\right\} + \mathrm{Tr}\left\{\rho(t)\ln\rho(t)\right\} + \sum_\nu \mathrm{Tr}_\nu\left\{\left[\rho_\nu(t)-\bar\rho_\nu\right]\ln\bar\rho_\nu\right\}\\
&= D\left(\rho(t)\middle|\middle|\rho_S(t)\bigotimes_\nu\bar\rho_\nu\right) - \sum_\nu \beta_\nu \mathrm{Tr}_\nu\left\{\left[\rho_\nu(t)-\bar\rho_\nu\right]\left[H_B^{(\nu)}-\mu_\nu N_B^{(\nu)}\right]\right\} ,
\end{aligned} \tag{4.7}$$

where the first term is nothing but the distance – expressed in terms of the quantum relative entropy – between the actual exact density matrix of the full universe $\rho(t)$ and the product state of the exact reduced system density matrix and the reservoir states. The first term is thus positive and vanishes if and only if the system and bath density matrices are not correlated, it will be denoted as the **entropy production**

$$\Delta_{\mathrm{i}} S(t) = D\left(\rho(t)\middle|\middle|\rho_S(t)\bigotimes_\nu\bar\rho_\nu\right) \ge 0 . \tag{4.8}$$

We see that the entropy production is large when the distance between the actual state and the product state is large, such that it can be seen as quantifying the correlations between system and reservoir. For finite-size reservoirs, recurrences can occur, and the entropy production can behave periodically. We therefore note that its production rate need not be positive. In particular, for periodically evolving universes we must observe times where $\frac{d}{dt}\Delta_{\mathrm{i}}S(t) < 0$.

By contrast, the second term in (4.7) can be expressed by the heat leaving the reservoirs (analogous to entropy flow)

$$\begin{aligned}
\Delta_e S(t) &= -\sum_\nu \beta_\nu \mathrm{Tr}_\nu\left\{\left[\rho_\nu(t)-\bar\rho_\nu\right]\left[H_B^{(\nu)}-\mu_\nu N_B^{(\nu)}\right]\right\}\\
&= \sum_\nu \beta_\nu \Delta Q_\nu(t) ,
\end{aligned} \tag{4.9}$$

where the the heat flowing out of the reservoir ν is defined as

$$\Delta Q_\nu(t) = \left\langle H_B^{(\nu)} - \mu_\nu N_B^{(\nu)}\right\rangle_0 - \left\langle H_B^{(\nu)} - \mu_\nu N_B^{(\nu)}\right\rangle_t . \tag{4.10}$$

Summarizing, the second law can be written in standard form

$$\Delta S(t) = \Delta_{\mathrm{i}} S(t) + \sum_\nu \beta_\nu \Delta Q_\nu(t) , \tag{4.11}$$

or equivalently as $\Delta_{\mathrm{i}} S(t) = \Delta S(t) - \sum_\nu \beta_\nu \Delta Q_\nu(t) \ge 0$, where only the definition of the heat has to be adapted. A few notes are in order.

- By performing the operation $\lim_{t\to\infty} \frac{1}{t}[\ldots]$ on Eq. (4.11), we find for a finite-sized system and a constant global Hamiltonian

$$-\sum_\nu \beta_\nu \lim_{t\to\infty} \frac{\langle H_\nu - \mu_\nu N_\nu\rangle_0 - \langle H_\nu - \mu_\nu N_\nu\rangle_t}{t} = \lim_{t\to\infty} \frac{\Delta_{\rm i} S(t)}{t} \geq 0\,. \tag{4.12}$$

  Now, if the currents leaving the reservoirs assume steady state values in the long-time limit (this is an assumption)

$$\lim_{t\to\infty} \frac{d}{dt} \langle H_\nu\rangle_t = -\bar{I}_E^\nu\,, \qquad \lim_{t\to\infty} \frac{d}{dt} \langle N_\nu\rangle_t = -\bar{I}_M^\nu\,, \tag{4.13}$$

  we can invoke the rule of l'Hospital to evaluate the limit, yielding

$$-\sum_\nu \beta_\nu \left(\bar{I}_E^\nu - \mu_\nu \bar{I}_M^\nu\right) \geq 0\,. \tag{4.14}$$

  This shows that under the assumption of stationary currents, the conventional form of the second law at steady state also holds beyond weak coupling and also if interactions are present inside the system.

- In general (for $t > 0$) the total entropy is not just the sum of system entropy (4.5) and reservoir entropies

$$S_\nu(t) = -\mathrm{Tr}\left\{\rho_\nu(t) \ln \rho_\nu(t)\right\}\,. \tag{4.15}$$

  Instead, it is modified by the correlations between system and reservoir (e.g. entanglement). The **correlation entropy** is therefore defined as

$$S_c(t) = \Sigma(t) - S(t) - \sum_\nu S_\nu(t)\,. \tag{4.16}$$

  Due to the assumption of an initial product state we have $S_c(0) = 0$, and therefore with $\Sigma(t) = \Sigma(0)$ the relation

$$S_c(t) = S_c(t) - S_c(0) = -\Delta S(t) - \sum_\nu \Delta S_\nu(t) \tag{4.17}$$

  However, by construction we also have

$$\begin{aligned} D\left(\rho(t)||\rho_S(t) \bigotimes_\nu \rho_\nu(t)\right) &= \mathrm{Tr}\left\{\rho(t)\ln\rho(t)\right\} - \mathrm{Tr}\left\{\rho(t)\left[\ln\rho_S(t) + \sum_\nu \ln\rho_\nu(t)\right]\right\} \\ &= -\Sigma(t) - \mathrm{Tr_S}\left\{\rho_S(t)\ln\rho_S(t)\right\} - \sum_\nu \mathrm{Tr}_\nu\left\{\rho_\nu(t)\ln\rho_\nu(t)\right\} \\ &= -\Sigma(t) + S(t) + \sum_\nu S_\nu(t) = -S_c(t) \geq 0\,. \end{aligned} \tag{4.18}$$

  The correlation entropy is thereby always negative. Now, since the sum of entropy production and correlation entropy

$$\Delta_{\rm i} S(t) + S_c(t) = -\sum_\nu \beta_\nu \Delta Q_\nu(t) - \sum_\nu \Delta S_\nu(t) = \sum_\nu D(\rho_\nu(t)||\bar{\rho}_\nu) \geq 0 \tag{4.19}$$

  is still positive, we get the hierarchy

$$\Delta_{\rm i} S(t) \geq -S_c(t) \geq 0\,. \tag{4.20}$$

- We can solve Eq. (4.7) for the entropy production

$$\Delta_{\rm i} S(t) = S(t) - S(0) - \sum_\nu \beta_\nu \Delta Q_\nu(t) \,. \tag{4.21}$$

Performing a time derivative on both sides yields

$$\frac{d}{dt}\Delta_{\rm i} S(t) = \dot{S}(t) - \sum_\nu \beta_\nu \Delta \dot{Q}_\nu(t) \,, \tag{4.22}$$

where $\dot{Q}_\nu(t)$ now denotes the heat current entering the system from reservoir ν. In general, this quantity will not be positive. However, assuming evolution under a Lindblad form, we know that also the entropy production rate $\frac{d}{dt}\Delta_{\rm i} S(t) \to \dot{S}_{\rm i} \geq 0$ is positive. Indeed, negative entropy production rates are sometimes used as a marker for a non-Markovian evolution [3].

Bibliography

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