Quantum Stochastic Thermodynamics

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May 10, 2023

The frist of many

These notes contain my solutions of the exercises and the examples provided in the book *"Quantum Stochastic Thermodynamics: Foundations and Selected Applications"* by Philip Strasberg.

I chose the names of examples and exercises to give an approximate idea of what they are about. Additionally, I changed the formualtion of most exercises to make them easier to understand without the whole book. Note that, while I tried to be as precise and complete as possible in the formulation of the exercises, in the solutions I often drop arguments or indices because they should be clear from the context.

Additionally, in some exercise some numerics were required. I included the codes, written in python or matlab, and the figures generated with them.

Contents

1 Quantum Stochastic Processes

Example 1.1: Evolution of an open quantum system

Consider n spins coupled with random strengths $g_{ij} \in [0, \Omega]$ evolving according to the Hamiltonian

$$H_{\text{tot}} = \sum_{i=1}^{n} \frac{\Omega}{2} \sigma_z^{(i)} + \sum_{i<j} \frac{g_{ij}}{2} \sigma_x^{(i)} \sigma_x^{(j)}.$$

Let's separate the spins into the "system" S made of a single spin, and the "bath" B made of the remaining spins. The Hamiltonian is then split into $H_{\text{tot}} = H_S + H_B + H_{SB}$, where H_{SB} is the interaction Hamiltonian between S and B.

Compute the evolution of the state when at $t = 0$ the system is prepared in

$$\rho_{\text{tot}}(0) = |+\rangle\langle+|_S \otimes \frac{e^{-\beta H_B}}{\mathcal{Z}_B}$$

```
import numpy as np
from qutip import *
import matplotlib.pyplot as plt
###############################
n = 7;      #Number of spins
Omega = 1;  #Energy gap of single spin
g = np.random.rand(n,n);    #Random coupling strengths
###############################
# Useful operators
eye= Qobj([[1,0], [0, 1]]); # Single spin identity
sx = Qobj([[0,1], [1, 0]]); # Single spin S_x
sy = sigmay();              # Single spin S_y
sz = Qobj([[1,0], [0,-1]]); # Single spin S_z
EYE= [eye]*n;               # n-spins identity
###############################
## Hamiltonians
H=0;    #Total
for i in range(n):
    tEYE = EYE*1;tEYE[i] = sz;
    H+= Omega/2*tensor(tEYE);
for i in range(n):
    for j in range(n-i-1):
        tz1 = EYE*1; tz2 = EYE*1;
        tz1[i] = sx; tz2[j] = sx;
        H+=g[i,j]/2*tensor(tz1)*tensor(tz2);

HB=0    #Bath
for i in range(n-1):
    tEYE = [eye]*(n-1);tEYE[i] = sz;
    HB+= Omega/2*tensor(tEYE);
for i in range(n-1):
    for j in range(n-i-2):
        tz1 = [eye]*(n-1); tz2 = [eye]*(n-1);
        tz1[i] = sx; tz2[j] = sx;
        HB+=g[i+1,j+1]/2*tensor(tz1)*tensor(tz2);

HS = Omega/2*sz;    #System
################################
def initial_states(beta):
    rhoS = Qobj([[1, 1],[1, 1]]);   rhoS/=rhoS.tr();
    rhoB = (-beta*HB).expm();   rhoB/=rhoB.tr();
    rSth = (-beta*HS).expm();   rSth/=rSth.tr();
    rhoI = tensor(rhoS, rhoB);
    return [rhoI, rSth]
################################
def calc_plot(beta, N):
    t = np.linspace(0, 60*Omega, N);

    states = initial_states(beta);
    rhoI = states[0]; rSth = states[1];

    SX = EYE*1; SX[0] = sx; SX = tensor(SX);
    SY = EYE*1; SY[0] = sy; SY = tensor(SY);
    SZ = EYE*1; SZ[0] = sz; SZ = tensor(SZ);
    result = mesolve(H, rhoI, t, [], [SX, SY, SZ])
    SSx = result.expect[0];
```

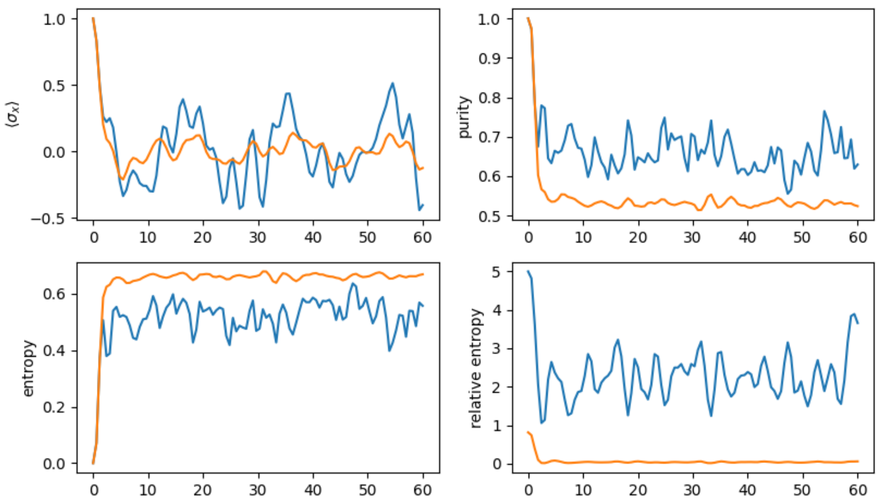


Figure 1: Output of code in Example 1.1. The blue line corresponds to $\beta\Omega = 10$, which means that the "bath" of $(n-1) = 6$ spins is initially cold. Instead, the orange line corresponds to $\beta\Omega = 1$, which means that the "bath" is initially hot.

```
    SSy = result.expect[1];
    SSz = result.expect[2];

    purity=np.zeros(N);entropy=np.zeros(N);relentr=np.zeros(N);

    for i in range(N):
        X = eye/2 + SSx[i]/2*sx + SSy[i]/2*sy + SSz[i]/2*sz
        purity[i] = (X*X).tr()
        entropy[i]=entropy_vn(X)
        relentr[i]=entropy_relative(X, rSth)

    #Plots
    plt.subplot(221)
    plt.plot(t, SSx);
    plt.ylabel(r"$\langle \sigma_x \rangle$");
    plt.subplot(222)
    plt.plot(t, purity);
    plt.ylabel("purity");
    plt.subplot(223)
    plt.plot(t, entropy);
    plt.ylabel("entropy");
    plt.subplot(224)
    plt.plot(t, relentr);
    plt.ylabel("relative entropy");

    return [t, X, purity, entropy, relentr]
######################################
N= 100;
beta = 10;
calc_plot(beta, N)
beta = 1;
calc_plot(beta, N)
######################################
plt.show();
```

Exercise 1.1: Time independent global Hamiltonian

Show that, if $\rho_{SB}(0) = \pi_{SB}$ and if H_{SB} is time independent, $\rho_{SB}(0) = \pi_{SB}$ for all t.

Solution:
The unitary evolution is $U(t) = e^{-iH_{SB}t}$ and determines the time evolution of the state through $\rho_{SB}(t) = U(t)\rho_{SB}(0)U(t)^\dagger$. Since the initial state and the unitary transformation commute, for all t we have

$\rho_{SB}(t) = \rho_{SB}(0)$

Exercise 1.2: Quantum Caldeira-Leggett model

Consider a harmonic oscillator with frequency ω and Hamiltonian $H_S = \frac{1}{2}(p_S^2 + \omega^2 x_S^2)$ coupled to a bath of one other harmonic oscillator with the same frequency. The global Hamiltonian is

$$H_{SB} = H_S + \frac{1}{2}\left[p_B^2 + \omega^2\left(x_B - \frac{c}{\omega^2}x_S\right)^2\right]. \tag{1}$$

The goal of this exercise is to show that, unlike the classical case, the local quantum state on S is not $\pi_S = e^{-\beta H_S}/Z_S$, but is actually $\pi_S^* = \mathrm{Tr}_B\left\{e^{-\beta H_{SB}}\right\}/Z_{SB}$.

1. Show that for a classical system $\pi_S^* = \pi_S$.
2. Show that for a quantum system $\pi_S^* \neq \pi_S$ by computing $\langle x_S^2\rangle$.

Solution:

1. Calculating the classical trace correponds to integrating over the phase space of the bath B, namely

$$\frac{1}{Z}\mathrm{Tr}_B\left\{e^{-\beta H_{SB}}\right\} = \int \frac{d^3x_B d^3p_B}{h^3}\frac{e^{-\beta H_{SB}}}{Z} = \frac{e^{-\beta H_{SB}}}{Z}\left(\frac{2\pi}{\beta}\right)^{3/2}\left(\frac{2\pi}{\beta\omega^2}\right)^{3/2} = \left(\frac{2\pi}{\beta\omega}\right)^3\frac{e^{-\beta H_S}}{Z}$$

. Remembering the partition function Z is just the trace over all the phase space of the Boltzmann exponential,

$$Z = \int \frac{d^3x_S d^3x_B d^3p_S d^3p_B}{h^6}e^{-\beta H_{SB}} = \left(\frac{2\pi}{\beta\omega}\right)^6,$$

we quickly realize that the reduced state on S coincides with the thermal state on S:

$$\pi_S^* = \left(\frac{\beta\omega}{2\pi}\right)^3 e^{-\beta H_S} = \frac{e^{-\beta H_S}}{Z_S} = \pi_S$$

2. Writing the Hamiltonian in full we get

$$H_{SB} = \frac{1}{2}\left[p_S^2 + p_B^2 + \omega^2 x_S^2 + \omega^2\left(x_B - \frac{c}{\omega^2}x_S\right)^2\right].$$

In particular, the potential energy (depending on the coordinates x_S, x_B) can be written as the scalar product

$$\frac{1}{2}\begin{pmatrix}x_S & x_B\end{pmatrix}\begin{pmatrix}\omega^2 + \frac{c^2}{\omega^2} & -c\\ -c & \omega^2\end{pmatrix}\begin{pmatrix}x_S\\ x_B\end{pmatrix} = \frac{1}{2}\vec{X}^\dagger A\vec{X}.$$

Since we want to diagonalize the Hamiltonian into its normal modes, we now diagonalize the potential energy of the system. The characteristic polynomial of A and its solutions read

$$(\omega^2 + \frac{c^2}{\omega^2} - \lambda)(\omega^2 - \lambda) - c^2 = \lambda^2 - \lambda(2\omega^2 + \frac{c^2}{\omega^2}) + \omega^4 = 0 \rightarrow \lambda_\pm = \omega^2 + \frac{c^2}{2\omega^2} \pm c\sqrt{1 + \frac{c^2}{4\omega^4}}$$

and the corresponding eigenvestors $\begin{pmatrix}\alpha^* & \beta^*\end{pmatrix}^\dagger$ satisfy

$$\begin{pmatrix}\frac{c^2}{2\omega^2} \mp c\sqrt{1 + \frac{c^2}{4\omega^4}} & -c\\ -c & -\frac{c^2}{2\omega^2} \mp c\sqrt{1 + \frac{c^2}{4\omega^4}}\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \vec{0} \rightarrow \vec{v}_\pm = \begin{pmatrix}1\\ \frac{c}{2\omega^2} \mp \sqrt{1 + \frac{c^2}{4\omega^4}}\end{pmatrix}.$$

We can now write the initial coordinates x_S, x_B in terms of the eigenmodes of the potential, namely

$$\begin{pmatrix}x_S\\ x_B\end{pmatrix} = q_+\vec{v}_+ + q_-\vec{v}_- \rightarrow \begin{cases} x_S = q_+ + q_-\\ x_B = \frac{c}{2\omega^2}(q_+ + q_-) + \sqrt{1 + \frac{c^2}{4\omega^4}}(q_- - q_+)\end{cases},$$

from which we can also find how the momenta transform by using the chain rule. In fact,

$$\begin{cases} p_+ = -i\hbar\partial_{q_+} = -i\hbar\left[\frac{\partial x_S}{\partial q_+}\partial_{x_S} + \frac{\partial x_B}{\partial q_+}\partial_{x_B}\right] = p_S + \left(\frac{c}{2\omega^2} - \sqrt{1+\frac{c^2}{4\omega^4}}\right)p_B \\ p_- = -i\hbar\partial_{q_-} = -i\hbar\left[\frac{\partial x_S}{\partial q_-}\partial_{x_S} + \frac{\partial x_B}{\partial q_-}\partial_{x_B}\right] = p_S + \left(\frac{c}{2\omega^2} + \sqrt{1+\frac{c^2}{4\omega^4}}\right)p_B \end{cases}$$

Invering these relations we get

$$\begin{cases} p_B = \frac{p_- - p_+}{2\sqrt{1+c^2/(4\omega^4)}} \\ p_S = p_+\left(\frac{1}{2} + \frac{c}{4\omega^2\sqrt{1+c^2/(4\omega^4)}}\right) - p_-\left(\frac{c}{4\omega^2\sqrt{1+c^2/(4\omega^4)}} - \frac{1}{2}\right) \end{cases}$$

A good consistency check is to calculate the commutators $[x_\alpha, p_\beta] = i\hbar\delta_{\alpha\beta}$. Now we can rewrite the Hamiltonian H_{SB} in terms of the normal modes. Let's start from the kinetic terms:

$$\begin{aligned}
\frac{1}{2}(p_S^2+p_B^2) = \frac{1}{2}\Bigg[&p_+^2\left(\frac{1}{4+c^2/\omega^4} + \left(\frac{1}{2} + \frac{c}{4\omega^2\sqrt{1+c^2/(4\omega^4)}}\right)^2\right) \\
&+ p_-^2\left(\frac{1}{4+c^2/\omega^4} + \left(\frac{1}{2} - \frac{c}{4\omega^2\sqrt{1+c^2/(4\omega^4)}}\right)^2\right) \\
&+ 2p_+p_-\left(\frac{1}{4+c^2/\omega^4} + \left(\frac{1}{2} + \frac{c}{4\omega^2\sqrt{1+c^2/(4\omega^4)}}\right)\left(\frac{1}{2} - \frac{c}{4\omega^2\sqrt{1+c^2/(4\omega^4)}}\right)\right)\Bigg] \\
\frac{1}{2}(p_S^2+p_B^2) = \frac{1}{2}\Bigg[&\frac{p_+^2}{4(1+c^2/(4\omega^4))}\left(1+1+\frac{c^2}{4\omega^4}+\frac{c^2}{4\omega^4}+\frac{c}{\omega^2}\sqrt{1+\frac{c^2}{4\omega^4}}\right) \\
&+ \frac{p_-^2}{4(1+c^2/(4\omega^4))}\left(1+1+\frac{c^2}{4\omega^4}+\frac{c^2}{4\omega^4}-\frac{c}{\omega^2}\sqrt{1+\frac{c^2}{4\omega^4}}\right) \\
&+ 2p_+p_-\left(\frac{1}{4+c^2/\omega^4} + \frac{1}{4} - \frac{1}{4}\frac{c^2}{4\omega^4(1+c^2/(4\omega^4))}\right)\Bigg] \\
\frac{1}{2}(p_S^2+p_B^2) = \frac{1}{2}\Bigg[&\frac{p_+^2}{4(1+c^2/(4\omega^4))}\left(\frac{\omega^2+\lambda_+}{\omega^2}\right) + \frac{p_-^2}{4(1+c^2/(4\omega^4))}\left(\frac{\omega^2+\lambda_-}{\omega^2}\right)\Bigg].
\end{aligned}$$

Now, let's look at the potential terms

$$\begin{aligned}
\frac{1}{2}\left[x_S^2 + \left(x_B - \frac{c}{\omega^2}x_S\right)^2\right] = \frac{1}{2}\Bigg[&q_+^2\left(1+\left(\frac{c}{2\omega^2} - \sqrt{1+\frac{c^2}{4\omega^4}} - \frac{c}{\omega^2}\right)^2\right) \\
&+ q_-^2\left(1+\left(\frac{c}{2\omega^2} + \sqrt{1+\frac{c^2}{4\omega^4}} - \frac{c}{\omega^2}\right)^2\right) \\
&+ 2q_+q_-\left(1+\left(\frac{c}{2\omega^2} + \sqrt{1+\frac{c^2}{4\omega^4}} - \frac{c}{\omega^2}\right)\left(\frac{c}{2\omega^2} - \sqrt{1+\frac{c^2}{4\omega^4}} - \frac{c}{\omega^2}\right)\right)\Bigg] \\
\frac{1}{2}\left[x_S^2 + \left(x_B - \frac{c}{\omega^2}x_S\right)^2\right] = \frac{1}{2}\Bigg[&q_+^2\left(1+\frac{c^2}{4\omega^4}+1+\frac{c^2}{4\omega^4}+\frac{c}{\omega^2}\sqrt{1+\frac{c^2}{4\omega^4}}\right) \\
&+ q_-^2\left(1+\frac{c^2}{4\omega^4}+1+\frac{c^2}{4\omega^4}-\frac{c}{\omega^2}\sqrt{1+\frac{c^2}{4\omega^4}}\right) \\
&+ 2q_+q_-\left(1-\left(1+\frac{c^2}{4\omega^4}\right)+\frac{c^2}{4\omega^4}\right)\Bigg] \\
\frac{1}{2}\left[x_S^2 + \left(x_B - \frac{c}{\omega^2}x_S\right)^2\right] = \frac{1}{2}\Bigg[&q_+^2\left(\frac{\omega^2+\lambda_+}{\omega^2}\right) + q_-^2\left(\frac{\omega^2+\lambda_-}{\omega^2}\right)\Bigg].
\end{aligned}$$

Therefore, we finally wrote the Hamiltonian in diagonal form and we can separate the two modes as follows

$$H_\pm = \frac{1}{2}\frac{\omega^2+\lambda_\pm}{4\omega^2(1+c^2/(4\omega^4))}\left(p_\pm^2 + 4\omega^2\left(1+\frac{c^2}{4\omega^4}\right)q_\pm^2\right)$$

Calling $\nu^2 = 4\omega^2(1 + c^2/(4\omega^4))$ we can decompose the coordinate and momentum in the creation and annihilation operators

$$q_\pm = \frac{\ell}{\sqrt{2}}(a_\pm^\dagger + a_\pm), \qquad p_\pm = \frac{i\hbar}{\ell\sqrt{2}}(a_\pm^\dagger - a_\pm), \qquad \ell^2 = \frac{\hbar}{\nu}.$$

Substituting this into the modes' Hamiltonians we get

$$H_\pm = \frac{1}{2}\frac{\omega^2 + \lambda_\pm}{4\omega^2(1 + c^2/(4\omega^4))}\hbar\left(2\omega\sqrt{1 + \frac{c^2}{4\omega^4}}\right)(a_\pm^\dagger a_\pm + a_\pm a_\pm^\dagger).$$

Here we can read the frequencies of the modes:

$$\Omega_\pm = \frac{\omega^2 + \lambda_\pm}{2\omega\sqrt{1 + c^2/(4\omega^4)}} \to \Omega_\pm^2 = \frac{\omega^4 + \lambda_\pm^2 + 2\omega^2\lambda_\pm}{4\omega^2(1 + c^2/(4\omega^4))} = \frac{\lambda_\pm(2\omega^2 + c^2/\omega^2 + 2\omega^2)}{(4\omega^2 + c^2/\omega^2)} = \lambda_\pm.$$

As expected, the normal modes frequencies are simply the roots of the eigenvalues of the potential matrix A. With these definitions the total Hamiltonian looks very simple, namely

$$H_{SB} = \hbar\Omega_+(a_+^\dagger a_+ + \frac{1}{2}) + \hbar\Omega_-(a_-^\dagger a_- + \frac{1}{2}).$$

Neglecting the constant $\hbar(\Omega_+ + \Omega_-)/2$, which is irrelavant for the statistical properties of the system, we can calculate the partition function of the global system

$$Z_{SB} = \sum_{n,m=0}^{\infty} e^{-\beta\hbar\Omega_+ n} e^{-\beta\hbar\Omega_- m} = \frac{1}{1 - e^{-\beta\hbar\Omega_+}}\frac{1}{1 - e^{-\beta\hbar\Omega_-}}.$$

To calculate $\langle x_S^2 \rangle$ we make use of $x_S = q_+ + q_-$ and the decomposition of the normal coordinates in the corresponding creation and annihilation operators. In particular, taking the square of $(a_+ + a_- + a_+^\dagger + a_-^\dagger)$ only the $a_\alpha a_\alpha^\dagger$ and $a_\alpha^\dagger a_\alpha$ give a non-vanishing contribution becuase they do not change the normal eigenmode. Therefore,

$$\langle x_S^2 \rangle = \frac{\ell^2}{2}\langle 2a_+^\dagger a_+ + 2a_-^\dagger a_- + 2\rangle = \ell^2\left[-\frac{\partial}{\partial(\beta\hbar\Omega_+)}\log Z_{SB} - \frac{\partial}{\partial(\beta\hbar\Omega_-)}\log Z_{SB} + 1\right]$$

Noticing that $\Omega_+ + \Omega_- = (4\omega^2 + c^2/\omega^2)/[2\omega\sqrt{1 + c^2/(4\omega^4)}] = 2\omega\sqrt{1 + c^2/(4\omega^4)} = \nu$, and calculating the trivial derivatives of the partition function, we obtain

$$\langle x_S^2 \rangle = \ell^2\left[\frac{1}{e^{\beta\hbar\Omega_+} - 1} + \frac{1}{e^{\beta\hbar\Omega_-} - 1} + 1\right] = \frac{\hbar}{\Omega_+ + \Omega_-}\left[\frac{e^{\beta\hbar(\Omega_+ + \Omega_-)} - 1}{(e^{\beta\hbar\Omega_+} - 1)(e^{\beta\hbar\Omega_-} - 1)}\right].$$

This is clearly different from the average $\langle x_S^2 \rangle_{\pi_S}$, which imples that the actual partial state π_S^* is *different* from the local thermal state π_S. Taking the classical limit, $\hbar \to 0$, we are left with

$$\langle x_S^2 \rangle = \frac{1}{\beta\Omega_-\Omega_+} = \frac{k_B T}{\sqrt{\omega^4 - c^2 + c^2}} = \frac{k_B T}{\omega^2}.$$

Exercise 1.3: Projective measurements with density matrices

Consider the rank 1 projectors $\Pi_S = |x\rangle\langle x|$ and the pure state $\rho_S = |\psi\rangle\langle\psi|$. What corresponds to the Born rule? Which equation describes the "collapse" of the wave function? When does the measurement reveal no information, i.e. $\rho'_S(x) = \rho_S$? Give a physical example where the projectors are not of rank 1.

Solution:
The Born rule is $p(x) = \mathrm{Tr}\{\Pi_S\rho_S\} = |\langle x|\psi\rangle|^2$ and the collapsed wave function is $\rho'_S(x) = \Pi_S\rho_S\Pi_S/p(x) = |x\rangle\langle x|$. The measurement does not give any information when the state is already in an eigenspace. A simple example consists of two spin 1/2 (distinguishable) systems. The total spin operator has three eigenvalues (-1, 0, 1) with non-trivial degeneracy (1, 2, 1).

Exercise 1.4: POVM $\Rightarrow$ probabilities

Show that any set of operators $\{M(r)\}_r$ satisfying

$$M(r) \geq 0, \qquad \sum_r M(r) = \mathbb{I}$$

gives rise to a set of well defined probabilities $p(r) = \mathrm{Tr}_S\{M(r)\rho_S\}$ for any state ρ_S.

Solution:
For any state ρ_S we can write the eigendecomposition $\rho_S = \sum_j \lambda_j |j\rangle\langle j|$, with $\lambda_j \geq 0$. The probability then reads

$$p(r) = \sum_j \lambda_j \langle j|M(r)|j\rangle \geq 0$$

where we used the positivity of $M(r)$, namely that, for all $|\psi\rangle$, $\langle\psi|M(r)|\psi\rangle \geq 0$.
Summing up all the probabilities we get

$$\sum_r p(r) = \mathrm{Tr}_S\left\{\sum_r M(r)\rho_S\right\} = \mathrm{Tr}_S\{\rho_S\} = 1.$$

Exercise 1.5: Imperfect quantum measurements on pure states

The operators $K(r) = \sum_x \sqrt{p(r|x)}\Pi_S(x)$ and $K_x(r) = \sqrt{p(r|x)}\Pi_S(x)$ induce the same measurement statistics $M(r) = \sum_x p(r|x)\Pi_S(x)$, but lead to different quantum states. Consider a pure initial state $\rho_S = |\psi\rangle\langle\psi|$. We now study how these different measurements affect the final state ρ'_S.

1. Show that the post-measurement state of $K(r) = \sum_x \sqrt{p(r|x)}\Pi_S(x)$ is pure.
2. Show that the post-measurement state of $K_x(r) = \sqrt{p(r|x)}\Pi_S(x)$ is generally not pure.

Solution:

1. The probability of observing the outcome r is

$$p(r) = \mathrm{Tr}_S\left\{\sum_x p(r|x)\Pi_S(x)\rho_S\right\} = \mathrm{Tr}_S\{M(r)|\psi\rangle\langle\psi|\}.$$

The final state is $\rho'_S(r) = K(r)\rho_S K^\dagger(r)/p(r)$. The state is pure iff $[\rho'_S(r)]^2 = \rho'_S(r)$. Without writing explicitely the summations and using $\Pi_S(x)\Pi_S(y) = \delta_{xy}\Pi_S(x)$, we get

$$[\rho'_S(r)]^2 = \frac{1}{p(r)^2}\sqrt{p(r|x)}\Pi_S(x)\rho_S\sqrt{p(r|y)}\Pi_S(y)\sqrt{p(r|x')}\Pi_S(x')\rho_S\sqrt{p(r|y')}\Pi_S(y')$$
$$[\rho'_S(r)]^2 = \frac{1}{p(r)}\sqrt{p(r|x)}\Pi_S(x)|\psi\rangle\frac{\langle\psi|M(r)|\psi\rangle}{p(r)}\langle\psi|\sqrt{p(r|y')}\Pi_S(y') = \rho'_S(r)$$

2. The post-measument state reads

$$\rho'_S(r) = \frac{1}{p(r)}\sum_x p(r|x)\Pi_S(x)\rho_S\Pi_S(x).$$

It is sufficient to find an example for which the state is not pure. Let $\rho_S = |+\rangle\langle+|$, with $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$, and $\Pi_S(0) = |0\rangle\langle 0|$, $Pi_S(1) = |1\rangle\langle 1|$. The final state then becomes

$$\rho'_S(r) = \frac{1}{p(r)}\sum_x p(r|x)\frac{1}{2}|x\rangle\langle x|,$$

which is clearly mixed when there is measurement error ($p(r|x) \notin \{0,1\}$).

Exercise 1.6: Classical measurements

Replace the notion of the densiti matrix with its classical counterpart, a probability vector $\mathbf{p}$. Calling $p(r|x)$ the condiitonal probability of obtaiing the measurement result r given that the system is in state x, we define the matrix $M_{xy}(r) = \delta_{xy}p(r|x)$.

What do $M(r)$ and a POVM have in common? What is the quantum counterpart of the classical expression $M(r)\mathbf{p}$? Relate the probability $p(r) = \sum_x p(r|x)p(x)$ to obtain the outcome r to the expression $M(r)\mathbf{p}$. Show that the (normalized) post-measurement state of the system given result r obeys **Bayes' rule** $p'(x|r) = p(r|x)p(x)/p(r)$. Verify that the average post-measurement state does not change: $\mathbf{p}' = \mathbf{p}$.

Solution:
Similarly to the POVM, the classical matrix $M(r)$ is non-negative and sum up to the identity:

$$\mathrm{Tr}\left\{M(r)\mathbf{p}\right\} = \sum_x p(r|x)p(x) \geq 0, \qquad \sum_r M(r) = \delta_{xy} = \mathbb{I}.$$

Additionally, the scalar $\mathrm{Tr}\left\{M(r)\mathbf{p}\right\} = p(r)$ is the probability of observing the outcome r. The quantum counterpart of $M(r)\vec{p}$ is the (non-normalized) post-measurement state $\bar{\rho}'_S(r) = \sum_x K_x(r)\rho_S K_x^\dagger(r)$. The normalized post-measurement state is $\mathbf{p}'(r) = M(r)\mathbf{p}/p(r)$, whose components are $p'(x|r) = p(r|x)p(x)/p(r)$, obeying Bayes' rules. The average post-measurement state is $\mathbf{p}' = \sum_r M(r)\mathbf{p} = \mathbb{I}\mathbf{p} = \mathbf{p}$.

Exercise 1.7: Transposition in not a quantum channel

Let $\rho = \rho_{00}\left|0\right\rangle\!\left\langle 0\right| + \rho_{10}\left|1\right\rangle\!\left\langle 0\right| + \rho_{01}\left|0\right\rangle\!\left\langle 1\right| + \rho_{11}\left|1\right\rangle\!\left\langle 1\right|$ be the density matrix of a qubit. The transpose operation with respect to the basis $\{\left|0\right\rangle, \left|1\right\rangle\}$ acts as $\mathcal{T}\rho = \rho_{00}\left|0\right\rangle\!\left\langle 0\right| + \rho_{10}\left|0\right\rangle\!\left\langle 1\right| + \rho_{01}\left|1\right\rangle\!\left\langle 0\right| + \rho_{11}\left|1\right\rangle\!\left\langle 1\right|$

Show that this map is positive, but not completely positive.

Solution:
For a matrix M, the transposed matrix M^T has the same spectrum. Therefore, if $M \geq 0$ then also $M^T \geq 0$. This means that the transposition $\mathcal{T}$ is indeed positive. However, we now consider the Bell state $(\left|00\right\rangle + \left|11\right\rangle)/\sqrt{2}$ in a larger Hilber space. The initial density matrix reads $\rho_{SB} = \frac{1}{2}(\left|00\right\rangle\!\left\langle 00\right| + \left|00\right\rangle\!\left\langle 11\right| + \left|11\right\rangle\!\left\langle 00\right| + \left|11\right\rangle\!\left\langle 11\right|)$, while the final one reads

$$\mathcal{T}_S\rho_{SB} = \frac{1}{2}(\left|00\right\rangle\!\left\langle 00\right| + \left|10\right\rangle\!\left\langle 01\right| + \left|01\right\rangle\!\left\langle 10\right| + \left|11\right\rangle\!\left\langle 11\right|) = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

which has one negative eigenvalue $(-1/2)$ with the eigenvector $\left|10\right\rangle - \left|01\right\rangle$. Therefore this transformation in not physical, meaning that it cannot be realized by an anctual physical system.

Exercise 1.8: Extending convex linear maps

Let $\mathcal{C}$ be a convex linear map acting on density matrices ρ of a Hilbert space with dimension $\dim\mathcal{H} = d$. Show that every complex matrix A on $\mathcal{H}$ can be written as a linear combination of density matrices ρ_i with complex coefficients $c_i \in \mathbb{C}$, i.e. $A = \sum_i C_i\rho_i$.

The extension $\bar{\mathcal{C}}$ is then defined via $\mathcal{C}A = \sum_i c_i\mathcal{C}\rho_i$.

Solution:
Since every matrix A can be written as a combination some hermitian matrices A_1, A_2 as $A = A_1 + iA_2$, and every hermitian B can be written as the difference $B = B_+ - B_-$ with $B_\pm$ hermitian positive matrices, all matrices A can be written as a linear combination of hermitian positive matrices. This means that every matrix A can be written as a linear combination of states ρ_i.

Exercise 1.9: Non-uniqueness of the operator-sum representation

Consider the map $\mathcal{C}\rho = \sum_\alpha K_\alpha\rho K_\alpha^\dagger$, and define $K_\alpha \equiv \sum_\beta u_{\alpha\beta}\bar{K}_\beta$ for an arbitrary unitary $U = \{u_{\alpha\beta}\}$.

Show that $\mathcal{C}\rho = \sum_\alpha \bar{K}_\alpha\rho\bar{K}_\alpha^\dagger$.

Solution:
Using the unitary of U, namely that $UU^\dagger = \mathbb{I}$, or equivalently $\sum_\beta u_{\alpha\beta}u^*_{\gamma\beta} = \delta\alpha\gamma$ we get

$$\mathcal{C}\rho = \sum_{\alpha\beta\gamma} u_{\alpha\beta}\bar{K}_\beta\rho\bar{K}^\dagger_\gamma u^*_{\alpha\gamma} = \sum_{\beta\gamma}\bar{K}_\beta\rho\bar{K}^\dagger_\gamma\delta_{\beta\gamma} = \sum_\beta \bar{K}_\beta\rho\bar{K}^\dagger_\beta$$

Exercise 1.10: Using the unitary dilation theorem

Use the unitary dilation theorem to derive

$$\bar{\rho}'_S(r) = \mathcal{C}(r)\rho_S = \sum_{\alpha_r} K_{\alpha_r}\rho_S K^\dagger_{\alpha_r}, \qquad \rho'_S = \mathcal{C}\rho_S = \sum_\alpha K_\alpha\rho_S K^\dagger_\alpha$$

and identify the operators K_{α_r}. Confirm that the maximum number of operators K_α is the dimansion of the ancilla $\mathcal{H}_A$, namely d^2.

Solution:
The unitary dilation therorem states that

$$\mathcal{C}(r)\rho_S = \mathrm{Tr}_A\left\{\Pi_A(r)U_{SA}(\rho_S\otimes|\phi\rangle\langle\phi|)U^\dagger_{SA})\right\} = \sum_j \langle j|_A\,\Pi_A(r)U_{SA}(\rho_S\otimes|\phi\rangle\langle\phi|_A)U^\dagger_{SA})\Pi_A(r)\,|j\rangle_A$$

$$\mathcal{C}(r)\rho_S = \sum_j \langle j|_A\,\Pi_A(r)U_{SA}\,|\phi\rangle\,\rho_S\,\langle\phi|_A\,U^\dagger_{SA}\Pi_A(r)\,|j\rangle_A\,.$$

In the sum there are terms that vanish because of the projector $\Pi_A(r)$. In particular, the surviving terms are those for which $\Pi_A(r)\,|j\rangle \neq 0$. Calling this set $\{j_r\}$ we identify the operator

$$K_{j_r} = \langle j_r|_A\,\Pi_A(r)U_{SA}\,|\phi\rangle_A\,.$$

Clearly, summing over all outcomes r yields $K_j = \langle j|_A\,U_{SA}\,|\phi\rangle_A$. Furthermore, since we labeled the operators with the basis of $\mathcal{H}_A$ (j), the maximum number of K_j is equal to the dimension of $\mathcal{H}_A$, i.e. d^2.

Exercise 1.11: Breaking the unitary dilation theorem

Consider the interaction of two qubits. The first one being the system and the second one being the ancilla. We consider the maximally entangled stated $|\pm\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}$ and the evolution governed by the unitary $U_{SA} = |+\rangle\langle+| + |-\rangle\langle 10| + |10\rangle\langle-| + |01\rangle\langle 01|$. Let the initial state $\rho_{SA} = |+\rangle\langle+|$ be entangled.

1. Confirm that U_{SA} is unitary.
2. The initial reduced state is $\rho_S = (|0\rangle\langle 0| + |1\rangle\langle 1|)/2$.
3. The final state ρ'_S coincides with the initial one, $\rho'_S = \rho_S$.
4. If we first perform a measurement of the initial system in its eigenbasis, the initial system state does not change on average, $|0\rangle\langle 0|\,\rho_S\,|0\rangle\langle 0| + |1\rangle\langle 1|\,\rho_S\,|1\rangle\langle 1| = \rho_S$, but the final system state now is $|0\rangle\langle 0|/4 + 3\,|1\rangle\langle 1|/4 \neq \rho_S$.

The same reduced initial system state gives rise to two different final states. Thus, we cannot associate any map $\mathcal{C}$ acting only on S with this input-output relation. This is because the global states are different. In particular, having an initial entangled states makes it impossible to mix different system states without influencing the dynamics.

Solution:

1. Using that $|\pm\rangle, |01\rangle, |10\rangle$ are orthogonal, we get

$$U_{SA}U^\dagger_{SA} = U^2_{SA} = |+\rangle\langle+| + |-\rangle\langle-| + |01\rangle\langle 01| + |10\rangle\langle 10| = \mathbb{I}$$

2.
$$\frac{1}{2}\text{Tr}_A \{|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\} = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \rho_S$$

3.
$$\rho'_{SA} = U_{SA}\rho_{SA}U^\dagger_{SA} = \rho_{SA} \Rightarrow \rho'_S = \rho_S.$$

4. After the measurement the global state becomes
$$\rho_{SA} \to \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|) = \frac{1}{2}(|+\rangle\langle +| + |-\rangle\langle -|)$$
whose reduced system state is $\rho_S = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$. After the evolution,
$$\rho'_{SA} = \frac{1}{2}U_{SA}(|+\rangle\langle +| + |-\rangle\langle -|)U^\dagger_{SA} = \frac{1}{2}(|+\rangle\langle +| + |10\rangle\langle 10|)$$
that has as the reduced state
$$\rho'_S = \frac{1}{4}|0\rangle\langle 0| + \frac{3}{4}|1\rangle\langle 1|.$$

Exercise 1.12: CPTP map between different Hilbert spaces

Verify that the following maps are CPTP by finding an operator-sum representation.

1. The trace map $\mathcal{C}\rho = \text{Tr}\{\rho\}$ discarding the system and destrying all the information contained within it.
2. The partial trace map $\mathcal{C}\rho_{12} = \text{Tr}_2\{\rho_{12}\} = \rho_1$.
3. The state creation $\mathcal{C}_\rho 1 = \rho$.
4. The state addition map $\mathcal{C}_{\rho_2}\rho_1 = \rho_1 \otimes \rho_2$

Solution:

1. Take the operators K_α to be vectors with the only non-zero coordinate being the α one, namely $K_\alpha = \delta_{\alpha i}$. The product satisfies $\sum_\alpha K^\dagger_\alpha K_\alpha = \sum_\alpha \delta_{\alpha j}\delta_{\alpha i} = \delta_{ij}$ and the corresponding map is
$$\mathcal{C}\rho = \sum_{\alpha,ij} \delta_{\alpha i}\rho_{ij}\delta_{\alpha j} = \sum_\alpha \rho_{\alpha\alpha} = \text{Tr}\{\rho\}.$$

2. Take the operators $K_\alpha = \mathbb{I}\otimes|\alpha\rangle$, which is the extension of the previous point. The sum $\sum_\alpha K^\dagger_\alpha K_\alpha = \mathbb{I}\otimes\sum_\alpha |\alpha\rangle\langle\alpha| = \mathbb{I}\otimes\mathbb{I}$ and the map is
$$\mathcal{C}\rho_{12} = \sum_\alpha \langle\alpha|_2\,\rho_{12}\,|\alpha\rangle_2 = \text{Tr}_2\{\rho_{12}\}.$$

3. Consider the eigendecomposition of ρ, namely $\rho = \sum_i p_i |i\rangle\langle i|$. Taking the operator $K_i = \sqrt{p_i}\,|i\rangle$, we can verify that the sum $\sum_i K^\dagger_i K_i = \sum_i p_i = 1 = \mathbb{I}_\mathbb{C}$. The corresponding operator reads
$$\mathcal{C}_\rho 1 = \sum_i K_i 1 K^\dagger_i = \rho.$$

4. Again, take the eigendecomposition of ρ and take the extended operators $K_i = \mathbb{I}_1 \otimes p_i\,|i\rangle_2$. The sum satisfies $\sum_i K^\dagger_i K_i = \mathbb{I}_1\otimes\mathbb{I}_\mathbb{C}$, and the corresponding map reads
$$\mathcal{C}_{\rho_2}\rho_1 = \sum_i K_i\rho_1 K^\dagger_i = \rho_1\otimes\rho_2.$$

Exercise 1.13: Classical mutual informations

Consider three binary random variables S, B, C with values s, b, c. On a given day, S described whether the sun shines, B whether the number of sunburns is high, C whether the number of ice cream salves is high. We set the conditional probabilities $p(b=1|s=1) = p(c=1|s=1) = p(b=0|s=0) = p(c=0|s=0) = \lambda \in [1/2, 1]$. By conservation of probabilities, $p(b=0|s=1) = p(c=0|s=1) = p(b=1|s=0) = p(c=1|s=0) = 1-\lambda$. Furthermore, we assume $p(s=1) = 1/2$.

1. Show that B and C are correlated unless $\lambda = 1/2$ by computing the mutual information
$$I_{B:C} \equiv \sum_{b,c} p(b,c) \ln \frac{p(b,c)}{p(b)p(c)}.$$
Using $p(b,c) = \sum_s p(b,c,s) = \sum_s p(b|s)p(c|s)p(s)$, show that $I_{B:C} = 0$ (no correlations) imples $\lambda = 1/2$, and $I_{B:C} = \ln 2$ (maximal correlations) implies $\lambda = 1$.
2. Show that $I_{B:S} = \ln 2 - S_{\text{Sh}}(\lambda)$ and find the values of λ for which S and B are maximally (un)correlated.
3. Introduce an intervention variable I_S labeling three actions: do nothing (i =idle), make the sun shine ($i=1$) or block sun shine ($i=0$). For i =idle, we set the conditional probabilities as before, $p(b|s, \text{idle}) = p(b|s)$. We further assume $p(b|s, i=1) = \lambda$ and $p(b|s, i=0) = 1-\lambda$ *independent* of s because we are intervening. Calculate the mutual information $I_{B:I_S}$. S is a **cause** of B is there are correlations between I_S and B. Find when S is not the cause of B.
4. Confirm that in general the Kolmogorov consistency condition is not satisfied $p(b,s) \neq \sum_i p(b,s,i)$.

Solution:

1. First, we calculate the probabilities of b and c: $p(b) = \sum_s p(b,s) = \sum_s p(b|s)p(s) = 1/2 = p(c)$. Then, noticing that $p(b,c) = [p(b|0)p(c|0) + p(b|1)p(c|1)]/2$ we can calculate the mutual information
$$I_{B:C} = (\lambda^2 + (1-\lambda)^2) \ln(2[\lambda^2 + (1-\lambda)^2]) + 2\lambda(1-\lambda)\ln(4\lambda[1-\lambda]) = \ln 2 - S_{\text{Sh}}(2\lambda[1-\lambda]).$$
To minimize the mutual information we need to maximize the Shannon entropy by setting $\lambda = 1/2$. In this case $I_{B:C} = 0$ the two variables are uncorrelated since it is all up to a coin flip. Instead, the maximum mutual information is obtained when the Shannon entropy is minimized, i.e. by setting $\lambda = 1$. In this case $I_{B:C} = \ln 2$ and b, c have always the same value.
2. The joint probability of b, s is $p(b,s) = p(b|s)p(s) = p(b|s)/2$, so we can calculate the mutual information
$$I_{B:S} = \lambda \ln(2\lambda) + (1-\lambda)\ln(2(1-\lambda)) = \ln 2 - S_{\text{Sh}}(\lambda).$$
Again, for $\lambda = 1/2$, $I_{B:S} = 0$ and the events are uncorrelated, whereas for $\lambda = 1$, $I_{B:S} = \ln 2$ and the events are maximally correlated.
3. The variable i has three possible outcomes. Let's list them
$$i = \begin{cases} \text{idle} & \to \quad p(b, \text{idle}) = \sum_s p(b|s)p(s)p(\text{idle}) = \frac{1}{2}p(\text{idle}) \\ 1 & \to \quad p(b,1) = p(b|i=1)p(i=1) = p(b|i=1)q_1 \\ 0 & \to \quad p(b,0) = p(b|i=0)p(i=0) = p(b|i=0)q_0 \end{cases}.$$
Now we can calculate the mutual information
$$I_{B:I_S} = \sum_{b,i} p(b,i) \ln \frac{p(b,i)}{p(b)p(i)} = S_{\text{Sh}}[p(b)] + p(\text{idle}) \ln \frac{1}{2} + \lambda q_1 \ln \frac{\lambda q_1}{q_1} + (1-\lambda) q_1 \ln \frac{(1-\lambda) q_1}{q_1} +$$
$$+ \lambda q_0 \ln \frac{\lambda q_0}{q_0} + (1-\lambda) q_0 \ln \frac{(1-\lambda) q_0}{q_0}$$
$$I_{B:I_S} = S_{\text{Sh}}[p(b)] - p(\text{idle}) \ln 2 - [1 - p(\text{idle})] S_{\text{Sh}}[\lambda]$$
We can minimize the mutual information by choosing (i) $p(\text{idle}) = 1$, such that $I_{B:I_S} = 0$, or (ii) $\lambda = 1/2$, such that $I_{B:I_S} = 0$. In the first case we are not intervening at all, in the second one S and B are uncorrelated in the first place.
4. It is sufficient to show an example. Let $p(i=0) = p(i=1) = 1/2$. Then, $\sum_i p(b,s,i) = (1-\lambda)/2 + \lambda/2 = 1/2$ is independent of both b and s. Now, the Kolmogorov consistency condition cannot be satisfied because, if it were, we would violate the probability conservation: $\sum_{b,s} p(b,s) = 2$, which is absurd.

Exercise 1.14: Quantum joint probability

The probability of observing the outcomes r_l at times t_l for a quantum system is given by

$$p(\mathbf{r}_n) = \mathrm{Tr}\left\{\mathcal{P}(r_n)\mathcal{U}(t_n, t_{n-1})\cdots\mathcal{P}(r_1)\mathcal{U}(t_1, t_0)\mathcal{P}(r_0)\rho\right\}$$

where $\mathcal{P}(r_l)\rho = \Pi(r_l)\rho\Pi(r_l)$ and $\mathcal{U}(t_l, t_k)\rho = U(t_l, t_k)\rho U^\dagger(t_l, t_k)$.

1. Show that the joint probability is non-negative and sums to 1.
2. Show that in general the joint probability does not satisfy the Kolmogorov consistency condition

$$p(r_n, \cdots, \not{r_l}, \cdots, r_0) \neq \sum_{r_l} p(r_n, \cdots, r_l, \cdots, r_0)$$

Solution:

1. Choosing a base $|j\rangle$ of the Hilbert space, we define the kets $|v_j\rangle$ as

$$|v_j\rangle \equiv \Pi(r_0)U^\dagger(t_1, t_0)\cdots U^\dagger(t_n, t_{n-1})\Pi(r_n)\,|j\rangle\,.$$

   Then the probability reads $p(\mathbf{r}_n) = \sum_j \langle v_j|\rho|v_j\rangle \geq 0$ which is non-negative by virtue of the non-negativity of ρ. Summing over all possible outcomes we get

$$\sum_{\mathbf{r}_n} p(\mathbf{r}_n) = \mathrm{Tr}\left\{\sum_{r_n}\mathcal{P}(r_n)\mathcal{U}(t_n, t_{n-1})\cdots\sum_{r_1}\mathcal{P}(r_1)\mathcal{U}(t_1, t_0)\sum_{r_0}\mathcal{P}(r_0)\rho\right\} = \mathrm{Tr}\left\{\mathcal{U}(t_n, t_0)\rho\right\} = 1$$

   where we used that the projectors sum to the identity.

2. It is sufficient to show an example. Let the initial state of a qubit be $\rho = |+\rangle\langle+|$. The first measurement is done on the $|0\rangle, |1\rangle$ basis. Then, the system evolves unitarily through the identity. Finally, the last measurement is done on the $|\pm\rangle$ basis. If we first measurement is not performed, then the probability of observing $+$ is $p(+) = 1$. Instead, when we do the first measurement and coarse-grain over the outcome, we get $p(+) = \frac{1}{2}$. This is basically the Stern-Gerlach experiment.

Exercise 1.15: Multi-linearity of the process tensor

Based on the definition of the process tensor:

$$\mathfrak{T}[\mathcal{C}(r_n), \cdots, \mathcal{C}(r_0)] \equiv \mathrm{Tr}_B\left\{\mathcal{C}(r_n)\mathcal{U}_{SB}(t_n, t_{n-1})\cdots\mathcal{C}(r_1)\mathcal{U}_{SB}(t_1, t_0)\mathcal{C}(r_0)\rho_{SB}(0)\right\}$$

show that, $\forall l \in \{0, 1, \cdots, n\}$,

$$\mathfrak{T}[\mathcal{A}_n, \cdots, a_l\mathcal{A}_l + b_l\mathcal{B}_l, \cdots, \mathcal{A}_0] = a_l\mathfrak{T}[\mathcal{A}_n, \cdots, \mathcal{A}_l, \cdots, \mathcal{A}_0] + b_l\mathfrak{T}[\mathcal{A}_n, \cdots, \mathcal{B}_l, \cdots, \mathcal{A}_0].$$

Consider a Hilbert space $\mathcal{H}_S$ of dimension d. The space of linear maps on $\mathcal{H}_S$ is $\mathcal{L}(\mathcal{H}_S)$. Furthermore, the space of superoperators is $\mathcal{L}(\mathcal{L}(\mathcal{H}_S))$. The tensor product acts as follows:

$$\mathfrak{T} : \underbrace{\mathcal{L}(\mathcal{L}(\mathcal{H}_S)) \otimes \cdots \otimes \mathcal{L}(\mathcal{L}(\mathcal{H}_S))}_{n+1\text{times}} \to \mathcal{L}(\mathcal{H}_S).$$

Deduce that the dimension of the input space of $\mathfrak{T}$ is $d^{4(n+1)}$.

Solution:
The multi-linearity of the process tensor follows directly from the linearity of the superoperators and of the trace. The Hilbert space has dimension d. $\mathcal{L}(\mathcal{H}_S)$ has dimension d^2. $\mathcal{L}(\mathcal{L}(\mathcal{H}_S))$ has dimension d^4. The tensor product of two spaces $\mathcal{A}\otimes\mathcal{B}$ has dimension $d_A d_B$. Therefore the dimension of the input space is $d^{4(n+1)}$.

Exercise 1.16: Quantum state tomography

Suppose you have sufficiently many copies of the state $\rho = p\,|0\rangle\langle 0| + (1-p)\,|1\rangle\langle 1| + c\,|0\rangle\langle 1| + c^*\,|1\rangle\langle 0|$, with $c \in \mathbb{C}$ satisfying $|c|^2 \le p(1-p)$.

Devise a measurement strategy yo determine ρ by using the Bloch sphere representation $\rho = (\mathbb{I} + \mathbf{r}\cdot\sigma)/2$.

This procedure can be generalized to arbitrary $d-$dimensional quantum systems using a generalized Bloch representation

$$\rho = \frac{1}{d}\left(\mathbb{I} + \sqrt{\frac{d(d-1)}{2}}\mathbf{r}\cdot\mathbf{\Lambda}\right)$$

with $\mathbf{\Lambda}$ a vector of d^2-1 traceless Hermitian matrices obeying $\mathrm{Tr}\left\{\Lambda_i \Lambda_j\right\} = 2\delta_{ij}$.

Solution:
The probability of observing $\sigma_z = 1$ is $p_{z=1} = p$. The probability of observing $\sigma_x = 1$ is $p_{x=1} = \mathrm{Tr}\left\{|+\rangle\langle +|\,\rho\right\} = \Re(c) + 1/2$. The probability of oserving $\sigma_y = 1$ is $p_{y=1} = \mathrm{Tr}\left\{|+_y\rangle\langle +_y|\,\rho\right\} = \Im(c) + 1/2$. Therefore, with these 3 independent mesurements we can reconstruct the 3 independent parameters of ρ.

Exercise 1.17: States spanning $\mathcal{L}(\mathcal{H}_S)$

Let $\{|n\rangle\}$ be a basis of $\mathcal{H}_S$. We consider the states $P_{(n,m)} = |\psi_{n,m}\rangle\langle\psi_{n,m}|$ defined through

$$|\psi_{n,m}\rangle = \begin{cases} \frac{|n\rangle + |m\rangle}{\sqrt{2}} & \text{if}\, n > m, \\ |n\rangle & \text{if}\, n = m, \\ \frac{i|n\rangle + |m\rangle}{\sqrt{2}} & \text{if}\, n < m, \end{cases}$$

Confirm that the set of states $P_{(n,m)}$ linearly spans the entire space of $d \times d$ matrices.

Solution:
Given the definition of $P_{(n,m)}$, we have a set of d^2 matrices. If these are linearly independent, then they form a basis for $\mathcal{L}(\mathcal{H}_S)$ (which has dimension d^2). Let's suppose they are not linearly independent. Then, we can write one of such states as a linear combination of the linearly independent others:

$$P_\alpha = \sum_\beta c_\beta P_\beta \to \mathrm{Tr}\left\{P_\alpha\right\} = 1 = \sum_\beta c_\beta$$

Using that these states are projectors we notice that $\mathrm{Tr}\left\{P_\beta P_\gamma\right\} = \langle\gamma|P_\beta|\gamma\rangle \le 1$ with the equality reached only when $\beta = \gamma$. Then, since $P_\alpha^2 = P_\alpha$, we have

$$\mathrm{Tr}\left\{P_\alpha^2\right\} = 1 = \sum_{\beta\gamma} c_\beta c_\gamma \mathrm{Tr}\left\{P_\beta P_\gamma\right\} < 1$$

which is absurd.

Exercise 1.18: Map linear decomposition

Every map $\mathcal{C}$ can be linearly expanded in the basis $\mathcal{C} = \sum_{\alpha,\beta} c_{\alpha\beta}\mathcal{B}_{\alpha\beta}$, where the superoperators $\mathcal{B}_{\alpha\beta}$ are defined through

$$\mathcal{B}_{\alpha\beta}\rho_S \equiv P_\alpha \mathrm{Tr}\left\{\Pi_\beta \rho_S\right\},$$

with $\{P_\alpha\}$ states that form a basis of $\mathcal{L}(\mathcal{H}_S)$, and $\{\Pi_\beta\}$ forming an informationally complete set of projectors.

Show that, if $\mathcal{C}$ preserves Hermiticity, then the coefficients $c_{\alpha\beta} \in \mathbb{R}$. If the map is trace-preserving, then $\sum_\alpha c_{\alpha\beta} = 1$.

Solution:
Let $A = A^\dagger$ a Hermitian matrix. The map acts as follows $\mathcal{C}A = \sum_{\alpha\beta} c_{\alpha\beta} P_\alpha \mathrm{Tr}\left\{\Pi_\beta A\right\}$. Taking the hermitian conjugate: $(\mathcal{C}A)^\dagger = \sum_{\alpha\beta} c^*_{\alpha\beta} P_\alpha \mathrm{Tr}\left\{\Pi_\beta A^\dagger\right\} = \sum_{\alpha\beta} c^*_{\alpha\beta} P_\alpha \mathrm{Tr}\left\{\Pi_\beta A\right\}$. If $\mathcal{C}$ preserves Hermiticity, then $(\mathcal{C}A)^\dagger = \mathcal{C}A$, which means that each coefficients must be equal: $c_{\alpha\beta} = c^*_{\alpha\beta} \Rightarrow c_{\alpha\beta} \in \mathbb{R}$.
Now we relax all the assumptions made on $\mathcal{C}$ and A to study the trace-preserving property. The trace of the mapped operator is $\mathrm{Tr}\left\{\mathcal{C}A\right\} = \sum_{\alpha\beta} c_{\alpha\beta} \mathrm{Tr}\left\{\Pi_\beta A\right\}$. If the operator is trace-preserving, then

$\forall A, \quad \mathrm{Tr}\{XA\} = \mathrm{Tr}\{\mathbb{I}A\}$, with $X = \sum_{\alpha\beta} c_{\alpha\beta}\Pi_\beta$. Since the trace is a scalar product the condition is satisfied $\forall A$ if and only if $X = \mathbb{I}$. By using the same projectors to decompose the identity operator we find $\sum_{\alpha\beta} c_{\alpha\beta}\Pi_\beta = \sum_\beta \Pi_\beta \Rightarrow \sum_\alpha c_{\alpha\beta} = 1$.

Exercise 1.19: Decorrelated interventions

The tensor product acts as follows:

$$\mathfrak{T} : \underbrace{\mathcal{L}(\mathcal{L}(\mathcal{H}_S)) \otimes \cdots \otimes \mathcal{L}(\mathcal{L}(\mathcal{H}_S))}_{n+1\text{times}} \to \mathcal{L}(\mathcal{H}_S).$$

An element $\mathbf{C}_{n:0}$ of the input space can be written using the base $\mathcal{B}_{\alpha\beta}\rho_S \equiv P_\alpha \mathrm{Tr}\{\Pi_\beta \rho_S\}$ as

$$\mathbf{C}_{n:0} = \sum_{\alpha_n\beta_n} \cdots \sum_{\alpha_0\beta_0} c_{\alpha_n\beta_n\cdots\alpha_0\beta_0} \mathcal{B}_{\alpha_n\beta_n} \otimes \cdots \otimes \mathcal{B}_{\alpha_0\beta_0},$$

with $c_{\alpha_n\beta_n\cdots\alpha_0\beta_0}$ not necesserally decoupled.

Confirm that the element $\mathbf{C}_{n:0}(\mathbf{r}_n)$ corresponding to applying a sequence of control operations $\mathcal{C}(r_n)\cdots\mathcal{C}(r_0)$ can be written as a tensor product $\mathbf{C}_{n:0}(\mathbf{r}_n) = \mathcal{C}(r_n) \otimes \cdots \otimes \mathcal{C}(r_0)$, which corresponds to a decorrelated intervention.

Solution:
The linear reconstruction of any set of intruments combined with the multi-linearity of the process tensor yields

$$\mathfrak{T}[\mathbf{C}_{n:0}(\mathbf{r}_n)] = \sum_{\alpha_n\beta_n} \cdots \sum_{\alpha_0\beta_0} c_{\alpha_n\beta_n} \cdots c_{\alpha_0\beta_0} \mathfrak{T}[\mathcal{B}_{\alpha_n\beta_n} \cdots \mathcal{B}_{\alpha_0\beta_0}] = \mathfrak{T}\left[\sum_{\alpha_n\beta_n} c_{\alpha_n\beta_n}\mathcal{B}_{\alpha_n\beta_n}, \cdots, \sum_{\alpha_0\beta_0} c_{\alpha_0\beta_0}\mathcal{B}_{\alpha_0\beta_0}\right]$$

From which we can identify

$$\mathbf{C}_{n:0}(\mathbf{r}_n) = \sum_{\alpha_n\beta_n} c_{\alpha_n\beta_n}\mathcal{B}_{\alpha_n\beta_n} \otimes \cdots \otimes \sum_{\alpha_0\beta_0} c_{\alpha_0\beta_0}\mathcal{B}_{\alpha_0\beta_0}$$

Exercise 1.20: Containment property of the process tensor

The process tensor $\mathfrak{T}$ was defined on the set of times $\{t_0, \cdots, t_n\}$. Consider any subset of times $T \subset \{t_0, \cdots, t_n\}$. Show that the process tensor $\mathfrak{T}_T$ defined on this subset is *contained* in the original $\mathfrak{T}$, meaning that all probabilities predictable from $\mathfrak{T}_T$ can also be recovered from $\mathfrak{T}$. Thus, process tensors $\mathfrak{T}_{T_1}, \cdots, \mathfrak{T}_{T_N}$ for discrete set of times $T_1 \subset \cdots \subset T_N$ form a hierarchy.

Solution:
Calling $\bar{T}$ the complementary set of times, the process tensor $\mathfrak{T}_T$ can be obtained from $\mathfrak{T}$ by using, for all $t \in \bar{T}$, the identity instrument. For example:

$$\mathfrak{T}_T[\mathcal{C}_{t_1}, \mathcal{C}_{t_3}] = \mathfrak{T}[\mathcal{I}_{t_0}, \mathcal{C}_{t_1}, \mathcal{I}_{t_2}, \mathcal{C}_{t_3}]$$

Exercise 1.21: Process tensor and state preparation

The process tensor does not depend linearly on the initial system state $\rho_S(0)$ in general. However, show that is does for an initial state of the form $\rho_{SB}(0) = \rho_S(0) \otimes \rho_B(0)$. In this case, the first control operation $\mathcal{C}(r_0)$ becomes redundant and one can define the process tensor are $\mathfrak{T}[\mathcal{C}(r_n), \cdots, \mathcal{C}(r_1), \rho_S(0)]$, with $\rho_S(0)$ arbitrary.

Solution:
By linearity of the superoperators and trace it is easy to verify that if the initial state is $\rho_S(0) = \alpha A + \beta B$, then

$$\begin{aligned}\mathfrak{T}[\mathcal{C}(r_n), \cdots, \mathcal{C}(r_0)] = \alpha \mathrm{Tr}_B\{\mathcal{C}(r_n)\mathcal{U}(t_n, t_{n-1})\cdots\mathcal{U}(t_1, t_0)\mathcal{C}(r_0)A \otimes \rho_B(0)\} + \\ + \beta \mathrm{Tr}_B\{\mathcal{C}(r_n)\mathcal{U}(t_n, t_{n-1})\cdots\mathcal{U}(t_1, t_0)\mathcal{C}(r_0)B \otimes \rho_B(0)\}.\end{aligned}$$

Exercise 1.22: Process tensor and correlations functions

Let A, B be arbitrary system observables. The process tensor can be used to compute correlations functions of the form

$$\langle A(t)B(0)\rangle = \mathrm{Tr}_{SB}\left\{AU_{SB}(t,0)B\rho_{SB}(0)U_{SB}^{\dagger}(t,0)\right\}.$$

Solution:
We write the spectral decomposition of A as $A = \sum_a a\,|a\rangle\langle a|$. Since

$$\langle A(t)B(0)\rangle = \sum_a a\mathrm{Tr}_{SB}\left\{|a\rangle\langle a|\,U_{SB}(t,0)B\rho_{SB}(0)U_{SB}^{\dagger}(t,0)\right\}$$

we can already identify the process tensor

$$\langle A(t)B(0)\rangle = \sum_a a\mathfrak{T}[\mathcal{P}_a, \mathcal{B}_0]$$

with $\mathcal{P}_a = |a\rangle\langle a|$ is a projector and $\mathcal{B}_0\rho_{SB}(0) = B\rho_{SB}(0)$. The latter superoperator is not necessarily CP, so it canno be implemented physically. However, we can decompose it in physical maps as $\mathcal{B}_0 = \sum_{\alpha\beta} c_{\alpha\beta}\mathcal{B}_{\alpha\beta}$:

$$\mathcal{B}_0\rho_{SB} = \sum_b b\,|b\rangle\langle b|\,\rho_{SB}\sum_{b'}|b'\rangle\langle b'| = \sum_{bb'} b\,|b\rangle\langle b'|\,\mathrm{Tr}_S\left\{|b'\rangle\langle b|\,\rho_{SB}\right\}.$$

To write this using the basis $\mathcal{B}_{\alpha\beta}$, one needs to decompose $|b\rangle\langle b'|$ in the P_α basis and $|b'\rangle\langle b|$ in the Π_β basis.

Exercise 1.23: Markovianity of closed systems

Verify that an isolated (i.e. unitarily evolving) system is Markovian.

Solution:
The process tensor for the isolated system reads

$$\mathfrak{T}[\mathcal{C}(r_n), \cdots, \mathcal{C}(r_0)] = \mathcal{C}(r_n)\mathcal{U}(t_n, t_{n-1})\cdots\mathcal{U}(t_1, t_0)\mathcal{C}(r_0)\rho_S(0)$$

Applying a causal break corresponds to

$$\mathfrak{T}[\mathcal{B}_{\alpha_k\beta_k}, \mathcal{C}(r_{k-1})\cdots, \mathcal{C}(r_0)] = \mathcal{U}(t_n, t_k)\sigma_S^{(\alpha_k)}\mathrm{Tr}_S\left\{P_\beta\tilde{\rho}_S(t_k)\right\}.$$

Then, the state after the causal break is

$$\rho_n[\mathcal{B}_{\alpha_k\beta_k}, \mathcal{C}(r_{k-1})\cdots, \mathcal{C}(r_0)] = \frac{\mathcal{U}(t_n, t_k)\sigma_S^{(\alpha_k)}\mathrm{Tr}_S\left\{P_\beta\tilde{\rho}_S(t_k)\right\}}{\mathrm{Tr}_S\left\{\mathcal{U}(t_n, t_k)\sigma_S^{(\alpha_k)}\mathrm{Tr}_S\left\{P_\beta\tilde{\rho}_S(t_k)\right\}\right\}} = \mathcal{U}(t_n, t_k)\sigma_S^{(\alpha_k)}$$

which is clearly independent of all previous interventions.

Exercise 1.24: Factorization of the process tensor

1. Show that if the process tensor factorizes as

   $$\mathfrak{T}[\mathcal{C}(r_n), \cdots, \mathcal{C}(r_0)] = \mathcal{C}(r_n)\mathcal{E}(t_n, t_{n-1})\cdots\mathcal{E}(t_1, t_0)\mathcal{C}(r_0)\rho_S(0),$$

   with $\rho_S(0) = \mathrm{Tr}_B\left\{\rho_{SB}\right\}$ and $\mathcal{E}(t_l, t_k)$ CPTP maps independent of the interventions $\mathcal{C}(r_n)\cdots\mathcal{C}(r_0)$, then the process is Markovian.

2. Consider a Markovian process in which the tensor product is obtained by applying only causal breaks, which decorrelate the system-bath state: $\mathcal{B}_{\alpha\beta}\rho_{SB} = \sigma_S^{(\alpha)} \otimes \mathrm{Tr}_S\left\{P_\beta\rho_{SB}\right\}$. One can therefore write

   $$\mathfrak{T}[\mathcal{B}_{\alpha_n\beta_n}\cdots\mathcal{B}_{\alpha_0\beta_0}] = \sigma_S^{(\alpha_n)}\mathrm{Tr}_S\left\{P_{\beta_n}\tilde{\mathcal{E}}(t_n, t_{n-1})\sigma_S^{(\alpha_{n-1})}\right\}\cdots\mathrm{Tr}_S\left\{P_{\beta_1}\tilde{\mathcal{E}}(t_1, t_0)\sigma_S^{(\alpha_0)}\right\}\mathrm{Tr}_S\left\{P_{\beta_0}\rho_S(0)\right\}.$$

   Using the Markovian property, prove that the CPTP maps $\tilde{\mathcal{E}}(t_l, t_k)$ are independent of the history of the system.

Solution:

1. Using a causal break at time t_k, the state at time t_n is

$$\rho_S(t_n) = \frac{\mathfrak{T}[\mathcal{B}_{\alpha_k\beta_k}, \mathcal{C}(r_{k-1}), \cdots, \mathcal{C}(r_0)]}{\mathrm{Tr}_S\left\{\mathfrak{T}[\mathcal{B}_{\alpha_k\beta_k}, \mathcal{C}(r_{k-1}), \cdots, \mathcal{C}(r_0)]\right\}} = \frac{\mathcal{E}(t_n, t_k)\sigma_S^{(\alpha_k)}\mathrm{Tr}_S\left\{P_\beta \tilde{\rho}_S(t_k)\right\}}{\mathrm{Tr}_S\left\{P_\beta \tilde{\rho}_S(t_k)\right\}} = \mathcal{E}(t_n, t_k)\sigma_S^{(\alpha_k)}$$

is independent of the interventions, which means that the process is Markovian.

2. Suppose there are two histories, $\mathbf{h} \equiv (\beta_k, \alpha_{k-1}, \beta_{k-1}, \cdots, \alpha_0, \beta_0)$, and $\mathbf{h}' \equiv (\beta'_k, \alpha'_{k-1}, \beta'_{k-1}, \cdots, \alpha'_0, \beta'_0) \neq \mathbf{h}$, such that they result in different propagations: $\tilde{\mathcal{E}}(t_l, t_k) \equiv \tilde{\mathcal{E}}(t_l, t_k|\mathbf{h}) \neq \tilde{\mathcal{E}}(t_l, t_k|\mathbf{h}') = \tilde{\mathcal{E}}'(t_l, t_k)$. We can now look at the definition of Markovianity with the causal break choosing the particular set of interventions according to $\mathbf{h}$ and $\mathbf{h}'$, respectively.

$$\rho_l[\mathcal{B}_{\alpha_k\beta_k} \cdots \mathcal{B}_{\alpha_0\beta_0}] = \tilde{\mathcal{E}}(t_l, t_k)\sigma_S^{(\alpha_k)}$$

$$\rho'_l[\mathcal{B}_{\alpha_k\beta'_k} \cdots \mathcal{B}_{\alpha'_0\beta'_0}] = \tilde{\mathcal{E}}'(t_l, t_k)\sigma_S^{(\alpha_k)}$$

which means that the state after a causal break depends on the history before it, which contradicts the Markov property. Therefore, by absurd, we have proven that $\tilde{\mathcal{E}}(t_l, t_k)$ do not depend on the prior history.

Exercise 1.25: Dynamical maps on classically correlated states

Consider a system-bath state with zero quantum discord with respect to a complete set of system projectors $|j\rangle\langle j|_S$ such that

$$\rho_{SB}(0) = \sum_j |j\rangle\langle j|\, \rho_{SB}\, |j\rangle\langle j| = \sum_j p_j\, |j\rangle\langle j| \otimes \rho_B(j),$$

with p_j probability distribution and $\rho_B(j)$ the state of the bath given the state $|j\rangle\langle j|_S$ of the system.

Show that the reduced system dynamics $\rho_S(t) = \mathrm{Tr}_B\left\{U_{SB}\rho_{SB}U_{SB}^\dagger\right\}$ is CPTP for any unitary U_{SB}.

Solution:
Introducing the spectral decomposition of $\rho_B(j) = \sum_b p(b|j)\, |b_j\rangle\langle b_j|$, we get

$$\rho_S(t) = \mathrm{Tr}_B\left\{U_{SB} \sum_j p_j\, |j\rangle\langle j|_S \otimes \sum_b p(b|j)\, |b_j\rangle\langle b_j|_B\, U_{SB}^\dagger\right\}$$

$$\rho_S(t) = \sum_{bb'j} \langle b'|U_{SB}\sqrt{p(b|j)}|b_j\rangle_B\, p_j\, |j\rangle\langle j|_S\, \langle b_j|U_{SB}^\dagger\sqrt{p(b|j)}|b'\rangle$$

We now introduce two $\mathbb{I}_S$ as follows

$$\rho_S(t) = \sum_{bb'j}\sum_{ki} \langle b'|U_{SB}\sqrt{p(b|j)}|b_j\rangle_B\, |k\rangle\langle k|_S\, p_j\, |j\rangle\langle j|_S\, |i\rangle\langle i|_S\, \langle b_j|U_{SB}^\dagger\sqrt{p(b|j)}|b'\rangle$$

which allow us to change the index inside the B brakets thanks to the orthonormality of the $|j\rangle_S$ basis, namely

$$\rho_S(t) = \sum_{bb'j}\sum_{ki} \langle b'|U_{SB}\sqrt{p(b|k)}|b_k\rangle_B\, |k\rangle\langle k|_S\, p_j\, |j\rangle\langle j|_S\, |i\rangle\langle i|_S\, \langle b_i|U_{SB}^\dagger\sqrt{p(b|i)}|b'\rangle_B\,.$$

We now recognize the structure $\rho'_S = \sum_\alpha K_\alpha \rho K_\alpha^\dagger$. In particular, the K operators are

$$K_{bb'} = \langle b'|U_{SB}\sqrt{p(b|k)}|b_k\rangle_B\, |k\rangle\langle k|_S\,.$$

For the evolution to be a CPTP map, these operators must satisfy the relation $\sum_\alpha K_\alpha^\dagger K_\alpha = \mathbb{I}$, so we have to check:

$$\sum_{bb'} K^\dagger_{bb'} K_{bb'} = \sum_{bb'}\sum_{ik} |i\rangle\langle i|_S \langle b_i|U^\dagger_{SB}\sqrt{p(b|i)}|b'\rangle_B \langle b'|U_{SB}\sqrt{p(b|k)}|b_k\rangle_B |k\rangle\langle k|_S$$
$$= \sum_{b}\sum_{ik} |i\rangle\langle i|_S \langle b_i|\sqrt{p(b|i)}\sqrt{p(b|k)}|b_k\rangle_B |k\rangle\langle k|_S$$
$$= \sum_{b}\sum_{ik} |i\rangle\langle k|_S \langle i|k\rangle_S \langle b_i|b_k\rangle_B \sqrt{p(b|i)}\sqrt{p(b|k)}$$
$$= \sum_{b}\sum_{i} |i\rangle\langle i|_S \langle b_i|b_i\rangle_B\, p(b|i) = \sum_i |i\rangle\langle i|_S = \mathbb{I}_S$$

So we have found the operator-sum representation of the map.

Exercise 1.26: Kolmogorov consistency condition on classically correlated states

Assuming that for all t_l the joint density matrix is

$$\rho_{SB}(t_l) = \sum_{r_l} p(r_l, t_l)\, |r_l\rangle\langle r_l|_S \otimes \rho_B(t_l|r_l),$$

show that the joint probabilities satisfy the Kolmogorov consistency condition.

Solution:
The joint probability is given by

$$p(\mathbf{r}_n) = \mathrm{Tr}\left\{\mathcal{P}(r_n)\mathcal{U}(t_n, t_{n-1})\cdots\mathcal{U}(t_1,t_0)\mathcal{P}(r_0)\rho_{SB}(0)\right\}.$$

Taking the marginal over the the outcome r_l we have

$$\sum_{r_l} p(\mathbf{r}_n) = \mathrm{Tr}\left\{\mathcal{P}(r_n)\mathcal{U}(t_n, t_{n-1})\cdots\left(\sum_{r_l}\mathcal{P}(r_l)\right)\cdots\mathcal{U}(t_1,t_0)\mathcal{P}(r_0)\rho_{SB}(0)\right\}.$$

Since the action of the projective measurement is $\mathcal{P}(r_l)\rho = |r_l\rangle\langle r_l|\,\rho\,|r_l\rangle\langle r_l|$, and, by hypotesis, the state at time t_l is classically correlated, we have

$$\sum_{r_l}\mathcal{P}(r_l)\rho_{SB}(t_l) = \sum_{r_l,s_l} |r_l\rangle\langle r_l|_S\, p(s_l,t_l)\, |s_l\rangle\langle s_l|_S \otimes \rho_B(t_l|s_l)\, |r_l\rangle\langle r_l|_S = \rho_{SB}(t_l),$$

which means that taking the marginal does not change the state. Therefore, the Kolmogorov consistency condition is satisfied:

$$p(r_0,\cdots,\not{p}_l,\cdots,r_n) = \sum_{r_l} p(r_0,\cdots,p_l,\cdots,r_n)$$

Exercise 1.27: Classicality imples incoherence

Prove that, if the hierarchy of probabilities $p(r_n,\cdots,r_1|\mathcal{C}_0)$ obeys the Kolmogorov consistency condition, then the process is incoherent.

Solution:
The joint probability given the initial state preparation is

$$p(r_n,\cdots,r_1|\mathcal{C}_0) = \mathrm{Tr}_S\left\{\mathfrak{T}[\mathcal{P}(r_n),\cdots,\mathcal{P}(r_1),\mathcal{C}_0]\right\}.$$

Since it satisfies the Kolmogorov consistency condition, we have

$$\mathrm{Tr}_S\left\{\mathfrak{T}[\mathcal{P}(r_n),\cdots,\mathcal{I}_l,\cdots\mathcal{P}(r_1),\mathcal{C}_0]\right\} = p(r_n,\cdots,\not{r}_l,r_1|\mathcal{C}_0) =$$
$$= \sum_l p(r_n,\cdots,r_l,\cdots r_1|\mathcal{C}_0) = \mathrm{Tr}_S\left\{\mathfrak{T}[\mathcal{P}(r_n),\cdots,\mathcal{D}_{R_l},\cdots,\mathcal{P}(r_1),\mathcal{C}_0]\right\},$$

where $\mathcal{D}_{R_l}$ is the marginal of the projective measurement, namely $\mathcal{D}_{R_l} = \sum_{r_l}\mathcal{P}(r_l)$. The two tensor product are actually the same because of how the projective measurement acts. Indeed, since R is non-degenerate the outcome of the last measurement fully determines the final state

$$\mathfrak{T}[\mathcal{P}(r_n), \cdots, \mathcal{P}(r_1), \mathcal{C}_0] = p(r_n, \cdots, r_1|\mathcal{C}_0) |r_n\rangle\langle r_n|_S ,$$

which means that, $\forall l$,

$$\mathfrak{T}[\mathcal{P}(r_n), \cdots, \mathcal{I}_l, \cdots \mathcal{P}(r_1), \mathcal{C}_0] = \mathfrak{T}[\mathcal{P}(r_n), \cdots, \mathcal{D}_{R_l}, \cdots, \mathcal{P}(r_1), \mathcal{C}_0].$$

Repeating this process and marginalizing the projective measurements we get the definition of $n-$incoherence, namely that the process tensors

$$\mathfrak{T}[\mathcal{D}_{R_n}, \left\{ \begin{array}{c} \mathcal{D}_{R_{n-1}} \\ \mathcal{I}_{n-1} \end{array} \right\} \cdots, \left\{ \begin{array}{c} \mathcal{D}_{R_1} \\ \mathcal{I}_1 \end{array} \right\}, \mathcal{C}_0]$$

are all the same. Furthermore, using the Kolmogorov consistency relation on the last intervention allows us to prove the $n-1$-incoherence, and so on. Therefore the process is incoherent.

Exercise 1.28: Non-classical Markovian processes

Find examples of non-classical process that are Markovian and incoherent with respect to a restricted set of preparations $\mathcal{C}_0$ or not invertible.

Solution:
Let $\rho_S(t_0) = (|0\rangle\langle 0| + |1\rangle\langle 1|)/2$, and let the dynamics be unitary. For the unitary $\mathcal{C}_0$: $\mathcal{C}_0\rho_S(t_0) = \rho_S(t_0)$. Therefore, if we take a unitary preparation and a unitary evolution on the maximally mixed state we get

$$\sum_{r_1} p(r_2, r_1|\mathcal{C}_0) = \mathrm{Tr}_S \left\{\mathcal{P}(r_2)\mathcal{U}_{2,1}\mathcal{D}_{R_1}\mathcal{U}_{1,0}\mathcal{C}_0\rho_S(t_0)\right\} = \mathrm{Tr}_S \left\{\mathcal{P}(r_2)\rho_S(t_0)\right\} = p(r_2, \not{r}_1),$$

as expected. Now, instead of taking a unitary preparation, we take $\mathcal{C}_0\rho_S(t_0) = |0\rangle\langle 0|$, and consider the following unitaries $\mathcal{U}_{2,1} = \mathcal{U}_{1,0}^\dagger$, and $\mathcal{U}_{1,0} |0\rangle\langle 0| = |+\rangle\langle +|$. In this case

$$\sum_{r_1} p(r_2, r_1|\mathcal{C}_0) = \mathrm{Tr}_S \left\{\mathcal{P}(r_2)\mathcal{U}_{2,1}\mathcal{D}_{R_1}\mathcal{U}_{1,0}\mathcal{C}_0\rho_S(t_0)\right\} = \mathrm{Tr}_S \left\{\mathcal{P}(r_2)(|0\rangle\langle 0| + |1\rangle\langle 1|)/2\right\} = 1/2,$$

whereas

$$p(r_2, \not{r}_1) = \mathrm{Tr}_S \left\{\mathcal{P}(r_2) |0\rangle\langle 0|\right\} = \delta_{0r_2}.$$

Therefore the Kolmogorov consistency condition is not satisfied for all preparations $\mathcal{C}_0$.

Exercise 1.29: Classical from quantum Markovianity

Consider a quantum stochastic process that yields for a fixed set of itnerventions the probabilities $p(\mathbf{r}_n)$. Then

1. If the quantum stochastic process is Markovian and if all interventions are causal breaks, then the probabilities $p(\mathbf{r}_n)$ satify the Markov property, namely $p(r_n|\mathbf{r_{n-1}}) = p(r_n|r_{n-1})$.
2. If we add to the assumptions of point (1) that the probabilities $p(\mathbf{r}_n)$ also satisfy the Kolmogorov consistency condition, then these probabilities describe a classical Markov process.

Solution:

1. The Markovianity condition of a quantum stochastic process reads

$$\rho_l[\mathcal{B}_{\alpha_k\beta_k}, \mathcal{C}_{k-1}, \cdots, \mathcal{C}_0] = \rho_l[\sigma^{(\alpha_k)}],$$

for $\mathcal{B}_{\alpha_k\beta_k}$ causal break. Then, when all interventions are causal breaks, we can write the probabilities as

$$p(\mathbf{r}_{n-1}) = \mathrm{Tr}\left\{\mathcal{B}_{\alpha_{n-1}\beta_{n-1}}\mathcal{U}_{SB}(t_{n-1}, t_{n-2})\cdots\mathcal{U}_{SB}(t_1, t_0)\mathcal{B}_{\alpha_0\beta_0}\rho_{SB}(0)\right\} = p(\mathbf{r}_{n-1})\mathrm{Tr}_S\left\{\sigma^{(\alpha_{k-1})}\right\}$$

$$p(\mathbf{r}_n) = \mathrm{Tr}\left\{\mathcal{B}_{\alpha_n\beta_n}\mathcal{U}_{SB}(t_n, t_{n-1})\cdots\mathcal{B}_{\alpha_0\beta_0}\rho_{SB}(0)\right\} = p(\mathbf{r}_{n-1})\mathrm{Tr}\left\{\mathcal{B}_{\alpha_n\beta_n}\mathcal{U}_{SB}(t_n, t_{n-1})\sigma^{(\alpha_{k-1})} \otimes \rho_B\right\}.$$

To calculate $p(r_n, r_{n-1})$ and $p(r_n)$ it is sufficient to not intervene in the first $n-1$ times, namely

$$p(r_{n-1}) = \mathrm{Tr}\left\{\mathcal{B}_{\alpha_{n-1}\beta_{n-1}}\rho_{SB}\right\} = p(r_{n-1})\mathrm{Tr}_S\left\{\sigma^{(\alpha_{k-1})}\right\}$$

$$p(r_n, r_{n-1}) = p(r_{n-1})\mathrm{Tr}\left\{\mathcal{B}_{\alpha_n\beta_n}\mathcal{U}_{SB}(t_n, t_{n-1})\sigma^{(\alpha_{k-1})} \otimes \rho_B\right\}.$$

From which we see that the classical Markov relation is satisfied

$$p(\mathbf{r}_n|\mathbf{r}_{n-1}) = \frac{p(\mathbf{r}_n)}{p(\mathbf{r}_{n-1})} = \frac{p(r_n)}{p(r_{n-1})} = p(r_n|r_{n-1})$$

2. A classical stochastic process is one that obeys the Kolmogorov consistency condition. Since it also satisfies the Markov condition then it is a classical Markov process.

2 Classical Stochastic Thermodynamics

Exercise 2.1: Heat engine efficiency

The first law for a system in contact with a work source and a hot and a cold bath reads

$$\Delta U_S = W + Q_H + Q_C,$$

where $Q_{H(C)}$ is the heat flow from the hot (cold) bath. Assuming that the baths are described throughout the process by constant temperatures $T_H > T_C$, the second law generalizes to

$$\Sigma = \Delta_S - \frac{Q_H}{T_H} - \frac{Q_C}{T_C} \geq 0.$$

For the set-up to act as a heat engine, we want to extract work from it $W < 0$. We further consider a *cyclically* working heat engine, which has entually reached a steady state characterized by $\Delta U_S = 0$ and $\Delta S_S = 0$ per cycle.

Show that, in this case, $W < 0 \Rightarrow Q_H > 0$, which implies that the heat engine's **efficiency** per cycle,

$$\eta \equiv -\frac{W}{Q_H} \geq 0.$$

Next, use $\Delta U_S = 0$ and $\Delta S_S = 0$ and the first and second laws of thermodynamics to show that the following relations hold:

$$\eta = 1 - \frac{T_C}{T_H} - \frac{T_C \Sigma}{Q_H} \leq 1 - \frac{T_C}{T_H} \equiv \eta_C.$$

Here, η_C is the **Carnot efficiency**, which is the maximum efficiency of any engine working between two heat baths with fixed temperatures. Thus, any excess in the entropy production Σ diminishes the efficiency of the engine.

Solution:

$$\Sigma = -\frac{Q_H}{T_H} - \frac{Q_C}{T_C} \geq 0 \to Q_H \left(\frac{1}{T_C} - \frac{1}{T_H} \right) \geq -\frac{W}{T_C} \geq 0$$

$$\eta \equiv -\frac{W}{Q_H} = \frac{Q_H + Q_C}{Q_H} = 1 - \frac{T_C}{T_H} - \frac{T_C \Sigma}{Q_H} \leq \eta_C$$

Exercise 2.2: Intrinsic entropies and energies and Landauer's principle

Generalize the magnetic memory example to the case where the two mesostates $x \in \{0, 1\}$ have different intrinsic entropy $\mathcal{S}_0 \neq \mathcal{S}_1$ and internal energies $\mathcal{U}_0 \neq \mathcal{U}_1$.

Show that the second law for an equilibration process (no external work supplied) starting with some p_x and ending with π_x becomes

$$\Sigma = k_B S_{\text{Sh}}(\pi_x) - k_B S_{\text{Sh}}(p_x) + \sum_x (\pi_x - p_x)\mathcal{S}_x - \frac{1}{T}\sum_x \mathcal{U}_x(\pi_x - p_x) \geq 0.$$

Solution:
Given the probability to be in a mesostate p_x and in a microstate $p(i_x|x)$, the Shannon entropy is

$$k_B S_{\text{Sh}} = -k_B \sum_x \sum_{i_x} p(i|x)p_x \ln[p(i|x)p_x] = -k_B \sum_x \sum_{i_x} p(i|x)p(x)[\ln p(x|i) + \ln p_x]$$

$$k_B S_{\text{Sh}} = k_B S_{\text{Sh}}(p_x) + \sum_x p_x S_{\text{Sh}}[p(i_x|x)] = k_B S_{\text{Sh}}(p_x) + \sum_x p_x \mathcal{S}_x.$$

For the process that maps $p_x \to \pi_x$ without requiring work $W = 0$, we can write the first and the second law of thermodynamics:

$$\Delta U_S = Q, \qquad \Sigma = \Delta S_S - \frac{Q}{T} \geq 0$$

which combined yield

$$\Sigma = k_B[S_{\rm Sh}(\pi_x) - S_{\rm Sh}(p_x)] + \sum_x (\pi_x - p_x)\mathcal{S}_x - \frac{1}{T}\sum_x (\pi_x - p_x)\mathcal{U}_x \geq 0.$$

Notably, one can have $\pi_0 > p_0 = \frac{1}{2}$ and still have the process happening spontaneusly. Indeed, taking $\mathcal{U}_0 = \mathcal{U}_\infty$, $\pi_0 = 1$, $\mathcal{S}_0 = \alpha\mathcal{S}_1$ we get

$$\Sigma = -k_B \ln 2 + \frac{1}{2}[\mathcal{S}_0 - \mathcal{S}_1] \to \frac{\mathcal{S}_0}{2}[\alpha - 1] \geq k_B \ln 2,$$

which is satisfied for a sufficiently large α.

Exercise 2.3: Rate master equation

Derive that the transition matrix $T_{l,k}$ for a finite time steo from t_k to t_l follows from the rate master equation $d_t\mathbf{p}(t) = R(t)\mathbf{p}(t)$ as the time-ordered exponential

$$T_{l,k} = \exp_+\left[\int_{t_k}^{t_l} R(t)dt\right].$$

If the rate matrix does not depend on time, show that $T_{l,k} = e^{(t_l - t_k)R}$. Then, under the assumption that the dynamics is Markovian, show that for any $n \in \mathbb{N}$

$$p(x_n, \cdots, x_0) = (T_{n,n-1})_{x_n,x_{n-1}} \cdots (T_{1,0})_{x_1,x_0} p_{x_0}(0),$$

where the joint probability $p(x_n, \cdots, x_0)$ completely characterizes the stochastic process.

Solution:
Rewriting the rate master equation we can write the solution of the differential equation in terms of the product of many steps, namely

$$\mathbf{p}(t + dt) \approx [\mathbb{I} + R(t)dt]\mathbf{p}(t) \to p(t_l) = \left[\lim_{N\to\infty}\prod_{i=0}^{N} e^{R(t_i)dt_i}\right]\mathbf{p}(t_k) = \exp_+\left[\int_{t_k}^{t_l} R(t)dt\right]\mathbf{p}(t)$$

which coincides with the time-ordered exponential.
If the rate matrix does not depend on t it is easy to check that $\mathbf{p}(t) = e^{Rt}\mathbf{p}(0)$ is a solution. Indeed, $\partial_t\mathbf{p}(t) = Re^{Rt}\mathbf{p}(0) = R\mathbf{p}(t)$.
Using the Markov property we can write the joint probability distribution as

$$p(x_n, \cdots, x_0) = p(x_n|\mathbf{x}_{n-1})p(x_{n-1}|\mathbf{x}_{n-2})\cdots p(x_1|x_0) = p(x_n|x_{n-1})p(x_{n-1}|x_{n-2})\cdots p(x_1|x_0)p(x_0),$$

where we recognize the conditional probabilities $p(x_l|x_k)$, which correspond to the transition matrices $(T_{l,k})_{x_l,x_k}$, therefore

$$p(x_n, \cdots, x_0) = (T_{n,n-1})_{x_n,x_{n-1}}(T_{n-1,n-2})_{x_{n-1},x_{n-2}} \cdots (T_{1,0})_{x_1,x_0} p(x_0).$$

Exercise 2.4: Steady state and equilibrium state

Use the rate master equation $d_t\mathbf{p}(t) = R(t)\mathbf{p}(t)$ and the local detailed balance

$$\frac{R_{x,x'}(\lambda_t)}{R_{x',x}(\lambda_t)} = \exp\left[\frac{E_{x'}(\lambda_t) - E_x(\lambda_t)}{k_B T}\right]$$

to show that the Gibbs state, $\pi_x = e^{-\beta E_x}/\mathcal{Z}_S$ is a steady-state, i.e. $R\pi = 0$.

A rate master equation has a unique steady-state solution if it is *fully connected* or *irreducible*, meaning that for any two states x, x' it is always possible to construct a path $x \to x_1 \to \cdots \to x'$ using other states $x_i, i \in \{1, \cdots, n\}$ such that the product $R_{x',x_n}R_{x_n,x_{n-1}}\cdots R_{x_1,x}$ does not vanish. Construct a rate matrix with multiple steady states and confirm that it is not irreducible. What kind of physical situation could be described by rate master equations with multiple steady states?

Solution:
Plugging the Gibbs state into the rate master equation and using the local detailed balance, we get (omitting the λ dependencies)

$$d_t \pi_x = \sum_{x'} R_{x,x'} \pi_{x'} = \sum_{x'} R_{x',x} e^{\beta(E_{x'} - E_x)} \frac{e^{-\beta E_{x'}}}{\mathcal{Z}_S} = \left(\sum_{x'} R_{x',x} \right) \frac{e^{-\beta E_x}}{\mathcal{Z}_S} = 0,$$

where in the last step we used the fact that the rate matrix R satisfies $\sum_x R_{x,x'} = 0$. Therefore, the Gibbs state is a steady state of the Markovian dynamics.
Let's consider two separate 2-dimensional systems that evolve with the rate matrix

$$R = \begin{pmatrix} -x & x & 0 & 0 \\ x & -x & 0 & 0 \\ 0 & 0 & -y & y \\ 0 & 0 & y & -y \end{pmatrix}$$

that has a 2-dimensional eigenspace of steady states, with basis

$$\frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \frac{1}{2} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}.$$

The rate matrix is not irreducible since it can be decomposed into two independent parts. In particular, we obtain such a rate matrix by considering completely independent systems that evolve separately.

Exercise 2.5: Out-of-equilibrium 2-level system

Consider a two-level system with states $0, 1$ described by the rate master equation

$$\frac{d}{dt} \begin{pmatrix} p_0(t) \\ p_1(t) \end{pmatrix} = \Gamma \begin{pmatrix} -e^{-\beta\Delta(\lambda_t)/2} & e^{\beta\Delta(\lambda_t)/2} \\ e^{-\beta\Delta(\lambda_t)/2} & -e^{\beta\Delta(\lambda_t)/2} \end{pmatrix} \begin{pmatrix} p_0(t) \\ p_1(t) \end{pmatrix},$$

with Γ an overall relaxation rate and $\Delta(\lambda_t)$ the time-dependent energy gap between 0 and 1. Assume the system starts in equilibrium, $\mathbf{p}(0) = \pi(\lambda_0)$. By considering a numerical parametrization of your choice, show that the system follows the instantaneous steady state, i.e. $\mathbf{p}(t) \approx \pi(\lambda_t)$ when the driving is slow, namely $\dot{\lambda}_t \ll \Gamma$.

Solution:
The rate matrix $R(\lambda_t)$ has eigenvalues and eigenvectors

$$\lambda = 0, \quad \pi(t) = \frac{1}{e^{\alpha} + e^{-\alpha}} \begin{pmatrix} e^{\alpha} \\ e^{-\alpha} \end{pmatrix}, \qquad \lambda = -2\Gamma \cosh(\alpha), \quad \mathbf{v} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

with $\alpha = \beta\Delta(\lambda_t)/2$ time-dependent. For all t, $\{\pi(t), \mathbf{v}\}$ span $\mathbb{R}^2$, so we can always write the probability vector at time t as $\mathbf{p}(t) = x_1(t)\pi(t) + \beta(t)\mathbf{v}$. Since $\mathbf{p}(t)$ is a probability vector, and $\sum_x v_x = 0$, the coefficient $x_1(t) = 1 \forall t$. Now, we can write the evolution of the probability vector through the rate matrix

$$\mathbf{p}(t + dt) = \boldsymbol{\pi}(t + dt) + \beta(t + dt)\mathbf{v} = \mathbf{p}(t) + dt R(\lambda_t)\mathbf{p}(t) = \boldsymbol{\pi}(t) + \beta(t)\mathbf{v} - dt\Gamma 2\cosh(\alpha)\beta(t)\mathbf{v},$$

which gives the following differential equation

$$\dot{\boldsymbol{\pi}} + \dot{\beta}\mathbf{v} = -2\Gamma \cosh(\alpha)\beta(t)\mathbf{v}.$$

The derivative of the Gibbs state follows from

$$d_t \pi_0 = \frac{e^{\alpha}\dot{\alpha}}{e^{\alpha} + e^{-\alpha}} - \frac{e^{\alpha}\dot{\alpha}}{(e^{\alpha} + e^{-\alpha})^2}(e^{\alpha} - e^{-\alpha}) = \pi_0 \dot{\alpha} \frac{2e^{-\alpha}}{e^{\alpha} + e^{-\alpha}} = \frac{2\dot{\alpha}}{(e^{\alpha} + e^{-\alpha})^2} \Rightarrow \dot{\boldsymbol{\pi}} = \frac{2\dot{\alpha}}{(e^{\alpha} + e^{-\alpha})^2}\mathbf{v}$$

where in the last step we used the conservation of probability is a 2-level system. Noticing that all terms in the differential equation are proportional to $\mathbf{v}$, we get

$$\dot{\beta} = -2\Gamma \cosh(\alpha)\beta(t) - \frac{2\dot{\alpha}}{(e^{\alpha} + e^{-\alpha})^2}$$

with $\dot{\alpha} \propto \dot{\lambda}_t$. When $\dot{\lambda}_t \ll \Gamma$, we can neglect the second term in the RHS, and the differential equation becomes

$$\dot{\beta} \approx -2\Gamma \cosh(\alpha)\beta(t).$$

Since $\Gamma > 0$ and $\cosh(\alpha) > 0 \forall t$, the product $\beta\dot{\beta} < 0$, meaning that $\dot{\beta^2} < 0$. This means that $\beta^2(t)$ is decreasing, and, at the same time, lower-bounded by 0. To conclude, we just need to check the initial condition: If the system starts in the Gibbs state, then $\beta(0) = 0$, and the system will stay close to $\boldsymbol{\pi}(t)$ when the driving is slow.

Exercise 2.6: Non-invariant Hamiltonian under time reversal

If $\Pi_{E,x} = |x\rangle\langle x|$ are projectors of rank 1, then the equation

$$\text{Tr}\left\{\Pi_{E,x} U(\delta t) \Pi_{E,x'} U(\delta t)^\dagger\right\} = \text{Tr}\left\{\Pi_{E,x'} U(\delta t) \Pi_{E,x} U(\delta t)^\dagger\right\}$$

becomes

$$|\langle x|Ux'\rangle|^2 = |\langle x'|Ux\rangle|^2,$$

meaning that the transition probability from x' to x equals the one from x to x'.

Consider a single spin 1/2 particle with Hamiltonian $H = B\sigma_z$, which is not invariant under time reversal, and construct an example where $|\langle x|Ux'\rangle|^2 \neq |\langle x'|Ux\rangle|^2$.

Solution:
The unitary evolution is

$$U = e^{-iHt/\hbar} = e^{-iBt\sigma_z/\hbar} = \begin{pmatrix} e^{-iBt/\hbar} & 0 \\ 0 & e^{iBt/\hbar} \end{pmatrix}$$

Choosing the states $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ and $|i_+\rangle = (|0\rangle + i\,|1\rangle)/\sqrt{2}$ we get

$$\langle i_+|U|+\rangle = \frac{1}{2}\left(e^{-iBt/\hbar} - ie^{iBt/\hbar}\right) \to |\langle i_+|U|+\rangle|^2 = \frac{1+\sin(2Bt/\hbar)}{2}$$

$$\langle +|U|i_+\rangle = \frac{1}{2}\left(e^{-iBt/\hbar} + ie^{iBt/\hbar}\right) \to |\langle +|U|i_+\rangle|^2 = \frac{1-\sin(2Bt/\hbar)}{2}$$

Exercise 2.7: Positive entropy production rate

1. Show that the entropy production rate $\dot{\Sigma}(t)$ can be alternatively expressed in terms of the relative entropy as follows:

$$\dot{\Sigma}(t) = -k_B \left.\frac{\partial}{\partial t}\right|_{\lambda_t} D[\mathbf{p}(t)|\boldsymbol{\pi}(\lambda_t)]$$

   where the derivative is taken with respect to a fixed λ_t. Use this expression to show that the entropy production rate is positive.

2. Confirm that the entropy production rate can be expressed as

$$\dot{\Sigma}(t) = \frac{k_B}{2}\sum_{xx'}[R_{xx'}(\lambda_t)p_{x'}(t) - R_{x'x}(\lambda_t)p_x(t)] \ln \frac{R_{xx'}(\lambda_t)p_{x'}(t)}{R_{x'x}(\lambda_t)p_x(t)}.$$

   Prove that $\dot{\Sigma}(t) \geq 0$ by using that $(a-b)\ln(a/b) \geq 0 \forall a, b \in \mathbb{R}^+$

Solution:

1. From the definitions, the average entropy production rate is

$$\dot{\Sigma} = k_B \frac{d}{dt} S_{\text{Sh}}[\mathbf{p}(t)] - \frac{\dot{Q}(t)}{T}, \qquad \dot{Q}(t) = \sum_x E_x(\lambda_t) \frac{d}{dt} p_x(t).$$

   Remembering that the Gibbs state is $\pi_x(\lambda_t) = e^{-\beta E_x(\lambda_t)}/Z(\lambda_t)$, we can write the average entropy production rate as

$$\dot{\Sigma} = k_B \left.\frac{\partial}{\partial t}\right|_{\lambda_t} \left[S_{\text{Sh}}[\mathbf{p}(t)] + \sum_x \left(\log[\pi_x(\lambda_t)] + \log[Z(\lambda_t)]\right) p_x(t) \right] = -k_B \left.\frac{\partial}{\partial t}\right|_{\lambda_t} D[\mathbf{p}(t)|\boldsymbol{\pi}(\lambda_t)].$$

Discretizing the derivative we get

$$\dot{\Sigma} = -k_B \frac{D[\mathbf{p}(t+dt)|\boldsymbol{\pi}(\lambda_t)] - D[\mathbf{p}(t)|\boldsymbol{\pi}(\lambda_t)]}{dt} = -k_B \frac{D[T(dt)\mathbf{p}(t)|\boldsymbol{\pi}(\lambda_t)] - D[\mathbf{p}(t)|\boldsymbol{\pi}(\lambda_t)]}{dt}$$

with $T(dt) = \mathbb{I} + dtR(t)$ the stochastic matrix governing the evolution of $\mathbf{p}(t)$. Importantly, we are studying a system obeying local detailed, which implies that the thermal state $\boldsymbol{\pi}(\lambda_t)$ is a steady state of $R(t)$, i.e. $R(t)\boldsymbol{\pi}(\lambda_t) = \boldsymbol{\pi}(\lambda_t)$. This means that $\boldsymbol{\pi}(\lambda_t)$ is a steady state of $T(dt)$ as well. Thus, we can write

$$\dot{\Sigma} = -k_B \frac{D[T(dt)\mathbf{p}(t)|T(dt)\boldsymbol{\pi}(\lambda_t)] - D[\mathbf{p}(t)|\boldsymbol{\pi}(\lambda_t)]}{dt} \geq 0,$$

where in the last step we used the monotonicity of the relative entropy, namely $D(T\mathbf{p}|T\mathbf{q}) \leq D(\mathbf{p}|\mathbf{q})$ $\forall \mathbf{p}, \mathbf{q}$ proability vectors, $\forall T$ stochastic matrix.

2. By using the definitions stated above, the average entropy production rate reads

$$\dot{\Sigma}(t) = -k_B \sum_x \dot{p}_x \left(\log p_x + \beta E_x\right) = -k_B \sum_x \dot{p}_x \log\left(p_x e^{\beta E_x}\right).$$

Splitting the sum into two copies and using the rate master equation $\dot{\mathbf{p}} = R\mathbf{p}$ we get

$$\dot{\Sigma}(t) = -\frac{k_B}{2} \sum_{xy} \left[R_{xy} p_y \log\left(p_x e^{\beta E_x}\right) + R_{yx} p_x \log\left(p_y e^{\beta E_y}\right)\right].$$

Notably, the quantity $\sum_x R_{xy} p_y \log\left(p_y e^{\beta E_y}\right) = 0$ because $\sum_x R_{xy} = 0$ since R is a rate matrix. Therefore, we can use it to write the entropy production rate as

$$\dot{\Sigma}(t) = -\frac{k_B}{2} \sum_{xy} \left[R_{xy} p_y \log\left(\frac{p_x e^{\beta E_x}}{p_y e^{\beta E_y}}\right) + R_{yx} p_x \log\left(\frac{p_y e^{\beta E_y}}{p_x e^{\beta E_x}}\right)\right].$$

Using the local detailed balance, namely

$$\frac{R_{xy}}{R_{yx}} = e^{\beta(E_y - E_x)}$$

the entropy production rate becomes

$$\dot{\Sigma}(t) = -\frac{k_B}{2} \sum_{xy} \left[R_{xy} p_y \log\left(\frac{R_{yx} p_x}{R_{xy} p_y}\right) + R_{yx} p_x \log\left(\frac{R_{xy} p_y}{R_{yx} p_x}\right)\right]$$

$$\dot{\Sigma}(t) = \frac{k_B}{2} \sum_{xy} \left[\left(R_{xy} p_y - R_{yx} p_x\right) \log\left(\frac{R_{xy} p_y}{R_{yx} p_x}\right)\right].$$

Since $(a-b)\log(a/b) \geq 0$ then it follows that also $\dot{\Sigma}(t) \geq 0$.

Exercise 2.8: Positive entropy production rate for multiple baths

Using the results from the previous exercise, prove that the entropy production rate for multiple baths,

$$\dot{\Sigma}(t) = k_B \frac{d}{dt} S_{\text{Sh}}[\mathbf{p}(t)] - \sum_\nu \frac{\dot{Q}_\nu}{T_\nu} \geq 0$$

is always positive by generalizing the previous exercise.

Solution:

1. We start from $R = \sum_\nu R^{(\nu)}$, $\dot{Q}_\nu = \sum_{xy} E_x(\lambda_t) R^{(\nu)}_{xy}(\lambda_t) p_y(t)$, $\pi_x(\beta_\nu, \lambda_t) = e^{-\beta_\nu E_x(\lambda_t)}/\mathcal{Z}_S(\beta_\nu, \lambda_t)$ to write

$$\dot{\Sigma}(t) = -k_B \left[\sum_x \dot{p}_x \log p_x + \sum_{\nu xy} \beta_\nu E_x R^{(\nu)}_{xy} p_y \right] = -k_B \sum_{\nu xy} \left[R^{(\nu)}_{xy} p_y \log \left(p_x e^{\beta_\nu E_x} \right) \right]$$

Calling $\partial_{t|\nu} \mathbf{p}(t) = R^{(\nu)}(\lambda_t)\mathbf{p}(t)$, we have

$$\dot{\Sigma}(t) = -k_B \sum_\nu \left. \frac{\partial}{\partial t} \right|_{\lambda_t|\nu} D[\mathbf{p}(t)|\boldsymbol{\pi}(\beta_\nu, \lambda_t)].$$

Using an arbitrarily small time-step dt, each bath contributes with

$$\frac{D[(\mathbb{I} + dt R^{(\nu)})\mathbf{p}(t)|\boldsymbol{\pi}(\beta_\nu, \lambda_t)] - D[\mathbf{p}(t)|\boldsymbol{\pi}(\beta_\nu, \lambda_t)]}{dt}$$

where the evolution happens due to the system being in contact with bath ν. Calling $T^{(\nu)}(dt) = \mathbb{I} + dt R^{(\nu)}(\lambda_t)$ the stochastic matrix that has $\boldsymbol{\pi}(\beta, \lambda_t)$ as a steady state (due to the local detailed balance), we have

$$\frac{D[T^{(\nu)}(\delta t)\mathbf{p}(t)|T^{(\nu)}(\delta t)\boldsymbol{\pi}(\beta_\nu, \lambda_t)] - D[\mathbf{p}(t)|\boldsymbol{\pi}(\beta_\nu, \lambda_t)]}{dt} \leq 0,$$

which is negative due to the monotonicity of the relative entropy. Therefore, the multi-bath entropy production rate is always positive $\dot{\Sigma}(t) \geq 0$.

2. Starting from the previous point, we can split the sum over xy into two copies as follows

$$\dot{\Sigma}(t) = -\frac{k_B}{2} \sum_{\nu xy} \left[R^{(\nu)}_{xy} p_y \log \left(p_x e^{\beta_\nu E_x} \right) + R^{(\nu)}_{yx} p_x \log \left(p_y e^{\beta_\nu E_y} \right) \right].$$

Since each $R^{(\nu)}$ is a rate matrix, the quantity $\sum_x R^{(\nu)}_{xy} p_y \log \left(p_y e^{\beta_\nu E_y} \right) = 0$, thus we can subtract it to the entropy production rate to obtain

$$\dot{\Sigma}(t) = -\frac{k_B}{2} \sum_{\nu xy} \left[R^{(\nu)}_{xy} p_y \log \left(\frac{p_x e^{\beta_\nu E_x}}{p_y e^{\beta_\nu E_y}} \right) + R^{(\nu)}_{yx} p_x \log \left(\frac{p_y e^{\beta_\nu E_y}}{p_x e^{\beta_\nu E_x}} \right) \right].$$

Since each rate matrix $R^{(\nu)}$ satisfies the local detailed balance for the corresponding bath, namely

$$\frac{R^{(\nu)}_{xy}}{R^{(\nu)}_{yx}} = \frac{e^{\beta_\nu E_y}}{e^{\beta_\nu E_x}},$$

the entropy production rate becomes

$$\dot{\Sigma}(t) = -\frac{k_B}{2} \sum_{\nu xy} \left[R^{(\nu)}_{xy} p_y \log \left(\frac{R^{(\nu)}_{yx} p_x}{R^{(\nu)}_{xy} p_y} \right) + R^{(\nu)}_{yx} p_x \log \left(\frac{R^{(\nu)}_{xy} p_y}{R^{(\nu)}_{yx} p_x} \right) \right],$$

$$\dot{\Sigma}(t) = \frac{k_B}{2} \sum_{\nu xy} \left[\left(R^{(\nu)}_{xy} p_y - R^{(\nu)}_{yx} p_x \right) \log \left(\frac{R^{(\nu)}_{xy} p_y}{R^{(\nu)}_{yx} p_x} \right) \right],$$

where each contribution of the sum is positive.

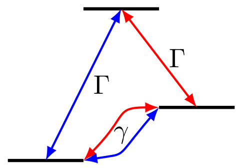


Figure 2: Sketch of the three-level system with the transitions regulated by the hot and cold baths.

Exercise 2.9: Equilibrium and non-equilibrium steady states

Consider a three-state system with energies $E_2 > E_1 > E_0$ coupled to a hot (H) and a cold (C) bath. THe following rate matrix with respect to the basis $\mathbf{p}(t) = [p_0(t), p_1(t), p_2(t)]^T$ fixes the dynamics:

$$R = \begin{pmatrix} -(\cdots) & \gamma[e^{\beta_C\Delta_{10}/2} + e^{\beta_H\Delta_{10}/2}] & \Gamma e^{\beta_C\Delta_{20}/2} \\ \gamma[e^{-\beta_C\Delta_{10}/2} + e^{-\beta_H\Delta_{10}/2}] & -(\cdots) & \Gamma e^{\beta_H\Delta_{21}/2} \\ \Gamma e^{-\beta_C\Delta_{20}/2} & \Gamma e^{-\beta_H\Delta_{21}/2} & -(\cdots) \end{pmatrix}$$

with $\Delta_{ij} = E_i - E_j$ is the energy difference while Γ and γ are rates. The diagonal matrix are fixed by the conservation of probability.

1. Confirm that this rate matrix has the additive structure $R = \sum_\nu R^{(\nu)}$.
2. Show that, if $\gamma = 0$ the steady state is a non-equilibrium state, but the heat flows are zero $\dot{Q}_H = \dot{Q}_C = 0$, which imples zero entropy production rate at steady state.
3. In contrast, if $\Gamma = 0$ and $p_2(0) = 0$, the steady state is an equilibrium state $\boldsymbol{\pi}(\beta)$. Find β.
4. By identifying non-equilibrium cycles in the 3-level system, argue why in 2. the heat currents are zero while in 3. they are not.

Solution:

1. It is easy to see that $R = R^{(H)} + R^{(C)}$ with

$$R^{(H)} = \begin{pmatrix} -(\cdots) & \gamma e^{\beta_H\Delta_{10}/2} & 0 \\ \gamma e^{-\beta_H\Delta_{10}/2} & -(\cdots) & \Gamma e^{\beta_H\Delta_{21}/2} \\ 0 & \Gamma e^{-\beta_H\Delta_{21}/2} & -(\cdots) \end{pmatrix}, \; R^{(C)} = \begin{pmatrix} -(\cdots) & \gamma e^{\beta_C\Delta_{10}/2} & \Gamma e^{\beta_C\Delta_{20}/2} \\ \gamma e^{-\beta_C\Delta_{10}/2} & -(\cdots) & 0 \\ \Gamma e^{-\beta_C\Delta_{20}/2} & 0 & -(\cdots) \end{pmatrix}$$

2. When $\gamma = 0$ the steady state satisfies

$$\begin{cases} p_0 = p_2 e^{\beta_C\Delta_{20}} \\ p_1 = p_2 e^{\beta_H\Delta_{21}} \\ p_0 + p_1 + p_2 = 1 \end{cases} \Rightarrow \mathbf{p} = \frac{1}{e^{\beta_C\Delta_{20}} + e^{\beta_H\Delta_{21}} + 1}\begin{pmatrix} e^{\beta_C\Delta_{20}} \\ e^{\beta_H\Delta_{21}} \\ 1 \end{pmatrix}$$

   which is clearly a nonequilibrium state for $\beta_C \neq \beta_H$.

   The heat flows are

$$\dot{Q}_H = \sum_{xy} E_x R^{(H)}_{xy} p_y = \Gamma\Delta_{21} e^{-\beta_H\Delta_{21}/2} p_1 - \Gamma\Delta_{21} e^{\beta_H\Delta_{21}/2} p_2 = 0$$

$$\dot{Q}_C = \sum_{xy} E_x R^{(C)}_{xy} p_y = \Gamma\Delta_{20} e^{\beta_C\Delta_{20}/2} p_0 - \Gamma\Delta_{20} e^{-\beta_C\Delta_{20}/2} p_2 = 0$$

   This means that, since at the steady state $d_t S_{\mathrm{Sh}}[\mathbf{p}(t)] = 0$, $\dot{\Sigma}(t) = -\dot{Q}_H/T_H - \dot{Q}_C/T_C = 0$.

3. When $\Gamma = 0$ the system effectively decomes 2-dimensional since $R_{x2} = R_{2y} = 0$ and the level-2 is unaffected by the dynamics. Therefore, if $p_2(0) = 0$, then $p_2(t) = 0\,\forall t$. Then, the 2D steady state reads

$$\begin{cases} p_0 = p_1 \frac{e^{\beta_C\Delta_{10}/2} + e^{\beta_H\Delta_{10}/2}}{e^{-\beta_C\Delta_{10}/2} + e^{-\beta_H\Delta_{10}/2}} \\ p_0 + p_1 = 1 \end{cases} \Rightarrow \mathbf{p} = \frac{1}{2[\cosh(\frac{\beta_C\Delta_{10}}{2}) + \cosh(\frac{\beta_H\Delta_{10}}{2})]}\begin{pmatrix} e^{\beta_C\Delta_{10}/2} + e^{\beta_H\Delta_{10}/2} \\ e^{-\beta_C\Delta_{10}/2} + e^{-\beta_H\Delta_{10}/2} \end{pmatrix}$$

whose effective temperature is given by $p_0/p_1 = e^{\beta^* \Delta_{10}}$, which yields

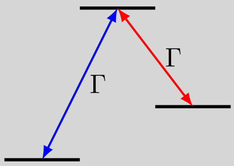
$$\beta^* = \frac{1}{\Delta_{10}} \ln\left(\frac{e^{\beta_C \Delta_{10}/2} + e^{\beta_H \Delta_{10}/2}}{e^{-\beta_C \Delta_{10}/2} + e^{-\beta_H \Delta_{10}/2}}\right)$$

The heat currents are

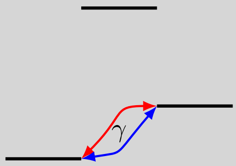
$$\dot{Q}_H = \gamma \Delta_{10} e^{-\beta_H \Delta_{10}/2} p_0 - \gamma \Delta_{10} e^{\beta_H \Delta_{10}/2} p_1 = \frac{\gamma \Delta_{10}[2\sinh[(\beta_C - \beta_H)\Delta_{10}/2]]}{2[\cosh(\frac{\beta_C \Delta_{10}}{2}) + \cosh(\frac{\beta_H \Delta_{10}}{2})]}$$

$$\dot{Q}_C = \gamma \Delta_{10} e^{-\beta_C \Delta_{10}/2} p_0 - \gamma \Delta_{10} e^{\beta_C \Delta_{10}/2} p_1 = \frac{\gamma \Delta_{10}[-2\sinh[(\beta_C - \beta_H)\Delta_{10}/2]]}{2[\cosh(\frac{\beta_C \Delta_{10}}{2}) + \cosh(\frac{\beta_H \Delta_{10}}{2})]}$$

4. We now sketch the two cases and consider a sequence of states forming a closed cycle $x_1 \to x_2 \to \cdots \to x_1$. Starting from any state, we write the possible transitions as u, d, u, d, with the color corresponding to the bath that caused the transition and the letter indicating the direction, u(p) or d(own) in energy.



Case (2): $\gamma = 0$.



Case (3): $\Gamma = 0$.

Any closed cycle in case (2) has the same number of u and d of each color because, for each $i \to j$, there is only one bath. For example, a closed cycle starting from 0 is $ududud$. To each transition there is some energy exchange with the corresponding bath. However, d and u exchange the opposite amount of energy. Since in case (2) $n_u = n_d$ for each color, the heat currents are zero.

By contrast, in case (3) there are closed cycles with $n_u \neq n_d$ but with $n_u + n_u = n_d + n_d$. For example, starting again from 0, the cycle ud exchanges finite heat with both baths.

Exercise 2.10: Coarsed-grained Markovianity

The microstate dynamics is Markovian and completely described by the conditional probabilities $p(i_x|i'_y) \equiv p(i_x, t + \delta t|i'_y, t)$ to jump from i'_y at t to i_x at $t + \delta t$. Thus, the joint probability distribution of ebserving a sequence of mesostates $\mathbf{x}_n = (x_n, \cdots, x_0)$ is

$$P(\mathbf{x}_n) = \sum_{i_{x_n}} \cdots \sum_{i_{x_0}} p(i_{x_n}|i_{x_{n-1}}) \cdots p(i_{x_1}|i_{x_0}) p(i_{x_0}|x_0) P_{x_0}(t_0).$$

Show that this described a Markov process if the probability of ending up in a mesostate is independent of the precise initial microstate, namely

$$\sum_{i_{x_l}} p(i_{x_l}|i'_{x_k}) = \sum_{i_{x_l}} p(i_{x_l}|i''_{x_k}) \quad \forall i'_{x_k} \neq i''_{x_k}.$$

Consider the transition matrix $p(i_x|i'_y)$ within time-scale separation for a time step $\delta\tau$ satisfying $F^{-1}_{i_x, i_{x'}} \ll \delta\tau \ll S^{-1}_{i_x, i'_y}$. Prove that

$$p(i_x|i'_y) = \delta_{xy} \pi_{i|x} \left(1 - \delta\tau \sum_{z \neq x} \sum_{k_z} S_{k_z, i_x}\right) + (1 - \delta_{xy}) \delta\tau \sum_{k_y} S_{i_x, k_y} \pi_{k|y},$$

which implies $p(i_x|i'_y) = p(i_x|i''_y) \quad \forall i'_y \neq i''_y$. The converse in not true: Markovianity does not imply time-scale separation.

Solution:
First, we notice that $\sum_{i_{x_n}} p(i_{x_n}|i_{x_{n-1}}) = C_{x_n, x_{n-1}}$ does not depend on $i_{x_{n-1}}$. This allows us to calculate

the sums one by one starting from the last one. The, the joint probability distribution becomes

$$P(\mathbf{x}_n) = C_{x_n,x_{n-1}} \cdots C_{x_1,x_0} \sum_{i_{x_0}} p(i_{x_0}|x_0) P_{x_0}(t_0) = C_{x_n,x_{n-1}} \cdots C_{x_1,x_0} P_{x_0}(t_0),$$

which is now decomposed in the Markovian form

$$P(\mathbf{x}_n) = P(x_n|x_{n-1}) \cdots P(x_1|x_0) P_{x_0}(t_0).$$

Given that we are consider the time scale $F\delta\tau \gg 1 \gg S\delta\tau$

$$\mathbf{p}(t+\delta\tau) = e^{L\delta\tau}\mathbf{p}(t) = e^{F\delta\tau + S\delta\tau}\mathbf{p}(t) \approx [\mathbb{I} + \delta\tau S] e^{F\delta\tau}\mathbf{p} = [\mathbb{I} + \delta\tau S]\boldsymbol{\pi}^*, \quad \forall \mathbf{p}.$$

Thus, for any initial condition the evolved probability reads

$$p_{i_x}(t+\delta\tau) = \left(1 - \delta\tau \sum_{z\neq x} \sum_{j_z} S_{j_z,i_x}\right) \pi_{i|x} P_x + \delta\tau \sum_{z\neq x} \sum_{k_z} S_{i_x,k_z} \pi_{k|z} P_z.$$

By choosing $[\mathbf{p}(t)]_{i_x} = \delta_{i_x,j_y}$ the evolution gives us directly the conditional probability $p(i_x|j_y)$. Crucially, this means $P_x(t) = \delta_{xy}$ since we are preparing the state in j_y at time t.
Therefore, the conditional probability reads

$$p(i_x|j_y) = \delta_{xy} \left(1 - \delta\tau \sum_{z\neq x} \sum_{j_z} S_{j_z,i_x}\right) \pi_{i|x} + (1 - \delta_{xy})\delta\tau \sum_{k_y} S_{i_x,k_y} \pi_{k|y} P_y.$$

Notably, this probability is independent of the specific microstate j_y in the same mesostate y because of the fast dynamics.

Exercise 2.11: Coarse-grained and strongly coupled equilibrium state

Show that the coarse-grained equilibrium state,

$$\pi_x^*(\lambda_t) = \frac{e^{-\beta \mathcal{F}_x(\lambda_t)}}{\mathcal{Z}(\lambda_t)},$$

and the reduced equilibrium state of a strongly coupled open system,

$$\pi_x^* = \sum_{i_x} \frac{e^{-\beta E_{i_x}}}{\mathcal{Z}},$$

coincide.

Solution:
We remember that the free-energy is

$$\mathcal{F}_x = -\frac{1}{\beta} \ln \mathcal{Z}_x, \quad \mathcal{Z}_x = \sum_{i_x} e^{-\beta E_{i_x}}.$$

Substituting into the coarse-grained equilibrium state we find

$$\pi_x^* = \frac{\sum_{i_x} e^{-\beta E_{i_x}}}{\mathcal{Z}}$$

which coincides with the reduced equilibrium state.

Exercise 2.12: Coarse-grained heat current and power

Using $p_{i_x}(t) = \pi_{i|x}(\lambda_t) P_x(t)$, derive

$$\dot{Q}(t) - \dot{Q}_{\rm cg}(t) = \dot{W}_{\rm cg}(t) - \dot{W}(t) = T \sum_x \frac{d\mathcal{S}_x(\lambda_t)}{dt} P_x(t)$$

where

$$\dot{Q}_{\rm cg}(t) \equiv \sum_x \mathcal{U}_x(\lambda_t)\frac{dP_x(t)}{dt}, \quad \dot{W}_{\rm cg}(t) \equiv \sum_x \frac{d\mathcal{U}_x(\lambda_t)}{dt}P_x(t),$$

are the coarse-grained heat flow and power.

Solution:
First, we remember that the mesostate intrinsic entropy is $\mathcal{S}_x = -\sum_{i_x}\pi_{i|x}\ln\pi_{i|x}$, with $\pi_{i|x} = e^{-\beta E_{i_x}}/\mathcal{Z}_x$. Writing the heat currents in terms of the microstates, we have

$$\dot{Q} = \sum_x\sum_{i_x} E_{i_x}\dot{\pi}_{i_x}, \quad \dot{Q}_{\rm cg} = \sum_x\sum_{i_x,j_x} E_{i_x}\pi_{i|x}\dot{\pi}_{j_x}.$$

Their difference reads

$$\dot{Q}-\dot{Q}_{\rm cg} = \sum_x\sum_{i_xj_x}\left(E_{i_x}\pi_{j|x}\dot{\pi}_{i_x} - E_{i_x}\pi_{i|x}\dot{\pi}_{j_x}\right) = \sum_x\sum_{i_xj_x}\left(E_{i_x}-E_{j_x}\right)\pi_{j|x}\dot{\pi}_{i_x} = -T\sum_x\sum_{i_xj_x}\ln\left(\frac{\pi_{i|x}}{\pi_{j|x}}\right)\pi_{j|x}\dot{\pi}_{i_x}.$$

We now use $\pi_{i_x} = \pi_{i|x}P_x$ to write the difference as

$$\begin{aligned}\dot{Q}-\dot{Q}_{\rm cg} &= -T\sum_x\sum_{i_xj_x}\ln\left(\frac{\pi_{i|x}}{\pi_{j|x}}\right)\pi_{j|x}(\dot{\pi}_{i|x}P_x + \pi_{i|x}\dot{P}_x)\\ &= T\sum_x\left(P_x\dot{\mathcal{S}}_x + \dot{P}_x\mathcal{S}_x - 0 - \dot{P}_x\mathcal{S}_x\right) = T\sum_x\frac{d\mathcal{S}_x(\lambda_t)}{dt}P_x(t).\end{aligned}$$

From the first law of thermodynamics we have that $\dot{U}_S = \dot{Q}+\dot{W} = \dot{Q}_{\rm cg}+\dot{W}_{\rm cg}$. Thus,

$$\dot{Q}(t)-\dot{Q}_{\rm cg}(t) = \dot{W}_{\rm cg}(t)-\dot{W}(t) = T\sum_x\frac{d\mathcal{S}_x(\lambda_t)}{dt}P_x(t).$$

Exercise 2.13: Intrinsic entropies and energies of mesostates

Assume λ_t = constant and consider a relaxation process from some nonequilibrium initial state $P_x(0)$ to the final equilibrium state π^*_x. Show that the entropy production coincides with the entropy production computed in Exercise 2.2, namely

$$\Sigma = k_B S_{\rm Sh}(\pi_x) - k_B S_{\rm Sh}(p_x) + \sum_x(\pi_x - p_x)\mathcal{S}_x - \frac{1}{T}\sum_x\mathcal{U}_x(\pi_x-p_x) \geq 0.$$

Solution:
The initial entorpy of the system is

$$S_i = -\sum_x P_x\ln P_x + \sum_x P_x\mathcal{S}_x,$$

whereas the final entropy is

$$S_f = -\sum_x \pi^*_x\ln\pi^*_x + \sum_x\pi^*_x\mathcal{S}_x.$$

Similarly, the initial and final internal energies are

$$U_i = \sum_x P_x\mathcal{U}_x, \qquad U_f = \sum_x\pi^*_x\mathcal{U}_x.$$

Therefore, the total entropy produced in the relaxation is

$$\Sigma = S_f - S_i - \frac{U_f-U_i}{T} = S_{\rm Sh}(\pi^*_x) - S_{\rm Sh}(P_x) + \sum_x(\pi^*_x - P_x)\mathcal{S}_x - \frac{1}{T}\sum_x(\pi^*_x-P_x)\mathcal{U}_x.$$

Exercise 2.14: Trajectory description of mesostates

Show that the average (with respect to the coarse-grained dynamics) of the following stochastic definitions gives rise to the following thermodynamics quantities

$$u_S(x_l, t_l) \equiv \mathcal{U}_{x_l}(\lambda_l)$$

$$s_S(x_l, t_l) \equiv \mathcal{S}_{x_l}(\lambda_l) - \ln p_{x_l}(t_l)$$

$$đq_{\mathrm{cg}}(t_l) \equiv \mathcal{U}_{x_{l+1}}(\lambda_{l+1}) - \mathcal{U}_{x_l}(\lambda_{l+1})$$

$$đw_{\mathrm{cg}}(t_l) \equiv \mathcal{U}_{x_l}(\lambda_{l+1}) - \mathcal{U}_{x_l}(\lambda_l)$$

where the mesostates are assumed to be x_l and x_{l+1} at times t_l and t_{l+1} respectively. Verify that the first law holds at the trajectory level.

Solution:
The average energy over the trajectory is

$$\langle u_S(x_l, t_l) \rangle = \sum_{\mathbf{P}} \mathcal{U}_{x_l}(\lambda_l) p(x_1, \cdots, x_n) = \sum_{x_l} \mathcal{U}_{x_l}(\lambda_l) p_{x_l} = U(t_l).$$

Similarly, the average entropy over the trajectory is

$$\langle s_S(x_l, t_l) \rangle = \sum_{\mathbf{P}} \left(\mathcal{S}_{x_l}(\lambda_l) - \ln p_{x_l}(t_l) \right) p(x_1, \cdots, x_n) = S_{\mathrm{Sh}}(p_{x_l}) + \sum_{x_l} p_{x_l} \mathcal{S}_{x_l}(\lambda_t) = S_S(t).$$

The average work at the coarse-grained level is

$$\langle đw_{\mathrm{cg}} \rangle = \sum_{x_l} p_{x_l}(t_l) \left(\mathcal{U}_{x_l}(\lambda_{l+1}) - \mathcal{U}_{x_l}(\lambda_l) \right) = dW_{\mathrm{cg}}(t_l),$$

while the average heat at the coarse-grained level is

$$\langle đq_{\mathrm{cg}} \rangle = \sum_{x_{l+1}} \mathcal{U}_{x_{l+1}}(\lambda_{l+1}) p_{x_{l+1}}(t_{l+1}) - \sum_{x_l} \mathcal{U}_{x_l}(\lambda_{l+1}) p_{x_l}(t_l) = \sum_{x_l} \mathcal{U}_{x_l}(\lambda_{l+1}) \left(p_{x_{l+1}}(t_{l+1}) - p_{x_l}(t_l) \right) = dQ_{\mathrm{cg}}(t_l)$$

The first law on the trajectory level reads

$$du_S = u_S(x_{l+1}, t_{l+1}) - u_S(x_l, t_l) = u_S(x_{l+1}, t_{l+1}) - u_S(x_l, t_{l+1}) + u_S(x_l, t_{l+1}) - u_S(x_l, t_l) = đq_{\mathrm{cg}}(t_l) + đw_{\mathrm{cg}}(t_l)$$

Exercise 2.15: Integral fluctuation theorem ⇒ 2$^{\text{nd}}$ law

Prove that the integral fluctuation theorem for entropy production, namely

$$\langle e^{-\sigma} \rangle_{\mathbf{x}_n} = 1,$$

imples $\Sigma = \langle \sigma \rangle_{\mathbf{x}_n} \geq 0$ and the existance of trajectories $\mathbf{x}_n$ with $\sigma(x_n) < 0$ unless $\sigma(\mathbf{x}_n) = 0 \, \forall \mathbf{x}_n$.

Solution:
Noticing that the exponential is a concave function, namely

$$e^{\alpha x + (1-\alpha) y} \leq \alpha e^x + (1-\alpha) e^y \qquad \forall \alpha \in [0,1], \forall x, y \in \mathbb{R},$$

we can use Jensen's inequality:

$$1 = \langle e^{-\sigma} \rangle_{\mathbf{x}_n} \geq e^{-\langle \sigma \rangle_{\mathbf{x}_n}} \Rightarrow \langle \sigma \rangle_{\mathbf{x}_n} \geq 0.$$

Suppose that there exists a trajectory $\mathbf{x}_n$ with positive entropy production $\sigma(\mathbf{x}_n) > 0$. If now no trajectory has negative entropy production this would violate the integral fluctuation theorem. Therefore, unless all trajectories produce zero entropy, there exists at least one trajectory with negative entropy production.

Exercise 2.16: Crooks' lemma on mesostates

Consider a stochastic trajectory of mesostates $\mathbf{x}_n$. Use time-scale separation to show that Crooks' lemma, namely

$$\ln \frac{p(\mathbf{x}_n|x_0)}{p_{\mathrm{tr}}(\mathbf{x}_n^\dagger|x_n)} = -\frac{q(\mathbf{x}_n)}{T},$$

generalizes to

$$\ln \frac{p(\mathbf{x}_n|x_0)}{p_{\mathrm{tr}}(\mathbf{x}_n^\dagger|x_n)} = -\frac{q_{\mathrm{cg}}(\mathbf{x}_n)}{T} - \sum_{l=0}^{n-1}[\mathcal{S}_{x_l}(\lambda_{l+1}) - \mathcal{S}_{x_l}(\lambda_l)] + \mathcal{S}_{x_n}(\lambda_n) - \mathcal{S}_{x_0}(\lambda_0).$$

Show that this imples

$$\ln \frac{p(\mathbf{x}_n)}{p_{\mathrm{tr}}(\mathbf{x}_n^\dagger)} = \sigma(\mathbf{x}_n) = \Delta s_S(t_n) - \beta q_{\mathrm{cg}}(\mathbf{x}_n) - \sum_{l=0}^{n-1}[\mathcal{S}_{x_l}(\lambda_{l+1}) - \mathcal{S}_{x_l}(\lambda_l)]$$

Solution:
The first steps are the same as in Crooks' lemma: first we split the probabilities into each step,

$$\frac{p(\mathbf{x}_n|x_0)}{p_{\mathrm{tr}}(\mathbf{x}_n^\dagger|x_n)} = \frac{p(x_n|x_{n-1},\lambda_n)\cdots p(x_1|x_0,\lambda_1)}{p(x_0|x_1,\lambda_1)\cdots p(x_{n-1}|x_n,\lambda_n)}.$$

Then, we reorganize the product and consider the single step

$$\frac{p(x_l|x_{l-1},\lambda_l)}{p(x_{l-1}|x_l,\lambda_l)} = \frac{\delta_{x_l,x_{l-1}} + R_{x_l x_{l-1}}(\lambda_l)}{\delta_{x_l,x_{l-1}} + R_{x_{l-1} x_l}(\lambda_l)}.$$

If $x_l = x_{l-1}$ the ratio is clearly 1. However, if $x_l \neq x_{l-1}$ we cannot use local detailed balance directly on R because it is the emergent dynamics. In fact, R describes the transitions between mesostates regardless of the microstate,

$$\dot{P}_x = \sum_y R_{xy}P_y = \sum_y \sum_{i_x,i_y} S_{i_x i_y} p_{i_y} = \sum_y \sum_{i_x,i_y} S_{i_x i_y}\pi_{i_y|y}P_y$$

from which we identify $R_{xy} = \sum_{i_x i_y} S_{i_x i_y}\pi_{i_y|y}$. Crucially, $S_{i_x i_y}$ satisfies local detailed balance. Therefore,

$$\frac{R_{xy}}{R_{yx}} = \frac{\sum_{i_x i_y} S_{i_x i_y}\pi_{i_y|y}}{\sum_{j_x j_y} S_{j_y j_x}\pi_{j_x|x}} = \frac{\mathcal{Z}_x}{\mathcal{Z}_y}\frac{\sum_{i_x i_y} S_{i_x i_y} e^{-\beta E_{i_y}}}{\sum_{j_x j_y} S_{j_y j_x} e^{-\beta E_{j_x}}} = \frac{\mathcal{Z}_x}{\mathcal{Z}_y}\frac{\sum_{i_x i_y} S_{i_y i_x} e^{\beta(E_{i_y}-E_{i_x})} e^{-\beta E_{i_y}}}{\sum_{j_x j_y} S_{j_y j_x} e^{-\beta E_{j_x}}}$$

fro, which we read

$$\frac{R_{xy}}{R_{yx}} = \frac{\mathcal{Z}_x}{\mathcal{Z}_y} = e^{\beta(F_y - F_x)}$$

where we used the free energy $F_x = \mathcal{U}_x - T\mathcal{S}_x$.
Thus, the ratio between the single step conditional probabilities reads

$$\frac{p(x_l|x_{l-1},\lambda_l)}{p(x_{l-1}|x_l,\lambda_l)} = e^{-\beta(\mathcal{U}_{x_l}(\lambda_l) - \mathcal{U}_{x_{l-1}}(\lambda_l))} e^{-\mathcal{S}_{x_{l-1}}(\lambda_l) + \mathcal{S}_{x_l}(\lambda_l)} = e^{-\beta đq_{\mathrm{cq}}(t_l)} e^{-\mathcal{S}_{x_{l-1}}(\lambda_l) + \mathcal{S}_{x_l}(\lambda_l)}$$

and we can write the mesolevel version of Crooks' lemma as

$$\begin{aligned}
\ln \frac{p(\mathbf{x}_n|x_0)}{p_{\mathrm{tr}}(\mathbf{x}_n^\dagger|x_n)} &= -\beta q_{\mathrm{cg}}(\mathbf{x}_n) + [\mathcal{S}_{x_n}(\lambda_n) - \mathcal{S}_{x_{n-1}}(\lambda_n) + \cdots + \mathcal{S}_{x_1}(\lambda_1) - \mathcal{S}_{x_0}(\lambda_1)] \\
&= -\beta q_{\mathrm{cg}}(\mathbf{x}_n) + \mathcal{S}_{x_n}(\lambda_n) - \sum_{l=1}^{n-1}[\mathcal{S}_{x_l}(\lambda_{l+1}) - \mathcal{S}_{x_l}(\lambda_l)] - \mathcal{S}_{x_0}(\lambda_1) \\
&= -\beta q_{\mathrm{cg}}(\mathbf{x}_n) + \mathcal{S}_{x_n}(\lambda_n) - \mathcal{S}_{x_0}(\lambda_0) - \sum_{l=0}^{n-1}[\mathcal{S}_{x_l}(\lambda_{l+1}) - \mathcal{S}_{x_l}(\lambda_l)].
\end{aligned}$$

Choosing the initial condition of the backward process to be equal to the final probability of the forward process, namely

$$p_{\mathrm{tr}}(x_n, 0) = p(x_n, t_n),$$

the logarithm of the ratio between the trajectory probabilities is

$$\ln \frac{p(\mathbf{x}_n)}{p_{\mathrm{tr}}(\mathbf{x}_n^\dagger)} = \ln \frac{p(\mathbf{x}_n|x_0)}{p_{\mathrm{tr}}(\mathbf{x}_n^\dagger|x_n)} + \ln \frac{p(x_0,0)}{p(x_n,t_n)} = \Delta s_S(t_n) - \beta q_{\mathrm{cg}}(\mathbf{x}_n) - \sum_{l=0}^{n-1}[\mathcal{S}_{x_l}(\lambda_{l+1}) - \mathcal{S}_{x_l}(\lambda_l)]$$

Exercise 2.17: Observing negative entropy production

Suppose the distribution $P(\sigma)$ is Gaussian with mean Σ and variance δ^2. Show that the integral fluctuation theorem fixes the variance to the value

$$\delta^2 = 2k_B\Sigma.$$

Show that this imples for the probability of observing a negative stochastic entropy production

$$\int_{-\infty}^{0} d\sigma P(\sigma) = \frac{1}{2}\text{erfc}\left(\frac{\sqrt{\Sigma/k_B}}{2}\right),$$

where erfc is the complementary error function.

Consider two ideal gases in a box at the same temperature and pressure initially separated by a dividing partition. After removing the partition, the average entropy production after the gases have finished mixing is $\Sigma = k_B N S_{\text{Sh}}[\{V_1/V, V_2/V\}]$ with V_1 (V_2) the volume initially occupied by gas 1 (2), $V = V_1 + V_2$ the total volume and N the number of particles. Estimate Σ and the probability of observing negative entropy production for a macroscopic system, $N \sim 10^{23}$.

Solution:
The Gaussian distribution reads

$$P(\sigma) = \frac{1}{\sqrt{2\pi}\delta}e^{-\frac{(\sigma-\Sigma)^2}{2\delta^2}}$$

and the integral fluctuatuin theorem states $\langle e^{-\sigma/k_B}\rangle = 1$. Combining them we get

$$1 = \int \frac{d\sigma}{\sqrt{2\pi}\delta}e^{-\sigma/k_B}e^{-\frac{(\sigma-\Sigma)^2}{2\delta^2}} = \int \frac{dx}{\sqrt{2\pi}\delta}e^{-(x+\Sigma)/k_B}e^{-\frac{x^2}{2\delta^2}} = e^{-\Sigma/k_B}\int \frac{dx}{\sqrt{2\pi}\delta}e^{-\frac{1}{2\delta^2}\left(x^2+2\frac{\delta^2}{k_B}+\frac{\delta^4}{k_B^2}-\frac{\delta^4}{k_B^2}\right)}$$

which results in

$$1 = e^{-\Sigma/k_B+\delta^2/(2k_B^2)}\int \frac{dy}{\sqrt{2\pi}\delta}e^{-y^2/(2\delta^2)} = e^{-\Sigma/k_B+\delta^2/(2k_B^2)} \Rightarrow \delta^2 = 2k_B\Sigma.$$

The probability of observing negative engtropy production is

$$\int_{-\infty}^{0} d\sigma P(\sigma) = \int_{-\infty}^{0}\frac{d\sigma}{\sqrt{2\pi}\delta}e^{-\frac{(\sigma-\Sigma)^2}{2\delta^2}} \overset{x=\frac{\sigma-\Sigma}{\sqrt{2}\delta}}{=} \int_{-\infty}^{-\frac{\Sigma}{\sqrt{2}\delta}}\frac{dx}{\sqrt{\pi}}e^{-x^2} = \int_{\frac{\Sigma}{\sqrt{2}\delta}}^{\infty}\frac{dx}{\sqrt{\pi}}e^{-x^2} = \frac{1}{2}\text{erfc}\left(\frac{1}{2}\sqrt{\frac{\Sigma}{k_B}}\right).$$

When the volumes are comparable, the average entropy produced $\Sigma \sim 10^{23}$, then, a rough overshoot of the probbaility of observing negative entropy production is $e^{-\Sigma} \sim 10^{-\Sigma/2} \sim 10^{-10^{22}}$, an incredibly small number.

Exercise 2.18: Crooks' lemma with multiple heat baths

Generalize Crooks' lemma to a sistem in contact with multiple heat baths.

Solution:
When dealing with multiple heat baths it is important to require the knowledge of which bath cased the stochastic jump. This means that, together with the list of system states x_i, there is also a list of baths ν_i. Then, the ratio between the forward and the backward conditional probabilities is

$$\frac{p(\mathbf{x}_n|x_0)}{p_{\text{tr}}(\mathbf{x}_n^\dagger|x_n)} = \frac{p(x_n|x_{n-1},\nu_n,\lambda_n)\cdots p(x_1|x_0,\nu_1,\lambda_1)}{p(x_0|x_1,\nu_1,\lambda_1)\cdots p(x_{n-1}|x_n,\nu_n,\lambda_n)}.$$

We now focus on the ratio of probabilities in a single step

$$\frac{p(x_l|x_{l-1},\nu_l,\lambda_l)}{p(x_{l-1}|x_l,\nu_l,\lambda_l)} = \frac{\delta_{x_l x_{l-1}} + \delta t R^{(\nu_l)}_{x_l x_{l-1}}(\lambda_l)}{\delta_{x_l x_{l-1}} + \delta t R^{(\nu_l)}_{x_{l-1} x_l}(\lambda_l)} = e^{\beta_{\nu_l}[E_{x_{l-1}}(\lambda_l)-E_{x_l}(\lambda_l)]_{\nu_l}} = e^{-\beta_{\nu_l} đq_{\nu_l}(t_l)},$$

where the notation $[\cdots]_\nu$ means that the energy was exchange to bath ν. Multiplying all these ratios together and taking the log we find Crooks' lemma formulated for multiple heat baths:

$$\ln\frac{p(\mathbf{x}_n|x_0)}{p_{\text{tr}}(\mathbf{x}_n^\dagger|x_n)} = -\sum_\nu \beta_\nu q_\nu(\mathbf{x}_n),$$

where $q_\nu(\mathbf{x}_n)$ is the heat exchanged with bath ν during the trajectory $\mathbf{x}_n$.

Exercise 2.19: Mathematics of integral and detailed fluctuation theorems

Integral and detailed fluctuation theorems can be trivially constructed if three mathematical requirements are met:

i) First, we have two probability distributions $p(x)$ and $q(x)$, $x \in X$.

ii) Second, let $p(x) = 0 \Leftrightarrow q(x) = 0$.

iii) Third, assume we have an involution $\dagger : X \to X$, which satisfies $(x^\dagger)^\dagger = x$.

Defining the 'entropy production' $\sigma(x) \equiv \ln[p(x)/q(x^\dagger)]$, show that it always satisfies an integral and detailed fluctuation theorem of the form $\langle e^{-\sigma}\rangle = 1$ and $P(\sigma)/Q(-\sigma) = e^\sigma$, with $P(\sigma) = \sum_x p(x)\delta[\sigma - \sigma(x)]$, $\quad Q(\sigma) = \sum_x q(x)\delta[\sigma - \sigma_{\rm tr}(x)]$, where $\sigma_{\rm tr}(x) = \ln[q(x)/p(x^\dagger)]$.

Solution:
Let's start from the integral fluctuation theorem:

$$\langle e^{-\sigma}\rangle = \sum_{x\in \mathrm{supp}(p)} \frac{q(x^\dagger)}{p(x)} p(x) = \sum_{x\in \mathrm{supp}(p)} q(x^\dagger) = 1$$

because p and q have the same support and $\dagger$ is a bijective map.
Now, let's move to the detailed fluctuation theorem:

$$Q(\sigma) = \sum_x q(x)\delta[\sigma - \sigma_{\rm tr}(x)] = \sum_x p(x^\dagger) e^{\sigma_{\rm tr}(x)}\delta[\sigma - \sigma_{\rm tr}(x)] = e^\sigma \sum_x p(x)\delta[\sigma - \sigma_{\rm tr}(x^\dagger)] = e^\sigma \sum_x p(x)\delta[\sigma + \sigma(x)]$$

from which the detailed fluctuation theorem $Q(\sigma) = e^\sigma P(-\sigma)$ follows.

Exercise 2.20: Which work works?

Consider a single particle with position vector $\mathbf{q}(t)$. If a force $\mathbf{F}(\mathbf{q})$ acts on the particle, the work done along the trajectory $\boldsymbol{\gamma}^\tau$ is

$$w'(\boldsymbol{\gamma}^\tau) \equiv \int_{\boldsymbol{\gamma}^\tau} \mathbf{F}\cdot d\mathbf{q}.$$

Use Newton's law $\mathbf{F} = m\ddot{\mathbf{q}}$ to deduce that $w' = \Delta T$, with $T = m\dot{\mathbf{q}}^2/2$ being the kinetic energy of the particle.
Assuming that the total energy is $T + V(\mathbf{q})$, with $V(\mathbf{q})$ potential energy, show that

$$w(\boldsymbol{\gamma}^\tau) - w'(\boldsymbol{\gamma}^\tau) = \Delta V.$$

This means that w' considers only the kinetic energy as the internal energy of the particle.
Consider the compression of a gas in a cylinder by a piston. If P is the pressure of the gas in volume V, the work done is $W = -\int PdV$. Let X be the position of the piston with mass M, which obey's Newton's law $M\ddot{X} = \sum_i F_i + F_{\rm ext}(\lambda_t)$. Here, F_i is the force excerted by the i-th particle on the piston.
Show that the work done on the gas is $W = -\int PdV = -\sum_i \int F_i dX$. Derive that $W = \Delta E_{\rm tot} - \Delta T_{\rm piston}$, where $E_{\rm tot}$ is the total energy of gas and piston. Deduce that W is identical to

$$w(\boldsymbol{\gamma}^\tau) \equiv H(\Gamma^\tau;\lambda_\tau) - H(\Gamma^0;\lambda_0) = \int_0^\tau dt\dot{\lambda}_t \frac{\partial H(\Gamma^t;\lambda_t)}{\partial \lambda_t}$$

if the system Hamiltonian contains the kinetic energy of the gas particles, the particle-particle potential and the particle-piston potential.

Solution:
The variation of the kinetic energy is

$$\Delta T = \int_0^\tau \dot{T} dt = \int_0^\tau m\ddot{\mathbf{q}}\cdot\dot{\mathbf{q}} dt = \int_{\boldsymbol{\gamma}^\tau} \mathbf{F}\cdot d\mathbf{q} = w'(\boldsymbol{\gamma}^\tau).$$

The work done along the trajectory corresponds to the variation of total energy:

$$w(\boldsymbol{\gamma}^\tau) = \Delta T + \Delta V = w'(\boldsymbol{\gamma}^\tau) + \Delta V.$$

Let's consider now the gas in a cylindrical volume. The work done on the gas is

$$W = -\int PdV = -\int PAdX = -\int \sum_i F_i dX$$

where A is the area of the piston. Crucially, the gas pressure is given only by the forces exerted by the gas particles. Then, the total work is

$$W = -\int \left[M\ddot{X} - F_{\text{ext}}(\lambda_t)\right] dX = -\Delta T_{\text{piston}} + \Delta E_{\text{tot}}.$$

If the system Hamiltonian is $H_S = T_{\text{p}} + V_{\text{pp}} + V_{\text{pP}}$, with T_{p} being the particles' kinetic energy, V_{pp} the particle-particle potential, V_{pP} the particle-piston potential, then the global Hamilonian $H_{\text{tot}} = H_S + T_{\text{P}}$ with T_{P} being the piston's kinetic energy. Then, $w(\boldsymbol{\gamma}^\tau) = \Delta H_S = \Delta H_{\text{tot}} - \Delta T_{\text{P}}$.

Exercise 2.21: Thermal state in the weak coupling regime

Consider the classical system-bath Hamiltonian

$$H_{SB}(\Gamma_{SB}; \lambda_t) = H_S(\Gamma_S; \lambda_t) + H_B(\Gamma_B) + V_{SB}(\Gamma_{SB}).$$

In the *weak coupling regime*, namely when $V_{SB}(\Gamma_{SB}) \ll H_S(\Gamma_S; \lambda_t), H_B(\Gamma_B)$, show that the canonical ensemble of the system-bath composite factorizes as

$$\pi_{SB}(\Gamma_{SB}, \lambda) \approx \pi_S(\Gamma_S, \lambda)\pi_B(\Gamma_B).$$

Solution:

$$\pi_{SB} = \frac{1}{h^{N_S+N_B}} \frac{e^{-\beta H_{SB}}}{\mathcal{Z}_{SB}} \approx \frac{1}{h^{N_S}} \frac{e^{-\beta H_S(\Gamma_S, \lambda)}}{\mathcal{Z}_S} \frac{1}{h^{N_B}} \frac{e^{-\beta H_B(\Gamma_B)}}{\mathcal{Z}_B} = \pi_S(\Gamma_S, \lambda)\pi_B(\Gamma_B)$$

Exercise 2.22: Work fluctuation theorems for open systems

Consider a driven system weakly coupled to a bath prepared in a canonical ensemble at temperature T. Let $p(w)$ [$p_{\text{tr}}(w)$] be the probability distribution of the fluctuating work, namely

$$w(\boldsymbol{\gamma}^\tau) = \int_0^\tau dt \dot{\lambda}_t \frac{\partial H_S(\Gamma_S^t; \lambda_t)}{\partial \lambda_t} = w(\boldsymbol{\gamma}_S^\tau),$$

in the forward [backward] process.

Prove that, for any driving protocol λ_t,

$$\langle e^{-\beta w} \rangle_{\boldsymbol{\gamma}_S} = e^{-\beta \Delta \mathcal{F}_S}, \qquad \frac{p(w)}{p_{\text{tr}}(-w)} = e^{\beta(w - \Delta \mathcal{F}_S)},$$

where $\Delta \mathcal{F}_S = \mathcal{F}_S(\lambda_t) - \mathcal{F}_S(\lambda_0)$ is the change is the system's equilibrium free energy with respect to temperature T.

Solution:
Let us first prove the detailed fluctuation theorem. The probability in the forward process is

$$p(w) = \int d\Gamma_S^0 d\Gamma_B^0 \delta[w - w(\boldsymbol{\gamma}_S^\tau)] \pi_S(\Gamma_S^0, \lambda_0) \pi_B(\Gamma_B^0).$$

Thanks to the weak coupling approximation, the bath traces out immediately, and we are left with the system only.

$$p(w) = \int d\Gamma_S^0 \delta[w - w(\boldsymbol{\gamma}_S^\tau)]\pi_S(\Gamma_S^0, \lambda_0) = \int \frac{d\Gamma_S^0}{h^{N_S}} \delta[w - \big(H_S(\Gamma_S^\tau, \lambda_\tau) - H_S(\Gamma_S^0, \lambda_0)\big)] \frac{e^{-\beta H_S(\Gamma_S^0, \lambda_0)}}{\mathcal{Z}(\lambda_0)}$$
$$= \frac{\mathcal{Z}(\lambda_\tau)}{\mathcal{Z}(\lambda_0)} e^{\beta w} \int \frac{d\Gamma_S^\tau}{h^{N_S}} \delta[w - \big(H_S(\Gamma_S^\tau, \lambda_\tau) - H_S(\Gamma_S^0, \lambda_0)\big)] \frac{e^{-\beta H_S(\Gamma_S^\tau, \lambda_\tau)}}{\mathcal{Z}(\lambda_\tau)}$$
$$= e^{\beta(w - \Delta \mathcal{F}_S)} \int d\Theta\Gamma_S^\tau \delta[w - \big(H_S(\Theta\Gamma_S^\tau, \lambda_\tau) - H_S(\Theta\phi^{-1}\Gamma_S^\tau, \lambda_0)\big)]\pi(\Theta\Gamma^\tau, \lambda_\tau)$$

with Θ being the time reversal operation, and $\phi\Gamma_S^0 = \Gamma_S^\tau$ being the evolution of the system trajectory. Crucially, this evolution is linked to the time-reversed one through $\Theta\phi^{-1} = \phi_{\rm tr}\Theta$. Using this and relabeling the phase space, we get

$$p(w) = e^{\beta(w - \Delta\mathcal{F})} \int d\Gamma_S^0 \delta[w - \big(H_S(\Gamma_S^0, \lambda_\tau) - H_S(\phi_{\rm tr}\Gamma_S^0, \lambda_0)\big)]\pi(\Gamma^0, \lambda_\tau) = e^{\beta(w - \Delta\mathcal{F}_S)} p_{\rm tr}(-w)$$

which is the detailed fluctuation theorem.
From the detailed fluctuation theorem the integral one follows directly as

$$\langle e^{-\beta w} \rangle_{\boldsymbol{\gamma}^\tau} = \int dw p(w) e^{-\beta w} = \int dw p_{\rm tr}(-w) e^{-\beta \Delta \mathcal{F}_S} = e^{-\beta \Delta \mathcal{F}_S}$$

Exercise 2.23: Work fluctuation theorems for open systems: The return of Markov and LDB

In the framework of a classical Markov process obeying local detailed balance, consider a forward and backward process by demanding that the initial state of the forward and backward process is described by a canonical ensemble, i.e. using $\pi_x(\lambda_0)$ and $\pi_x(\lambda_t)$, respectively.

Use Crooks' lemma to derive

$$\ln \frac{p(\mathbf{x}_n)}{p_{\rm tr}(\mathbf{x}_n^\dagger)} = \frac{w(\mathbf{x}_n) - \Delta\mathcal{F}_S}{k_B T},$$

where $w(\mathbf{x}_n) = u(x_n, t_n) - u(x_0, 0) - q(\mathbf{x}_n)$ is the stochastic work during the forward process. Use this result to prove Exercise 2.22 after identifying $\boldsymbol{\gamma}_S$ with $\mathbf{x}_n$.

Solution:
The ratio between the probabilities of the forward and backward process reads

$$\frac{p(\mathbf{x}_n)}{p_{\rm tr}(\mathbf{x}_n^\dagger)} = \frac{p(\mathbf{x}_n|x_0)\pi_{x_0}(\lambda_0)}{p_{\rm tr}(\mathbf{x}_n^\dagger|x_n)\pi_{x_n}(\lambda_n)} \overset{\text{Crooks'}}{=} e^{-\beta q(\mathbf{x}_n)} \frac{\mathcal{Z}_S(\lambda_n)}{\mathcal{Z}_S(\lambda_0)} e^{-\beta(E_{x_0}(\lambda_0) - E_{x_n}(\lambda_n))} = e^{\beta(w - \Delta\mathcal{F}_S)}.$$

The probability of obsering the work w is then

$$p(w) = \sum_{\mathbf{x}_n} \delta[w - w(\mathbf{x}_n)] p(\mathbf{x}_n) = e^{\beta(w - \Delta\mathcal{F}_S)} \sum_{\mathbf{x}_n} \delta[w - w(\mathbf{x}_n)] p_{\rm tr}(\mathbf{x}_n^\dagger) = e^{\beta(w - \Delta\mathcal{F}_S)} \sum_{\mathbf{x}_n} \delta[w + w_{\rm tr}(\mathbf{x}_n^\dagger)] p_{\rm tr}(\mathbf{x}_n^\dagger)$$

from which follows the detailed fluctuation theorem

$$p(w) = e^{\beta(w - \Delta\mathcal{F}_S)} p_{\rm tr}(-w).$$

Exercise 2.24: Nonequilibrium free energy and relative entropy

Given the nonequilibrium F_S and equilibrium $\mathcal{F}_S$ free energy with respect to the same temperature T, namely

$$F_S \equiv U_S - TS_S, \qquad \mathcal{F}_S = -k_B T \ln \mathcal{Z}_S,$$

prove that

$$F_S(t) - \mathcal{F}_S(\lambda_t) = k_B T D[\mathbf{p}(t)|\boldsymbol{\pi}(\lambda_t)] \geq 0$$

Solution:
Let's start from the nonequilibrium free energy:

$$F_S = \sum_i (E_i p_i + k_B T p_i \ln p_i) = k_B T \sum_i p_i \ln \left(p_i e^{\beta E_i} \frac{\mathcal{Z}}{\mathcal{Z}} \right) = k_B T \sum_i p_i \ln \left(\frac{p_i}{\pi_i} \right) - k_B T \ln \mathcal{Z}.$$

Moving things around we have

$$F_S - \mathcal{F}_S = k_B T D[\mathbf{p}(t)|\boldsymbol{\pi}(\lambda_t)].$$

Exercise 2.25: Equilibrium internal energy and entropy at strong coupling

At strong coupling, the Hamiltonian of mean force is defined through

$$\pi_S^*(\Gamma_S;\lambda) = \int d\Gamma_B \pi_{SB}(\Gamma_{SB};\lambda) \equiv \frac{e^{-\beta H_S^*(\Gamma_S;\lambda)}}{\mathcal{Z}_S^*(\lambda)}, \quad \mathcal{Z}_S^*(\lambda) \equiv \frac{\mathcal{Z}_{SB}(\lambda)}{\mathcal{Z}_B}.$$

Show that, in the classical case, the Hamiltonian of mean force reads

$$H_S^*(\Gamma_S;\lambda) = H_S(\Gamma_S;\lambda) - \frac{1}{\beta} \ln \int d\Gamma_B e^{-\beta V_{SB}(\Gamma_{SB})} \pi_B(\Gamma_B).$$

Postulating that the equilibrium internal energy and entropy are obtained, in analogy with standard statistical mechanics, as

$$\mathcal{U}_S^*(\lambda) \equiv \frac{\partial}{\partial \beta}[\beta \mathcal{F}_S^*(\lambda)], \quad \mathcal{S}_S^*(\lambda) \equiv k_B \beta^2 \frac{\partial}{\partial \beta} \mathcal{F}_S^*(\lambda),$$

derive

$$\mathcal{U}_S^*(\lambda) = \int d\Gamma_S \pi_S^*(\Gamma_S;\lambda) \left[H_S^*(\Gamma_S;\lambda) + \beta \frac{\partial}{\partial \beta} H_S^*(\Gamma_S;\lambda) \right]$$

$$\mathcal{S}_S^*(\lambda) = \int d\Gamma_S \pi_S^*(\Gamma_S;\lambda) \left\{ -\ln \left[h^{N_S f} \pi_S^*(\Gamma_S;\lambda) \right] + \beta^2 \frac{\partial}{\partial \beta} H_S^*(\Gamma_S;\lambda) \right\}$$

Solution:
From the definition,

$$-\beta H_S^* = \ln \mathcal{Z}_S^* + \ln \int d\Gamma_B \frac{e^{-\beta(H_S + H_B + V_{SB})}}{\mathcal{Z}_{SB}} = \ln \frac{\mathcal{Z}_{SB}}{\mathcal{Z}_B} - \ln \mathcal{Z}_{SB} - \beta H_S + \ln \int d\Gamma_B e^{-\beta H_B} e^{-\beta V_{SB}}$$

a from which we get

$$H_S^* = H_S - \frac{1}{\beta} \ln \int d\Gamma_B \pi_B e^{-\beta V_{SB}}.$$

Then, we remember that the equilibrium free energy at strong coupling is defined as

$$\mathcal{F}_S^* = -k_B T \ln \mathcal{Z}_S^* = -\frac{1}{\beta} \ln \int d\Gamma_S e^{-\beta H_S^*}.$$

Now we can take the derivatives with respect to β:

$$\mathcal{U}_S^* = -\frac{1}{\mathcal{Z}_S^*} \int d\Gamma_S e^{-\beta H_S^*} \left[-H_S^* - \beta \frac{\partial}{\partial \beta} H_S^* \right] = \int d\Gamma_S \pi_S^* \left[H_S^* + \beta \frac{\partial}{\partial \beta} H_S^* \right].$$

Similarly, for the entropy we get

$$\mathcal{S}_S^* = k_B \beta^2 \left[\frac{1}{\beta^2} \ln \mathcal{Z}_S^* + \frac{1}{\beta} \mathcal{U}_S^* \right] = k_B \left[\ln \mathcal{Z}_S^* + \beta \mathcal{U}_S^* \right] = k_B \int d\Gamma_S \pi_S^* \left[\beta H_S^* + \ln \mathcal{Z}_S^* + \beta^2 \frac{\partial}{\partial \beta} H_S^* \right]$$

which gives

$$\mathcal{S}_S^* = k_B \int d\Gamma_S \pi_S^* \left[-\ln[h^{N_S f} \pi_S^*] + \beta^2 \frac{\partial}{\partial \beta} H_S^* \right].$$

Exercise 2.26: Extensivity at strong coupling

The system S is split into two subsystems, X and Y, such that $S = XY$. Let us introduce the partition functions $\mathcal{Z}_X^* \equiv \mathcal{Z}_{XYB}/\mathcal{Z}_{YB}$ and $\mathcal{Z}_Y^* \equiv \mathcal{Z}_{XYB}/\mathcal{Z}_{XB}$. For both partition functions we have

$$\mathcal{F}_X^* = \mathcal{F}_{XYB} - \mathcal{F}_{YB}, \quad \mathcal{F}_Y^* = \mathcal{F}_{XYB} - \mathcal{F}_{XB}.$$

To show extensivity, one needs to confirm that $\mathcal{F}_S^* = \mathcal{F}_{XY}^* = \mathcal{F}_X^* + \mathcal{F}_Y^*$. Show that this is only possible at weak coupling, where one can neglect the interactions V_{XY}, V_{XB}, V_{YB}.

Solution:
The entensivity in $\mathcal{F}$ correponds to the factorization of the partition functions, namely

$$\mathcal{F}_{XY}^* = \mathcal{F}_X^* + \mathcal{F}_Y^* \Leftrightarrow \mathcal{Z}_{XY}^* = \mathcal{Z}_X^* \mathcal{Z}_Y^*.$$

Now, the partition functions are

$$\mathcal{Z}_{XYB} = \int \frac{d\Gamma_X d\Gamma_Y d\Gamma_B}{h^{N_X+N_Y+N_B}} e^{-\beta(H_X+H_Y+H_B+V_{XY}+V_{XB}+V_{YB})}$$

$$\mathcal{Z}_{XB} = \int \frac{d\Gamma_X d\Gamma_B}{h^{N_X+N_B}} e^{-\beta(H_Y+H_B+V_{XB})}$$

and to get the decomposition

$$\mathcal{Z}_{YB}\mathcal{Z}_{XB} = \mathcal{Z}_B \mathcal{Z}_{XYB}$$

one needs to neglect the interactions.

Exercise 2.27: Integral fluctuation theorem at strong coupling

The stochastic entropy production at strong coupling is defined as

$$\sigma^*(\gamma_S^t) \equiv \Delta s_S^* - \frac{q_S^*(\gamma_S^t)}{T}.$$

Show that, if the initial state is in the form $\rho_{SB}(\Gamma_{SB};0) = \rho_S(\Gamma_S;0)\pi(\Gamma_B|\Gamma_S)$, with

$$\pi(\Gamma_B|\Gamma_S) = \frac{\pi_{SB}(\Gamma_S,\Gamma_B;\lambda_0)}{\pi_S^*(\Gamma_S;\lambda_0)} = \frac{e^{-\beta[H_B(\Gamma_B)+V_{SB}(\Gamma_{SB})]}}{\int d\Gamma_B e^{-\beta[H_B(\Gamma_B)+V_{SB}(\Gamma_{SB})]}},$$

the stochastic entropy production can be written as

$$\sigma^*(t)/k_B = \ln\left[\frac{\rho_S(\Gamma_S^0;0)\pi_B(\Gamma_B^0|\Gamma_S^0)}{\rho_S(\Gamma_S^t;t)\pi_B(\Gamma_B^t|\Gamma_S^t)}\right].$$

Using Liouville's theorem, derive the integral fluctuation theorem at strong coupling, namely

$$\langle e^{-\sigma^*/k_B}\rangle_{\gamma_S^t} = 1.$$

Solution:
Let us first recall all the necessary ingredients:

$$s_S^* = -\ln[h^{N_Sf}\rho_S(\Gamma_S^t;t)] + \beta^2\partial_\beta H_S^*(\Gamma_S^t;\lambda_t), \quad u_S^* = H_S^*(\Gamma_S^t;\lambda_t) + \beta\partial_\beta H_S^*(\Gamma_S^t;\lambda_t)$$
$$q_S^* = \Delta u_S^* - w, \quad w = H_{SB}(\Gamma_{SB}^t;\lambda_t) - H_{SB}(\Gamma_S^0;\lambda_0)$$
$$H_S^*(\Gamma_S;\lambda) = H_S(\Gamma_S;\lambda) - \frac{1}{\beta}\ln\int d\Gamma_B e^{-\beta V_{SB}(\Gamma_{SB})}\pi(\Gamma_B)$$

Let's start from the system's entropy and energy

$$\Delta s_S^* = \ln\frac{\rho_S(0)}{\rho_S(t)} + \beta^2\partial_\beta\Delta H_S^*, \quad \Delta u_S^* = \Delta H_S^* + \beta\partial_\beta\Delta H_S^*.$$

From this we can write the global entropy productions as

$$\sigma^* = \ln\frac{\rho_S(0)}{\rho_S(t)} + \beta^2\partial_\beta\Delta H_S^* + \beta(w - \Delta H_S^* - \beta\partial_\beta\Delta H_S^*) = \ln\frac{\rho_S(0)}{\rho_S(t)} + \beta(w - \Delta H_S^*).$$

Now, we write the difference of the Hamiltonian of mean force as

$$H_S^*(\Gamma_S^t;\lambda_t) - H_S^*(\Gamma_S^0;\lambda_0) = \Delta H_S - \frac{1}{\beta}\ln\left(\frac{\mathcal{Z}_{B|S}(\Gamma_S^t)}{\mathcal{Z}_{B|S}(\Gamma_S^0)}\right), \quad \mathcal{Z}_{B|S}(\Gamma_S^t) = \int d\Gamma_B e^{-\beta[H(\Gamma_B)+V_{SB}(\Gamma_{SB}^t)]}.$$

Substituting into the total entropy we get

$$\sigma^* = \ln\frac{\rho_S(0)}{\rho_S(t)} + \beta(\Delta H_{SB} - \Delta H_S) + \ln\left(\frac{\mathcal{Z}_{B|S}(\Gamma_S^t)}{\mathcal{Z}_{B|S}(\Gamma_S^0)}\right) = \ln\left(\frac{\rho_S(0)\pi_B(\Gamma_B^0|\Gamma_S^0)}{\rho_S(t)\pi_B(\Gamma_B^t|\Gamma_S^t)}\right).$$

We can now use this expression for the entropy production combined with Liouville's theorem to prove the integral fluctuation theorem. In fact,

$$\langle e^{-\sigma^*/k_B}\rangle = \int d\Gamma_S^0 d\Gamma_B^0 \rho_S(t)\pi_B(\Gamma_B^t|\Gamma_S^t) = 1.$$

Exercise 2.28: Entropy production rate at strong coupling

Using the relation $\partial_t H_S^*(\lambda_t) = \partial_t H_S(\lambda_t)$, derive

$$\dot{\Sigma}^* = -k_B \left.\frac{\partial}{\partial t}\right|_{\lambda_t} D[\rho_S(\Gamma_S;t)|\pi_S^*(\Gamma_S;\lambda_t)].$$

Solution:
We have seen previously that

$$\sigma^* = \ln\frac{\rho_S(0)}{\rho_S(t)} + \beta(w - \Delta H_S^*).$$

Since $\Sigma^* = \langle\sigma^*\rangle$, the time derivative gives

$$\dot{\Sigma}^* = \partial_t\langle -\ln\rho_S(t)\rangle + \beta(\partial_t\langle w\rangle - \partial_t\langle H_S^*(\lambda_t)\rangle) = \partial_t S_S + \beta\partial_t\langle w\rangle - \beta\partial_t\langle H_S^*\rangle.$$

Now, let's look at the relative entropy.

$$-\left.\frac{\partial}{\partial t}\right|_{\lambda_t} D[\rho_S(\Gamma_S;t)|\pi_S^*(\Gamma_S;\lambda_t)] = -\int d\Gamma_S\dot{\rho}_S\ln\frac{\rho_S}{\pi_S^*} = -\int d\Gamma_S\dot{\rho}_S(\ln\rho_S + \beta H_S^*)$$
$$= \partial_t S_S - \beta\int d\Gamma_S\left[\partial_t(\rho_S H_S^*) - \rho_S\partial_t H_S^*\right] = \partial_t S_S - \beta\partial_t\langle H_S^*\rangle + \beta\langle\partial_t H_S.\rangle$$

Recognizing that the average work is

$$\langle w\rangle = \int ds\langle\partial_t H_S(s)\rangle \to \partial_t\langle w\rangle = \langle\partial_t H_S\rangle,$$

we easily see that the two expressions coincide.

Exercise 2.29: Strong coupling from coarse-graining: Hamiltonian of mean force

Consider the system X strongly coupled to $Y \subset B$ such that XY is weakly coupled to $R = B \setminus Y$. The energy of XY are

$$E_{xy}(\lambda_t) = E_x(\lambda_t) + E_y + V_{xy},$$

and the equilibrium state of XY (which is reached thanks to the weak coupling to the residual bath R) is $\pi_{xy}(\lambda_t)$.

Derive the Hamiltonian of mean force

$$E_x^*(\lambda_t) = E_x - \frac{1}{\beta}\ln\langle e^{-\beta V_{xy}}\rangle_Y,$$

and the following relation

$$E_x^*(\lambda_t) = \mathcal{F}_x(\lambda_t) - \mathcal{F}_Y,$$

where $\mathcal{F}_x(\lambda_t) = -k_B T\ln\sum_y e^{-\beta E_{xy}(\lambda_t)}$.

Solution:
Starting from the thermal state of XY, the Hamiltonian of mean force is defined through

$$\pi_{xy} = \frac{e^{-\beta E_{xy}}}{\mathcal{Z}_{XY}} \to \pi_x^* = \sum_y \pi_{xy} \equiv \frac{e^{-\beta E_x^*}}{\mathcal{Z}_X^*}$$

from which we read

$$-\beta E_x^* = \ln \frac{\mathcal{Z}_X^*}{\mathcal{Z}_{XY}} + \ln\left(e^{-\beta E_x}\sum_y e^{-\beta(E_y+V_{xy})}\right) = -\beta E_x + \ln\left(\sum_y e^{-\beta V_{xy}}\pi_y\right) + \ln\left(\frac{\mathcal{Z}_X^*\mathcal{Z}_Y}{\mathcal{Z}_{XY}}\right).$$

Since the last term is just a constant, we can disregard it and we are left with

$$E_x^* = E_x - \frac{1}{\beta}\ln\langle e^{-\beta V_{xy}}\rangle_Y.$$

Alternatively,

$$E_x^* = -\frac{1}{\beta}\ln\left(e^{-\beta E_x}\sum_y e^{-\beta V_{xy}}\frac{e^{-\beta E_y}}{\mathcal{Z}_Y}\right) = -k_B T\left[\ln\left(\sum_y e^{-\beta E_{xy}}\right) - \ln \mathcal{Z}_Y\right] = \mathcal{F}_x^* - \mathcal{F}_Y$$

Exercise 2.30: Strong coupling from coarse-graining: internal energy and entropy

Starting from the setting of Exercise 2.29, assume that Y evolves fast, such that one can apply time-scale separation. This means that $p_{xy}(t) \approx \pi_{y|x}p_x(t)$. Using the definitions of stochastic internal energy and system entropy,

$$u_x(t) = E_x(\lambda_t) + \sum_y (V_{xy} + E_y)\pi_{y|x}(\lambda_t), \quad s_x(t) = -k_B \ln p_x(t) - k_B \sum_y \pi_{y|x}(\lambda_t)\ln \pi_{y|x}(\lambda_t),$$

derive

$$u_x(t) - u_x^*(t) = \mathcal{U}_Y, \quad s_x(t) - s_x^*(t) = \mathcal{S}_Y.$$

Here, $\mathcal{U}_Y$ and $\mathcal{S}_Y$ are the equilibrium internal energy and entropy of Y alone, and u_x^*, s_x^* follow from the definitions of Exercise 2.25.

Solution:
From Exercise 2.25 we have

$$\mathcal{U}_S^* = \int d\Gamma_S \rho_S \left[H_S^* + \beta\partial_\beta H_S^*\right], \quad \mathcal{S}_S^* = \int d\Gamma_S \rho_S \left[-\ln\left(h^{N_S f}\rho_S\right) + \beta^2\partial_\beta H_S^*\right]$$

from which we have the stochastic internal energy and entropy at strong coupling

$$u_S^* \equiv H_S^* + \beta\partial_\beta H_S^*, \quad s_S^* \equiv -\ln\left(h^{N_S f}\rho_S\right) + \beta^2\partial_\beta H_S^*.$$

In the previous exercise we have seen that $E_x^* = \mathcal{F}_x - \mathcal{F}_Y$, so we have

$$u_x^* = (\mathcal{F}_x - \mathcal{F}_Y) + \beta\partial_\beta(\mathcal{F}_x - \mathcal{F}_Y) = \partial_\beta[\beta(\mathcal{F}_x - \mathcal{F}_Y)].$$

The derivative of $\mathcal{F}_x$ gives

$$\partial_\beta[\beta\mathcal{F}_x] = \frac{\sum_y E_{xy}e^{-\beta E_{xy}}}{\sum_y e^{-\beta E_{xy}}} = E_x + \frac{\sum_y (E_y + V_{xy})e^{-\beta(E_y+V_{xy})}}{\sum_y e^{-\beta(E_y+V_{xy})}} = E_x + \sum_y (E_y + V_{xy})\pi_{y|x} = u_x$$

Therefore

$$u_x - u_x^* = \partial_\beta[\beta\mathcal{F}_Y] = \frac{\sum_y E_y e^{-\beta E_y}}{\sum_y e^{-\beta E_y}} = \mathcal{U}_Y$$

Similarly, the stochastic entropy at strong coupling is

$$s_x^* = -\ln p_x + \beta^2\partial_\beta(\mathcal{F}_x - \mathcal{F}_Y).$$

The β-derivative on $\mathcal{F}_x$ acts as

$$\begin{aligned}
\partial_\beta \mathcal{F}_x &= \frac{1}{\beta^2}\ln\left(\sum_y e^{-\beta E_{xy}}\right) + \frac{1}{\beta}\frac{\sum_y E_{xy}e^{-\beta E_{xy}}}{\sum_y e^{-\beta E_{xy}}} \\
&= -\frac{E_x}{\beta} + \frac{1}{\beta^2}\ln\left(\sum_y e^{-\beta(E_y+V_{xy})}\right) + \frac{E_x}{\beta} + \frac{1}{\beta}\sum_y (E_y+V_{xy})\pi_{y|x} \\
&= \frac{1}{\beta^2}\sum_y \left[\beta(E_y+V_{xy}) + \ln \mathcal{Z}_{Y|x}\right]\pi_{y|x} = -\frac{1}{\beta^2}\sum_y \pi_{y|x}\ln\pi_{y|x}.
\end{aligned}$$

To calculate the derivative of $\mathcal{F}_Y$ we can simply set $E_x = 0 = V_{xy}$ in the previous calculation, and leads to $\beta^2\partial_\beta\mathcal{F}_Y = \mathcal{S}_Y$.
Therefore, the difference between the entropies reads

$$s_x - s_x^* = -\beta^2\partial_\beta\mathcal{F}_Y = \mathcal{S}_Y$$

Exercise 2.31: Strong coupling from coarse-graining: non-separable time-scales

Let $\Sigma_{XY}(t) \equiv [W(t) - \Delta F_{XY}(t)]/T$ be the entropy production emerging from the joint description of X and Y in weak contact with the residual bath R. Here, $F_{XY}(t) = \sum_{xy} p_{xy}(t)[E_{xy}(\lambda_t) + k_B T \ln p_{xy}(t)]$ is the nonequilibrium free energy.

Assuming that the initial state is $p_{xy}(0) = \pi_{y|x}p_x(0)$, show that

$$\Sigma^*(t) - \Sigma_{XY} = k_B D[p_{xy}|\pi_{y|x}p_x(t)] \geq 0,$$

where $\Sigma^*(t)$ is the entropy production calculated in the framework of the Hamiltonian of mean force.

Solution:
Let's start from the relative entropy:

$$D[p_{xy}(t)|\pi_{y|x}p_x(t)] = -S[p_{xy}(t)] + S[p_x(t)] + \sum_{xy} p_{xy}(t)\left[\beta(E_y+V_{xy}) + \ln\mathcal{Z}_{Y|x}\right].$$

Using the definition of the nonequilibrium free energy, $F_{XY} = U_{XY} - TS_{XY}$ and the entropy production Σ_{XY}, we have

$$\begin{aligned}
D[p_{xy}(t)|\pi_{y|x}p_x(t)] + \Sigma_{XY} &= \beta W + \beta F_{XY}(0) + S[p_x(t)] - \beta\langle E_x(t)\rangle + \sum_x p_x(t)\ln\mathcal{Z}_{Y|x} \\
&= \beta W + \beta U_{XY}(0) - S[p_{xy}(0)] + S[p_x(t)] - \beta\langle E_x(t)\rangle + \sum_x p_x(t)\ln\mathcal{Z}_{Y|x} \\
&= \beta W - \beta\Delta U_X + \beta\sum_{xy} p_x(0)\pi_{y|x}(E_y+V_{xy}) + \\
&+ \sum_{xy} p_x(0)\pi_{y|x}\left[\ln p_x(0) - \beta(E_y+V_{xy}) - \ln\mathcal{Z}_{Y|x}\right] + S[p_x(t)] + \sum_x p_x(t)\ln\mathcal{Z}_{Y|x} \\
&= \beta(W - \Delta U_X) + \Delta S_X + \sum_x [p_x(t) - p_x(0)]\ln\mathcal{Z}_{Y|x}.
\end{aligned}$$

Now we can move to the entropy produced in the Hamiltonian of mean force framework, namely

$$\Sigma^* = \langle\sigma^*\rangle = \langle\Delta s_x^* - \beta q_x^*\rangle = \langle\Delta s_x^* - \beta\Delta u_x^* + \beta w\rangle$$

Crucially, the stochastic entropy and energy in the Hamiltonian of mean force read

$$s_x^* = -\ln p_x + \beta^2\partial_\beta E_x^*, \quad u_x^* = E_x^* + \beta\partial_\beta E_x^*, \quad E_x^* = E_x - \frac{1}{\beta}\ln\frac{\mathcal{Z}_{Y|x}}{\mathcal{Z}_Y},$$

such that the difference

$$s_x^* - \beta u_x^* = -\ln p_x - \beta E_x^* = -\ln p_x - \beta E_x + \ln\frac{\mathcal{Z}_{Y|x}}{\mathcal{Z}_Y}.$$

Finally, we can calculate the average as

$$\langle \sigma^* \rangle = \Delta S_X - \beta \Delta U_X + \sum_x [p_x(t) - p_x(0)] \ln \frac{\mathcal{Z}_{Y|x}}{\mathcal{Z}_Y} + \beta W.$$

Since $\mathcal{Z}_Y$ does not depend on x, it cancels out, and we are left with the same expression as $D[p_{xy}(t)|\pi_{y|x}p_x(t)] + \Sigma_{XY}$, thereby proving the relation we were looking for.

Exercise 2.32: A lower bound on entropy production

The entropy production of the joint system XY can be expressed as

$$\Sigma_{XY}(t) = k_B D[p(\mathbf{xy}_n)|p_{\mathrm{tr}}(\mathbf{xy}_n^\dagger)]$$

by means of local detailed balance (Crooks' lemma). Here, $\mathbf{xy}_n$ is a trajectory of microstates in XY and $\mathbf{xy}_n^\dagger$ is the corresponding time-reversed trajectory.

Defining the 'trajectory entropy production' as

$$\Sigma_{\mathrm{traj}}(t) \equiv k_B D[p(\mathbf{x}_n)|p_{\mathrm{tr}}(\mathbf{x}_n^\dagger)],$$

prove that

$$\Sigma_{\mathrm{traj}}(t) \leq \Sigma_{XY}(t)$$

by constructing a stochastic matrix T that maps $p_{xy} \to p_x$ and use the monotonicity of the relative entropy, namely

$$D[T\mathbf{p}|T\mathbf{q}] \leq D[\mathbf{p}|\mathbf{q}].$$

Solution:
The most general stochastic matrix relating the probabilities p_{xy} and q_x is

$$q_{x'} = \sum_{xy} T_{x',xy} p_{xy}.$$

Choosing $T_{x',xy} = \delta_{x'x}$ is a valid choice for a stochastic matrix. Indeed, all entries are non-negative and $\sum_{x'} \delta_{x'x} = 1$. The outcome of this choice is

$$p_x = \sum_{xy} p_{xy}.$$

Now that we have the transitio matrix that maps the joint trajectory into the marginal one, we can use the monotonicity of the relative entropy:

$$\Sigma_{XY}(t) = D[p(\mathbf{xy}_n)|p_{\mathrm{tr}}(\mathbf{xy}_n^\dagger)] \geq D[Tp(\mathbf{xy}_n)|Tp_{\mathrm{tr}}(\mathbf{xy}_n^\dagger)] = D[p(\mathbf{x}_n)|p_{\mathrm{tr}}(\mathbf{x}_n^\dagger)] = \Sigma_{\mathrm{traj}}(t)$$

Example 2.1: Free energies of complex molecules

Using the stochastic work, namely

$$w(\boldsymbol{\gamma}_S^\tau) = H_{SB}(\Gamma_{SB}^\tau, \lambda_\tau) - H_{SB}(\Gamma_{SB}^0, \lambda_0)$$

we can derive

$$\int d\Gamma_{SB}^0 \delta(\Gamma_S - \Gamma_S^\tau) \pi_{SB}(\Gamma_{SB}^0, \lambda_0) e^{-\beta w(\boldsymbol{\gamma}_S^\tau)} = \int d\Gamma_{SB}^0 \delta(\Gamma_S - \Gamma_S^\tau) \frac{e^{-\beta H_{SB}(\Gamma_{SB^\tau}, \lambda_\tau)}}{\mathcal{Z}_{SB}(\lambda_0)}$$

$$\text{Liouville's theorem} \rightarrow = \int d\Gamma_{SB}^\tau \delta(\Gamma_S - \Gamma_S^\tau) \frac{e^{-\beta H_{SB}(\Gamma_{SB^\tau}, \lambda_\tau)}}{\mathcal{Z}_{SB}(\lambda_0)}$$

$$= e^{-\beta H_S(\Gamma_S, \lambda_\tau)} \int d\Gamma_B^\tau \frac{e^{-\beta[H_B(\Gamma_B^\tau) + V_{SB}(\Gamma_S, \Gamma_B^\tau)]}}{\mathcal{Z}_{SB}(\lambda_0)} = \pi_S^*(\Gamma_S; \lambda_\tau) \frac{\mathcal{Z}_S^*(\lambda_\tau)}{\mathcal{Z}_S^*(\lambda_0)} = \pi_S^*(\Gamma_S; \lambda_\tau) e^{-\beta \Delta \mathcal{F}_S^*}.$$

This can be summarised as

$$\pi_S^*(\Gamma_S; \lambda_\tau) e^{-\beta \Delta \mathcal{F}_S^*} = \langle \delta(\Gamma_S - \Gamma_S^\tau) e^{-\beta w(\boldsymbol{\gamma}_S^\tau)} \rangle_{\boldsymbol{\gamma}_S^\tau}.$$

Interestingly, integrating over Γ_S gives the integral fluctuation theorem at strong coupling.

Let the Hamiltonian of mean force be

$$H_S^*(\Gamma_S;\lambda_t) = \tilde{H}_S^*(\Gamma_S) + \frac{k}{2}(x-\lambda_t)^2,$$

with $\tilde{H}_S^*(\Gamma_S)$ being the undriven Hamiltonian of mean force. Taking the distribution $\delta[x'-x(\Gamma_S)]$ and integrating over Γ_S we get

$$\int d\Gamma_S \delta[x'-x(\Gamma_S)]\frac{e^{-\beta H_S^*(\Gamma_S,\lambda_\tau)}}{\mathcal{Z}_S^*(\lambda_0)} = e^{-\beta\frac{k}{2}(x'-\lambda_\tau)^2}\int d\Gamma_S \delta[x'-x(\Gamma_S)]\frac{e^{-\beta \tilde{H}_S^*(\Gamma_S,\lambda_\tau)}}{\mathcal{Z}_S^*(\lambda_0)}$$

from which we can define $\tilde{w}(\boldsymbol{\gamma}_S^\tau) = w(\boldsymbol{\gamma}_S^\tau) - \frac{k}{2}(x(\Gamma_S)-\lambda_\tau)^2$ and write

$$\int d\Gamma_S \delta[x'-x(\Gamma_S)]\frac{e^{-\beta \tilde{H}_S^*(\Gamma_S,\lambda_\tau)}}{\mathcal{Z}_S^*(\lambda_0)} = \int d\Gamma_S \delta[x'-x(\Gamma_S)]\langle \delta(\Gamma_S-\Gamma_S^\tau)e^{-\beta\tilde{w}(\boldsymbol{\gamma}_S^\tau)}\rangle_{\boldsymbol{\gamma}_S^\tau}.$$

Deining the equilibrium free energy at fixed extension x' as

$$\tilde{\mathcal{F}}_S^*(x') = -k_BT\ln\tilde{\mathcal{Z}}_S^*(x'), \quad \tilde{\mathcal{Z}}_S^*(x') = \int d\Gamma_S \delta[x'-x(\Gamma_S)]e^{-\beta\tilde{H}_S^*(\Gamma_S)},$$

we have

$$\tilde{\mathcal{F}}_S^*(x') = -k_BT\ln\langle\delta[x'-x(\Gamma_S^\tau)]e^{-\beta\tilde{w}(\boldsymbol{\gamma}_S^\tau)}\rangle_{\boldsymbol{\gamma}_S^\tau} + \tilde{\mathcal{F}}_S^*(\lambda_0).$$

3 Quantum Thermodynamics Without Measurements

Exercise 3.1: Time-dependent Hamiltonian from a time-independent one

Consider an atom interacting with a single mode of the electromagnetic field, whose dynamics is described by the **Jaynes-Cummings Hamiltonian**

$$H_{\rm JC} = \frac{\hbar\Omega}{2}\sigma_z + \hbar\omega a^\dagger a + \hbar g(\sigma_+ a + a^\dagger \sigma_-).$$

The atom is a two-level system with energy gap $\hbar\Omega$ between the ground ($|g\rangle$) and excited ($|e\rangle$) states. The EM field is described by a single harmonic oscillator with freuqncy ω and ladder operators $a, a^\dagger$. The atom-field interaction with strength g describes emission (absorption) of a photon by the atom using the lowering (raising) operators $\sigma_- = |g\rangle\langle e|$ ($\sigma_+ = |e\rangle\langle g|$).

Assume that the atom is on resonance with the EM field, $\Omega = \omega$, and write the unitary time evolution operator in the interaction picture.

Consider an initially pure state of the form $|\psi(0)\rangle_S \otimes |\alpha\rangle_W$, where $|\psi(0)\rangle_S$ is an arbitrary atom state and $|\alpha\rangle_W \equiv e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}|n\rangle$ is a coherent state of the field with amplitude $\alpha \in \mathbb{C}$. For simplicity, assume $\alpha > 0$. Show that if the amplitude of the coherent state is large enough, $\alpha \gg 1$, the EM field acts as a work reservoir.

Calculate the time-dependent Hamiltonian acting on S.

Assuming that the atom is initially in the ground state, calculate the proability of finding the fild at time t still in the same coherent state $|\alpha\rangle$.

Solution:

The interaction picture is useful to work with simpler Hamiltonians. It is based on using a different reference frame, which is reached through the unitary transformation U_0 as

$$|\tilde\psi\rangle = U_0|\psi\rangle \to \partial_t|\tilde\psi\rangle = \dot U_0|\psi\rangle - \frac{i}{\hbar}U_0 H|\psi\rangle = -\frac{i}{\hbar}\left(U_0 H U_0^\dagger - \frac{\hbar}{i}\dot U_0 U_0^\dagger\right)U_0|\psi\rangle = -\frac{i}{\hbar}\tilde H|\tilde\psi\rangle.$$

Choosing $U_0 = \exp(itH_0/\hbar)$ we have

$$\tilde H = U_0 H U_0^\dagger - U_0 H_0 U_0^\dagger = U_0(H - H_0)U_0^\dagger.$$

Choosing H_0 to be the non-interacting Hamiltonian $H_0 = \hbar\Omega(\sigma_z/2 + a^\dagger a)$ we are left with

$$\tilde H = e^{it\Omega(\sigma_z/2 + a^\dagger a)}\left(\hbar g(\sigma_+ a + a^\dagger\sigma_-)\right)e^{-it\Omega(\sigma_z/2+a^\dagger a)}.$$

To write this in a clean way we have to calculate some (anti-)commutators. Let's start from the Pauli matrices:

$$|e\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |g\rangle = \begin{pmatrix}0\\1\end{pmatrix}, \quad \sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}, \quad \sigma_+ = \sigma_-^\dagger = \begin{pmatrix}0 & 1\\0 & 0\end{pmatrix}$$

$$\sigma_z\sigma_+ = \sigma_+, \quad \sigma_+\sigma_z = -\sigma_+, \quad \sigma_z\sigma_- = -\sigma_-, \quad \sigma_-\sigma_z = \sigma_-$$

From which we have

$$e^{ix\sigma_z}\sigma_+ e^{-ix\sigma_z} = \sum_{nm}\frac{(ix)^n\sigma_z^n}{n!}\sigma_+\frac{(-1)^m(ix)^m\sigma_z^m}{m!} = \sum_{nm}\frac{(ix)^n}{n!}\sigma_+\frac{(ix)^m}{m!} = \sigma_+ e^{2ix}$$

$$e^{ix\sigma_z}\sigma_- e^{-ix\sigma_z} = \left(\sigma_+ e^{2ix}\right)^\dagger = \sigma_- e^{-2ix}.$$

Now, let's move on to the bosonic operators $[a, a^\dagger] = 1$.

$$aa^\dagger a = (a^\dagger a + 1)a \to a(a^\dagger a)^n = (a^\dagger a + 1)a(a^\dagger a)^{n-1} = (a^\dagger a + 1)^n a$$
$$a^\dagger a a^\dagger = a^\dagger(1 + a^\dagger a) \to (a^\dagger a)^n a^\dagger = (a^\dagger a)^{n-1}a^\dagger(1 + a^\dagger a) = a^\dagger(1 + a^\dagger a)^n$$

From which we have

$$e^{ixa^\dagger a}ae^{-ixa^\dagger a} = e^{ixa^\dagger a}a\sum_n\frac{(-ix)^n(a^\dagger a)^n}{n} = e^{ixa^\dagger a}\sum_n\frac{(-ix)^n(a^\dagger a+1)^n}{n!}a = e^{-ix}a$$

$$e^{ixa^\dagger a}a^\dagger e^{-ixa^\dagger a} = [e^{-ix}a]^\dagger = e^{ix}a^\dagger$$

Using these relations we can write the Hamiltonian in the interaction picture as

$$\tilde H = \hbar g(\sigma_+ e^{it\Omega}ae^{-it\Omega} + \sigma_- e^{-it\Omega}a^\dagger e^{it\Omega} = \hbar g(\sigma_+ a + a^\dagger\sigma_-).$$

The unitary time evolution operator in the interaction picture is

$$\tilde{U}(t) = e^{-it\tilde{H}/\hbar} = e^{-itg(\sigma_+ a + a^\dagger \sigma_-)}.$$

Using the matrix representation on the atom Hilbert space, the Hamiltonian becomes

$$\tilde{H} = \hbar g \begin{pmatrix} 0 & a \\ a^\dagger & 0 \end{pmatrix} = \hbar g A.$$

Notice that A has some nice powers:

$$A^2 = \begin{pmatrix} aa^\dagger & 0 \\ 0 & a^\dagger a \end{pmatrix} = \begin{pmatrix} N+1 & 0 \\ 0 & N \end{pmatrix} \Rightarrow A^{2n} = \begin{pmatrix} (N+1)^n & 0 \\ 0 & N^n \end{pmatrix}, \quad A^{2n+1} = \begin{pmatrix} 0 & (N+1)^n a \\ N^n a^\dagger & 0 \end{pmatrix}.$$

Thus, we can expand the time evolution operator is series as

$$\begin{aligned}
\tilde{U}(t) &= \sum_{n=0}^{\infty} \frac{(-itg)^n}{n!} A^n = \sum_{n=0}^{\infty} \frac{(-itg)^{2n}}{(2n)!} A^{2n} + \sum_{n=0}^{\infty} \frac{(-itg)^{2n+1}}{(2n+1)!} A^{2n+1} \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n (tg)^{2n}}{(2n)!} \begin{pmatrix} (N+1)^n & 0 \\ 0 & N^n \end{pmatrix} + \sum_{n=0}^{\infty} \frac{i(-1)^{n+1}(tg)^{2n+1}}{(2n+1)!} \begin{pmatrix} 0 & (N+1)^n a \\ N^n a^\dagger & 0 \end{pmatrix} \\
&= \begin{pmatrix} \cos(tg\sqrt{N+1}) & 0 \\ 0 & \cos(tg\sqrt{N}) \end{pmatrix} - i \begin{pmatrix} 0 & \frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}} a \\ \frac{\sin(tg\sqrt{N})}{\sqrt{N}} a^\dagger & 0 \end{pmatrix} \\
&= \cos(tg\sqrt{N+1}) |e\rangle\langle e| + \cos(tg\sqrt{N}) |g\rangle\langle g| - i \left(\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}} a |e\rangle\langle g| + a^\dagger \frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}} |g\rangle\langle e| \right)
\end{aligned}.$$

We now consider the initial state in the separable form $|\psi(0)\rangle \otimes |\alpha\rangle$ with $|\alpha\rangle$ a coherent state. Remembering that the ladder operators act on the $\{|n\rangle\}$ basis as

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger |n\rangle = \sqrt{n+1}|n+1\rangle,$$

we notice that

$$a|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} a|n\rangle = e^{-|\alpha|^2/2} \sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{(n-1)!}} |n-1\rangle = \alpha|\alpha\rangle.$$

We can this when calculating the reduced state after the evolution took place:

$$\rho_S(t) = \mathrm{Tr}_W \left\{ \tilde{U}(t) |\psi(0)\alpha\rangle\langle\psi(0)\alpha| \tilde{U}^\dagger(t) \right\} = \sum_n \langle n|\tilde{U}(t)|\alpha\rangle |\psi(0)\rangle\langle\psi(0)| \langle\alpha|\tilde{U}^\dagger(t)|n\rangle$$

with

$$\begin{aligned}
\langle n|\tilde{U}(t)|\alpha\rangle = &\left(\cos(tg\sqrt{n+1}) |e\rangle\langle e| + \cos(tg\sqrt{n}) |g\rangle\langle g| - i\frac{\sin(tg\sqrt{n+1})}{\sqrt{n+1}} \alpha |e\rangle\langle g| \right) \langle n|\alpha\rangle + \\
&+ \left(-i\sqrt{n} \frac{\sin(tg\sqrt{n})}{\sqrt{n}} |g\rangle\langle e| \right) \langle n-1|\alpha\rangle.
\end{aligned}$$

Therefore, the sum in the reduced density matrix $\rho_S(t)$ will contain terms proportional to $|\langle n|\alpha\rangle|^2, |\langle n-1|\alpha\rangle|^2, \langle\alpha|n-1\rangle\langle n|\alpha\rangle$ and the complex conjugate. Since the scalar product $\langle n|\alpha\rangle = e^{-|\alpha|^2/2}\alpha^2/\sqrt{n!}$, the probability of finding n photons in the coherent state $|\alpha\rangle$ is

$$p_n = |\langle n|\alpha\rangle|^2 = e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!} \to \langle n\rangle = \sum_n n p_n = e^{-|\alpha|^2} \alpha^2 \sum_n \frac{|\alpha|^{2(n-1)}}{(n-1)!} = \alpha^2.$$

To calculate the variance we can look at

$$\langle n(n-1)\rangle = e^{-|\alpha|^2} \alpha^4 \sum_n \frac{|\alpha|^{2(n-2)}}{(n-2)!} = \alpha^4 \to \langle n^2\rangle = \alpha^2 + \alpha^4 \to \langle \Delta n^2\rangle = \alpha^2.$$

Since the ratio between the variance and the mean photon number is $1/\alpha$, the photon distribution becomes peaked around its mean at large α. Therefore, when taking the sum over n in the partial trace

$\rho_S(t)$ we can approximate it with the contribution of the mean value $\langle n \rangle = \alpha^2$. Additionally, since the Poisson distribution is highly peaked around its mean, we can approximate everything but the Poisson distribution p_n with the mean value:

$$\langle n|\tilde{U}(t)|\alpha\rangle \to [\cos(tg\alpha)\,(|e\rangle\langle e| + |g\rangle\langle g|) - i\sin(tg\alpha)\,(|e\rangle\langle g| + |g\rangle\langle e|)]\,\langle n|\alpha\rangle$$

$$\langle n|\tilde{U}(t)|\alpha\rangle \to \langle n|\alpha\rangle \begin{pmatrix} \cos(tg\alpha) & -i\sin(tg\alpha) \\ -i\sin(tg\alpha) & \cos(tg\alpha) \end{pmatrix} = \langle n|\alpha\rangle \sum_k (-1)^k \left(\frac{(tg\alpha)^{2k}}{(2k)!}\mathbb{I} - i\frac{(tg\alpha)^{2k+1}}{(2k+1)!}\sigma_x \right)$$

Noticing that

$$e^{-ix\sigma_x} = \sum_k \frac{(-ix)^k \sigma_x^k}{k!} = \sum_k \left(\frac{(-1)^k x^{2k}}{(2k)!}\mathbb{I} - i\frac{(-1)^k x^{2k+1}}{(2k+1)!}\sigma_x \right)$$

we can write the matrix element of the unitary evolution as

$$\langle n|\tilde{U}(t)|\alpha\rangle \to \langle n|\alpha\rangle\, e^{-itg\alpha\sigma_x}.$$

Thus, the reduced density matrix reads

$$\rho_S(t) \approx \sum_n |\,\langle n|\alpha\rangle\,|^2 e^{-itg\alpha\sigma_x}\,|\psi(0)\rangle\langle\psi(0)|\,e^{itg\alpha\sigma_x} = e^{-itg\alpha\sigma_x}\,|\psi(0)\rangle\langle\psi(0)|\,e^{itg\alpha\sigma_x}.$$

This gives the effective Hamiltonian $\tilde{V} = \hbar g\alpha\sigma_x$ in the interaction picture. Going back to the Schrödinger picture with $V = U_0^\dagger \tilde{V} U_0$ we get

$$V = H_0 + e^{-itH_0/\hbar}\hbar g\alpha\sigma_x e^{itH_0/\hbar} = H_0 + \hbar g\alpha e^{-it\Omega\sigma_z/2}(\sigma_+ + \sigma_-)e^{it\Omega\sigma_z/2} = H_0 + \hbar g\alpha\left(\sigma_+ e^{-i\Omega t} + \sigma_- e^{i\Omega t}\right),$$

where we used the commutation relations proved before. Therefore, we have the effective time-dependent hamiltonian acting on the system:

$$H_{\text{eff}}(\lambda_t) = \frac{\hbar\Omega}{2}\sigma_z + \hbar g\alpha\left(\sigma_+ e^{-i\Omega t} + \sigma_- e^{i\Omega t}\right).$$

Conversly, to find the probability of finding the field in the same state we need to trace over the atom's Hilbert space:

$$p_\alpha(t) = \mathrm{Tr}_A\left\{\langle\alpha|\,\tilde{U}(t)\,|g\alpha\rangle\langle g\alpha|\,\tilde{U}^\dagger(t)\,|\alpha\rangle\right\}.$$

Remembering that

$$\langle n|\tilde{U}(t)|g\alpha\rangle = \left(\cos(tg\sqrt{n})\,|g\rangle - i\frac{\sin(tg\sqrt{n+1})}{\sqrt{n+1}}\alpha\,|e\rangle\right)\langle n|\alpha\rangle$$

the partial trace over the atom's HIlbert space reads

$$p_\alpha(t) = \sum_{n,m} e^{-\alpha^2}\frac{\alpha^n\alpha^m}{n!m!}\,\langle n|\alpha\rangle\,\langle\alpha|m\rangle\left[\cos(tg\sqrt{n})\cos(tg\sqrt{m}) + \alpha^2\frac{\sin(tg\sqrt{n+1})}{\sqrt{n+1}}\frac{\sin(tg\sqrt{m+1})}{\sqrt{m+1}}\right].$$

Once again we use that the Poisson distribution becomes peaked at the mean value and approximate n and m in the square brackets with α^2, their mean value. This simplifies the summations considerably, as both sums reduce to the coherent state and we are left with

$$p_\alpha(t) \approx \left[\cos^2(tg\alpha) + \alpha^2\frac{\sin^2(tg\sqrt{\alpha^2+1})}{\alpha^2+1}\right] = 1 + \mathcal{O}\left(\frac{tg}{\alpha}\right) + \mathcal{O}\left(\frac{1}{\alpha^2}\right).$$

Exercise 3.2: Simplifying the master equation with a thermal bath

Assuming that the system-bath is initially in

$$\rho_{SB}(0) = \rho_S(0)\otimes\pi_B(\beta), \quad \pi_B(\beta) = \frac{e^{-\beta H_B}}{\mathcal{Z}_B},$$

show that one can set

$$\mathrm{Tr}_B\left\{\tilde{V}_{SB}(t)\pi(\beta)\right\} = 0$$

without loss of generality by introducing a redefined system Hamiltonian H'_S. Here, $\tilde{V}_{SB}$ is the interaction Hamiltonian between system and bath in the interaction picture.

Solution:
We call the operator acting on S as

$$\tilde{K}_S = \mathrm{Tr}_B \left\{ \tilde{V}_{SB} \pi_B(\beta) \right\}$$

and notice that it cal also be written as

$$\tilde{K}_S = \mathrm{Tr}_B \left\{ e^{it(H_S+H_B)/\hbar} V_{SB} e^{-it(H_S+H_B)/\hbar} \pi_B(\beta) \right\} = e^{itH_S/\hbar} \mathrm{Tr}_B \left\{ V_{SB} \pi_B \right\} e^{-itH_S/\hbar} = e^{itH_S/\hbar} K_S e^{-itH_S/\hbar}.$$

Now we can write the Hamiltonian in the interaction picture as

$$\tilde{H} = \tilde{K}_S + \left(\tilde{V}_{SB} - \tilde{K}_S \right) = \tilde{K}_S + \tilde{V}'_{SB}$$

Where we introduced the new interaction $\tilde{V}'_{SB}$. Going back to the Schrödinger picture we have

$$H = H_0 + U^\dagger \tilde{H} U = H_S + H_B + K_S + (V_{SB} - K_S) = H'_S + H_B + V'_{SB}.$$

With these redefined system and interaction Hamiltonian, we use the new interaction picture, indicated as $\tilde{\tilde{\bullet}}$, that is obtained with the unitary transformation $U = e^{it(H'_S+H_B)/\hbar}$ and get

$$\tilde{\tilde{H}}' = U V'_{SB} U^\dagger = \tilde{\tilde{V}}'_{SB}.$$

Calculating the trace over B yields

$$\mathrm{Tr}_B \left\{ \tilde{\tilde{V}}'_{SB} \pi_B \right\} = e^{itH'_S} \mathrm{Tr}_B \left\{ V'_{SB} \pi_B \right\} e^{-itH'_S} = e^{itH'_S} \mathrm{Tr}_B \left\{ (V_{SB} - K_S) \pi_B \right\} e^{-itH'_S} = 0.$$

Exercise 3.3: Hermitian decomposition of operators

It is always possible to write the interaction Hamiltonias as

$$V_{SB} = \sum_\alpha A_\alpha \otimes B_\alpha.$$

Show that one can assume A_α, B_α to be Hermitian without loss of generality, namely, if they are not, show that you can find Hermitian operatos A'_α, B'_α such that $V_{SB} = \sum_\alpha A'_\alpha \otimes B'_\alpha$ by using that any operator can be written as $A = A_1 + iA_2$ with $A_{1/2}$ Hermitian.

Solution:
Let A be an operator and $A^\dagger$ be its hermitian conjugate. From these we can build two hermitian operators, A_1, A_2 as

$$A_1 = \frac{1}{2} \left(A + A^\dagger \right), \quad A_2 = \frac{i}{2} \left(A^\dagger - A \right) \longrightarrow A = A_1 + iA_2.$$

Now, the interaction Hamiltonian is hermitian itself, $V_{SB}^\dagger = V_{SB}$, therefore

$$V_{SB} = \sum_\alpha A_\alpha \otimes B_\alpha = \sum_\alpha (A_{\alpha 1} + iA_{\alpha 2}) \otimes (B_{\alpha 1} + iB_{\alpha 2}) = \sum_\alpha (A_{\alpha 1} - iA_{\alpha 2}) \otimes (B_{\alpha 1} - iB_{\alpha 2}) = V_{SB}^\dagger.$$

Taking the average between V_{SB} and $V_{Sb}^\dagger$ we get

$$V_{SB} = \frac{V_{SB} + V_{SB}^\dagger}{2} = \sum_\alpha (A_{\alpha 1} \otimes B_{\alpha 1} - A_{\alpha 2} \otimes B_{\alpha 2}) = \sum_\beta A'_\beta \otimes B'_\beta$$

with $A'_\beta \equiv (-1)^{i+1} A_{\alpha i}$ and $B'_\beta \equiv B_{\alpha i}$ with $i = 1, 2$.

Exercise 3.4: Markov approximation in the Caldeira-Leggett model

Consider the Caldeira-Legget model introduced in Exercise 1.2. The interaction Hamiltonian is of the form $V_{SB} = S \otimes B$ with $B = \sum_k c_k x_k$.

Show that the bath correlation function reads

$$C(t) = \mathrm{Tr}_B \{B(t) B \pi_B\} = \sum_k \frac{\hbar c_k^2}{2\omega_k} \left[\cos(\omega_k t) \coth\left(\frac{\beta\hbar\omega_k}{2}\right) - i \sin(\omega_k t)\right].$$

Defining the spectral density $J(\omega) \equiv \pi/2 \sum_k (c_k^2/\omega_k)\delta(\omega - \omega_k)$, the bath correlation function becomes

$$C(t) = \frac{\hbar}{\pi} \int_0^\infty d\omega J(\omega) \left[\cos(\omega t) \coth\left(\frac{\beta\hbar\omega}{2}\right) - i \sin(\omega t)\right].$$

A spectral density of the form $J(\omega) = \gamma\omega\Theta(\omega_C - \omega)$ is called *Ohmic*. Here, γ is a damping constant and ω_C is a cut-off frequency. In the limit $\omega_C \to \infty$, show that the spectral density $J(\omega) \sim \omega$ leads to $C(t) \sim \delta(t) + \mathcal{O}(\hbar)$.

Solution:
The bath Hamiltonian reads

$$H_B = \sum_k \hbar\omega_k a_k^\dagger a_k$$

with a_k being the annihilation operator of the k-th bath. The positions x_k entering the interaction Hamiltonian can be decomposed as

$$x_k = \frac{\ell_k}{\sqrt{2}}(a_k + a_k^\dagger), \quad \ell_k^2 = \frac{\hbar}{\omega_k}.$$

We want the bath correlation functions, namely

$$C(t) = \mathrm{Tr}_B \{B(t) B \pi_B\} = \mathrm{Tr}_B \left\{e^{itH_B/\hbar} B e^{-itH_B/\hbar} B \pi_B\right\},$$

therefore we need to use the commutation relation $[a, a^\dagger] = 1$ to find $B(t)$. Noticing that

$$a(a^\dagger a)^n = (aa^\dagger)^n a = (1 + a^\dagger a)^n a, \quad (a^\dagger a)^n a^\dagger = a^\dagger (aa^\dagger)^n = a^\dagger (1 + a^\dagger a)^n$$

we have

$$a e^{xa^\dagger a} = e^{x(a^\dagger a + 1)} a, \quad e^{xa^\dagger a} a^\dagger = a^\dagger e^{x(a^\dagger a+1)}$$

the operator $B(t)$ becomes

$$B(t) = \sum_k \frac{\ell_k c_k}{\sqrt{2}} e^{it\omega_k a_k^\dagger a_k}(a_k + a_k^\dagger) e^{-it\omega_k a_k^\dagger a_k} = \sum_k \frac{\ell_k c_k}{\sqrt{2}} \left(a_k e^{-it\omega_k} + a_k^\dagger e^{it\omega_k}\right)$$

which makes the bath correlation function

$$\begin{aligned}
C(t) &= \sum_{\alpha\beta} \frac{\ell_\alpha c_\alpha \ell_\beta c_\beta}{2} \mathrm{Tr}_B \left\{\left(a_\alpha a_\beta e^{-it\omega_\alpha} + a_\alpha a_\beta^\dagger e^{-it\omega_\alpha} + a_\alpha^\dagger a_\beta^\dagger e^{it\omega_\alpha} + a_\alpha^\dagger a_\beta e^{it\omega_\alpha}\right)\pi_B\right\} \\
&= \sum_{\alpha\beta} \frac{\ell_\alpha c_\alpha \ell_\beta c_\beta}{2} \mathrm{Tr}_B \left\{\left(a_\alpha a_\beta^\dagger e^{-it\omega_\alpha} + a_\alpha^\dagger a_\beta e^{it\omega_\alpha}\right)\pi_B\right\} = \sum_\alpha \frac{\ell_\alpha^2 c_\alpha^2}{2} \mathrm{Tr}_B \left\{\left(e^{-it\omega_\alpha} + a_\alpha^\dagger a_\alpha 2\cos(t\omega_\alpha)\right)\pi_B\right\} \\
&= \sum_\alpha \frac{\ell_\alpha^2 c_\alpha^2}{2} \left(e^{-it\omega_\alpha} - 2\cos(t\omega_\alpha) \frac{\partial \ln \mathcal{Z}_B}{\partial(\beta\hbar\omega_\alpha)}\right) \\
&= \sum_\alpha \frac{\ell_\alpha^2 c_\alpha^2}{2} \left(e^{-it\omega_\alpha} - 2\cos(t\omega_\alpha) \frac{\partial}{\partial(\beta\hbar\omega_\alpha)} \ln\left(\frac{1}{1 - e^{-\beta\hbar\omega_\alpha}}\right)\right) \\
&= \sum_\alpha \frac{\ell_\alpha^2 c_\alpha^2}{2} \left(e^{-it\omega_\alpha} - 2\cos(t\omega_\alpha) \frac{1}{e^{\beta\hbar\omega_\alpha} - 1}\right) = \sum_\alpha \frac{\hbar c_\alpha^2}{2\omega_\alpha} \left(\cos(t\omega_\alpha)\left[1 - 2\frac{1}{e^{\beta\hbar\omega_\alpha} - 1}\right] - i\sin(t\omega_\alpha)\right) \\
C(t) &= \sum_\alpha \frac{\hbar c_\alpha^2}{2\omega_\alpha} \left(\cos(t\omega_\alpha) \coth\left(\frac{\beta\hbar\omega_\alpha}{2}\right) - i\sin(t\omega_\alpha)\right).
\end{aligned}$$

We now consider an Ohmic spectral density in the limit on large bandwidth. Using that the hyperbolic cotangent is

$$\coth(x) = \frac{e^{2x} + 1}{e^{2x} - 1} = \frac{1 + e^{-2x}}{1 - e^{-2x}} \begin{cases} \approx 1 + 2e^{-2x} & \text{at large } x \\ \approx \frac{1}{x} + \mathcal{O}(x) & \text{at small } x \end{cases}$$

$$C(t) \sim \int_0^{\omega_C} d\omega\omega \left[\cos(\omega t)\left(\frac{2}{\beta\hbar\omega} + \mathcal{O}(\beta\hbar\omega) - i\sin(t\omega)\right)\right] \sim \delta(t)$$

Exercise 3.5: Fourier components of system coupling operators

Consider the system coupling operators A_α in the interaction picture. Decomposing the system Hamiltonian in its eigenspaces as $H_S = \sum_s \epsilon_n \Pi(\epsilon_s)$, we have

$$\tilde{A}_\alpha(t) = \sum_{ss'} e^{-i(\epsilon_{s'}-\epsilon_s)t/\hbar}\Pi(\epsilon_s)A_\alpha\Pi(\epsilon_{s'}) \equiv \sum_\omega e^{-i\omega t}A_\alpha(\omega).$$

with $\hbar\omega = \epsilon_s - \epsilon_{s'}$ the transisition frequency and $A_\alpha(\omega) = \sum_{\epsilon_{s'}-\epsilon_s=\hbar\omega}\Pi(\epsilon_s)A_\alpha\Pi(\epsilon_{s'})$ the Fourier component of the system coupling operator.

Prove that

$$A_\alpha^\dagger(\omega) = A_\alpha(-\omega), \quad [A_\alpha(\omega), H_S] = \hbar\omega A_\alpha(\omega), \quad A_\alpha(\omega)\pi_S = e^{-\beta\hbar\omega}\pi_S A_\alpha(\omega).$$

Solution:
The first property follows from the definition:

$$A_\alpha^\dagger(\omega) = \sum_{\epsilon_{s'}-\epsilon_s=\hbar\omega}\Pi(\epsilon_{s'})A_\alpha\Pi(\epsilon_s) = \sum_{\epsilon_x-\epsilon_y=-\hbar\omega}\Pi(\epsilon_y)A_\alpha\Pi(\epsilon_x) = A_\alpha(-\omega).$$

The commutator can be calculated explicitely:

$$[A_\alpha(\omega), H_S] = A_\alpha(\omega)H_S - H_S A_\alpha(\omega) = \sum_{\epsilon_x-\epsilon_y=\hbar\omega}\Pi(\epsilon_y)A_\alpha\Pi(\epsilon_x)(\epsilon_x - \epsilon_y) = \hbar\omega A_\alpha(\omega).$$

From this commutation rule we have

$$A_\alpha(\omega)H_S^n = A_\alpha(\omega)H_S H_S^{n-1} = (H_S + \hbar\omega)A_\alpha(\omega)H_S^{n-1} = (H_S + \hbar\omega)^n A_\alpha(\omega).$$

Therefore,

$$A_\alpha(\omega)e^{-\beta H_S} = e^{-\beta(H_S+\hbar\omega)}A_\alpha(\omega) \rightarrow A_\alpha(\omega)\pi_S = e^{-\beta\hbar\omega}\pi_S A_\alpha(\omega).$$

Exercise 3.6: Kubo-Martin-Schwinger condition and local detailed balance.

Show that the bath correlation functions,

$$C_{\alpha\beta}(t) = \mathrm{Tr}_B\left\{B_\alpha(t)B_\beta\pi_B\right\}$$

satisfy the Kubo-Martin-Schwinger condition, namely

$$C_{\alpha\beta}(t) = C_{\beta\alpha}(-t - i\beta\hbar)$$

and use it to derive the local detailed balance condition on the rates

$$\gamma_{\alpha\beta}(\omega) = e^{\beta\hbar\omega}\gamma_{\beta\alpha}(-\omega),$$

where the rates are defined as

$$\gamma_{\alpha\beta}(\omega) = \frac{1}{\hbar^2}\int_{-\infty}^{\infty} d\tau e^{i\omega\tau}C_{\alpha\beta}(\tau)$$

assuming that the bath correlation function is analytic in the complex τ plane for $\Im(\tau) \in [-i\beta\hbar, 0]$ and decays quickly to zero for $|\tau| \to \infty$.

Solution:
Remembering that the bath correlation function is defined as

$$C_{\alpha\beta}(t) = \mathrm{Tr}_B\left\{B_\alpha(t)B_\beta\pi_B\right\} = \mathrm{Tr}_B\left\{e^{iH_Bt/\hbar}B_\alpha e^{-iH_Bt/\hbar}B_\beta\pi_B\right\}$$

we verify the Kubo-Martin-Schwinger condition with

$$\begin{aligned}C_{\alpha\beta}(-t-i\beta\hbar) &= \mathrm{Tr}_B\left\{e^{-iH_Bt/\hbar+\beta H_B}B_\alpha e^{iH_Bt/\hbar-\beta H_B}B_\beta\pi_B\right\}\\ &= \frac{1}{\mathcal{Z}_B}\mathrm{Tr}_B\left\{e^{-iH_Bt/\hbar+\beta H_B}B_\alpha e^{iH_Bt/\hbar-\beta H_B}B_\beta e^{-\beta H_B}\right\} = \mathrm{Tr}_B\left\{e^{-iH_Bt/\hbar}B_\alpha e^{iH_Bt/\hbar}\pi_B B_\beta\right\}\\ &= \mathrm{Tr}_B\left\{e^{iH_Bt/\hbar}B_\beta e^{-iH_Bt/\hbar}B_\alpha\pi_B\right\} = C_{\beta\alpha}(t).\end{aligned}$$

Now we can use it to derive the local detailed balance condition.

$$\begin{aligned}\gamma_{\alpha\beta}(\omega) &= \frac{1}{\hbar^2}\int_{-\infty}^{\infty}d\tau e^{i\omega\tau}C_{\alpha\beta}(\tau) = \frac{1}{\hbar^2}\int_{-\infty}^{\infty}d\tau e^{i\omega\tau}C_{\beta\alpha}(-\tau-i\beta\hbar)\\ &= \frac{1}{\hbar^2}e^{\beta\hbar\omega}\int_{-\infty-i\beta\hbar}^{\infty-i\beta\hbar}dz e^{-i\omega z}C_{\beta\alpha}(z) = e^{\beta\hbar\omega}\gamma_{\beta\alpha}(-\omega).\end{aligned}$$

where in the last step we made use of the assumptions on the analyticity and decay of the bath correlation function, which makes the integral over the $\tau - i\beta\hbar$ line equal to the one on the τ line.

Exercise 3.7: Stationarity of the thermal state

Recalling that the evolution of the system state is given by

$$\partial_t\rho = \mathcal{L}\rho = -\frac{i}{\hbar}[H_S,\rho_S] + \mathcal{D}\rho_S,$$

with the dissipator in the Born-Markov secular master equation given by

$$\mathcal{D}\rho_S = \sum_{\alpha\beta\omega}\gamma_{\alpha\beta}(\omega)\left[2A_\beta(\omega)\rho_S A_\alpha^\dagger(\omega) - \left\{A_\alpha^\dagger(\omega)A_\beta(\omega),\rho_S\right\}\right],$$

demonstrate that the thermal state π_S is a stationary state,

$$\mathcal{L}\pi_S = 0.$$

Solution:
Since the Liouvillian containes two terms, let's look at them one at the time: First, the Hamiltonian evolution given by the commutator $[H_S,\rho_S]$. If $\rho_S = \pi_S = e^{-\beta H_S}/\mathcal{Z}_S \Rightarrow [H_S,\pi_S] = 0$. Therefore, the Hamiltonian evolution does not contribute to the time derivative.
Now, let's look at the dissipator. Remembering from Exercise 3.5 that the Fourier components of the interaction satisfy

$$A_\alpha^\dagger(\omega) = A_\alpha(-\omega), \quad [A_\alpha(\omega),H_S] = \hbar\omega A_\alpha(\omega), \quad A_\alpha(\omega)\pi_S = e^{-\beta\hbar\omega}\pi_S A_\alpha(\omega),$$

we can use them to work out the action of the dissipator. Noticing that

$$A_\beta(\omega)\pi_S A_\alpha^\dagger(\omega) = e^{-\beta\hbar\omega}\pi_S A_\beta(\omega)A_\alpha^\dagger(\omega) = e^{-\beta\hbar\omega}A_\beta(\omega)A_\alpha^\dagger(\omega)\pi_S$$

we can write

$$\mathcal{D}\pi_S = \sum_{\alpha\beta\omega}\gamma_{\alpha\beta}(\omega)\left[e^{-\beta\hbar\omega}\left\{A_\beta(\omega)A_\alpha^\dagger(\omega),\pi_S\right\} - \left\{A_\alpha^\dagger(\omega)A_\beta(\omega),\pi_S\right\}\right].$$

Using local detailed balance, which we proved in Exercise 3.6, we have

$$\mathcal{D}\pi_S = \sum_{\alpha\beta\omega}\left[\gamma_{\beta\alpha}(-\omega)\left\{A_\beta(\omega)A_\alpha^\dagger(\omega),\pi_S\right\} - \gamma_{\alpha\beta}(\omega)\left\{A_\alpha^\dagger(\omega)A_\beta(\omega),\pi_S\right\}\right].$$

Relabeling the first anti-commutator and using $A_\alpha^\dagger(\omega) = A_\alpha(-\omega)$ we get

$$\begin{aligned}\mathcal{D}\pi_S &= \sum_{\alpha\beta\omega}\left[\gamma_{\alpha\beta}(\omega)\left\{A_\alpha(-\omega)A_\beta^\dagger(-\omega),\pi_S\right\} - \gamma_{\alpha\beta}(\omega)\left\{A_\alpha^\dagger(\omega)A_\beta(\omega),\pi_S\right\}\right]\\ &= \sum_{\alpha\beta\omega}\left[\gamma_{\alpha\beta}(\omega)\left\{A_\alpha^\dagger(\omega)A_\beta(\omega),\pi_S\right\} - \gamma_{\alpha\beta}(\omega)\left\{A_\alpha^\dagger(\omega)A_\beta(\omega),\pi_S\right\}\right] = 0.\end{aligned}$$

Combining these we have that the action of the Liouvillian on the thermal state is

$$\mathcal{L}\pi_S = 0.$$

Exercise 3.8: Positivity of the rate matrix

The rate matrix is obtained through the Fourier transform of the bath correlationfunction, namely

$$\gamma_{\alpha\beta}(\omega) = \frac{1}{\hbar^2}\int_{-\infty}^{\infty} d\tau e^{i\omega\tau} C_{\alpha\beta}(\tau), \quad C_{\alpha\beta}(t) = \mathrm{Tr}_B\left\{B_\alpha(t)B_\beta\pi_B\right\}.$$

Show that $\{\gamma_{\alpha\beta}(\omega)\}$ is a positive matrix by showing that $\mathbf{v}^\dagger\gamma\mathbf{v} \geq 0\,\forall\mathbf{v}$.

Solution:
The scalar product reads

$$v^*_\alpha\gamma_{\alpha\beta}v_\beta = \frac{1}{\hbar^2}\int d\tau e^{i\omega\tau} v^*_\alpha C_{\alpha\beta}(\tau)v_\beta.$$

Thus, we now write explicitely the bath correlation function in the energy eigenbasis as

$$C_{\alpha\beta}(t) = \sum_{nm} e^{i\epsilon_n t/\hbar} B^{nm}_\alpha e^{-i\epsilon_m t/\hbar} B^{mn}_\beta \frac{e^{-\beta\epsilon_n}}{\mathcal{Z}_B}$$

$$\begin{aligned}
\sum_{\alpha\beta} v^*_\alpha\gamma_{\alpha\beta}v_\beta &= \frac{1}{\hbar^2}\sum_{nm\alpha\beta}\int d\tau e^{i\omega\tau} v^*_\alpha e^{i\epsilon_n\tau/\hbar} B^{nm}_\alpha e^{-i\epsilon_m\tau/\hbar} B^{mn}_\beta \frac{e^{-\beta\epsilon_n}}{\mathcal{Z}_B} v_\beta \\
&= \frac{1}{\hbar^2}\sum_{nm\alpha\beta} v^*_\alpha B^{nm}_\alpha B^{mn}_\beta \frac{e^{-\beta\epsilon_n}}{\mathcal{Z}_B} v_\beta \int d\tau e^{i\omega\tau} e^{i\epsilon_n\tau/\hbar} e^{-i\epsilon_m\tau/\hbar} \\
&= \frac{1}{\hbar^2}\sum_{nm\alpha\beta} v^*_\alpha B^{nm}_\alpha B^{mn}_\beta \frac{e^{-\beta\epsilon_n}}{\mathcal{Z}_B} v_\beta \delta(\omega - [\epsilon_m - \epsilon_n]/\hbar)
\end{aligned}$$

Remembering that the bath operators B_α are hermitian, namely $B^{nm}_\alpha = B^{mn*}_\alpha$, we can introduce the vectors $V^{mn} = \sum_\beta B^{mn}_\beta v_\beta$, thus obtaining

$$\sum_{\alpha\beta} v^*_\alpha\gamma_{\alpha\beta}v_\beta = \frac{1}{\hbar^2}\sum_{nm} V^{mn*}V^{mn}\frac{e^{-\beta\epsilon_n}}{\mathcal{Z}_B}\delta(\omega - [\epsilon_m - \epsilon_n]/\hbar) = \frac{1}{\hbar^2}\sum_{nm}|V^{mn}|^2\frac{e^{-\beta\epsilon_n}}{\mathcal{Z}_B}\delta(\omega - [\epsilon_m - \epsilon_n]/\hbar) \geq 0$$

Therefore, the eigenvalues of γ are non-negative.

Exercise 3.9: Classical behaviour of the Born-Markov secular master equation

Consider sequential projective measurements of an open system in its energy eigenbasis $H_S = \sum_s \epsilon_s\Pi(\epsilon_s)$. Assume that in between the measurements the Born-Markov secular approximation is justified and we can use the master equation $\partial_t\rho_S = \mathcal{L}\rho_S$, with $\mathcal{L}$ the Liouvillian.

Show that the non-normalized state conditioned on receiving the measurement outcomes $\epsilon_{s(n)}, \cdots, \epsilon_{s(1)}$ at times $t_n > \cdots > t_1 > 0$ reads

$$\tilde{\rho}_S(\epsilon_{s(n)}, \cdots, \epsilon_{s(1)}) = \mathcal{P}(\epsilon_{s(n)})e^{\mathcal{L}(t_n - t_{n-1})}\cdots\mathcal{P}(\epsilon_{s(1)})e^{\mathcal{L}t_1}\rho_S(0),$$

where $\mathcal{P}(\epsilon_{s(k)})$ is the projection superoperator associated with measurement result $\epsilon_{s(k)}$.

Show that the measurement probabilities $p(\epsilon_{s(n)}, \cdots, \epsilon_{s(1)}) = \mathrm{Tr}_S\left\{\tilde{\rho}_S(\epsilon_{s(n)}, \cdots, \epsilon_{s(1)})\right\}$ satisfy the Kolmogorov consistency condition, therefore making it undistinguishable from a classical stochastic process.

Solution:
The measurements act through the projection superoperators

$$\mathcal{P}(\epsilon_k)\rho = \Pi(\epsilon_k)\rho\Pi(\epsilon_k).$$

Therefore, the final non-normalized state is given by the sequence of Liouvillian evolution and projective measurements as

$$\tilde{\rho}_S(\epsilon_{s(n)},\cdots,\epsilon_{s(1)}) = \mathcal{P}(\epsilon_{s(n)})e^{\mathcal{L}(t_n-t_{n-1})}\cdots\mathcal{P}(\epsilon_{s(1)})e^{\mathcal{L}t_1}\rho_S(0),$$

for time-independent Liouvillian superoperator.
The Kolmogorov consistency condition reads

$$p(r_n,\cdots,\not{r_k},\cdots,r_1) = \sum_k p(r_n,\cdots,r_k,\cdots,r_1).$$

Applying the RHS to the sequence of projective measurements we get

$$\mathrm{Tr}_S\left\{\mathcal{P}(\epsilon_{s(n)})e^{\mathcal{L}(t_n-t_{n-1})}\cdots\mathcal{D}_{H_S}e^{\mathcal{L}(t_k-t_{k-1})}\cdots\mathcal{P}(\epsilon_{s(1)})e^{\mathcal{L}t_1}\rho_S(0),\right\}$$

with the dephasing superoperator defined as

$$\mathcal{D}_{H_S}\rho = \sum_k \Pi(\epsilon_k)\rho\Pi(\epsilon_k)$$

Notice that

$$e^{-iH_St/\hbar}\rho_S e^{iH_St/\hbar} = \sum_{mn} e^{-i(\omega_m-\omega_n)t}\Pi(\epsilon_m)\rho_S\Pi(\epsilon_n) \Rightarrow \frac{1}{T}\int_0^T dt\sum_{mn} e^{-i(\omega_m-\omega_n)t}\Pi(\epsilon_m)\rho_S\Pi(\epsilon_n) \to D_{H_S}\rho_S.$$

Notice that

$$\mathcal{L}\mathcal{D}_{H_S}\rho_S = \lim_{T\to\infty}\int_0^T\left(-\frac{i}{\hbar}[H_S,U\rho_SU^\dagger] + \sum_{n\omega}k_n(\omega)\left[S_n(\omega)U\rho_SU^\dagger S_n^\dagger(\omega) - \frac{1}{2}\left\{S_n^\dagger(\omega)S_n(\omega),U\rho_SU^\dagger\right\}\right]\right)$$

with $U = e^{-iH_St/\hbar}$. Obviously $[H_S,U]=0$. Furthermore, we remember that $[S_n(\omega),H_S] = \hbar\omega S_n(\omega) \Rightarrow S_n(\omega)U = e^{-i(H_S+\hbar\omega)t/\hbar}S_n(\omega) = e^{-i\omega t}US_n(\omega)$. Using these properties, we have

$$\mathcal{L}\mathcal{D}_{H_S}\rho_S = \lim_{T\to\infty}\int_0^T\left(-\frac{i}{\hbar}U[H_S,\rho_S]U^\dagger + \sum_{n\omega}k_n(\omega)\left[US_n(\omega)\rho_SS_n^\dagger(\omega)U^\dagger - \frac{1}{2}U\left\{S_n^\dagger(\omega)S_n(\omega),\rho_S\right\}U^\dagger\right]\right)$$

which implies

$$[\mathcal{L},\mathcal{D}_{H_S}] = 0.$$

Furthermore,

$$\mathcal{P}(\epsilon_k)\mathcal{D}_{H_S}\rho_S = \sum_n \Pi(\epsilon_k)\Pi(\epsilon_n)\rho_S\Pi(\epsilon_n)\Pi(\epsilon_k) = \sum_n \Pi(\epsilon_n)\Pi(\epsilon_k)\rho_S\Pi(\epsilon_k)\Pi(\epsilon_n) = \mathcal{D}_{H_S}\mathcal{P}(\epsilon_k)\rho_S$$

which means $[\mathcal{P}(\epsilon_k),\mathcal{D}_{H_S}]=0$. Therefore, we can move the dephasing operator from the k-th position to the n-th position:

$$\begin{aligned}
\sum_k p(r_n,\cdots,r_1) &= \mathrm{Tr}_S\left\{\mathcal{P}(\epsilon_{s(n)})e^{\mathcal{L}(t_n-t_{n-1})}\cdots\mathcal{D}_{H_S}e^{\mathcal{L}(t_k-t_{k-1})}\cdots\mathcal{P}(\epsilon_{s(1)})e^{\mathcal{L}t_1}\rho_S(0)\right\}\\
&= \mathrm{Tr}_S\left\{\mathcal{D}_{H_S}\mathcal{P}(\epsilon_{s(n)})e^{\mathcal{L}(t_n-t_{n-1})}\cdots\mathbb{I}e^{\mathcal{L}(t_k-t_{k-1})}\cdots\mathcal{P}(\epsilon_{s(1)})e^{\mathcal{L}t_1}\rho_S(0)\right\}\\
&= \sum_{i,j}\langle\epsilon_i|\,\Pi(\epsilon_j)\left[\mathcal{P}(\epsilon_{s(n)})e^{\mathcal{L}(t_n-t_{n-1})}\cdots\mathbb{I}e^{\mathcal{L}(t_k-t_{k-1})}\cdots\mathcal{P}(\epsilon_{s(1)})e^{\mathcal{L}t_1}\rho_S(0)\right]\Pi(\epsilon_j)\,|\epsilon_i\rangle\\
&= \sum_i\langle\epsilon_i|\left[\mathcal{P}(\epsilon_{s(n)})e^{\mathcal{L}(t_n-t_{n-1})}\cdots\mathbb{I}e^{\mathcal{L}(t_k-t_{k-1})}\cdots\mathcal{P}(\epsilon_{s(1)})e^{\mathcal{L}t_1}\rho_S(0)\right]|\epsilon_i\rangle\\
p(r_n,\cdots,\not{r_k},\cdots,r_1) &= \mathrm{Tr}_S\left\{\mathcal{P}(\epsilon_{s(n)})e^{\mathcal{L}(t_n-t_{n-1})}\cdots\mathbb{I}e^{\mathcal{L}(t_k-t_{k-1})}\cdots\mathcal{P}(\epsilon_{s(1)})e^{\mathcal{L}t_1}\rho_S(0)\right\}
\end{aligned}$$

which proves that the Born-Markov secular master equation satisfies the Kolmogorov consistency condition.

Exercise 3.10: Entropy production rate in the Born-Markov secular approximation

Show that the entropy production rate

$$\dot{\Sigma}(t) = \frac{d}{dt}S_S(t) - \frac{\dot{Q}(t)}{T}$$

can be written as $\dot{\Sigma}(t) = -k_B \partial_t D[\rho_S(t)|\pi_S]$.

Using the theorem about the CPTP master equation of Example 3.1, stating that there exists a CPTP map $\mathcal{E}(dt)$ propagating the state forwards in time: $\rho_S(t+dt) = \mathcal{E}(dt)\rho_S(t)$, and that the thermal state in stationary, $\mathcal{E}(dt)\pi_S = \pi_S$, show that

$$\dot{\Sigma}(t) = k_B \lim_{dt \searrow 0} \frac{D[\rho_S(t)|\pi_S] - D[\mathcal{E}(dt)\rho_S(t)|\mathcal{E}(dt)\pi_S]}{dt},$$

and use it to prove the positivity of $\dot{\Sigma}(t)$.

Solution:
The entropy, internal energy, and heat current are defined as

$$S_S \equiv -\mathrm{Tr}_S\left\{\rho_S \ln \rho_S\right\}, \quad U_S = \mathrm{Tr}_S\left\{H_S \rho_S\right\}, \quad \dot{Q} \equiv \mathrm{Tr}_S\left\{H_S \dot{\rho}_S\right\}.$$

Therefore, we can write the entropy production rate as

$$\dot{\Sigma} = -\mathrm{Tr}_S\left\{\dot{\rho}_S\left(\ln \rho_S + \beta H_S\right)\right\} = -\partial_t \mathrm{Tr}_S\left\{\rho_S\left(\ln \rho_S - \ln \pi_S\right)\right\} = -\partial_t D[\rho_S(t)|\pi_S].$$

Writing the derivative explicitely, we have

$$\dot{\Sigma} = \lim_{dt \to 0} \frac{D[\rho_S(t)|\pi_S] - D[\rho_S(t+dt)|\pi_S]}{dt} = \lim_{dt \to 0} \frac{D[\rho_S(t)|\pi_S] - D[\mathcal{E}(dt)\rho_S(t)|\mathcal{E}(dt)\pi_S]}{dt} \geq 0$$

where the last inequality follows from the monotonicity of the relative entropy.

Exercise 3.11: Born-Markov secular master eq. with multiple baths and driving

Considering the global Hamiltonian

$$H_{SB}(\lambda_t) = H_S(\lambda_t) + \sum_\nu \left(V_{SB}^{(\nu)} + H_B^{(\nu)}\right)$$

and the initial state

$$\rho_{SB}(0) = \rho_S(0) \bigotimes_\nu \pi_\nu(\beta_\nu),$$

show that the Born-Markov secular master equation for slow driving is

$$\partial_t \rho_S(t) = -\frac{i}{\hbar}[H_S(\lambda_t), \rho_S(t)] + \sum_\nu \mathcal{D}_\nu(\lambda_t)\rho_S(t).$$

This requires from the vanishment of the cross-terms

$$\mathrm{Tr}_{\nu,\mu}\left\{\tilde{V}_{SB}^{(\nu)}(t)\tilde{V}_{SB}^{(\mu)}(t)\pi_\nu(\beta_\nu)\pi_\mu(\beta_\mu)\right\} = 0,$$

which follows from Exercise 3.2.

Solution:
First, we go into the interaction picture through the unitary transformation $U_{\mathrm{int}} = \mathcal{T}\exp\left(-i\int_0^t ds[H_S(\lambda_s) + \sum_\nu H_\nu]\frac{dt}{\hbar}\right)$, which transform an operator A into $\tilde{A}(t) = U_{\mathrm{int}}^\dagger A U_{\mathrm{int}}$. In the interaction picture, the global state evolves according to

$$\partial_t \tilde{\rho}_{SB} = -\frac{i}{\hbar}\sum_\nu [\tilde{V}_\nu(t), \tilde{\rho}_{SB}].$$

Integrating this differential equation we get

$$\tilde{\rho}_{SB}(t) = \tilde{\rho}_{SB}(0) - \frac{i}{\hbar}\int_0^t ds_1 \sum_\nu [\tilde{V}_\nu(s_1), \tilde{\rho}_{SB}(0)] - \frac{1}{\hbar^2}\int_0^t ds_1 \int_0^{s_1} ds_2 \sum_{\nu\mu}[\tilde{V}_\nu(s_1), [\tilde{V}_\mu(s_2), \tilde{\rho}_{SB}(s_2)]].$$

Now we can take the trace over the baths to find the evolution of the system alone. Notably, the first-order term contains the operators

$$\tilde{K}_S^\nu = \mathrm{Tr}_\nu \left\{ \tilde{V}_\nu \pi_\nu \right\}$$

which can be set to 0 without loss of generality as demonstrated in Exercise 3.2:

$$\mathrm{Tr}_\nu \left\{ \tilde{V}_\nu \pi_\nu \right\} = 0.$$

Therefore, tracing out the baths makes the first order in $\tilde{V}_\nu$ vanish.
To tackle the second order term we now assume that the baths are very large and their state is not perturbed by the system evolution. Mathematically:

$$\tilde{\rho}_{SB}(t) \approx \tilde{\rho}_S(t) \bigotimes_\nu \pi_\nu.$$

Furthermore, we consider a decomposition of the interaction Hamiltonians as

$$V_\nu = \sum_\alpha A_\alpha^\nu \otimes B_\alpha^\nu \to \tilde{V}_\nu(t) = \sum_\alpha A_\alpha^\nu(t) \otimes B_\alpha^\nu(t)$$

where A_α^ν acts on S whereas B_α^ν acts on bath ν. The double commutator contains terms of the form

$$C_{\alpha\beta}^{\nu\mu}(t) = \mathrm{Tr}_{\nu\mu}\left\{ B_\alpha^\nu(t) B_\beta^\mu (\pi_\nu \otimes \pi_\mu) \right\}$$

which is the generalization of the bath correlation function to multiple heat baths. This allows us to write the double commutator as

$$\mathrm{Tr}_B \left\{ \sum_{\nu\mu} [\tilde{V}_\nu(s_1), [\tilde{V}_\mu(s_2), \tilde{\rho}_{SB}(s_2)]] \right\} = \sum_{\mu\nu\alpha\beta} \Big(C_{\alpha\beta}^{\nu\mu}(s_1 - s_2) \left[A_\alpha^\nu(s_1) A_\beta^\mu(s_2) \tilde{\rho}_S - A_\beta^\mu(s_2) \tilde{\rho}_S A_\alpha^\nu(s_1) \right] + \\ + C_{\beta\alpha}^{\mu\nu}(s_2 - s_1) \left[\tilde{\rho}_S A_\beta^\mu(s_2) A_\alpha^\nu(s_1) - A_\alpha^\nu(s_1) \tilde{\rho}_S A_\beta^\mu(s_2) \right] \Big).$$

Crucially, if $\mu \neq \nu$ we can separate the trace as

$$C_{\alpha\beta}^{\nu\mu}(t) = \mathrm{Tr}_\nu \left\{ B_\alpha^\nu(t) \pi_\nu \right\} \mathrm{Tr}_\mu \left\{ B_\beta^\mu \pi_\mu \right\}$$

and we can perform the sum over the indices α, β, yielding the operators

$$\sum_{\alpha\beta} C_{\alpha\beta}^{\nu\mu}(s_1 - s_2) A_\alpha^\nu(s_1) A_\beta^\mu(s_2) = \tilde{K}_S^\nu(s_1) \tilde{K}_S^\mu(s_2) = 0.$$

Therefore, only the diagonal $\mu = \nu$ terms contribute. Using $C_{\alpha\beta}^{\nu\nu}(t) = C_{\alpha\beta}^\nu(t)$ the time evolution of the partial state $\tilde{\rho}_S$ is

$$\partial_t \tilde{\rho}_S = -\frac{1}{\hbar^2}\int_0^t ds \sum_{\nu\alpha\beta} \Big(C_{\alpha\beta}^\nu(t - s) \left[A_\alpha^\nu(t) A_\beta^\nu(s) \tilde{\rho}_S(s) - A_\beta^\nu(s) \tilde{\rho}_S(s) A_\alpha^\nu(t) \right] + \\ + C_{\beta\alpha}^\nu(s - t) \left[\tilde{\rho}_S(s) A_\beta^\nu(s) A_\alpha^\nu(t) - A_\alpha^\nu(t) \tilde{\rho}_S(s) A_\beta^\nu(s) \right] \Big).$$

In the weak coupling regime we can approximate $\tilde{\rho}_S(t) = \tilde{\rho}_S(s) + \mathcal{O}(V)$ reducing the equation to

$$\partial_t \tilde{\rho}_S = \frac{1}{\hbar^2}\int_0^t ds \sum_{\nu\alpha\beta} C_{\alpha\beta}^\nu(t - s) \left[A_\beta^\nu(s) \tilde{\rho}_S(t) A_\alpha^\nu(t) - A_\alpha^\nu(t) A_\beta^\nu(s) \tilde{\rho}_S(t) \right] + \mathrm{h.c.}$$

$$\partial_t \tilde{\rho}_S = \frac{1}{\hbar^2}\int_0^t d\tau \sum_{\nu\alpha\beta} C_{\alpha\beta}^\nu(\tau) \left[A_\beta^\nu(t - \tau) \tilde{\rho}_S(t) A_\alpha^\nu(t) - A_\alpha^\nu(t) A_\beta^\nu(t - \tau) \tilde{\rho}_S(t) \right] + \mathrm{h.c.}$$

$$\partial_t \tilde{\rho}_S = \frac{1}{\hbar^2}\int_0^\infty d\tau \sum_{\nu\alpha\beta} C_{\alpha\beta}^\nu(\tau) \left[A_\beta^\nu(t - \tau) \tilde{\rho}_S(t) A_\alpha^\nu(t) - A_\alpha^\nu(t) A_\beta^\nu(t - \tau) \tilde{\rho}_S(t) \right] + \mathrm{h.c.}$$

where in the last step we used the Markov approximation to extend the integration up to ∞.
In order to approach the secular approximation, we first need to decompose the system operators $A^\nu_\alpha(t)$ into their Fourier components, which is obtained by noticing that

$$A^\nu_\alpha(t) = \sum_{mn} \Pi(\epsilon_m) A^\nu_\alpha(t) \Pi(\epsilon_n) = \sum_{mn} \Pi(\epsilon_m) U^\dagger_{\rm int} A^\nu_\alpha U_{\rm int} \Pi(\epsilon_n)$$

in the non-driven case one calculates directly $U_{\rm int}\Pi(\epsilon_n) = e^{-i\omega_n t}\Pi(\epsilon_n)$. However, in the driven case we need the driving to be slow. Then, we can approximate the system Hamiltonian as $H_S(\lambda_t) \approx H_S(\lambda_0) + \dot{\lambda}_t \mathcal{H}_S$, and the unitary becomes

$$U_{\rm int} \approx \mathcal{T}\exp\left(-i\int_0^t H_S(\lambda_0)\frac{dt}{\hbar} - i\int_{\lambda_0}^{\lambda_t} \mathcal{H}_S \frac{d\lambda}{\hbar}\right) = \exp\left[-i\left(H_S(\lambda_0) + \mathcal{H}\frac{\lambda_t - \lambda_0}{t}\right)\frac{t}{\hbar}\right] = \exp\left[-iH_S^{\rm slow}\frac{t}{\hbar}\right]$$

Choosing the eigenspaces of $H_S^{\rm slow}$ determined by the projectors $\Pi(\epsilon_n(\lambda_t))$ we have

$$A^\nu_\alpha = \sum_{mn} e^{-i[\omega_n(\lambda_t) - \omega_m(\lambda_t)]t} \Pi(\epsilon_m(\lambda_t)) A^\nu_\alpha \Pi(\epsilon_n(\lambda_t)) = \sum_\omega e^{-i\omega(\lambda_t)t} A^\nu_\alpha(\omega(\lambda_t)).$$

Dropping the argument (λ_t) for the sake of conciseness, we write the Born-Markov equation as

$$\partial_t \tilde{\rho}_S = \frac{1}{\hbar^2}\int_0^\infty d\tau \sum_{\nu\alpha\beta}\sum_{\omega\omega'} C^\nu_{\alpha\beta}(\tau) e^{i\omega'\tau} e^{-i(\omega+\omega')t}\left[A^\nu_\beta(\omega')\tilde{\rho}_S(t) A^\nu_\alpha(\omega) - A^\nu_\alpha(\omega)A^\nu_\beta(\omega')\tilde{\rho}_S(t)\right] + \text{h.c.}$$

and we now use the secular approximation, which states that the $(\omega+\omega')t$ components oscillate rapidly compared to the state dynamics and therefore we can approximate $e^{-i(\omega+\omega')t} \approx \delta_{\omega,-\omega'}$ (rotating wave approximation). Then, the Born-Markov secular master equation reads

$$\partial_t \tilde{\rho}_S = \frac{1}{\hbar^2}\int_0^\infty d\tau \sum_{\nu\alpha\beta}\sum_{\omega'} C^\nu_{\alpha\beta}(\tau) e^{i\omega'\tau}\left[A^\nu_\beta(\omega')\tilde{\rho}_S(t) A^\nu_\alpha(-\omega') - A^\nu_\alpha(-\omega')A^\nu_\beta(\omega')\tilde{\rho}_S(t)\right] + \text{h.c.}$$

$$\partial_t \tilde{\rho}_S = \frac{1}{\hbar^2}\int_0^\infty d\tau \sum_{\nu\alpha\beta}\sum_{\omega} C^\nu_{\alpha\beta}(\tau) e^{i\omega\tau}\left[A^\nu_\beta(\omega)\tilde{\rho}_S(t) A^{\nu\,\dagger}_\alpha(\omega) - A^{\nu\,\dagger}_\alpha(\omega)A^\nu_\beta(\omega)\tilde{\rho}_S(t)\right] + \text{h.c.}$$

Carrying out the integration we can introduce the Fourier transform of the bath correlation function

$$\gamma^\nu_{\alpha\beta}(\omega) \equiv \frac{1}{\hbar^2}\int_{-\infty}^\infty d\tau C^\nu_{\alpha\beta}(\tau)e^{i\omega\tau}, \quad \lambda_{\alpha\beta}(\omega) \equiv \frac{1}{2i\hbar}\int_{-\infty}^\infty d\tau\, \text{sgn}(\tau) C^\nu_{\alpha\beta}(\tau)e^{i\omega\tau}$$

which satisfy $\gamma^{\nu\,*}_{\alpha\beta}(\omega) = \gamma^\nu_{\beta\alpha}(\omega)$, $\lambda^{\nu\,*}_{\alpha\beta}(\omega) = \lambda^\nu_{\beta\alpha}(\omega)$ and combine to

$$\frac{1}{\hbar^2}\int_0^\infty d\tau C^\nu_{\alpha\beta}(\tau)e^{i\omega\tau} = \frac{\gamma^\nu_{\alpha\beta}(\omega)}{2} + \frac{i}{\hbar}\lambda_{\alpha\beta}(\omega).$$

Then, the BMS master equation can be written as

$$\partial_t \tilde{\rho}_S = \sum_{\nu\alpha\beta}\sum_\omega \left[\frac{\gamma^\nu_{\alpha\beta}(\omega)}{2} + \frac{i}{\hbar}\lambda_{\alpha\beta}(\omega)\right]\left[A^\nu_\beta(\omega)\tilde{\rho}_S(t)A^{\nu\,\dagger}_\alpha(\omega) - A^{\nu\,\dagger}_\alpha(\omega)A^\nu_\beta(\omega)\tilde{\rho}_S(t)\right] + \text{h.c.}$$

$$\partial_t \tilde{\rho}_S = \sum_{\nu\alpha\beta}\sum_\omega \left(\frac{1}{2}\gamma^\nu_{\alpha\beta}(\omega)\left[2A^\nu_\beta(\omega)\tilde{\rho}_S(t)A^{\nu\,\dagger}_\alpha(\omega) - \left\{A^{\nu\,\dagger}_\alpha(\omega)A^\nu_\beta(\omega), \tilde{\rho}_S(t)\right\}\right] + \right.$$
$$\left. -\frac{i}{\hbar}\lambda_{\alpha\beta}(\omega)\left[A^{\nu\,\dagger}_\alpha(\omega)A^\nu_\beta(\omega), \tilde{\rho}_S\right]\right)$$

where we recognize the dissipator and the Lamb shift. Neglecting the latter and going back to the Schrödinger picture (using the properties of the Fourier components, see Exercise 3.5), we finally find

$$\partial_t \rho_S = -\frac{i}{\hbar}[H_S(\lambda_t), \rho_S] + \sum_\nu \mathcal{D}_\nu(\lambda_t)\rho_S$$

where the dissipator generated by bath ν is

$$\mathcal{D}_\nu(\lambda_t)\rho_S(t) = \sum_{\alpha\beta}\sum_{\omega=\epsilon_n(\lambda_t)-\epsilon_m(\lambda_t)} \frac{1}{2}\gamma^\nu_{\alpha\beta}(\omega)\left[2A^\nu_\beta(\omega)\rho_S(t)A^{\nu\,\dagger}_\alpha(\omega) - \left\{A^{\nu\,\dagger}_\alpha(\omega)A^\nu_\beta(\omega), \rho_S(t)\right\}\right].$$

Exercise 3.12: From BMS master eq. to classical master eq. and decoherence

Consider a non-degenerate system Hamiltonian $H_S = \sum_x \epsilon_x |x\rangle\langle x|$ with $\epsilon_x = \epsilon_y \Leftrightarrow x = y$. Show that the populations $p_x(t) = \langle x|\rho_S(t)|x\rangle$ of the energy eigenstates obey a closed equation of the form

$$\partial_t p_x(t) = \sum_y \left[R_{xy} p_y(t) - R_{yx} p_x(t)\right],$$

with rates $R_{xy} \equiv \sum_{\alpha\beta} \gamma_{\alpha\beta}(\epsilon_y - \epsilon_x) \langle x|A_\beta|y\rangle \langle y|A_\alpha|x\rangle$.

Use Exercise 3.6 to confirm that the rates obey the local detailed balance condition, namely

$$\frac{R_{xy}}{R_{yx}} = e^{-\beta(\epsilon_x - \epsilon_y)}.$$

Assuming that the set of transition frequencies is also non-degenerate, namely $\epsilon_x - \epsilon_y = \epsilon_k - \epsilon_l \Leftrightarrow x = k \wedge y = l$, the coherences $\rho_{xy}(t) \equiv \langle x|\rho_S(t)|y\rangle$ evolve according to

$$\partial_t \rho_{xy}(t) = -\frac{i}{\hbar}(\epsilon_x - \epsilon_y)\rho_{xy}(t) - \sum_z \frac{R_{zx} + R_{zy}}{2} \rho_{xy}(t)$$

which is an exponentially dumped oscillation, causing decoherence.

Solution:
Let's start from the Born-Markov secular master equation:

$$\partial_t \rho_S = -\frac{i}{\hbar}[H_S, \rho_S] + \mathcal{D}\rho_S \rightarrow \partial_t \langle x|\rho_S|y\rangle = -\frac{i}{\hbar}(\epsilon_x - \epsilon_y) \langle x|\rho_S|y\rangle + \langle x|\mathcal{D}\rho_S|y\rangle$$

The dissipator acts as

$$\mathcal{D}\rho = \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega) \left[2A_\beta(\omega)\rho_S A_\alpha^\dagger(\omega) - \left\{A_\alpha^\dagger(\omega)A_\beta(\omega), \rho_S\right\}\right]$$

with $A_\alpha(\omega) = \sum_{\epsilon_x - \epsilon_y = \omega} \Pi(\epsilon_y) A_\alpha \Pi(\epsilon_x)$ which satisfies $A_\alpha^\dagger(\omega) = A_\alpha(-\omega)$, $[A_\alpha(\omega), H_S] = \hbar\omega A_\alpha(\omega)$. SInce we are considering a non-degenerate Hamiltonian, the Fourier component of the system interaction operators read $A_\alpha(\omega) = \sum_{\epsilon_x - \epsilon_y = \omega} |\epsilon_y\rangle\langle\epsilon_y| A_\alpha |\epsilon_x\rangle\langle\epsilon_x|$.
Let's look first the diagonal terms:

$$\begin{aligned}\langle x|\mathcal{D}\rho_S|x\rangle = \sum_{\alpha\beta}\sum_\omega \gamma_{\alpha\beta}(\omega) \, [2 \langle x|A_\beta|x+\omega\rangle\langle x+\omega|\rho_S|x+\omega\rangle\langle x+\omega|A_\alpha|x\rangle + \\ - \langle x|A_\alpha|x-\omega\rangle\langle x-\omega|A_\beta|x\rangle\langle x|\rho_S|x\rangle - \langle x|\rho_S|x\rangle\langle x|A_\alpha|x-\omega\rangle\langle x-\omega|A_\beta|x\rangle]\end{aligned}$$

where the summation over ω selects the transitions involving x. In particular, calling in the first line $y = x + \omega$ and $y = x - \omega$ in the second line, we find

$$\begin{aligned}\langle x|\mathcal{D}\rho_S|x\rangle = \sum_{\alpha\beta}\sum_y \{\gamma_{\alpha\beta}(\epsilon_y - \epsilon_x) \, [2 \langle x|A_\beta|y\rangle\langle y|\rho_S|y\rangle\langle y|A_\alpha|x\rangle] + \\ -\gamma_{\alpha\beta}(\epsilon_x - \epsilon_y) \, [\langle x|A_\alpha|y\rangle\langle y|A_\beta|x\rangle\langle x|\rho_S|x\rangle + \langle x|\rho_S|x\rangle\langle x|A_\alpha|y\rangle\langle y|A_\beta|x\rangle]\}.\end{aligned}$$

Introducing the populations $p_x = \langle x|\rho_S|x\rangle$ and the rates $R_{xy} = \sum_{\alpha\beta} 2\gamma_{\alpha\beta}(\epsilon_y - \epsilon_x) \langle x|A_\beta|y\rangle\langle y|A_\alpha|x\rangle$ we have

$$\langle x|\mathcal{D}\rho_S|x\rangle = \sum_y [R_{xy}p_y - R_{yx}p_x]$$

which, when plugged into the BMS master equation yields the classical master equation

$$\partial_t p_x = \sum_y [R_{xy}p_y - R_{yx}p_x].$$

Now ket's focus on the coherences:

$$\begin{aligned}\langle x|\mathcal{D}\rho_S|y\rangle = \sum_{\alpha\beta}\sum_\omega \gamma_{\alpha\beta}(\omega) \, [2 \langle x|A_\beta|x+\omega\rangle\langle x+\omega|\rho_S|y+\omega\rangle\langle y+\omega|A_\alpha|y\rangle + \\ - \langle x|A_\alpha|x-\omega\rangle\langle x-\omega|A_\beta|x\rangle\langle x|\rho_S|y\rangle - \langle x|\rho_S|y\rangle\langle y|A_\alpha|y-\omega\rangle\langle y-\omega|A_\beta|y\rangle].\end{aligned}$$

This scalar product can be simplified notably thanks to the assumption on the non-degeneracy of the transition frequencies. In fact, in the first line we have that the transition frequency ω must link both x and $x' = x + \omega$, and y and $y' = y + \omega$. However, since we are looking at $x \neq y$, the non-degeneracy of ω implies that there are no frequencies that make the first line finite. Therefore, the first line does not contribute to the dynamics. Nonetheless, the second line does because the transition frequency ω links only one between x, x' and y, y'. Therefore, calling $z = x - \omega$ for the first term and $z = y - \omega$ for the second, we have

$$\begin{aligned}\langle x|\mathcal{D}\rho_S|y\rangle &= -\sum_{\alpha\beta}\sum_{z}\left(\gamma_{\alpha\beta}(\epsilon_x - \epsilon_z)\langle x|A_\alpha|z\rangle\langle z|A_\beta|x\rangle\rho_{xy} + \gamma_{\alpha\beta}(\epsilon_y - \epsilon_z)\langle y|A_\alpha|z\rangle\langle z|A_\beta|y\rangle\rho_{xy}\right)\\ &= -\sum_z \frac{R_{zx} + R_{zy}}{2}\rho_{xy}.\end{aligned}$$

Plugging this into the master equation we finally get

$$\partial_t \rho_{xy} = -\frac{i}{\hbar}(\epsilon_x - \epsilon_y)\rho_{xy} - \sum_z \frac{R_{zx} + R_{zy}}{2}\rho_{xy}.$$

Exercise 3.13: Ergotropy and passive states

For an isolated system with Hamiltonian H in the state ρ we define the maximum *extractable* work or **ergotropy** as

$$E(\rho) \equiv \max_U \mathrm{Tr}\left\{H(\rho - U\rho U^\dagger)\right\} \geq 0$$

where the maximization is over all possible unitaries U. In this case, the Hamiltonian is the same at the beginning and at the end of the process, which means that the process is cyclic.

Show that $E(\rho) = 0$ whenever ρ is *passive*: Writing $H = \sum_k \epsilon_k |k\rangle\langle k|$ with ordered energies $\epsilon_{k+1} \geq \epsilon_k$ then a state $\rho = \sum_k \lambda_k |k\rangle\langle k|$ is passive when $\lambda_{k+1} \leq \lambda_k\ \forall k$.

Solution:
Notice that the maximum is achieved when, for a fixed $\mathrm{Tr}\{H\rho\}$, $\mathrm{Tr}\left\{HU\rho U^\dagger\right\}$ is minimum. Let's focus on the latter.

$$\mathrm{Tr}\left\{HU\rho U^\dagger\right\} = \sum_{kls}\epsilon_k U_{kl}\rho_{ls}U^*_{ks} = \sum_{kls\alpha}\epsilon_k p_\alpha U_{kl}U^*_{ks}\langle l|\alpha\rangle\langle\alpha|s\rangle = \sum_{k\alpha}\epsilon_k p_\alpha|\langle v_k|\alpha\rangle|^2$$

where $|v_k\rangle = \sum_s U^*_{ks}|s\rangle$. The ergotropy is

$$E(\rho) = \max_U \sum_{k\alpha}\epsilon_k p_\alpha\left(|\langle k|\alpha\rangle|^2 - |\langle v_k|\alpha\rangle|^2\right).$$

When $E(\rho) = 0 \to \forall U : \mathrm{Tr}\left\{H(\rho - U\rho U^\dagger)\right\} \leq 0$, namely

$$\sum_{k\alpha}\epsilon_k p_\alpha(|\langle k|\alpha\rangle|^2 - |\langle v_k|\alpha\rangle|^2) \leq 0.$$

Assuming that the state ρ is **not** passive but still diagonal in the Hamiltonian eigenbasis it means that there exists two energies $\epsilon_i > \epsilon_j$ that have probabilities $p_i > p_j$. Then, by choosing the unitary transformation that swaps $i \leftrightarrow j$ and leaves every other eigenstate untouched, we find

$$\mathrm{Tr}\left\{H(\rho - U\rho U^\dagger)\right\} = (\epsilon_i - \epsilon_j)(p_i - p_j) > 0$$

which is absurd. Now, let's look at the case in which ρ is not diagonal in the Hamiltonian eigenbasis. Let's consider the passive state $\tilde{\rho} = \sum_k p_{\alpha_k}|k\rangle\langle k|$, which is diagonal in the Hamiltonian eigenbasis by construction. This state can be reached by applying a unitary transformation on ρ:

$$\rho = \sum_\alpha p_\alpha |\alpha\rangle\langle\alpha| \to \tilde{\rho} = \sum_k p_{\alpha_k}|k\rangle\langle k|$$

by using the unitary $U = \sum_k |k\rangle\langle\alpha_k|$. Since $\tilde{\rho}$ is passive we have

$$E(\rho) = \sum_{k\alpha}\epsilon_k p_\alpha|\langle k|\alpha\rangle|^2 - \sum_k \epsilon_k p_{\alpha_k}.$$

Notably, $S_{k\alpha} = |\langle k|\alpha\rangle|^2$ is a bi-stochastic matrix since $\sum_k S_{k\alpha} = \sum_\alpha S_{k\alpha} = 1$ and $S_{k\alpha} \geq 0$. Furthermore, the set of bi-stochastic matrices is convex: if A, B are bi-stochastic, then also $qA + (1-q)B$ with $q \in [0,1]$ is also bi-stochastic. Let's look at the minimum over the set of bi-stochastic matrices of $\sum_{k\alpha} \epsilon_k S_{k\alpha} p_\alpha$. Suppose that the minimum is **not** an extremal points: then it can be decomposed as $S = qA + (1-q)B$ with $q \in (0,1)$. However, this means that A, B are minima as well, which is absurd. Therefore the minimum happens only at the extremal points of the set. These points are the permutation matrices: namey matrices in which all entries are either $0, 1$. Importantly, we have already constructed the bistochastic matric that yields the global minimum by studying $\tilde{\rho}$. Thus, since $S_{k\alpha} = |\langle k|\alpha\rangle|^2$ is not an extremal point of the set we have $E(\rho) > 0$. In conclusion, this means that if the state does not commute with the Hamiltonian it is always possible to extract energy from it by applying the unitary transformation that ends in the passive state.

Exercise 3.14: Extracting work with unitaries

Consider an unitary process with three steps:

(i) Transform the eigenbasis of $\rho_S(0)$ to the energy eigenbasis of $H_S(\lambda_0)$;

(ii) Reorder the populations of the energy eigenstates so that the new populations, denoted by q_s, decrease monotonically with increasing energy;

(iii) adjust the Hamiltonian, i.e. switch $\lambda_0 \to \lambda_0'$, such that the separations between adjacent energy levels are set as $q_s = e^{-\beta\epsilon_s(\lambda_0')/\mathcal{Z}_S(\lambda_0')}$, while the eigenvectors $|\epsilon_s\rangle$ remain fixed.

After these steps, the state is a thermal equilibrium state with respect to $H_S(\lambda_0')$.

Calculate the amount of extracted work, and verify that, after completing the cycle with an isothermal transformation the extracted work reads

$$-W_{\text{tot}} = F_S[\rho_S(0), \lambda_0] - \mathcal{F}(\lambda_0) > 0.$$

Solution:
The initial energy is $U_0 = \text{Tr}\{H(\lambda_0)\rho_S(0)\}$. Instead, the energy after step (iii) is

$$U_f = \text{Tr}\left\{H(\lambda_0')\sum_s q_s |\epsilon_s\rangle\langle\epsilon_s|\right\} = \sum_s \epsilon_s' q_s = \sum_s -T\ln(q_s \mathcal{Z}_S')q_s.$$

Splitting the log we find

$$U_f = TS[\rho_S(0)] - T\ln \mathcal{Z}_S' = TS[\rho_S(0)] + \mathcal{F}(\lambda_0').$$

Therefore, the extracted work after the unitary steps (i-iii) is

$$-W = -(U_f - U_0) = \text{Tr}\{H(\lambda_0)\rho(0)\} - TS[\rho(0)] - \mathcal{F}(\lambda_0') = F[\rho_S(0), \lambda_0] - \mathcal{F}(\lambda_0').$$

Now we make an isothermal transformation to get back to the initial state. Importantly, the total entropy reads $\Sigma(t) = S[\rho_S(\lambda_t)] - \frac{Q(t)}{T}$ so we can write the entropy production in a time interval δt as

$$\delta\Sigma = \dot{\lambda}_t \delta t \frac{\partial}{\partial\lambda} S[\rho_S(\lambda)] - \beta\delta Q.$$

Since the process is isothermal, $\rho_S(\lambda_t) = e^{-\beta H_S(\lambda_t)}/\mathcal{Z}_S(\lambda_t)$, which means that

$$\frac{\partial}{\partial\lambda} S[\rho_S(\lambda)] = -\text{Tr}\left\{\frac{\partial\rho_S(\lambda_t)}{\partial\lambda}\log\rho_S(\lambda_t)\right\} = -\text{Tr}\{(-\beta\partial_\lambda H - \partial_\lambda \log\mathcal{Z}_S(\lambda_t))\rho(\lambda_t)\log\rho_S(\lambda_t)\}$$

$$\delta S = \dot{\lambda}\delta t\text{Tr}\{(\beta\partial_\lambda H + \partial_\lambda\log\mathcal{Z}_S)\rho_S(-\beta H - \log\mathcal{Z}_S)\}$$

while the increase in heat is

$$\delta Q = \text{Tr}\{H(-\beta\partial_\lambda H - \partial_\lambda\log\mathcal{Z}_S)\rho_S\}\dot{\lambda}\delta t$$

Combining them we get

$$\delta\Sigma = -\dot{\lambda}\delta t\text{Tr}\{(\beta\partial_\lambda H + \partial_\lambda\log\mathcal{Z}_S)\rho_S\log\mathcal{Z}_S\} = -\dot{\lambda}\delta t\log\mathcal{Z}_S\text{Tr}\left\{(\beta\partial_\lambda H + \text{Tr}\left\{\frac{-\beta(\partial_\lambda H)e^{-\beta H}}{\mathcal{Z}_S}\right\})\rho_S\right\}$$

from which we see that the isothermal process is reversible:

$$\delta\Sigma = -\dot{\lambda}\delta t \log \mathcal{Z}_S \left[\text{Tr}\left\{(\beta\partial_\lambda H + \text{Tr}\left\{-\beta(\partial_\lambda H)\rho_S\right\})\rho_S\right\}\right] = -\dot{\lambda}\delta t \log \mathcal{Z}_S \left[\text{Tr}\left\{\beta(\partial_\lambda H)\rho_S\right\} + \text{Tr}\left\{-\beta(\partial_\lambda H)\rho_S\right\}\right]$$

$$\delta\Sigma = 0 \Rightarrow \delta S = \frac{\delta Q}{T}$$

Now we can calcuate the change in internal energy of the system, and, htrough the first law, the work done on it.

$$U_0 - U_0' = \text{Tr}\left\{H(\lambda_0)\pi(\lambda_0)\right\} - \text{Tr}\left\{H(\lambda_0')\pi(\lambda_0')\right\} = TS[\pi(\lambda_0)] + \mathcal{F}(\lambda_0) - TS[\pi(\lambda_0')] - \mathcal{F}(\lambda_0') = Q + W_{\text{isothermal}}$$

Since $\beta Q = \Delta S$ we find

$$W_{\text{isothermal}} = \mathcal{F}(\lambda_0) - \mathcal{F}(\lambda_0')$$

which means that the work extracted from a single cycle is

$$-W_{\text{cycle}} = -W - W_{\text{isothermal}} = F[\rho_S(0), \lambda_0] - \mathcal{F}(\lambda_0).$$

Exercise 3.15: Work extraction from quantum coherence

The dephasing operation $\mathcal{D}_{H_S}$ is defined through

$$\mathcal{D}_{H_S}\rho \equiv \sum_k \Pi(\epsilon_k)\rho\Pi(\epsilon_k),$$

where $\Pi(\epsilon_k)$ is the projector onto the k-th eigenspace of the Hamiltonian H_S.

Consider a state ρ_S with coherences in the energy eigenbasis, i.e. $\mathcal{D}_{H_S}\rho_S \neq \rho_S$. Show that $F_S(\mathcal{D}_{H_S}\rho_S) < F_S(\rho_S)$, which means that is it possible to extract work when transforming ρ_S to $\mathcal{D}_{H_S}\rho_S$.

Solution:
The nonequilibrium free energy is

$$F(\rho) = \text{Tr}\left\{H\rho\right\} + T\text{Tr}\left\{\rho\ln\rho\right\} = \sum_{\alpha k} \epsilon_k p_\alpha |\langle k|\alpha\rangle|^2 + \sum_\alpha T p_\alpha \ln p_\alpha.$$

Instead, the dephased state $\mathcal{D}\rho = \sum_k q_k |k\rangle\langle k|$ with $q_k = \sum_\alpha p_\alpha |\langle k|\alpha\rangle|^2$, which means that its nonequilibrium free energy is

$$F(\mathcal{D}\rho) = \sum_{\alpha k} \epsilon_k p_\alpha |\langle k|\alpha\rangle|^2 + T\sum_{k\alpha} p_\alpha |\langle k|\alpha\rangle|^2 \ln(p_\alpha |\langle k|\alpha\rangle|^2)$$

Thus, the difference between the noneuqilibrium free energies reads

$$F(\rho) - F(\mathcal{D}\rho) = -T\sum_\alpha p_\alpha \sum_k |\langle k|\alpha\rangle|^2 \ln(|\langle k|\alpha\rangle|^2) \geq 0$$

Exercise 3.16: Quantum Carnot cycle

Consider a two-level system with Hamiltonian $H = \Delta_t |e\rangle\langle e|$ as the working medium of a heat engine. Here, $|e\rangle$ denotes the excited state and Δ_t the controllable energy spacing of the medium.

Construct an example of a quantum Carnot cycle and find the conditions to achieve zero entropy production.

Solution:
We can consider the cycle made of two thermalization processes and two unitaries such that, after the thermalization with the hot bath, the probability of finding the qubit in the excited state is

$$p_1 = \frac{1}{e^{\beta_h\Delta_1} + 1}.$$

Afterwards, we disconnect the qubit from the bath and change the energy separation to Δ_2 while keeping the probability of finding the qubit in the excited state fixed, $p_2 = p_1$.
Then, we let the qubit thermalize with the cold bath while the energy separation is Δ_3, and the excited

probability changes to

$$p_3 = \frac{1}{e^{\beta_c \Delta_3} + 1}.$$

We then disconnected again the qubit from the bath and change the energy separation to Δ_4 while keeping $p_4 = p_3$.
Finally, we thermalize again with the hot bath, completing the cycle.
In the first step, there is no heat exchange, and the work extracted is

$$W_{h\to c} = \frac{\Delta_2 - \Delta_1}{e^{\beta_h \Delta_1} + 1}.$$

To have an isothermal process with the bath, we need the state to be thermal. Thus, we first quench the Hamiltonian $\Delta_2 \to \Delta_2' = \frac{\beta_h \Delta_1}{\beta_c}$. This requires the work

$$W_{\text{quench},c} = \left(\frac{T_c}{T_h}\Delta_1 - \Delta_2\right) p_1.$$

Then, we can proceed with the isothermal process with the bath, where the work and heat exchanged are

$$Q_c = T_c \Delta S, \quad W_c = \Delta F_c$$

In particular, the heat reads

$$\beta_c Q_c = p_1 \log p_1 + (1-p_1)\log(1-p_1) - p_3 \log p_3 - (1-p_3)\log(1-p_3) = \log\frac{1-p_1}{1-p_3} + p_1 \log\frac{p_1}{1-p_1} - p_3 \log\frac{p_3}{1-p_3}$$

noticing that $1 - p_1 = e^{\beta_h \Delta_1} p_1$ we find

$$\beta_c Q_c = (\beta_h \Delta_1 - \beta_c \Delta_3) + \log\frac{p_1}{p_3} - p_1 \beta_h \Delta_1 + p_3 \beta_c \Delta_3 = \beta_h \Delta_1 (1-p_1) - \beta_c \Delta_3 (1-p_3) + \log\frac{p_1}{p_3}.$$

The energy difference gives the work done:

$$\Delta U = \Delta_3 p_3 - \Delta_2' p_1 \to W = \Delta U - Q_c.$$

Then, the second unitary process exerts the work

$$W_{c\to h} = (\Delta_4 - \Delta_3) p_3 = \frac{\Delta_4 - \Delta_3}{e^{\beta_c \Delta_3} + 1}.$$

Before the last isothermal process we once again qucnh the system Hamiltonian $\Delta_4 \to \Delta_4' = \frac{\beta_c \Delta_3}{\beta_h}$ such that the state is thermal with respect to the hot bath. This requires the work

$$W_{\text{quench},h} = \left(\frac{T_h}{T_c}\Delta_3 - \Delta_4\right) p_3.$$

Finally, we can do the isothermal process with the hot bath, exchanging both heat and work. In particular, the heat is

$$\beta_h Q_h = \Delta S = -p_1 \log p_1 - (1-p_1)\log(1-p_1) + p_3 \log p_3 + (1-p_3)\log(1-p_3) = -\beta_c Q_c.$$

From this we can calculate the entropy production in one cycle

$$\Delta S_{cycle} = -\beta_h Q_h - \beta_c Q_c = 0$$

which means that the cycle is reversible.
The total work extracted is

$$\begin{aligned}
-W_{tot} &= -W_{h\to c} - W_c - W_{c\to h} - W_h - W_{\text{quench},c} - W_{\text{quench},h} \\
&= -\Bigg(\frac{\Delta_2 - \Delta_1}{e^{\beta_h \Delta_1} + 1} + \Delta_3 p_3 - \Delta_2' p_1 - Q_c + \frac{\Delta_4 - \Delta_3}{e^{\beta_c \Delta_3} + 1} + \Delta_1 p_1 - \Delta_4' p_3 - Q_h + \\
&\qquad + \left[\frac{T_c}{T_h}\Delta_1 - \Delta_2\right] p_1 + \left[\frac{T_h}{T_c}\Delta_3 - \Delta_4\right] p_3\Bigg) \\
-W_{tot} &= -(\Delta_2 - \Delta_2' + \Delta_2' - \Delta_2) p_1 + -Q_c + (\Delta_4 - \Delta_4' + \Delta_4' - \Delta_4) p_3 - Q_h) \\
&= Q_c + Q_h = Q_h\left(1 - \frac{T_c}{T_h}\right)
\end{aligned}$$

which is performed at Carnot efficiency $\eta_{\text{Carnot}} = 1 - \frac{T_c}{T_h}$.

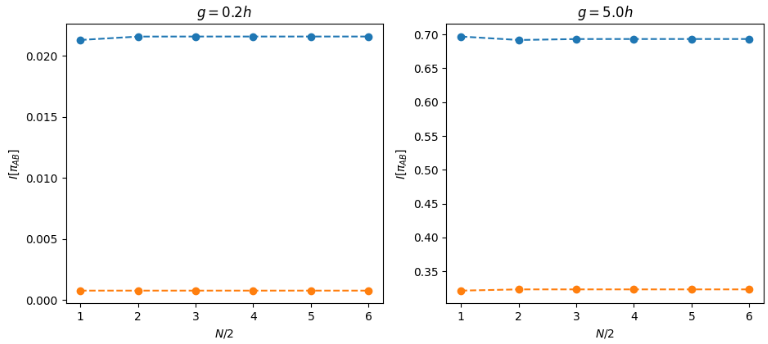


Figure 3: Mutual information $I[\pi_{AB}]$ of the two halves of the spin chain at the thermal state π_{AB}. We fixed $h = 1$, and considered weak (left, $g = 0.2$) and strong (right, $g = 5$) coupling for a cold (blue, $T = 0.5$) and a hot (orange, $T = 5$) temperature. Note the difference in two order of magnitudes between the weak and the strong coupling.

Exercise 3.17: Numerical calculation of many-body thermal state

Consider a one-dimensional Ising model, described by the Hamiltonian

$$H_{\text{Ising}} = -h \sum_{i=1}^{N} \sigma_z^{(i)} - g \sum_{i=1}^{N-1} \sigma_x^{(i)} \sigma_x^{(i+1)},$$

with N the number of sites, h the coupling to the external magnetic field, and g the strength of the nearest-neighbour interaction.

Verify numerically the relation

$$\pi_{AB} \approx \pi_A \otimes \pi_B$$

for $N = 2, 4, 6$, and 8 by separating the chain in the middle.

Solution:

```
import numpy as np
from qutip import *
import matplotlib.pyplot as plt
######################################################################
eye= Qobj([[1,0], [0, 1]]); # Single spin identity
sz = sigmaz();            # Single spin S_z
sx = sigmax();            # Single spin S_x
######################################################################
def Hamiltonian(h, g, N):
    Hh=0; Hg=0;
    EYE = [eye]*N
    for i in range(N):
        tEYE = EYE*1; tEYE[i] = sz;
        Hh+=tensor(tEYE);
    for i in range(N-1):
        tEYE = EYE*1; tEYE[i] = sx; tEYE[i+1] = sx;
        Hg+= tensor(tEYE);
    return -h*Hh-g*Hg

def initial_states(beta, h, g, N):
    H = Hamiltonian(h, g, N);
    rhoAB = (-beta*H).expm();   rhoAB/=rhoAB.tr();

    A=[]; B=[];
    for i in range(int(N/2)):
        A.append(i); B.append(int(N/2)+i)
    rhoA = rhoAB.ptrace(A); rhoB = rhoAB.ptrace(B);
    rhoArhoB = tensor(rhoA, rhoB)
    return [rhoAB, rhoArhoB]

def mutual_information(beta, h, g, N):
    X = initial_states(beta, h, g, N);
    return entropy_vn(X[1]) - entropy_vn(X[0])
######################################################################
def calc_plot(T, h, g, N):
```

```
    k = len(g);
    for i in range(k):
        plt.subplot(1,k,i+1)
        plt.xlabel("$N/2$"); plt.ylabel("$I[\pi_{AB}]$")
        plt.title("$g=%.1f h$" %g[i])
        for j in range(len(T)):
            I = np.zeros(len(N));
            for s in range(len(N)):
                I[s] = mutual_information(1/T[j], h, g[i], N[s])
            print(N, I)
            plt.plot(np.array(N)/2, I, '--o')
    return
########################################################################
h=1
N = [2,4,6, 8, 10, 12]
T = [.5, 5]
g = [.2, 5]
calc_plot(T, h, g, N)
plt.show()
```

Exercise 3.18: Dissipation inequality at strong coupling

By defining the strong coupling internal energy as

$$U_S(t) \equiv \mathrm{Tr}_{SB}\left\{\left[H_S(\lambda_t) + \sum_\nu V_{SB}^{(\nu)(\lambda_t)}\right]\rho_{SB}(t)\right\}$$

and thus the heat as $Q_\nu(t) = -\mathrm{Tr}_\nu\left\{H_B^{(\nu)}[\rho_\nu(t) - \rho_\nu(0)]\right\}$, show that the following expressions are equivalent:

$$\Sigma \equiv \Delta S[\rho_S(t)] - \sum_\nu \frac{Q_\nu(t)}{T_\nu}, \qquad \Sigma(t) = D\left[\rho_{SB}(t)\middle|\rho_S(t)\bigotimes_\nu \pi_\nu(\beta_\nu)\right] = \sum_\nu D[\rho_\nu(t)|\pi_\nu(\beta_\nu)] + I_{\mathrm{tot}}[\rho_{SB}(t)],$$

where the total information is defined as $I_{\mathrm{tot}}(\rho_{1\cdots N}) \equiv \sum_i S(\rho_i) - S(\rho_{1\cdots N})$.

Solution:

$$\begin{aligned}\Sigma &= \mathrm{Tr}\left\{\rho_{SB}(t)(\ln\rho_{SB}(t) - \ln[\rho_S(t)\bigotimes_\nu \pi_\nu])\right\} = -S[\rho_{SB}(t)] + S[\rho_S(t)] - \sum_\nu \mathrm{Tr}\left\{\rho_\nu(t)\ln\pi_\nu\right\}\\ &= -S[\rho_{SB}(0)] + S[\rho_S(t)] - \sum_\nu \mathrm{Tr}\left\{\rho_\nu(t)\ln\pi_\nu\right\} = -S[\rho_S(0)] - \sum_\nu S[\pi_\nu] + S[\rho_S(t)] - \sum_\nu \mathrm{Tr}_\nu\left\{\rho_\nu(t)\ln\pi_\nu\right\}\\ &= \Delta S[\rho_S(t)] - \sum_\nu \mathrm{Tr}_\nu\left\{(\rho_\nu(t) - \pi_\nu)\ln\pi_\nu\right\} = \Delta S[\rho_S(t)] + \sum_\nu \beta_\nu \mathrm{Tr}_\nu\left\{(\rho_\nu(t) - \pi_\nu)H_B^{(\nu)}\right\}\\ &= \Delta S[\rho_S(t)] - \sum_\nu \frac{Q_\nu(t)}{T_\nu}.\end{aligned}$$

The entropy change has two positive contributions: $D[\rho_\nu(t)|\pi_\nu(\beta_\nu)]$, which represent the amount of information that is lost when describing the baths with the thermal states π_ν, in fact, during the evolution the baths' states change; and $I_{\mathrm{tot}}[\rho_{SB}(t)]$ which accounts for the correlations that build up between system and baths, and, in particular, the amount of information that is lost when describing the global state with a product state.

Exercise 3.19: Quantum thermodynamic properties at strong coupling

Defining $\mathcal{F}_S^*(\lambda) \equiv -k_B T \ln \mathcal{Z}_S^*(\lambda)$, with $\mathcal{Z}_S^*(\lambda) \equiv \mathcal{Z}_{SB}/\mathcal{Z}_B$ and $e^{-\beta H_S^*(\lambda)}/\mathcal{Z}_S^*(\lambda) \equiv \mathrm{Tr}_B\left\{\pi_{SB}(\beta,\lambda)\right\}$, show that

$$\mathcal{U}_S^*(\lambda) \equiv \mathrm{Tr}_S\left\{\pi_S^*[H_S^*(\lambda) + \beta\partial_\beta H_S^*(\lambda)]\right\} = \partial_\beta[\beta\mathcal{F}_S^*(\lambda)] = \mathcal{U}_{SB}(\lambda) - \mathcal{U}_B,$$

$$\mathcal{S}_S^*(\lambda) \equiv k_B \mathrm{Tr}_S\left\{\pi_S^*[-\ln\pi_S^* + \beta^2\partial_\beta H_S^*(\lambda)]\right\} = k_B\beta^2\partial_\beta\mathcal{F}_S^*(\lambda) = \mathcal{S}_{SB}(\lambda) - \mathcal{S}_B.$$

Note that in the book one finds π_S instead of π_S^*, which is—I believe—a mistake.

Solution:
From $\beta\mathcal{F}_S^* = -\ln \mathrm{Tr}\left\{e^{-\beta H_S^*}\right\}$ we can calculate the derivative as

$$\partial_\beta(\beta\mathcal{F}_S^*) = -\frac{1}{\mathcal{Z}_S^*}\mathrm{Tr}\left\{\partial_\beta e^{-\beta H_S^*}\right\}$$

Since in general $[H_S^*, \partial_\beta H_S^*] \neq 0$ we have to be careful with the derivative. Thankfully, the linearity and cyclicity of the trace allows us to write

$$\begin{aligned}\mathrm{Tr}\left\{\partial_\beta e^{-\beta H_S^*}\right\} &= \sum_n \mathrm{Tr}\left\{\frac{(-1)^n\beta^{n-1}(H_S^*)^n}{(n-1)!} + \frac{(-\beta)^n}{n!}\left([\partial_\beta H_S^*](H_S^*)^{n-1} + \cdots + (H_S^*)^{n-1}[\partial_\beta H_S^*]\right)\right\} \\ &= \mathrm{Tr}\left\{-H_S^* e^{-\beta H_S^*} - \beta[\partial_\beta H_S^*]e^{-\beta H_S^*}\right\}\end{aligned}$$

from which we have

$$\partial_\beta(\beta\mathcal{F}_S^*) = \mathrm{Tr}\left\{\pi_S^*[H_S^* + \beta\partial_\beta H_S^*]\right\} = \partial_\beta[-\ln \mathcal{Z}_{SB} + \mathcal{Z}_B] = \mathcal{U}_{SB} - \mathcal{U}_B.$$

From $\beta^2\partial_\beta\mathcal{F}_S^* = \beta\partial_\beta(\beta\mathcal{F}_S^*) - \beta\mathcal{F}_S^*$ we have

$$\beta^2\partial_\beta\mathcal{F}_S^* = \mathrm{Tr}\left\{\pi_S^*[\beta H_S^* + \beta^2\partial_\beta H_S^* + \ln \mathcal{Z}_S^*]\right\} = \mathrm{Tr}\left\{\pi_S^*[-\ln \pi_S^* + \beta^2\partial_\beta H_S^*]\right\}$$

Using the definition of $\mathcal{Z}_S^*$ we finally have

$$\beta^2\partial_\beta\mathcal{F}_S^* = \beta(\mathcal{U}_{SB} - \mathcal{U}_B) - \beta(\mathcal{F}_{SB} - \mathcal{F}_B) = S_{SB} - S_B$$

Exercise 3.20: Positivity of entropy production at strong coupling

Using the Hamiltonian of mean force H_S^* defined through the relations

$$\frac{e^{-\beta H_S^*(\lambda_t)}}{\mathcal{Z}_S^*(\lambda_t)} \equiv \mathrm{Tr}_B\left\{\pi_{SB}(\lambda_t)\right\}, \quad \mathcal{Z}_S^*(\lambda_t) \equiv \frac{\mathcal{Z}_{SB}(\lambda_t)}{\mathcal{Z}_B}$$

and defining internal energy and system entropy as

$$U_S^*(t) \equiv \mathrm{Tr}_S\left\{\rho_S(t)\left[H_S^*(\lambda_t) + \beta\partial_\beta[H_S^*(\lambda_t)]\right]\right\}, \qquad S_S^*(t) \equiv \mathrm{Tr}_S\left\{\rho_S(t)\left[-\ln \rho_S(t) + \beta^2\partial_\beta[H_S^*(\lambda_t)]\right]\right\}$$

use the following definitionm of heat $Q^*(t) \equiv \Delta U_S^*(t) - W(t)$ to show that the entropy production

$$\Sigma^*(t) = \Delta S_S^*(t) - \frac{Q^*(t)}{T}$$

can be written as

$$\Sigma^*(t) = D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] - D[\rho_S(t)|\pi_S^*(\lambda_t)].$$

Finally, use the monotonity of the relative entropy to show that $\Sigma^*(t) \geq 0$.

Solution:
Using the definitions and the fact that the entropy of the global state does not change due to the unitary evolution we have

$$\begin{aligned}\Sigma^* &= \mathrm{Tr}\left\{\rho_{SB}[\ln \rho_{SB} - \ln \pi_{SB}]\right\} - \mathrm{Tr}\left\{\rho_S[\ln \rho_S - \ln \pi_S^*]\right\} \\ &= -S[\rho_{SB}(t)] + S[\rho_S(t)] + \beta\mathrm{Tr}\left\{\rho_{SB}(t)H_{SB}(\lambda_t)\right\} + \ln \mathcal{Z}_{SB}(\lambda_t) - \beta\mathrm{Tr}\left\{\rho_S(t)H_S^*(\lambda_t)\right\} - \ln \mathcal{Z}_S^*(\lambda_t) \\ &= -S[\rho_{SB}(0)] + S[\rho_S(t)] + \beta\mathrm{Tr}\left\{\rho_{SB}(t)H_{SB}(\lambda_t)\right\} - \beta\mathrm{Tr}\left\{\rho_S(t)H_S^*(\lambda_t)\right\} + \ln \mathcal{Z}_B \\ &= -\beta\mathrm{Tr}\left\{\pi_{SB}(\lambda_0)H_{SB}(\lambda_0)\right\} - \ln\frac{\mathcal{Z}_{SB}(\lambda_0)}{\mathcal{Z}_B} + S[\rho_S(t)] + \beta\mathrm{Tr}\left\{\rho_{SB}(t)H_{SB}(\lambda_t)\right\} - \beta\mathrm{Tr}\left\{\rho_S(t)H_S^*(\lambda_t)\right\} \\ &= \beta W(t) - \ln \mathcal{Z}_S^*(\lambda_0) + S[\rho_S(t)] - \beta\mathrm{Tr}\left\{\rho_S(t)H_S^*(\lambda_t)\right\} \\ &= \beta W(t) + \beta\mathcal{F}_S^*(\lambda_0) - \beta\mathrm{Tr}\left\{\rho_S(t)[H_S^*(\lambda_t) + T\ln \rho_S(t)]\right\} = \beta W(t) + \beta\mathcal{F}_S^*(\lambda_0) - \beta[U_S^*(t) - TS_S^*(t)] \\ &= \beta W(t) - \beta[F_S^*(t) - \mathcal{F}_S^*(\lambda_0)] = \beta\Delta U_S^* - \beta Q^*(t) - \beta\Delta U_S^* + \Delta S_S^* = \Delta S_S^*(t) - \beta Q^*(t).\end{aligned}$$

In particular, using that $D[\mathrm{Tr}_A\left\{\rho_{AB}\right\}|\mathrm{Tr}_A\left\{\sigma_{AB}\right\}] \leq D[\rho_{AB}|\sigma_{AB}]$ one finds that $\Sigma^*(t) \geq 0$.

Exercise 3.21: Comparing the strong coupling entropies

Both exercises 3.18 and 3.20 study the entropy production at strong coupling. However, while the former includes the coupling energy into the system's energy, the latter studies the effects of the interaction through the Hamiltonian of mean force. Here, we compare these two cases.

First, consider the case $V_{SB}(\lambda_0) = 0$, such that $H_S(\lambda_0) = H_S^*(\lambda_0)$. Show that this imples

$$\Sigma^*(t) - \Sigma(t) = D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] - D[\rho_{SB}(t)|\pi_S^*(\lambda_t) \otimes \pi_B].$$

Thus, if $\pi_{SB} \approx \pi_S \otimes \pi_B$, we have $\Sigma^*(t) = \Sigma(t)$.

Now, assume $V_{SB}(\lambda_0) \neq 0$ and an initial state of the form $\rho_{SB}(0) = \pi_{SB}(\beta, \lambda_0)$. Show that

$$\Sigma^*(t) - \Sigma(t) = D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] - D[\rho_{SB}(t)|\pi_S^*(\lambda_t) \otimes \pi_B] + I[\pi_{SB}(\lambda_0)] + D[\pi_B^*(\lambda_0)|\pi_B].$$

Confirm that this is related to a boundary term and that $\Sigma^*(t) = \Sigma(t)$ if the zeroth law holds, namely $\pi_{SB} \approx \pi_S \otimes \pi_B$.

Solution:
Let us do the second point immediately since the first one follows from it. From Exercise 3.18 we have

$$\Sigma(t) \equiv \Delta S[\rho_S(t)] - \beta Q(t), \qquad Q(t) \equiv -\mathrm{Tr}_B \{H_B[\rho_B(t) - \rho_B(0)]\}.$$

Notice that the result of Exercise 3.18, namely writing this entropyproduction in terms of some relative entropy, *requires* a separable initial state. Thus we do not use it.
Instead, we use the result of Exercise 3.20 since we are interested in the states in the form π_{AB}.

$$\begin{aligned}
\Sigma^*(t) - \Sigma(t) &= D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] - D[\rho_S(t)|\pi_S^*(\lambda_t)] - \Delta S[\rho_S(t)] - \beta \mathrm{Tr}_B \{H_B[\rho_B(t) - \rho_B(0)]\} \\
&= D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] + S[\rho_S(t)] + \mathrm{Tr}\{\rho_S(t) \ln \pi_S^*(\lambda_t)\} - S[\rho_S(t)] + S[\rho_S(0)] \\
&\qquad - \beta \mathrm{Tr}_B \{H_B[\rho_B(t) - \rho_B(0)]\} \\
&= D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] + \mathrm{Tr}\{\rho_S(t) \ln \pi_S^*(\lambda_t)\} + \mathrm{Tr}\{\rho_B(t) \ln \pi_B\} - \mathrm{Tr}\{\rho_B(0) \ln \pi_B\} + S[\rho_S(0)] \\
&= D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] + \mathrm{Tr}\{\rho_{SB}(t) \ln[\pi_S^*(\lambda_t) \otimes \pi_B]\} - \mathrm{Tr}\{\rho_B(0) \ln \pi_B\} + S[\rho_S(0)] \\
&= D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] - D[\rho_{SB}(t)|\pi_S^*(\lambda_t) \otimes \pi_B] - S[\rho_{SB}(t)] - \mathrm{Tr}\{\rho_B(0) \ln \pi_B\} + S[\rho_S(0)] \\
&= D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] - D[\rho_{SB}(t)|\pi_S^*(\lambda_t) \otimes \pi_B] - S[\rho_{SB}(0)] - \mathrm{Tr}\{\rho_B(0) \ln \pi_B\} + S[\rho_S(0)] \\
&= D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] - D[\rho_{SB}(t)|\pi_S^*(\lambda_t) \otimes \pi_B] + I[\rho_{SB}(0)] - \mathrm{Tr}\{\rho_B(0) \ln \pi_B\} - S[\rho_B(0)] \\
&= D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] - D[\rho_{SB}(t)|\pi_S^*(\lambda_t) \otimes \pi_B] + I[\rho_{SB}(0)] - D[\rho_B(0)|\pi_B] \\
&= D[\rho_{SB}(t)|\pi_{SB}(\lambda_t)] - D[\rho_{SB}(t)|\pi_S^*(\lambda_t) \otimes \pi_B] + I[\pi_{SB}(\lambda_0)] - D[\pi_B^*(\lambda_0)|\pi_B]
\end{aligned}$$

Now, if the initial state is separable, $I[\rho_S \otimes \pi_B] = 0$, and, if at the beginning there is no interaction $\pi_B^*(\lambda_0) = \pi_B \to D[\pi_B|\pi_B] = 0$ and we are left with the first case. If the zeroth law holds, the first two relative entropies cancel out because $\pi_S^* \approx \pi_S$ since the interaction is affects negligibly the state. On top of that, the mutual information $I[\pi_{SB}]$ vanishes because the state is separable, and the last relative entropy vanishes as well because $\pi_B^* \approx \pi_B$. Thus, when the zeroth law holds, we have $\Sigma^*(t) = \Sigma(t)$.

Exercise 3.22: Special coarse-graining for the observational entropy

Given a *coarse-graining* X, namely a complete set of projectors $\{\Pi(x)\}$, the observational entropy is defined as

$$S_{\mathrm{obs}}^X(\rho) \equiv \sum_x p_x [-\ln p_x + \ln V(x)]$$

where $p_x \equiv \mathrm{Tr}\{\Pi(x)\rho\}$ is the probability of observing x and $V(x) \equiv \mathrm{Tr}\{\Pi(x)\}$.

Find the coarse-graining such that $S_{\mathrm{obs}}^X(\rho) = S_{\mathrm{Sh}}(\rho)$, namely the observational entropy becomes the Shannon entropy.

Find the coarse-graining such that $S_{\mathrm{obs}}^X(\rho) = S_B(\rho)$, namely the observational entropy becomes the Boltzmann entropy.

Solution:
If all projectors have rank 1, namely $\mathrm{Tr}\{\Pi(x)\} = 1$, we can associate an orthonormal basis to the

coarse-graining, and the observational entropy becomes

$$S_{\text{obs}}^{X}(\rho) = -\sum_x \langle x|\rho|x\rangle \ln \langle x|\rho|x\rangle = -\text{Tr}\left\{\rho \ln \rho\right\}.$$

This means that the observations performed on the system are perfect: in fact, we are able to completely distinguish any two microstates.
If the coarse graining is made of only one proectors, namely $\Pi(x) = \mathbb{I}$, the probability becomes $p_x = 1$, and we are left with

$$S_{\text{obs}}^{X}(\rho) = \ln d,$$

with d the dimension of the Hilbert space. This corresponds to the Boltzmann entropy since the number of microstates is d. This corresponds to the case in which our observations are useless: we only know that the system is in some state, and, given our ignorance, all possible states are equally likely.

Exercise 3.23: Observational entropy and Shannon entropy

Let $\rho(x) \equiv \Pi(x)\rho\Pi(x)/p(x)$ be the post-measurement state given outcome x, $\omega(x) \equiv \Pi(x)/V(x)$ be the generalized microcanonical ensemble, and $\mathcal{D}_X\rho \equiv \sum_x \Pi(x)\rho\Pi(x)$ be tha average post-measurement state.

Show that

$$S_{\text{obs}}^{X}(\rho) - S_{\text{Sh}}(\rho) = D[\rho|\mathcal{D}_X\rho] + \sum_x p(x) D[\rho(x)|\omega(x)].$$

Solution:

$$\begin{aligned}
S_{\text{obs}}^{X}(\rho) - S_{\text{Sh}}(\rho) &= \sum_x p_x[-\ln p_x + \ln V(x)] + \text{Tr}\left\{\rho\ln\rho\right\} \\
&= \sum_x \text{Tr}\left\{\Pi(x)\rho\Pi(x)\right\}[-\ln p_x + \ln V(x)] + \text{Tr}\left\{\rho\ln\rho\right\} \\
&= -\sum_x \left[\text{Tr}\left\{\Pi(x)\rho\Pi(x)\ln\left(\frac{\Pi(x)}{V(x)}\right)\right\} + p_x\ln p_x\right] + \text{Tr}\left\{\rho\ln\rho\right\} \\
&= -\sum_x \left[\text{Tr}\left\{p_x\rho(x)\ln\left(\omega(x)\right)\right\} + p_x\ln p_x\right] + \text{Tr}\left\{\rho\ln\rho\right\} \\
&= \sum_x \left[p_x D[\rho(x)|\omega(x)] - p_x\ln p_x - p_x\text{Tr}\left\{\rho(x)\ln\rho(x)\right\}\right] + \text{Tr}\left\{\rho\ln\rho\right\} \\
&= \sum_x \left[p_x D[\rho(x)|\omega(x)] - p_x\text{Tr}\left\{\rho(x)\ln[p_x\rho(x)]\right\}\right] + \text{Tr}\left\{\rho\ln\rho\right\}
\end{aligned}$$

Using the fact that $\Pi(x)$ are projectors, we have

$$\text{Tr}\left\{\rho\ln\mathcal{D}_X\rho\right\} = \sum_x \text{Tr}\left\{\rho\ln[\Pi(x)\rho\Pi(x)]\right\} = \sum_x \text{Tr}\left\{\Pi(x)\rho\Pi(x)\ln[\Pi(x)\rho\Pi(x)]\right\} = \sum_x \text{Tr}\left\{p_x\rho(x)\ln[p_x\rho(x)]\right\}$$

Therefore, we find

$$S_{\text{obs}}^{X}(\rho) - S_{\text{Sh}}(\rho) = \sum_x p_x D[\rho(x)|\omega(x)] + D[\rho|\mathcal{D}_X\rho].$$

Exercise 3.24: Non-equilibrium temperature and associated entropy

Defining the nonequilibrium temperature T_t^* through

$$\text{Tr}\left\{H(\lambda_t)\rho(t)\right\} \equiv \text{Tr}\left\{H(\lambda_t)\pi(\beta_t^*)\right\},$$

show that the associated equilibrium entropy satisfies

$$T_t^* d\mathcal{S}(\beta_t^*, \lambda_t) = dU(t) - \text{Tr}\left\{[dH(\lambda_t)]\pi(\beta_t^*, \lambda_t)\right\},$$

where $dU(t) = \text{Tr}\left\{H(\lambda_{t+dt})\rho(t+dt) - H(\lambda_t)\rho(t)\right\}$.

Solution:
Let's start from the energy variation and use the definition of nonequilibrium temperature

$$\begin{aligned} dU(t) &= \mathrm{Tr}\left\{H(\lambda_{t+dt})\rho(t+dt) - H(\lambda_t)\rho(t)\right\} = \mathrm{Tr}\left\{H(\lambda_{t+dt})\pi(\beta^*_{t+dt},\lambda_{t+dt}) - H(\lambda_t)\pi(\beta^*_t,\lambda_t)\right\} \\ &= \mathrm{Tr}\left\{[dH(\lambda_t)]\pi(\beta^*_t,\lambda_t) + H(\lambda_{t+dt})d[\pi(\beta^*_t,\lambda_t)]\right\} = \mathrm{Tr}\left\{[dH(\lambda_t)]\pi(\beta^*_t,\lambda_t)\right\} + T^*_t d\mathcal{S}(\beta^*_t,\lambda_t). \end{aligned}$$

Shuffling things around we get the identity we were looking for.

Exercise 3.25: Recoverable work or how to extract work in a macroscopic way

Consider a process where the system at time τ is put into contact with an infinitely large bath at temperature T^*_τ, and afterwards the temperature T^*_t and the driving protocol λ_t are *slowly* (i.e. reversibly) changed back to their initial values T^*_0 and λ_0. Importantly, we know *only* the average energy of the system (equivalently, its nonequilibrium temperature), and cannot implement arbitrary unitary operations. Show that the extracted work during this process is $-\int_0^\tau đW^{\mathrm{rec}}(t)$, where the recoverable work is defined as

$$đW^{\mathrm{rec}}(t) \equiv \mathrm{Tr}\left\{[dH(\lambda_t)]\pi(\beta^*_t,\lambda_t)\right\}.$$

Solution:
Since the process is reversible, the entropy change in the system and the heat exchanged with the bath are related though the second law as

$$đQ(t) = T^*_t \mathcal{S}(\beta^*_t,\lambda_t).$$

Crucially, here the entropy is simply the equilibrium entropy of the effective thermal state because we *only* know the average energy, and thus the least assuming state is exactly the thermal one. Using the first law and the result of Exercise 3.24 we find

$$dW(t) = dU(t) - đQ = dU(t) - T^*_t d\mathcal{S}(\beta^*_t,\lambda_t) = \mathrm{Tr}\left\{[dH(\lambda_t)]\pi(\beta^*_t,\lambda_t)\right\} = đW^{\mathrm{rec}}(t)$$

and, integrating over time

$$W = \int_\tau^0 đW^{\mathrm{rec}}(t) = -\int_0^\tau đW^{\mathrm{rec}}(t)$$

Exercise 3.26: Observational entropy of classical system coupled to a bath

Consider the coarse-graining $X = S \otimes E_B$, with $S = \{|s\rangle\langle s|\}$ a set of rank 1 projectors on the system and $E_B = \{\Pi(E_B)\}$, $\Pi(E_B) = \sum_{\epsilon\in[E,E+\delta)} |\epsilon\rangle\langle\epsilon|$ the energy projectors on the bath. The observatgional entropy then reads

$$S^{S\otimes E_B}_{\mathrm{obs}}(\rho_{SB}) = \sum_{s,E_B} p_{s,E_B}[-\ln p_{s,E_B} + \ln V(E_B)].$$

Consider a classical nondegenerate system and label $s = E_x$, where x denotes a microstate of the system. Assuming that the global energy E is fixed such that $E_B = E - E_x$ if the system is found in state x, identify the observational entropy with the entropy production.

Solution:
Substituting the given choice of coarse-graining with the condition of fixed global energy we are left with

$$S^{S\otimes E_B}_{\mathrm{obs}}(\rho_{SB}) = \sum_s p_s[-\ln p_s + \ln V(E-E_s)] = S_{\mathrm{Sh}}[p_s] + \sum_s p_s S_B[E-E_s]$$

which contains a contribution accounting for the system's entropy, $S_{\mathrm{Sh}}[p_s]$, and a contibution accounting for the bath's entropy, $\sum_s p_s S_B[E-E_s]$.

Exercise 3.27: Hierarchy of second laws

Using the relation between the remaining heat bath and the equilibrium entropy difference

$$\mathcal{S}_B(\beta^*_\tau) - \mathcal{S}_B(\beta^*_0) = \int \frac{đQ^{\mathrm{rem}}_B(t)}{T^*_t},$$

prove that

$$\Delta S_S(\tau) - \frac{Q(\tau)}{T_0} - \left[\Delta S_S(\tau) - \int \frac{đQ(t)}{T_t^*}\right] = k_B D[\pi_B(\beta_t^*)|\pi_B(\beta_0)] \geq 0.$$

Solution:

$$-\frac{Q(\tau)}{T_0} + \int \frac{đQ(t)}{T_t^*} = -\frac{Q(\tau)}{T_0} + \mathcal{S}_B(\beta_0^*) - \mathcal{S}_B(\beta_\tau^*) = \mathcal{S}_B(\beta_0^*) - \mathcal{S}_B(\beta_\tau^*) + \beta_0 \int_0^\tau \mathrm{Tr}_B \left\{H_B[\rho_B(t+dt) - \rho(t)]\right\}$$
$$= \mathcal{S}_B(\beta_0^*) - \mathcal{S}_B(\beta_\tau^*) + \beta_0 \mathrm{Tr}_B \left\{H_B[\rho_B(\tau) - \rho_B(0)]\right\}$$
$$= \mathcal{S}_B(\beta_0^*) - \mathcal{S}_B(\beta_\tau^*) + \beta_0 \mathrm{Tr}_B \left\{H_B[\pi_B(\beta_\tau^*) - \pi_B(\beta_0^*)]\right\}$$
$$= \mathcal{S}_B(\beta_0^*) - \mathcal{S}_B(\beta_\tau^*) + \beta_0 \mathcal{U}_B(\beta_\tau^*) - \beta_0 \mathcal{U}_B(\beta_0^*)$$

Assuming that the initial bath state is a Gibbs state at inverse temperature β_0 we find

$$-\frac{Q(\tau)}{T_0} + \int \frac{đQ(t)}{T_t^*} = \mathcal{S}_B(\beta_0) - \mathcal{S}_B(\beta_\tau^*) + \beta_0 \mathcal{U}_B(\beta_\tau^*) - \beta_0 \mathcal{U}_B(\beta_0) = \beta_0 F[\pi(\beta_\tau^*)] - \beta_0 \mathcal{F}[\beta_0] \geq 0$$

Alternatively, we can write it in terms of a relative entropy as

$$-\mathcal{S}_B(\beta_\tau^*) + \mathrm{Tr}\left\{\pi_B(\beta_0)[\beta_0 H_B + \ln \mathcal{Z}_B]\right\} + \beta_0 \mathcal{U}_B(\beta_\tau^*) - \beta_0 \mathcal{U}_B(\beta_0) = -\mathcal{S}_B(\beta_\tau^*) + \ln \mathcal{Z}_B + \beta_0 \mathcal{U}_B(\beta_\tau^*)$$
$$-\mathcal{S}_B(\beta_\tau^*) + \mathrm{Tr}\left\{\pi_B(\beta_\tau^*)[\beta_0 H_B + \ln \mathcal{Z}_B]\right\} = -\mathcal{S}_B(\beta_\tau^*) - \mathrm{Tr}\left\{\pi_B(\beta_\tau^*) \ln \pi_B(\beta_0)\right\}$$
$$= D[\pi_B(\beta_\tau^*|\pi_B(\beta_0))] \geq 0$$

Exercise 3.28: Cavity master equation

We model the photon echanges between the system with Hamiltonian $H_S = \hbar\omega_c a^\dagger a$ and its environment with the Hamiltonian

$$H_{SB} = H_S + \hbar \sum_k g_k (a + a^\dagger)(b_k + b_k^\dagger) + \hbar \sum_k \omega_k b_k^\dagger b_k.$$

The operators $b_k^\dagger, b_k$ are the bosonic field operators of the bath.

Derive the cavity master equation by using the Born-Markov-secular approximation (neglecting any Lamb shift terms). Show that the cavity lifetime is

$$\frac{1}{\tau_c} = 4\pi \sum_k g_k^2 \delta(\omega_c - \omega_k) = 4\pi \int_0^\infty d\omega \rho(\omega) g(\omega)^2 \delta(\omega_c - \omega)$$

with $\rho(\omega)$ the density of field modes. Do the rates obey local detailed balance?

Solution:

First we calculate the Hamiltonian in the interaction picture through the unitary $U_I = e^{i(H_S+H_B)t/\hbar}$. Noticing that

$$a(a^\dagger a)^n = (aa^\dagger)^n a = (1 + a^\dagger a)^n a \to a e^{x a^\dagger a} = e^{x(a^\dagger a + 1)} a$$

we find

$$\tilde{V}_{SB} = \hbar \sum_k g_k (e^{-i\omega_c t} a + e^{i\omega_c t} a^\dagger)(e^{-i\omega_k t} b_k + e^{i\omega_k t} b_k^\dagger) = A \otimes B$$

which is decomposed as $A = e^{-i\omega_c t} a + e^{i\omega_c t} a^\dagger$, $B = \hbar \sum_k g_k (e^{-i\omega_k t} b_k + e^{i\omega_k t} b_k^\dagger)$. We can now calculate the bath correlation function

$$C(t) = \mathrm{Tr}_B\left\{B(t)B(0)\pi_B\right\} = \sum_k \hbar^2 g_k^2 \mathrm{Tr}\left\{(e^{-i\omega_k t} b_k b_k^\dagger + e^{i\omega_k t} b_k^\dagger b_k) \frac{e^{-\beta\hbar\omega_k b_k^\dagger b_k}}{\mathcal{Z}_k}\right\}$$

with $\mathcal{Z}_k = \frac{1}{1 - e^{-\beta\hbar\omega_k}}$, $\mathcal{Z}_k(x) = [1 - e^{-x}]^{-1}$

$$C(t) = \sum_k \hbar^2 g_k^2 \left[e^{i\omega_k t} \frac{1}{\mathcal{Z}_k}(-\partial_x)\mathcal{Z}_k + e^{-i\omega_k t}(1 - \frac{\partial_x \mathcal{Z}_k}{\mathcal{Z}_k})\right] = \sum_k \hbar^2 g_k^2 \left[e^{i\omega_k t} N_k + e^{-i\omega_k t}(N_k + 1)\right]$$

with $N_k = [e^{\beta\hbar\omega_k} - 1]^{-1}$ is the Bose-Einstein distribution at ω_k. The rates are given by the Fourier transform of the bath correlation function

$$\Gamma(\omega) = 2\pi \sum_k \hbar^2 g_k^2 [N_k \delta(\omega + \omega_k) + [N_k + 1]\delta(\omega - \omega_k)]$$

We can now use the secular approximation to write the master equation as

$$\partial_t \tilde{\rho}_S(t) = \frac{1}{\hbar^2} \left\{\Gamma(\omega_c) \left(2a\tilde{\rho}_S a^\dagger - \{a^\dagger a, \tilde{\rho}_S(t)\}\right) + \Gamma(-\omega_c) \left(2a^\dagger \tilde{\rho}_S a - \{aa^\dagger, \tilde{\rho}_S(t)\}\right)\right\}.$$

Notice that since both $\omega_c, \omega_k \geq 0$, only the delta distribution with the difference of the frequencies contributes. Therefore, calling the cavity lifetime

$$\frac{1}{\tau_c} = 4\pi \sum_k g_k^2 \delta(\omega_c - \omega_k),$$

we have

$$\partial_t \tilde{\rho}_S(t) = \frac{1}{\tau_c} \left\{[N_c + 1] \left(a\tilde{\rho}_S a^\dagger - \frac{1}{2}\{a^\dagger a, \tilde{\rho}_S(t)\}\right) + N_c \left(a^\dagger \tilde{\rho}_S a - \frac{1}{2}\{aa^\dagger, \tilde{\rho}_S(t)\}\right)\right\}.$$

Going back to the Schrödinger picture we finally have

$$\partial_t \rho_S = -i[\omega_c a^\dagger a, \rho_S] + \frac{1}{\tau_c} \left\{[N_c + 1] \left(a\rho_S a^\dagger - \frac{1}{2}\{a^\dagger a, \rho_S(t)\}\right) + N_c \left(a^\dagger \rho_S a - \frac{1}{2}\{aa^\dagger, \rho_S(t)\}\right)\right\}.$$

We can also verify that the rates satisfy the local detailed balance condition: when the system interacts with one bath k, it can either absorb or emit the energy $\hbar\omega_k$. The ratio between absorption end emission is

$$\frac{N_k}{N_k + 1} = e^{-\beta\hbar\omega_k} = e^{-\beta\Delta E},$$

as expected.

Exercise 3.29: Positivity of strong coupling non-equilibrium entropy

Shot that the non-equilibrium strong coupling entropy production of the system and ancilla, namely

$$\Sigma_{SA}^*(t) = \Delta S_{SA}^*(t) - \frac{Q^*(t)}{T} = \frac{W(t) - \Delta F_{SA}^*(t)}{T} \geq 0$$

is equivalent to

$$\Sigma_{SA}^*(t) = D[\rho_{SAB}(t)|\pi(SAB)(\lambda_t)] - D[\rho_{SA}(t)|\pi_{SA}^*(\lambda_t)]$$

Solution:
This is identical to Exercise 3.20: we first call $SA = X$.
Using the definitions and the fact that the entropy of the global state does not change due to the unitary evolution we have

$$\begin{aligned}
\Sigma_X^* &= \mathrm{Tr}\left\{\rho_{XB}[\ln \rho_{XB} - \ln \pi_{XB}]\right\} - \mathrm{Tr}\left\{\rho_X[\ln \rho_X - \ln \pi_X^*]\right\} \\
&= -S[\rho_{XB}(t)] + S[\rho_X(t)] + \beta \mathrm{Tr}\left\{\rho_{XB}(t) H_{XB}(\lambda_t)\right\} + \ln \mathcal{Z}_{XB}(\lambda_t) - \beta \mathrm{Tr}\left\{\rho_X(t) H_X^*(\lambda_t)\right\} - \ln \mathcal{Z}_X^*(\lambda_t) \\
&= -S[\rho_{XB}(0)] + S[\rho_X(t)] + \beta \mathrm{Tr}\left\{\rho_{XB}(t) H_{XB}(\lambda_t)\right\} - \beta \mathrm{Tr}\left\{\rho_X(t) H_X^*(\lambda_t)\right\} + \ln \mathcal{Z}_B \\
&= -\beta \mathrm{Tr}\left\{\pi_{XB}(\lambda_0) H_{XB}(\lambda_0)\right\} - \ln \frac{\mathcal{Z}_{XB}(\lambda_0)}{\mathcal{Z}_B} + S[\rho_X(t)] + \beta \mathrm{Tr}\left\{\rho_{XB}(t) H_{XB}(\lambda_t)\right\} - \beta \mathrm{Tr}\left\{\rho_X(t) H_X^*(\lambda_t)\right\} \\
&= \beta W(t) - \ln \mathcal{Z}_X^*(\lambda_0) + S[\rho_X(t)] - \beta \mathrm{Tr}\left\{\rho_X(t) H_X^*(\lambda_t)\right\} \\
&= \beta W(t) + \beta \mathcal{F}_X^*(\lambda_0) - \beta \mathrm{Tr}\left\{\rho_X(t)[H_X^*(\lambda_t) + T \ln \rho_X(t)]\right\} = \beta W(t) + \beta \mathcal{F}_X^*(\lambda_0) - \beta[U_X^*(t) - T S_X^*(t)] \\
&= \beta W(t) - \beta[F_X^*(t) - \mathcal{F}_X^*(\lambda_0)] = \beta \Delta U_X^* - \beta Q^*(t) - \beta \Delta U_X^* + \Delta S_X^* = \Delta S_X^*(t) - \beta Q^*(t).
\end{aligned}$$

In particular, using that $D[\mathrm{Tr}_A\{\rho_{AB}\}|\mathrm{Tr}_A\{\sigma_{AB}\}] \leq D[\rho_{AB}|\sigma_{AB}]$ one finds that $\Sigma_X^*(t) \geq 0$.

Exercise 3.30: Thermodynamics of a micromaser

To model the cavity dynamics under the influence of atoms we make use of the fact that the arom-cavity interaction time τ' is much smaller than the cavity lifetime τ_c, namely $\tau' \ll \tau_c$. Thus, we treat the atom-cavity dynamics as a CPTP map $\rho_S^+ = \mathrm{Tr}_A\left\{U_{\mathrm{JC}} \rho_S^- \otimes |e\rangle\langle e|_A U_{\mathrm{JC}}^\dagger\right\}$, where $\rho_S^\pm$ are the cavity state before or after

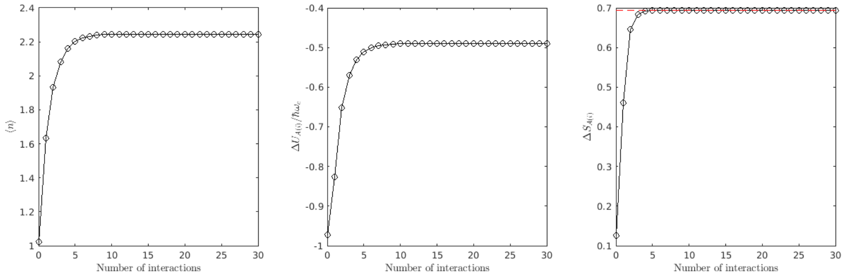


Figure 4: Average cavity photon number, atom i energy difference and atom i entropy difference as a function of the number i of atoms that have interacted with the cavity.

the interaction, $|e\rangle$ is the initially excited state of the atom, and U_{JC} is the unitary time evolution from the Jaynes-Cummings Hamiltonian, studied in Exercise 3.1.

(i) Assume the atom and cavity to be at exact resonance, and use the interaction picture time evolution operator to derive

$$\rho^+ = \sum_{mn} e^{-iH_S\tau'/\hbar} \left\{ \sin(gt\sqrt{m+1}) \sin(gt\sqrt{n+1}) \, |m+1\rangle\langle n+1| + \right. \\ \left. + \cos(gt\sqrt{m+1}) \cos(gt\sqrt{n+1}) \, |m\rangle\langle n| \right\} e^{iH_S\tau'/\hbar} \rho^-_{mn},$$

with $\rho^-_S = \sum_{mn} \rho^-_{mn} |m\rangle\langle n|$.

(ii) Consider the initial cavity state $\rho_{mn}(0) = \delta_{mn} P_n(0)$, i.e. without coherences in the Fock basis, and show that this CPTP map does not generate any coherence.

(iii) From here, show that the the cavity master equation derived in Exercise 3.28 reduces to a rate master equation $\partial_t P_m(t) = \sum_n R_{mn} P_n(t)$ with rate matrix

$$R_{mn} = \frac{1+N_c}{\tau_c}[(m+1)\delta_{m+1,n} - m\delta_{m,n}] + \frac{N_c}{\tau_c}[m\delta_{m-1,n} - (m+1)\delta_{m,n}],$$

and the CPTP map can be written as $P^+_m = \sum_n T_{mn} P^-_n$ with transition matrix

$$T_{mn} = \delta_{mn} \cos^2(g\tau'\sqrt{n+1}) + \delta_{m,n+1} \sin^2(g\tau'\sqrt{n+1}),$$

which makes the probability vector $\mathbf{P}$ evolve according to

$$\mathbf{P}(k\tau) = \underbrace{e^{R\tau} T \cdots e^{R\tau} T}_{k \text{ times}} \mathbf{P}(0).$$

(iv) Use that the cavity state contains no coherences in the Fock basis to show that the atom state after the interaction is

$$\rho^+_A = \mathrm{Tr}_S \left\{ U_{\mathrm{JC}} \rho^-_S \otimes |e\rangle\langle e|_A \, U^\dagger_{\mathrm{JC}} \right\} \\ = \sum_n \left[\cos^2(g\tau'\sqrt{n+1}) \, |e\rangle\langle e| + \sin^2(g\tau'\sqrt{n+1}) \, |h\rangle\langle h| \right] P^-_n .$$

(v) Study the dynamics numerically using $\omega_c/2\pi = 51.1$ GHz, $T = 0.8$ K, which results in the mean occupation number of the cavity $N_c \approx 0.05$. Take the cavity lifetime to be $\tau_c = 65$ ms, the atom-cavity interaction time to be $\tau' = 9.55$ µs, which satisfies $\tau' \ll \tau_c$, the atom-cavity coupling strength to be $g/\pi = 47.9$ kHz, and the waiting time between two atoms to be $\tau = 16.4$ ms. As the initial state, take the thermal state $P_n(0) = \pi_n$.

Solution:

(i) Translating the state into the interaction picture we have $\tilde{\rho}^+_S = \mathrm{Tr}_A \left\{ \tilde{U}_{\mathrm{JC}} \rho^-_S \otimes |e\rangle\langle e|_A \, \tilde{U}^\dagger_{\mathrm{JC}} \right\}$. In

Exercise 3.1 we calculated $\tilde{U}_{\mathrm{JC}}$, which reads

$$\tilde{U}_{\mathrm{JC}} = \cos(tg\sqrt{N+1})\,|e\rangle\!\langle e| + \cos(tg\sqrt{N})\,|g\rangle\!\langle g| - i\left[\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}}a\,|e\rangle\!\langle g| + a^\dagger\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}}\,|g\rangle\!\langle e|\right],$$

where $N = a^\dagger a$ is the cavity number operator. Then, we can use it to calculate the partial trace:

$$\mathrm{Tr}_A\left\{\tilde{U}_{\mathrm{JC}}\rho_S^- \otimes |e\rangle\!\langle e|_A\,\tilde{U}_{\mathrm{JC}}^\dagger\right\} = \mathrm{Tr}_A\left\{\left[\cos(tg\sqrt{N+1})\rho_S^- \otimes |e\rangle\!\langle e| - ia^\dagger\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}}\rho_S^- \otimes |g\rangle\!\langle e|\right]\tilde{U}_{\mathrm{JC}}^\dagger\right\}$$

which leads to

$$\tilde{\rho}_S^+ = \cos(tg\sqrt{N+1})\rho_S^- \cos(tg\sqrt{N+1}) + a^\dagger\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}}\rho_S^-\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}}a.$$

Using the decomposition $\rho_S^- = \sum_{mn}\rho_{mn}^-\,|m\rangle\!\langle n|$, and remembering that $a^\dagger\,|m\rangle = \sqrt{m+1}\,|m+1\rangle$ and $\tilde{\rho}_S = e^{iH_St/\hbar}\rho_S e^{-iH_St/\hbar}$ we finally arrive at the relation we were looking for:

$$\rho_S^+ = e^{-iH_St/\hbar}\sum_{mn}\rho_{mn}^-[\cos(tg\sqrt{m+1})\cos(tg\sqrt{n+1})\,|m\rangle\!\langle n| + \\ + \sin(tg\sqrt{m+1})\sin(tg\sqrt{n+1})\,|m+1\rangle\!\langle n+1|]e^{iH_St/\hbar}$$

(ii) Considering the initial state $\rho_{mn}^- = \delta_{mn}P_n$, after the CPTP map we have

$$\begin{aligned}\rho_S^+ &= e^{-iH_St/\hbar}\sum_n\left[\cos^2(tg\sqrt{n+1})\,|n\rangle\!\langle n| + \sin^2(tg\sqrt{n+1})\,|n+1\rangle\!\langle n+1|\right]P_n e^{iH_St/\hbar}\\ &= \sum_n\left[\cos^2(tg\sqrt{n+1})\,|n\rangle\!\langle n| + \sin^2(tg\sqrt{n+1})\,|n+1\rangle\!\langle n+1|\right]P_n\end{aligned}$$

where it is easy to check that $\langle n|\rho_S^+|m\rangle = 0$ if $n \neq m$. Therefore the CPTP map does not generate any coherence.

(iii) The cavity master equation reads

$$\partial_t\rho_S = -i[\omega_c a^\dagger a, \rho_S] + \frac{1}{\tau_c}\left\{[N_c+1]\left(a\rho_S a^\dagger - \frac{1}{2}\{a^\dagger a, \rho_S(t)\}\right) + N_c\left(a^\dagger\rho_S a - \frac{1}{2}\{aa^\dagger, \rho_S(t)\}\right)\right\}.$$

Taking the matrix element mn of this differential equation we find

$$\partial_t\rho_{mn} = -i\omega_c(m-n)\rho_{mn} + \frac{1}{\tau_c}\left\{[N_c+1]\left(\sqrt{(m+1)(n+1)}\rho_{m+1,n+1} - \frac{1}{2}(m+n)\rho_{mn}\right)\right. \\ \left. + N_c\left(\sqrt{mn}\rho_{m-1,n-1} - \frac{1}{2}(m+n+2)\rho_{mn}\right)\right\}.$$

If $\rho_{mn} = \delta_{mn}P_n(t)$, for $m \neq n$ the evolution gives $\partial_t\rho_{mn} = 0$ which means that no coherences are generated. Then, we can write all the evolution in terms of a classical rate equation.

$$\partial_t P_n = \frac{1}{\tau_c}\left\{[N_c+1]\left((n+1)P_{n+1} - nP_n\right) + N_c\left(nP_{n-1} - (n+1)P_n\right)\right\} = \sum_m R_{nm}P_m$$

with rates

$$R_{nm} = \frac{N_c+1}{\tau_c}\left[(n+1)\delta_{n+1,m} - n\delta_{n,m}\right] + \frac{N_c}{\tau_c}\left[n\delta_{n-1,m} - (n+1)\delta_{n,m}\right].$$

Instead, the CPTP map is determined by the transitions

$$P_n^+ = \cos^2(tg\sqrt{n+1})P_n^- + \sin^2(tg\sqrt{n})P_{n-1} = \sum_m T_{nm}P_m$$

with

$$T_{nm} = \cos^2(tg\sqrt{n+1})\delta_{nm} + \sin^2(tg\sqrt{n})\delta_{n-1,m}.$$

(iv) We can use the same procedure done in point (i): we go in the interaction picture first and using $\tilde{U}_{\rm JC}$ we find

$$\mathrm{Tr}_S\left\{\tilde{U}_{\rm JC}\rho_S^-\otimes|e\rangle\langle e|_A\,\tilde{U}_{\rm JC}^\dagger\right\}=\mathrm{Tr}_S\left\{\left[\cos(tg\sqrt{N+1})\rho_S^-\otimes|e\rangle\langle e|-ia^\dagger\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}}\rho_S^-\otimes|g\rangle\langle e|\right]\tilde{U}_{\rm JC}^\dagger\right\}$$

Crucially ρ_S^- does not contain any coherence in the Fock basis, which means that only the diagonal terms contribute after the trace over S. This leads to

$$\tilde{\rho}_A^+=\mathrm{Tr}_S\left\{\cos(tg\sqrt{N+1})\rho_S^-\cos(tg\sqrt{N+1})\otimes|e\rangle\langle e|+a^\dagger\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}}\rho_S^-\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}}a\otimes|g\rangle\langle g|\right\}$$
$$=\sum_n\left[\cos^2(tg\sqrt{n+1})P_n^-\,|e\rangle\langle e|+\sin^2(tg\sqrt{n+1})P_n^-\,|g\rangle\langle g|\right]$$
$$\rho_A^+=\sum_n\left[\cos^2(tg\sqrt{n+1})\,|e\rangle\langle e|+\sin^2(tg\sqrt{n+1})\,|g\rangle\langle g|\right]P_n^-$$

(v)
```
clc; clear all; format compact;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%    Initial data
par.wc = 2*pi*51.1e9;   %Hz
par.Nc = 0.05;
par.tc = 65e-3; %s cavity relaxation time
par.ti = 9.55e-6;   %s interaction time
par.tw = 16.4e-3;   %s waiting time
par.g = pi*47.9e3;  %Hz
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
n = 20;  %Hilbert space cut
P = initial_state(n, par);

N = 30;
[NPH, DUA, DSA] = calc_plot(n, N, par);

subplot(131)
plot(0:N, NPH, 'k-o')
xlabel("Number of interactions", 'Interpreter','latex');ylabel("$\langle n \rangle$
    ", 'Interpreter','latex');
subplot(132)
plot(0:N, DUA, 'k-o')
xlabel("Number of interactions", 'Interpreter','latex');ylabel("$\Delta U_{A(i)}/\
    hbar\omega_c$", 'Interpreter','latex');
subplot(133)
plot(0:N, DSA, 'k-o'); hold on
plot(0:N, log(2)*ones([N+1, 1]), 'r--')
xlabel("Number of interactions", 'Interpreter','latex');ylabel("$\Delta S_{A(i)}$",
     'Interpreter','latex');

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function PP = initial_state(n, par)
    %Nc = 1/(exp(wc/T) - 1 ) ->  exp(wc/T) = 1/Nc +1
    z = par.Nc/(par.Nc +1);
    ind = 1:n;
    PI = z.^(ind - 1);
    PP = PI'/sum(PI);
end

function T = atom_cavity_interaction(n, par)
    ind = 1:n;
    mainD = cos(par.g*par.ti*sqrt(ind)).^2;
    mainD(n) = 1;
    secoD = sin(par.g*par.ti*sqrt(ind(1:n-1))).^2;
    T = diag(mainD) + diag(secoD, -1);
    %check = sum(T(ind, :))
end

function TT = cavity_evolution(n, par)
    ind = 1:n;
    R = -(1+par.Nc)/par.tc* diag(ind-1) - par.Nc/par.tc*diag(ind);
    R = R + (1+par.Nc)/par.tc*diag(ind(1:n-1), 1) + par.Nc/par.tc*diag(ind(1:n-1),
    -1);
    R(n,n) = -R(n-1,n);
```

```
    %check = sum(R(ind, :))
    TT = expm(R*par.tw);
end

function PP = Nevolution(N, n, P, par)
    T = atom_cavity_interaction(n, par);
    TT = cavity_evolution(n, par);
    M = (TT*T)^N;
    PP = M*P;
    %check = sum(PP)
end

function pe = atom_state(n, P, par)
    ind = 1:n;
    x = cos(par.g*par.ti*sqrt(ind)).^2;
    pe = sum(x.*P');
end

function [nph, Ua, Sa] = observables(n, P, par)
    pe = atom_state(n, P, par);
    ind = 1:n;
    T = atom_cavity_interaction(n, par);
    P = T*P;
    nph = sum((ind-1).*P');
    Ua = pe-1;
    Sa = -pe*log(pe) - (1-pe)*log(1-pe);
end

function [NPH, DUA, DSA] = calc_plot(n, Ni, par)
    IND = 0:(Ni+1);
    P = initial_state(n, par);
    for i=0:Ni
        [NPH(i+1), DUA(i+1), DSA(i+1)] = observables(n, Nevolution(IND(i+1), n, P,
    par), par);
    end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

Exercise 3.31: Second law with particle transport

When the system exchanges both energy and particles with the baths, the heat flowing in bath ν is defined as

$$\dot{Q}_\nu \equiv -\left[d_t U_\nu(t) - \nu d_t N_\nu(t)\right]$$

and the entropy production (for infinitely large baths) then reads

$$\Sigma(t) = \Delta S_S(t) - \sum_\nu \frac{Q_\nu(t)}{T_\nu}.$$

Show that it can also be written as

$$\Sigma(t) = D\left[\rho_{SB}(t)\middle|\rho_S(t)\bigotimes_\nu \Xi_\nu(\beta_\nu,\mu_\nu)\right]$$

Solution:

$$
\begin{aligned}
D\left[\rho_{SB}(t)\middle|\rho_S(t)\bigotimes_\nu \Xi_\nu(\beta_\nu,\mu_\nu)\right] &= -S[\rho_{SB}(t)] - \mathrm{Tr}\left\{\rho_S(t)\ln\rho_S(t)\right\} - \mathrm{Tr}\left\{\rho_B(t)\ln\bigotimes_\nu \Xi_\nu\right\} \\
&= -S[\rho_{SB}(0)] + S[\rho_S(t)] + \sum_\nu \mathrm{Tr}\left\{\rho_\nu(t)[\beta_\nu(H_\nu - \mu_\nu\hat{N}_\nu) + \ln\mathcal{Z}_\nu]\right\} \\
&= \Delta S_S(t) - S[\bigotimes_\nu \Xi_\nu] + \sum_\nu [\beta_\nu[U_\nu(t) - \mu_\nu N_\nu(t)] + \ln\mathcal{Z}_\nu] \\
&= \Delta S_S(t) + \sum_\nu [-\beta_\nu[U_\nu(0) - \mu_\nu N_\nu(0)] + \beta_\nu[U_\nu(t) - \mu_\nu N_\nu(t)]] \\
&= \Delta S_S(t) + \sum_\nu \beta_\nu\left[\Delta U_\nu(t) - \mu_\nu\Delta N_\nu(t)\right] = \Delta S_S(t) - \sum_\nu \beta\nu Q_\nu(t) = \Sigma(t)
\end{aligned}
$$

which imples $\Sigma(t) \geq 0$.

Exercise 3.32: Jordan-Wigner transformation

The Jordan-Wigner transformation maps a set of N fermions with annihilation operators f_i to a set of Pauli matrices $\tilde{f}_i$ acting on different spins with a tensor product structure.

Show that the operators

$$\tilde{f}_i = \underbrace{\sigma_z \otimes \cdots \otimes \sigma_z}_{i-1} \otimes \sigma_- \otimes \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{N-i}$$

satisfy the anti-commutation relations $\{\tilde{f}_i, \tilde{f}_j^\dagger\} = \delta_{ij}$, $\{\tilde{f}_i, \tilde{f}_j\} = 0$.

Use the identity $\sum_{k=0}^N \binom{N}{k} = 2^N$ to show that the Hilbert space dimension of N spins equals the Fock space dimension of N fermions.

Finally, confirm that the system-bath Hamiltonian

$$H_{SB} = H_S + \sum_k \epsilon_k c_k^\dagger c_k + \hbar\sum_{sk}\left(t_{sk} d_s^\dagger c_k + t_{sk}^* c_k^\dagger d_s\right)$$

has the desired tensor product structure after the Jordan-Wigner transformation as

$$H_{SB} = H_S \otimes \mathbb{I}_B + \mathbb{I}_S \otimes \sum_k \epsilon_k \tilde{c}_k^\dagger \tilde{c}_k - \hbar\sum_{sk}\left(t_{sk}\tilde{d}_s^\dagger \otimes \tilde{c}_k + t_{sk}^*\tilde{d}_s \otimes \tilde{c}_k^\dagger\right).$$

Solution:
Remembering that the Pauli matrices are

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

we have $\{\sigma_z, \sigma_\pm\} = 0$ and $\{\sigma_-, \sigma_+\} = \mathbb{I}$. Then, we can calculate, for $i < j$:

$$
\begin{aligned}
\{\tilde{f}_i, \tilde{f}_j\} = &\underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{i-1} \otimes \sigma_-\sigma_z \otimes \sigma_z \otimes \cdots \otimes \sigma_z \otimes \sigma_- \otimes \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{N-j} + \\
&+ \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{i-1} \otimes \sigma_z\sigma_- \otimes \sigma_z \otimes \cdots \otimes \sigma_z \otimes \sigma_- \otimes \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{N-j} = 0
\end{aligned}
$$

$$
\begin{aligned}
\{\tilde{f}_i, \tilde{f}_j{}^\dagger\} = &\underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{i-1} \otimes \sigma_-\sigma_z \otimes \sigma_z \otimes \cdots \otimes \sigma_z \otimes \sigma_+ \otimes \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{N-j} + \\
&+ \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{i-1} \otimes \sigma_z\sigma_- \otimes \sigma_z \otimes \cdots \otimes \sigma_z \otimes \sigma_+ \otimes \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{N-j} = 0
\end{aligned}
$$

And we are left with the case $i = j$.

$$\{\tilde{f}_i, \tilde{f}_i\} = \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{i-1} \otimes \{\sigma_-, \sigma_-\} \otimes \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{N-i} = 0$$

$$\{\tilde{f}_i, \tilde{f}_i{}^\dagger\} = \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{i-1} \otimes \{\sigma_-, \sigma_+\} \otimes \underbrace{\mathbb{I} \otimes \cdots \otimes \mathbb{I}}_{N-i} = \mathbb{I}^{\otimes N}$$

The Fock space of N ferrmions is determined by the direct sum $\mathcal{F} = \bigoplus_{n=0}^N \mathcal{H}_{n|N}$ where $\mathcal{H}_{n|N}$ is the Hilbert space with n fermions out of the N initial ones. The dimension on this Hilbert space, since the particles are industinguishable, is equal to the number of ways to select the n fermions, namely $N!/(n!(N-n)!)$. Then, the dimension of the Fock space is $d_{\mathcal{F}} = \sum_{n=0}^N \binom{N}{n} = 2^N$ which coincides with the dimension of the Hilbert space of N spins. Therefore, the Jordan-Wigner transformation is an isomorphism bewtween these Hilbert spaces.
We order the spins Hilbert spaces such that all the d_s come before the c_k. Then, the terms $d_s^\dagger d_s$ and $c_k^\dagger c_k$ become

$$d_s^\dagger d_s \to \mathbb{I}^{\otimes(s-1)} \otimes \sigma_z \otimes \mathbb{I}^{\otimes(s_{\max}-s)} \otimes \mathbb{I}^{\otimes k_{\max}}, \quad c_k^\dagger c_k \to \mathbb{I}^{\otimes s_{\max}} \otimes \mathbb{I}^{\otimes(k-1)} \otimes \sigma_z \otimes \mathbb{I}^{\otimes(k_{\max}-k)}$$

while the other terms become

$$d_s^\dagger c_k = \left[\sigma_z^{\otimes(s-1)} \otimes \sigma_+ \otimes \mathbb{I}^{\otimes S-s+K}\right]\left[\sigma_z^{\otimes S+k-1} \otimes \sigma_- \otimes \mathbb{I}^{\otimes K-k}\right] = \mathbb{I}^{\otimes s-1} \otimes \sigma_+\sigma_z \otimes \sigma_z^{\otimes x} \otimes \sigma_- \otimes \mathbb{I}^{\otimes K-k}$$

which leads to

$$d_s^\dagger c_k = -\mathbb{I}^{\otimes s-1} \otimes \sigma_+ \otimes \sigma_z^{\otimes x} \otimes \underbrace{\sigma_-}_{S+k} \otimes \mathbb{I}^{\otimes K-k} = -\tilde{d}_s^\dagger \otimes \tilde{c}_k$$

with $\tilde{d}_s$ acting only on the first S spins and $\tilde{c}_k$ acting only on the last K spins. This separation is similar to the system-bath separation, with the difference that now the operators $\tilde{d}_s$ and $\tilde{c}_k$ commute.

Exercise 3.33: Single-electron transistor: master equation

Given the system-bath Hamiltonian

$$H_{SB} = \epsilon_0 d^\dagger d + \sum_{\nu=L,R} \sum_k \left[\epsilon_{\nu k} c_{\nu k}^\dagger c_{\nu k} + \hbar\left(t_{\nu k} d^\dagger c_{\nu k} + t_{\nu k}^* c_{\nu k}^\dagger d\right)\right]$$

derive the following master equation for the empty (filled) E (F) probabilities

$$\frac{d}{dt}\begin{pmatrix} p_F(t) \\ p_E(t)\end{pmatrix} = \sum_\nu \Gamma_\nu(\epsilon_0)\begin{pmatrix} -[1-f_\nu(\epsilon_0)] & f_\nu(\epsilon_0) \\ 1-f_\nu(\epsilon_0) & -f_\nu(\epsilon_0)\end{pmatrix}\begin{pmatrix} p_F(t) \\ p_E(t)\end{pmatrix}$$

by employing the weak coupling and Markov approximation.

Solution:
First, we need to go in the interaction picture. For fermionic operators we have

$$(d^\dagger d)^n d^\dagger = d^\dagger (dd^\dagger)^n = d^\dagger(1-d^\dagger d)^n \to e^{ixd^\dagger d} d^\dagger = d^\dagger e^{ix} e^{-ixd^\dagger d}$$

Additionally,

$$(d^\dagger)^2 = 0 \to d^\dagger e^{-ixd^\dagger d} = d^\dagger \to e^{ixd^\dagger d} d^\dagger e^{-ixd^\dagger d} = d^\dagger e^{ix}.$$

We can use these relations to calculate the Hamiltonian in the intaction picture by transforming it with the unitary $U_I = e^{i(H_S+H_B)t/\hbar}$:

$$\tilde{V} = \hbar \sum_{\nu k}\left(t_{\nu k} d^\dagger c_{\nu k} e^{i(\omega_0-\omega_{\nu k})t} + t_{\nu k}^* c_{\nu k}^\dagger d e^{-i(\omega_0-\omega_{\nu k})t}\right).$$

We want to decompose this Hamiltonian as $A_S \otimes B_B$, so we Jordan-Wigner transform it, see Exercise 3.32, and obtain

$$\tilde{V} = -\hbar \sum_{\nu k}\left(t_{\nu k} \tilde{d}^\dagger \otimes \tilde{c}_{\nu k} e^{i(\omega_0-\omega_{\nu k})t} + t_{\nu k}^* \tilde{d} \otimes \tilde{c}_{\nu k}^\dagger e^{-i(\omega_0-\omega_{\nu k})t}\right),$$

in which we identify

$$A_S = \tilde{d}^\dagger e^{i\omega_0 t} + \tilde{d} e^{-i\omega_0 t}, \quad B_B = -\hbar \sum_{\nu k}\left(t_{\nu k} \tilde{c}_{\nu k} e^{-i\omega_{\nu k} t} + t_{\nu k}^* \tilde{c}_{\nu k}^\dagger e^{i\omega_{\nu k} t}\right).$$

We can now calculate the bath correlation function by remembering that only the terms $\tilde{c}_{\nu k}\tilde{c}^\dagger_{\nu k}$ and $\tilde{c}^\dagger_{\nu k}\tilde{c}_{\nu k}$ contribute after the partial trace.

$$C(t) = \hbar^2 \sum_{\nu k} |t_{\nu k}|^2 \mathrm{Tr}_B \left\{ \left(e^{-i\omega_{\nu k} t}\tilde{c}_{\nu k}\tilde{c}^\dagger_{\nu k} + e^{i\omega_{\nu k} t}\tilde{c}^\dagger_{\nu k}\tilde{c}_{\nu k} \right) \pi_B \right\}.$$

Using that

$$\mathrm{Tr}_B \left\{ \tilde{c}^\dagger \tilde{c} \frac{e^{-\beta(\epsilon-\mu)\tilde{c}^\dagger \tilde{c}}}{\mathcal{Z}} \right\} = -\frac{1}{\beta}\partial_\epsilon \ln \mathcal{Z} = -\frac{1}{\beta}\partial_\epsilon \ln(1+e^{-\beta(\epsilon-\mu)}) = \frac{1}{1+e^{\beta(\epsilon-\mu)}} = f(\epsilon)$$

gives the Fermi distribution, the bath correlaiton function becomes

$$C(t) = \hbar^2 \sum_{\nu k} |t_{\nu k}|^2 \left[e^{-i\omega_{\nu k} t}(1-f_{\nu k}) + e^{i\omega_{\nu k} t} f_{\nu k} \right].$$

Now we can calculate the Fourier transform

$$\Gamma(\omega) = \frac{1}{\hbar^2}\int C(t) e^{i\omega t} dt = 2\pi \sum_{\nu k} |t_{\nu k}|^2 \left[(1-f_{\nu k})\delta(\omega-\omega_{\nu k}) + f_{\nu k}\delta(\omega+\omega_{\nu k}) \right]$$

which determines the relaxation rates of the dynamics. Now we can look at the Born-Markov master equation *before* the secular approximation:

$$\partial_t \tilde{\rho}_S = \sum_{\omega\omega'} \Gamma(\omega') e^{i(\omega-\omega')t} \left[A(\omega')\tilde{\rho}_S A^\dagger(\omega) - A^\dagger(\omega)A(\omega')\tilde{\rho}_S \right] + \text{h.c.}$$

where we use the Fourier components of $A_S = \sum_\omega A(\omega)e^{-i\omega t}$. In particular, since $A(\omega_0) = \tilde{d}$ and $A(-\omega_0) = \tilde{d}^\dagger$, the product $A^\dagger(\omega_0)A(-\omega_0) = \tilde{d}^\dagger \tilde{d}^\dagger = 0$ vanishes because of the fermionic nature of the operators. Furthermore, decomposing $\tilde{\rho}_S$ into the fermionic operators we have $\tilde{\rho}_S = \alpha d^\dagger d + \beta d d^\dagger$, which means that $A(\omega_0)\tilde{\rho}_S A^\dagger(-\omega_0) = 0$. Therefore, having only one fermionic operator d selects the frequencies $\omega = \omega'$ without requiring the secular approximation.
Then, neglecting the Lamb shift, the master equation becomes

$$\partial_t \tilde{\rho}_S = \Gamma(\omega_0)\left[2\tilde{d}\tilde{\rho}_S \tilde{d}^\dagger - \{\tilde{d}^\dagger \tilde{d}, \tilde{\rho}_S\} \right] + \Gamma(-\omega_0)\left[2\tilde{d}^\dagger \tilde{\rho}_S \tilde{d} - \{\tilde{d}\tilde{d}^\dagger, \tilde{\rho}_S\} \right]$$

Calling the bath-induced relaxation time

$$\frac{1}{\tau_\nu} = \sum_k 4\pi |t_{\nu k}|^2 \delta(\omega_0 - \omega_{\nu k})$$

we can write the master equation as

$$\partial_t \tilde{\rho}_S = \sum_\nu \left(\frac{1-f_\nu(\epsilon_0)}{\tau_\nu} \left[\tilde{d}\tilde{\rho}_S \tilde{d}^\dagger - \frac{1}{2}\{\tilde{d}^\dagger \tilde{d}, \tilde{\rho}_S\} \right] + \frac{f_\nu(\epsilon_0)}{\tau_\nu} \left[\tilde{d}^\dagger \tilde{\rho}_S \tilde{d} - \frac{1}{2}\{\tilde{d}\tilde{d}^\dagger, \tilde{\rho}_S\} \right] \right)$$

Since there cannot be coherences between states of different fermionic number, the master equation reduces to a classical rate equation. Calling the empty (filled) state $|E\rangle$ ($|F\rangle$) we get

$$\partial_t p_E = \sum_\nu \left(\frac{1-f_\nu(\epsilon_0)}{\tau_\nu} p_F - \frac{f_\nu(\epsilon_0)}{\tau_\nu} p_E \right)$$

$$\partial_t p_F = \sum_\nu \left(-\frac{1-f_\nu(\epsilon_0)}{\tau_\nu} p_F + \frac{f_\nu(\epsilon_0)}{\tau_\nu} p_E \right)$$

which can be summarized as

$$\frac{d}{dt}\begin{pmatrix} p_F(t) \\ p_E(t) \end{pmatrix} = \sum_\nu \frac{1}{\tau_\nu} \begin{pmatrix} -[1-f_\nu(\epsilon_0)] & f_\nu(\epsilon_0) \\ 1-f_\nu(\epsilon_0) & -f_\nu(\epsilon_0) \end{pmatrix} \begin{pmatrix} p_F(t) \\ p_E(t) \end{pmatrix}.$$

Exercise 3.34: Local detailed balance with particles exchange

Consider a rate master equation $d_t p_x = \sum_y R_{xy} p_y$ describing both energy and particles exchanges. Assume R_{xy} was derived from a system in contact with an ideal single heat bath with temperature T and chemical potential μ. Prove that the following relations are identical

$$\frac{R_{xy}}{R_{yx}} = e^{-\beta[\epsilon_x - \epsilon_y - \mu(n_x - n_y)]}, \quad \frac{R_{xy}}{R_{yx}} = \exp\left[\frac{S_B(E-\epsilon_x, N-n_x) - S_B(E-\epsilon_y, N-n_y)}{k_B}\right].$$

Solution:
The differential form of the first law states that

$$dU = TdS + \mu dN \to TdS = dU - \mu dN.$$

Taking the partial derivatives we can determine the temperature and chemical potential, indeed

$$\frac{1}{T} = \partial_U S_B|_N, \quad -\frac{\mu}{T} = \partial_N S_B|_U.$$

Then, we have

$$\begin{aligned} S_B(E-\epsilon_x, N-n_x) - S_B(E-\epsilon_y, N-n_x) + S_B(E-\epsilon_y, N-n_x) - S_B(E-\epsilon_y, N-n_y) = \\ = \partial_U S_B|_N(\epsilon_y - \epsilon_x) + \partial_N S_B|_U(n_y - n_x) = -\beta[\epsilon_x - \epsilon_y - \mu(n_x - n_y)]. \end{aligned}$$

Exercise 3.35: Single-electron transistor: entropy production

Consider the single-electron transistor described by the rate master equation found in Exercise 3.33, and prove that then entropy production rate $\dot{\Sigma}$ is non-negative in the steady state.

More generally, assume that you have a quantum master equation of the form

$$\partial_t \rho_S(t) = -\frac{i}{\hbar}[H_S, \rho_S(t)] + \sum_\nu \mathcal{D}_\nu \rho_S(t),$$

with $\mathcal{D}_\nu \Xi_{\mathcal{S}}(\beta_\nu, \mu_\nu) = 0$. Show that the entropy production rate

$$\dot{\Sigma}(t) = \frac{d}{dt} S[\rho_S(t)] - \sum_\nu \frac{\dot{Q}_\nu(t)}{T_\nu} \geq 0.$$

Solution:
From Exercise 3.33 we know the rate master equation:

$$\frac{d}{dt}\begin{pmatrix} p_F(t) \\ p_E(t) \end{pmatrix} = \sum_\nu \frac{1}{\tau_\nu}\begin{pmatrix} -[1-f_\nu(\epsilon_0)] & f_\nu(\epsilon_0) \\ 1-f_\nu(\epsilon_0) & -f_\nu(\epsilon_0) \end{pmatrix}\begin{pmatrix} p_F(t) \\ p_E(t) \end{pmatrix},$$

from which we can find the steady state:

$$p_E = \frac{\sum_\nu \Gamma_\nu (1-f_\nu)}{\sum_\nu \Gamma_\nu}, \quad p_F = \frac{\sum_\nu \Gamma_\nu f_\nu}{\sum_\nu \Gamma_\nu}.$$

The particle current from bath L is then

$$I_M^L = \Gamma_L(f_L p_E - [1-f_L]p_F) = \Gamma_L \frac{\Gamma_R f_L[1-f_R] - \Gamma_R[1-f_L]f_R}{\sum_\nu \Gamma_\nu} = \Gamma_L \Gamma_R \frac{f_L - f_R}{\Gamma_L + \Gamma_R}.$$

Because of tight-coupling, the energy crrent from bath L is simply $I_U^L = \epsilon_0 I_M^L$. Then, we can calculate the entropy production in the steady state:

$$\dot{\Sigma} = -\sum_\nu \beta_\nu \dot{Q}_\nu = -[\beta_L(\epsilon_0 - \mu_L) I_M^L + \beta_R(\epsilon_0 - \mu_R) I_M^R] = [\beta_R(\epsilon_0 - \mu_R) - \beta_L(\epsilon_0 - \mu_L)]\, I_M^L.$$

The sign of the entropy production rate is determined by the product

$$(x-y)[f(y) - f(x)] \geq 0 \quad \forall x, y \quad \text{because } f(x) \text{ is decreasing.}$$

$$
\begin{aligned}
\dot{\Sigma} &= -\mathrm{Tr}\left\{\partial_t \rho \ln \rho\right\} - \sum_\nu \beta_\nu \mathrm{Tr}\left\{(H_S - \mu_\nu N_S)\mathcal{D}_\nu \rho\right\} \\
&= +\cancel{\frac{i}{\hbar}\mathrm{Tr}\left\{[H_S,\rho]\ln\rho\right\}} - \sum_\nu \mathrm{Tr}\left\{\mathcal{D}_\nu \ln \rho\right\} + \sum_\nu \left[\mathrm{Tr}\left\{\mathcal{D}_\nu \rho \ln \Xi_\nu\right\} + \ln \mathcal{Z}_\nu \cancel{\mathrm{Tr}\left\{\mathcal{D}_\nu \rho\right\}}\right] \\
&= \sum_\nu \mathrm{Tr}\left\{\mathcal{D}_\nu \rho \left[\ln \Xi_\nu - \ln \rho\right]\right\}.
\end{aligned}
$$

We now define the CPTP map $\mathcal{E}_\nu \rho \equiv e^{dt\mathcal{D}_\nu}\rho$ such that $\mathcal{E}_\nu \Xi_\nu = \Xi_\nu$ and $\mathcal{E}_\nu\rho - \rho \approx dt\mathcal{D}_\nu\rho$. Then, we have

$$
\begin{aligned}
\dot{\Sigma} &= \sum_\nu \mathrm{Tr}\left\{\mathcal{D}_\nu \rho \left[\ln \Xi_\nu - \ln \rho\right]\right\} = \lim_{dt\searrow 0}\frac{1}{dt}\sum_\nu \mathrm{Tr}\left\{[\mathcal{E}_\nu\rho - \rho][\ln \Xi_\nu - \ln\rho]\right\} \\
&= \lim_{dt\searrow 0}\frac{1}{dt}\sum_\nu \left(D[\rho|\Xi_\nu] + \mathrm{Tr}\left\{\mathcal{E}_\nu\rho[\ln \mathcal{E}_\nu\Xi_\nu - \ln \mathcal{E}_\nu\rho + \ln \mathcal{E}_\nu \rho - \ln \rho]\right\}\right) \\
&= \lim_{dt\searrow 0}\frac{1}{dt}\sum_\nu \left(D[\rho|\Xi_\nu] - D[\mathcal{E}_\nu\rho|\mathcal{E}_\nu\Xi_\nu] + \mathrm{Tr}\left\{(\rho + dt\mathcal{D}_\nu\rho)\frac{dt\mathcal{D}_\nu\rho}{\rho} + \mathcal{O}(dt^2)\right\}\right) \\
&= \lim_{dt\searrow 0}\frac{1}{dt}\sum_\nu \left(D[\rho|\Xi_\nu] - D[\mathcal{E}_\nu\rho|\mathcal{E}_\nu\Xi_\nu] + \cancel{\mathrm{Tr}\left\{dt\mathcal{D}_\nu\rho\right\}} + \mathcal{O}(dt^2)\right) = \lim_{dt\searrow 0}\frac{1}{dt}\sum_\nu \left(D[\rho|\Xi_\nu] - D[\mathcal{E}_\nu\rho|\mathcal{E}_\nu\Xi_\nu]\right).
\end{aligned}
$$

Now we can use the monotonicity of the relative entropy under CPTP maps: $D[\rho|\sigma] \geq D[\mathcal{E}\rho|\mathcal{E}\sigma]$ to prove $\dot{\Sigma}(t) \geq 0$.

Exercise 3.36: Coulomb-coupled quantum dots

Consider tha system Hamiltonian

$$
H_S = \epsilon_S d_S^\dagger d_S + \epsilon_D d_D^\dagger d_D^\dagger + U d_S^\dagger d_S d_D^\dagger d_D^\dagger
$$

describing two Coulomb-coupled quantum dots. These dots are coupled to baths as follows

$$
V_{SB}^S + H_B^S = \sum_{\nu=L,R}\sum_k \left[\epsilon_{\nu k} c_{\nu k}^\dagger c_{\nu k} + \hbar\left(t_{\nu k} d_S^\dagger c_{\nu k} + t_{\nu k}^* c_{\nu k}^\dagger d_S\right)\right],
$$

$$
V_{SB}^D + H_B^D = \sum_k \left[\epsilon_{Dk} c_{Dk}^\dagger c_{Dk} + \hbar\left(t_{Dk} d_D^\dagger c_{Dk} + t_{Dk}^* c_{Dk}^\dagger d_D\right)\right].
$$

Derive the rate master equation and check whether local detailed balance is satisfied.

Solution:
First we perform a Jordan-Wigner transformation as done in Exercise 3.32

$$
\begin{aligned}
H_S &= \epsilon_S \tilde{d}_S^\dagger \tilde{d}_S + \epsilon_D \tilde{d}_D^\dagger \tilde{d}_D^\dagger + U \tilde{d}_S^\dagger \tilde{d}_S \tilde{d}_D^\dagger \tilde{d}_D^\dagger, \\
V_{SB}^S + H_B^S &= \sum_{\nu=L,R}\sum_k \left[\epsilon_{\nu k} \tilde{c}_{\nu k}^\dagger \tilde{c}_{\nu k} - \hbar\left(t_{\nu k} \tilde{d}_S^\dagger \tilde{c}_{\nu k} + t_{\nu k}^* \tilde{c}_{\nu k}^\dagger \tilde{d}_S\right)\right], \\
V_{SB}^D + H_B^D &= \sum_k \left[\epsilon_{Dk} \tilde{c}_{Dk}^\dagger \tilde{c}_{Dk} - \hbar\left(t_{Dk} \tilde{d}_D^\dagger \tilde{c}_{Dk} + t_{Dk}^* \tilde{c}_{Dk}^\dagger \tilde{d}_D\right)\right],
\end{aligned}
$$

so that now the operators acting on different subsystems commute (instead of anticommuting). Then, we go to the interaction picture through the unitary $U_I = e^{i(H_S+H_B)t/\hbar}$, remembering that

$$
e^{ix\tilde{d}^\dagger\tilde{d}}\tilde{d}e^{-ix\tilde{d}^\dagger\tilde{d}} = \tilde{d}e^{-ix}
$$

we can write the interactions as

$$
\tilde{V}_{SB}^S = -\hbar\sum_{\nu=L,R}\sum_k \left(t_{\nu k}\tilde{d}_S^\dagger \tilde{c}_{\nu k} e^{i(\omega_S + \Omega \tilde{d}_D^\dagger \tilde{d}_D - \omega_{\nu k})t} + t_{\nu k}^* \tilde{c}_{\nu k}^\dagger \tilde{d}_S e^{-i(\omega_S + \Omega\tilde{d}_D^\dagger\tilde{d}_D - \omega_{\nu k})t}\right)
$$

$$
\tilde{V}_{SB}^D = -\hbar\sum_k \left(t_{Dk}\tilde{d}_D^\dagger \tilde{c}_{Dk} e^{i(\omega_D + \Omega\tilde{d}_S^\dagger\tilde{d}_S - \omega_{Dk})t} + t_{Dk}^* \tilde{c}_{Dk}^\dagger \tilde{d}_D e^{i(\omega_D + \Omega\tilde{d}_S^\dagger\tilde{d}_S - \omega_{Dk})t}\right)
$$

where $\hbar\Omega = U$. Luckily, the interaction Hamiltonians are already decomposed as $A_S^{S/D} \otimes B_B^{S/D}$, with

$$A_S^x = \tilde{d}_x^\dagger e^{i\omega_x t}\left(\tilde{d}_{\bar{x}}\tilde{d}_{\bar{x}}^\dagger + e^{i\Omega t}\tilde{d}_{\bar{x}}^\dagger\tilde{d}_{\bar{x}}\right) + \tilde{d}_x e^{-i\omega_x t}\left(\tilde{d}_{\bar{x}}\tilde{d}_{\bar{x}}^\dagger + e^{-i\Omega t}\tilde{d}_{\bar{x}}^\dagger\tilde{d}_{\bar{x}}\right)$$

with $x, \bar{x} \in \{S, D\}$ and $\bar{x} \neq x$.

$$B_B^x = -\hbar\sum_{\nu\in\mathcal{B}_x}\sum_k\left(t_{\nu k}\tilde{c}_{\nu k}e^{-i\omega_{\nu k}t} + t_{\nu k}^*\tilde{c}_{\nu k}^\dagger e^{i\omega_{\nu k}t}\right)$$

with $\mathcal{B}_S = \{L, R\}$ and $\mathcal{B}_D = \{D\}$. Then, we can calculate the bath correlation function

$$C_{xy}(t) = \mathrm{Tr}_B\left\{B_B^x(t)B_B^y(0)\pi_B\right\} = \delta_{xy}C_{xx}(t)$$

because $\mathrm{Tr}_B\left\{\tilde{c}_{xk}^\dagger\tilde{c}_{yk}\pi_B\right\} = 0$ for $x \neq y$. Then, we have for the S part

$$\begin{aligned}C_{SS}(t) &= \sum_{\nu=L,R}\sum_k\hbar^2|t_{\nu k}|^2\mathrm{Tr}\left\{\left(\tilde{c}_{\nu k}^\dagger\tilde{c}_{\nu k}e^{i\omega_{\nu k}t} + \tilde{c}_{\nu k}\tilde{c}_{\nu k}^\dagger e^{-i\omega_{\nu k}t}\right)\pi_B\right\}\\ &= \sum_{\nu=L,R}\sum_k\hbar^2|t_{\nu k}|^2\left(f_{\nu k}e^{i\omega_{\nu k}t} + [1-f_{\nu k}]e^{-i\omega_{\nu k}t}\right)\end{aligned}$$

with $f_{\nu k} = f_\nu(\hbar\omega_{\nu k})$ is the Fermi function of bath ν. Similarly, we have

$$C_{DD}(t) = \sum_k\hbar^2|t_{Dk}|^2\left(f_{Dk}e^{i\omega_{Dk}t} + [1-f_{Dk}]e^{-i\omega_{Dk}t}\right).$$

The Fourier transforms of the bath correlation functions are straightforward and read

$$\Gamma_{SS}(\omega) = 2\pi\sum_{\nu=L,R}\sum_k|t_{\nu k}|^2\left(f_{\nu k}\delta(\omega+\omega_{\nu k}) + [1-f_{\nu k}]\delta(\omega-\omega_{\nu k})\right)$$

$$\Gamma_{DD}(\omega) = 2\pi\sum_k|t_{Dk}|^2\left(f_{Dk}\delta(\omega+\omega_{Dk}) + [1-f_{Dk}]\delta(\omega-\omega_{Dk})\right).$$

We can now use the frequency decomposition of the A_S^x operators, $A_S^x(t) = \sum_\omega A_S^x(\omega)e^{-i\omega t}$, and in particular the fermionic nature of the $A_S^x(\omega)$ operators to reach the master equation

$$\partial_t\tilde{\rho} = \sum_{x,\omega}\Gamma_{xx}(\omega)\left[2A_S^x(\omega)\tilde{\rho}A_S^{x\dagger}(\omega) - \{A_S^{x\dagger}(\omega)A_S^x(\omega), \tilde{\rho}\}\right],$$

without the need for the secular approximation. Calling

$$\Gamma_x \equiv 4\pi\sum_k|t_{xk}|^2\delta(\omega_x-\omega_{xk}), \quad \Gamma_x^U \equiv 4\pi\sum_k|t_{xk}|^2\delta(\omega_x+\Omega-\omega_{xk}),$$

$$f_x \equiv f_x(\hbar\omega_x), \quad f_x^U \equiv f_x(\hbar\omega_x + \hbar\Omega)$$

we can write the master equation as

$$\begin{aligned}\partial_t\tilde{\rho} = \sum_{x=L,R,D}\Bigg(&\Gamma_x[1-f_x]\left[\tilde{d}_x[1-\tilde{n}_{\bar{x}}]\tilde{\rho}[1-\tilde{n}_{\bar{x}}]\tilde{d}_x^\dagger - \frac{1}{2}\{\tilde{d}_x^\dagger\tilde{d}_x[1-\tilde{n}_{\bar{x}}], \tilde{\rho}\}\right] +\\ &+\Gamma_x f_x\left[\tilde{d}_x^\dagger[1-\tilde{n}_{\bar{x}}]\tilde{\rho}[1-\tilde{n}_{\bar{x}}]\tilde{d}_x - \frac{1}{2}\{\tilde{d}_x\tilde{d}_x^\dagger[1-\tilde{n}_{\bar{x}}], \tilde{\rho}\}\right] +\\ &+\Gamma_x^U[1-f_x^U]\left[\tilde{d}_x\tilde{n}_{\bar{x}}\tilde{\rho}\tilde{n}_{\bar{x}}\tilde{d}_x^\dagger - \frac{1}{2}\{\tilde{d}_x^\dagger\tilde{d}_x\tilde{n}_{\bar{x}}, \tilde{\rho}\}\right] + \Gamma_x^U f_x^U\left[\tilde{d}_x^\dagger\tilde{n}_{\bar{x}}\tilde{\rho}\tilde{n}_{\bar{x}}\tilde{d}_x - \frac{1}{2}\{\tilde{d}_x\tilde{d}_x^\dagger\tilde{n}_{\bar{x}}, \tilde{\rho}\}\right]\Bigg)\end{aligned}$$

Focusing only on the diagonal terms we find the set of equations

$$\begin{aligned}\partial_t p_{0E} &= \left(\Gamma_L[1-f_L] + \Gamma_R[1-f_R]\right)p_{0F} + \Gamma_D[1-f_D]p_{1E} - \left(\Gamma_L f_L + \Gamma_R f_L + \Gamma_D f_D\right)p_{0E}\\ \partial_t p_{1E} &= \Gamma_D f_D p_{0E} - \Gamma_D[1-f_D]p_{1E} + \left(\Gamma_L^U[1-f_L^U] + \Gamma_R^U[1-f_R^U]\right)p_{1F} - \left(\Gamma_L^U f_L^U + \Gamma_R^U f_R^U\right)p_{1E}\\ \partial_t p_{0F} &= \left(\Gamma_L f_L + \Gamma_R f_R\right)p_{0E} - \left(\Gamma_L f_L + \Gamma_R f_R\right)p_{0F} + \Gamma_D^U[1-f_D^U]p_{1F} - \Gamma_D^U f_D^U p_{0F}\\ \partial_t p_{1F} &= \left(\Gamma_L^U f_L^U + \Gamma_R^U f_R^U\right)p_{1E} + \Gamma_D f_D p_{0F} - \left(\Gamma_L^U[1-f_L^U] + \Gamma_R^U[1-f_L^U] + \Gamma_D^U[1-f_D^U]\right)p_{1F}\end{aligned}$$

which can be summarized using the vector $\mathbf{p}^T = (p_{0E}, p_{1E}, p_{0F}, p_{1F})$ with the matrices

$$R^{L/R} = \begin{pmatrix} -\Gamma_{L/R} f_{L/R} & 0 & \Gamma_{L/R}[1 - f_{L/R}] & 0 \\ 0 & -\Gamma^U_{L/R} f^U_{L/R} & 0 & \Gamma^U_{L/R}[1 - f^U_{L/R}] \\ \Gamma_{L/R} f_{L/R} & 0 & -\Gamma_{L/R} f_{L/R} & 0 \\ 0 & \Gamma^U_{L/R} f^U_{L/R} & 0 & -\Gamma^U_{L/R}[1 - f^U_{L/R}] \end{pmatrix}$$

$$R^D = \begin{pmatrix} -\Gamma_D f_D & \Gamma_D[1 - f_D] & 0 & 0 \\ \Gamma_D f_D & -\Gamma_D[1 - f_D] & 0 & 0 \\ 0 & 0 & -\Gamma^U_D f^U_D & \Gamma^U_D[1 - f^U_D] \\ 0 & 0 & \Gamma^U_D f^U_D & -\Gamma^U_D[1 - f^U_D] \end{pmatrix}$$

in the rate equation

$$\partial_t \mathbf{p} = (R^L + R^R + R^D)\mathbf{p}.$$

Since $f_x(\epsilon)/[1 - f_x(\epsilon)] = e^{\beta_x(\epsilon - mu_x)}$, detailed balance is satisfied.

4 Quantum Fluctuation Theorems

Exercise 4.1: Two point measurement: Abstract integral fluctuation theorem

In the framework of the two point measurement scheme with the observable $X(\lambda_t) = \sum_x x_t \Pi(x_t)$, with $\Pi(x_t)$ projectors, consider the initial state

$$\rho(0) = \sum_{x_0} \mu(x_0)\Pi(x_0),$$

and an arbitrary set of weights $\mu(x_\tau)$ such that $\sum_\tau \mu(x_\tau)\mathrm{Tr}\left\{\Pi(x_\tau)\right\} = 1$. Show that

$$\langle e^{-\ln[\mu(x_0)/\mu(x_\tau)]}\rangle_{x_0 x_\tau} = 1.$$

Solution:
The joint probability distribution reads

$$p(x_\tau, x_0) = \mathrm{Tr}\left\{\Pi(x_\tau)U\Pi(x_0)\rho(0)\Pi(x_0)U^\dagger\Pi(x_\tau)\right\}$$

where U is the unitary evolution from $0 \to \tau$.

$$\begin{aligned}\langle e^{-\ln[\mu(x_0)/\mu(x_\tau)]}\rangle_{x_0 x_\tau} &= \sum_{x_0 x_\tau} \frac{\mu(x_\tau)}{\mu(x_0)} p(x_\tau, x_0) = \sum_{x_0 x_\tau} \frac{\mu(x_\tau)}{\mu(x_0)} \mathrm{Tr}\left\{\Pi(x_\tau)U\mu(x_0)\Pi(x_0)U^\dagger\right\} \\ &= \sum_{x_\tau} \mu(x_\tau)\mathrm{Tr}\left\{\Pi(x_\tau)\right\} = 1\end{aligned}$$

Exercise 4.2: Two point measurement: Time-reversed probability distribution

Consider the forward process discussed in Exercise 4.1 and its time-reversed process that begins with the system being in the initial state

$$\rho_{\mathrm{tr}}(\tau) = \sum_{x_\tau} \mu(x_\tau)\Pi_\Theta(x_\tau),$$

where the projectors $\Pi_\Theta(x_\tau) = \Theta\Pi(x_\tau)\Theta^{-1}$ define the time-reversed observable $X_\Theta(\lambda_t) = \sum_{x_t} x_t \Pi_\Theta(x_t)$. The weights are taken to satisfy $\sum_{x_\tau} \mu(x_\tau)\mathrm{Tr}\left\{\Pi_\Theta(x_\tau)\right\} = \sum_{x_\tau} \mu(x_\tau)\mathrm{Tr}\left\{\Pi(x_\tau)\right\} = 1$.

Then, the joint probability distribution in the time-reversed process is

$$p_{\mathrm{tr}}(x_0, x_\tau) = \mathrm{Tr}\left\{\Pi_\Theta(x_0)U_\Theta(\tau,0)\Pi_\Theta(x_\tau)\rho_{\mathrm{tr}}(0)\Pi_\Theta(x_\tau)U_\Theta^\dagger(\tau,0)\right\},$$

with $U_\Theta(\tau, 0)$ being the time-reversed unitary evolution operator.

Show that

$$p_{\mathrm{tr}}(x_0, x_\tau) = \frac{\mu(x_\tau)}{\mu(x_0)} p(x_\tau, x_0).$$

Solution:

$$\begin{aligned}p_{\mathrm{tr}}(x_0, x_\tau) &= \mathrm{Tr}\left\{\Pi_\Theta(x_0)U_\Theta(\tau,0)\mu(x_\tau)\Pi_\Theta(x_\tau)U_\Theta^\dagger(\tau,0)\right\} = \mu(x_\tau)\mathrm{Tr}\left\{\Pi(x_\tau)U(\tau,0)\Pi(x_0)U^\dagger(\tau,0)\right\} \\ &= \frac{\mu(x_\tau)}{\mu(x_0)}\mathrm{Tr}\left\{\Pi(x_\tau)U(\tau,0)\Pi(x_0)\left(\sum_{y_0}\mu(y_0)\Pi(y_0)\right)\Pi(x_0)U^\dagger(\tau,0)\right\} \\ &= \frac{\mu(x_\tau)}{\mu(x_0)}\mathrm{Tr}\left\{\Pi(x_\tau)U(\tau,0)\Pi(x_0)\rho(0)\Pi(x_0)U^\dagger(\tau,0)\right\} = \frac{\mu(x_\tau)}{\mu(x_0)} p(x_\tau, x_0)\end{aligned}$$

Exercise 4.3: Two point measurement: Abstract detailed fluctuation theorem

Taking $f(x) = -\ln\mu(x)$, the probabilities of observing Δf in the forward and backward process are

$$P(\Delta f) = \sum_{x_0 x_\tau} \delta\left(\Delta f - [f(x_\tau) - f(x_0)]\right) p(x_\tau, x_0), \quad P_{\mathrm{tr}}(\Delta f) = \sum_{x_0 x_\tau} \delta\left(\Delta f - [f(x_0) - f(x_\tau)]\right) p_{\mathrm{tr}}(x_0, x_\tau),$$

respectively. From Exercise 4.2, these are related through

$$\frac{P(\Delta f)}{P_{\rm tr}(-\Delta f)} = e^{\Delta f},$$

which is called *abstract detailed fluctuation theorem.*

Show that, if

(a) $\rho_{\rm tr}(\tau) = \rho(0)$,

(b) the measured observable is invariant under time reversal, i.e. $X_\Theta(\lambda_0) = X(\lambda_0)$ and $X_\Theta(\lambda_\tau) = X(\lambda_\tau)$,

(c) the Hamiltonian in invariant under time reversal,

(d) the driving protocol is time-symmetric, i.e. $\lambda_t = \lambda_{\tau-t}\,\forall t \in [0,\tau]$,

then $P(\Delta f) = P_{\rm tr}(\Delta f)$.

Solution:
Let's first look at the definitions of the joint probabilities:

$$p(x_\tau, x_0) = \mathrm{Tr}\left\{\Pi(x_\tau)U\Pi(x_0)\rho(0)\Pi(x_0)U^\dagger\right\}, \quad p_{\rm tr}(x_0, x_\tau) = \mathrm{Tr}\left\{\Pi_\Theta(x_0)U_\Theta\Pi_\Theta(x_\tau)\rho_{\rm tr}(\tau)\Pi_\Theta(x_\tau)U_\Theta^\dagger\right\}.$$

Then, using the hypothesis given, we can write the time reversed probability as

$$p_{\rm tr}(x_0, x_\tau) = \mathrm{Tr}\left\{\Pi(x_0)U\Pi(x_\tau)\rho(0)\Pi(x_\tau)U^\dagger\right\} = p(x_0, x_\tau),$$

where we used that $U_\Theta = \exp_+\left[-\frac{i}{\hbar}\int_0^\tau H_\Theta(\lambda_{\tau-s})\right] = \exp_+\left[-\frac{i}{\hbar}\int_0^\tau H(\lambda_s)\right] = U$. Finally, lokking at the probability $P_{\rm tr}(\Delta f)$ we have

$$P_{\rm tr}(\Delta f) = \sum_{x_0 x_\tau} \delta\left(\Delta f - [f(x_0) - f(x_\tau)]\right) p(x_0, x_\tau) = P(\Delta f)$$

after a simple relabeling of the sum indices.

Exercise 4.4: Integral fluctuation theorem and entropy production

During the driving protocol the internal energy changes *on average* from the initial equilibrium values $\mathcal{U}(0) = \mathrm{Tr}\left\{H(\lambda_0)\pi(\lambda_0)\right\}$ to some final non-equilibrium value $U(\tau) = \mathrm{Tr}\left\{H(\lambda_\tau)\rho(\tau)\right\} = W(\tau) + \mathcal{U}(0)$, where $W(\tau) = \int_0^\tau dt \mathrm{Tr}\left\{[\partial_t H(\lambda_t)]\rho(t)\right\}$ is the work done on the system.

Let β^*_τ be the inverse temperature of a fictitious Gibbs ensemble $\pi(\beta^*_\tau, \lambda_\tau)$ having the same internal energy as the final non-equilibrium state $\rho(\tau)$, i.e. $U(\tau) = \mathcal{U}(\beta^*_\tau, \tau) \equiv \mathrm{Tr}\left\{H(\lambda_\tau)\pi(\beta^*_\tau, \lambda_\tau)\right\}$, and choose the weights $\mu(\epsilon_\tau) = e^{-\beta^*_\tau[\epsilon_\tau - \mathcal{F}(\beta^*_\tau, \lambda_\tau)]}$.

Show that

$$\langle e^{-\beta^*_\tau[\epsilon_\tau - \mathcal{F}(\beta^*_\tau, \lambda_\tau)] + \beta[\epsilon_0 - \mathcal{F}(\beta, \lambda_0)]}\rangle_{\epsilon_\tau, \epsilon_0} = 1,$$

and use it to show that $\mathcal{S}(\beta^*_\tau, \lambda_\tau) \geq \mathcal{S}(\beta, \lambda_0)$.

Solution:
Let $f(\epsilon_\tau) = -\ln\mu(\epsilon_\tau) = \beta^*_\tau[\epsilon_\tau - \mathcal{F}(\beta^*_\tau, \lambda_\tau)]$. The detailed fluctuation theorem then reads

$$P(\Delta f)e^{-\Delta f} = P_{\rm tr}(-\Delta f) \Rightarrow \langle e^{-\Delta f}\rangle = 1$$

$$\left\langle e^{-\beta^*_\tau[\epsilon_\tau - \mathcal{F}(\beta^*_\tau, \lambda_\tau)] + \beta^*_0[\epsilon_0 - \mathcal{F}(\beta^*_0, \lambda_0)]}\right\rangle = \left\langle e^{-\beta^*_\tau[\epsilon_\tau - \mathcal{F}(\beta^*_\tau, \lambda_\tau)] + \beta_0[\epsilon_0 - \mathcal{F}(\beta_0, \lambda_0)]}\right\rangle = 1.$$

Since the exponential is a convex function $e^{qx+(1-q)y} \leq qe^x + (1-q)e^y\,\forall q \in [0,1]$, then

$$e^{\langle -\beta^*_\tau[\epsilon_\tau - \mathcal{F}(\beta^*_\tau, \lambda_\tau)] + \beta_0[\epsilon_0 - \mathcal{F}(\beta_0, \lambda_0)]\rangle} \leq 1 \to \langle -\beta^*_\tau[\epsilon_\tau - \mathcal{F}(\beta^*_\tau, \lambda_\tau)] + \beta_0[\epsilon_0 - \mathcal{F}(\beta_0, \lambda_0)]\rangle \leq 0$$

$$-\beta^*_\tau\mathcal{U}(\beta^*_\tau, \tau) + \beta^*_\tau\mathcal{F}(\beta^*_\tau, \tau) + \beta_0\mathcal{U}(0) - \beta_0\mathcal{F}(\beta_0, \lambda_0) = \mathcal{S}(\beta_0, \lambda_0) - \mathcal{S}(\beta^*_\tau, \lambda_\tau) \leq 0.$$

Therefore, the detailed fluctuation theorem implies the second law: when we start from a thermal state and we only know the average energy of the system, the entropy increases.

Exercise 4.5: Fluctuation theorems for strongly coupled open quantum system

Consider an arbitrary system-bath Hamiltonian of the form $H_{SB}(\lambda_t) = H_S(\lambda_t)+V_{SB}(\lambda_t)+H_B$, with $V_{SB}(\lambda_0) = V_{SB}(\lambda_\tau) = 0$. Use the Hamiltonian of mean force $H_S^*(\lambda_t)$ to confirm that $\mathcal{F}_{SB}(\lambda_t) = \mathcal{F}_S^*(\lambda_t) + \mathcal{F}_B$, where $\mathcal{F}_S^*(\lambda_t) \equiv -k_B T \ln \mathcal{Z}_S^*(\lambda_t)$ is the strong coupling equilibrium free energy.

Show that the strong coupling quantum work fluctuation theorems

$$\left\langle e^{-\beta w} \right\rangle = e^{-\beta \Delta \mathcal{F}_S^*}, \quad \frac{P(w)}{P_{\mathrm{tr}}(-w)} = e^{\beta(w-\Delta\mathcal{F}_S^*)}$$

hold.

Solution:
The Hamiltonian of mean force is defined by

$$\mathcal{Z}_S^* \equiv \frac{\mathcal{Z}_{SB}}{\mathcal{Z}_B}, \quad \frac{e^{-\beta H_S^*}}{\mathcal{Z}_S^*} \equiv \mathrm{Tr}_B\left\{\pi_{SB}\right\},$$

from which it follows immediately that $\mathcal{F}_{SB}(\lambda_t) = \mathcal{F}_S^*(\lambda_t)+\mathcal{F}_B$. Then, plugging this into the fluctuation theorems for closed systems, namely

$$\left\langle e^{-\beta w} \right\rangle = e^{-\beta \Delta \mathcal{F}}, \quad \frac{P(w)}{P_{\mathrm{tr}}(-w)} = e^{\beta(w-\Delta\mathcal{F})}$$

we have

$$\left\langle e^{-\beta w} \right\rangle = e^{-\beta \Delta \mathcal{F}_S^*}, \quad \frac{P(w)}{P_{\mathrm{tr}}(-w)} = e^{\beta(w-\Delta\mathcal{F}_S^*)}$$

since $\Delta\mathcal{F} = \mathcal{F}_{SB}(\lambda_\tau) - \mathcal{F}_{SB}(\lambda_0) = \Delta\mathcal{F}_S^*$. Note that we required the interaction at the beginning and at the end of the driving protocol to vanish so that we can write the initial states of the forward and backward protocols as product states, $\pi_{SB} = \pi_S \otimes \pi_B$.

Exercise 4.6: Integral entropy production fluctuation theorems and second laws

Show that the integral entropy production fluctuation theorem

$$\left\langle e^{-\sigma/k_B} \right\rangle_{\mathbf{x}_\tau,\mathbf{x}_0} = 1, \quad \sigma \equiv \Delta s_S - \sum_\nu \beta_\nu q_\nu,$$

imlpes the second laws:

$$\Sigma(t) \equiv k_B \Delta S[\rho_S(t)] - \sum_\nu \frac{Q_\nu(t)}{T_\nu} \geq 0, \quad Q_\nu(t) = -\mathrm{Tr}_\nu \left\{ H_B^{(\nu)}[\rho_\nu(t) - \rho_\nu(0)] \right\};$$

$$\Sigma(t) = \Delta S_S(t) - \sum_\nu \frac{Q_\nu(t)}{T_\nu} \geq 0, \quad \dot{Q}_\nu(t) \equiv -\left(d_t U_\nu(t) - \mu_\nu d_t N_\nu(t)\right).$$

Solution:
We use the convexity of the exponential to find the inequality

$$\langle\sigma\rangle = \langle \Delta s_S - \sum_\nu \beta_\nu q_\nu \rangle \geq 0.$$

Since $\Delta s_S = -\ln \frac{p_S(s_\tau)}{p_S(s_0)}$, the average over all initial and final outcomes gives $\langle \Delta s_S\rangle = \Delta S_S$. Additionally,

$$\langle q_\nu \rangle = -\langle \epsilon_\nu^\tau - \epsilon_\nu^0 - \mu_\nu[n_\nu^\tau - n_\nu^0]\rangle = -\left(U_\nu(\tau) - U_\nu(0) - \mu_\nu[N_\nu(\tau) - N_\nu(0)]\right).$$

If the bath and the system do not exchange particles $N_\nu(\tau) = N_\nu(0)$, and we recover the second law

$$\Sigma(t) \equiv k_B \Delta S[\rho_S(t)] - \sum_\nu \frac{Q_\nu(t)}{T_\nu} \geq 0, \quad Q_\nu(t) = -\mathrm{Tr}_\nu \left\{ H_B^{(\nu)}[\rho_\nu(t) - \rho_\nu(0)] \right\}.$$

If instead we allow the system and the baths to exchange particles we recover the second law

$$\Sigma(t) = \Delta S_S(t) - \sum_\nu \frac{Q_\nu(t)}{T_\nu} \geq 0, \quad \dot{Q}_\nu(t) \equiv -\left(d_t U_\nu(t) - \mu_\nu d_t N_\nu(t)\right).$$

Exercise 4.7: Exchange fluctuation theorem and particle conservation

Consider two interacting baths with Hamiltonian $H(\lambda_t) = \sum_\nu H_B^{(\nu)} + V(\lambda_t)$ in the time-symmetric case, namely $\Theta H_B^{(\nu)} \Theta^{-1} = H_B^{(\nu)}$ and $\Theta V(\lambda_t)\Theta^{-1} = V(\lambda_{\tau-t})$.

Then, the *exchange fluctuation theorem* holds

$$\frac{P(\Delta\epsilon_1, \Delta\epsilon_2, \Delta n_1, \Delta n_2)}{P(-\Delta\epsilon_1, -\Delta\epsilon_2, -\Delta n_1, -\Delta n_2)} = e^{\sum_\nu \beta_\nu(\Delta\epsilon_\nu - \mu_\nu \Delta n_\nu)}.$$

Show that, if the total number operator $\hat{N}_{\text{tot}}$ commutes with the Hamiltonian at all times, $[H(\lambda_t), \hat{N}_{\text{tot}}] = 0$, then

$$P(\Delta\epsilon_1, \Delta\epsilon_2, \Delta n_1, \Delta n_2) = P(\Delta\epsilon_1, \Delta\epsilon_2, \Delta n_1, -\Delta n_1)\delta(\Delta n_1 + \Delta n_2).$$

Solution:
The joint probability of the outcomes is

$$p(\vec{\epsilon}^\tau \vec{n}^\tau, \vec{\epsilon}^0 \vec{n}^0) = \text{Tr}\left\{\Pi(\vec{\epsilon}^\tau \vec{n}^\tau) U \Pi(\vec{\epsilon}^0 \vec{n}^0)\rho(0)\Pi(\vec{\epsilon}^0 \vec{n}^0) U^\dagger\right\}$$

We now look at the total number of particles in a specific trajectory, and use the fact that the total particle number operator commutes with the Hamiltnian at all times to find

$$\begin{aligned}(n_1^\tau + n_2^\tau) p(\vec{\epsilon}^\tau \vec{n}^\tau, \vec{\epsilon}^0 \vec{n}^0) &= \text{Tr}\left\{\hat{N}_{\text{tot}}\Pi(\vec{\epsilon}^\tau \vec{n}^\tau) U \Pi(\vec{\epsilon}^0 \vec{n}^0)\rho(0)\Pi(\vec{\epsilon}^0 \vec{n}^0) U^\dagger\right\} \\ &= \text{Tr}\left\{\Pi(\vec{\epsilon}^\tau \vec{n}^\tau) U \hat{N}_{\text{tot}} \Pi(\vec{\epsilon}^0 \vec{n}^0)\rho(0)\Pi(\vec{\epsilon}^0 \vec{n}^0) U^\dagger\right\} = (n_1^0 + n_2^0) p(\vec{\epsilon}^\tau \vec{n}^\tau, \vec{\epsilon}^0 \vec{n}^0)\end{aligned}$$

From which we have

$$(\Delta n_1 + \Delta n_2) p(\vec{\epsilon}^\tau \vec{n}^\tau, \vec{\epsilon}^0 \vec{n}^0) = 0 \to p(\vec{\epsilon}^\tau \vec{n}^\tau, \vec{\epsilon}^0 \vec{n}^0) = p(\vec{\epsilon}^\tau \vec{n}^\tau, \vec{\epsilon}^0 \vec{n}^0)\delta_{n_1^\tau - n_1^0, -(n_2^\tau - n_2^0)}.$$

Finally, we can now look at the the joint probability distribution

$$\begin{aligned}P(\Delta\boldsymbol{\epsilon}, \Delta\mathbf{n}) = \sum_{\vec{\epsilon}^\tau \vec{n}^\tau, \vec{\epsilon}^0 \vec{n}^0} &\delta(\Delta\epsilon_1 - [\epsilon_1^\tau - \epsilon_1^0])\delta(\Delta\epsilon_2 - [\epsilon_2^\tau - \epsilon_2^0])\delta(\Delta n_1 - [n_1^\tau - n_1^0]) \times \\ &\times \delta(\Delta n_2 - [n_2^\tau - n_2^0]) p(\vec{\epsilon}^\tau \vec{n}^\tau, \vec{\epsilon}^0 \vec{n}^0)\delta_{n_1^\tau - n_1^0, -(n_2^\tau - n_2^0)}\end{aligned}$$

From which we recognize that $P(\Delta\boldsymbol{\epsilon}, \Delta\mathbf{n}) \propto \delta(\Delta n_1 + \Delta n_2)$ from which we can conclude that

$$P(\Delta\epsilon_1, \Delta\epsilon_2, \Delta n_1, \Delta n_2) = P(\Delta\epsilon_1, \Delta\epsilon_2, \Delta n_1, -\Delta n_1)\delta(\Delta n_1 + \Delta n_2).$$

Exercise 4.8: Dyson series solution to the BMS master equation

In the interaction picture, the Born-Markov secular master equation of a system in contact with one bath reads

$$\partial_t \tilde{\rho}_S(t) = \sum_{\omega\alpha} r_\alpha(\omega)\left[S_\alpha(\omega)\tilde{\rho}_S(t)S_\alpha^\dagger(\omega) - \frac{1}{2}\{S_\alpha^\dagger(\omega)S_\alpha, \tilde{\rho}_S(t)\}\right] = \mathcal{D}\tilde{\rho}_S(t).$$

Defining the jump (super)operator as

$$\mathcal{J}(\omega)\tilde{\rho}_S(t) \equiv \sum_\alpha r_\alpha(\omega) S_\alpha(\omega)\tilde{\rho}_S(t)S_\alpha^\dagger(\omega),$$

the Born-Markov secular master equation can be casted as follows

$$\partial_t \tilde{\rho}_S = \mathcal{L}_0 \tilde{\rho}_S(t) + \sum_\omega \mathcal{J}(\omega)\tilde{\rho}_S(t).$$

Show that the *Dyson series*

$$\tilde{\rho}_S(t) = \sum_{n=0}^\infty \sum_{\omega_n \cdots \omega_1} \int_0^t dt_n \cdots \int_0^{t_2} dt_1 e^{\mathcal{L}_0(t-t_n)}\mathcal{J}(\omega_n)e^{\mathcal{L}_0(t_n - t_{n-1})} \cdots \mathcal{J}(\omega_2)e^{\mathcal{L}_0(t_2-t_1)}\mathcal{J}(\omega_1)e^{\mathcal{L}_0 t_1}\rho_S(0)$$

is the solution of the Born-Markov secular master equation.

Solution:
We can take the time derivative of the DYson series and verify that it satisfies the BMS master equation:

$$\partial_t \tilde{\rho}_S(t) = \sum_{n=0}^{\infty} \sum_{\omega_n \cdots \omega_1} \left[\int_0^t dt_n \cdots \int_0^{t_2} dt_1 \mathcal{L}_0 e^{\mathcal{L}_0(t-t_n)} \mathcal{J}(\omega_n) e^{\mathcal{L}_0(t_n - t_{n-1})} \cdots \mathcal{J}(\omega_2) e^{\mathcal{L}_0(t_2-t_1)} \mathcal{J}(\omega_1) e^{\mathcal{L}_0 t_1} \rho_S(0) + \right.$$
$$\left. + \int_0^t dt_{n-1} \cdots \int_0^{t_2} dt_1 \mathcal{J}(\omega_n) e^{\mathcal{L}_0(t-t_{n-1})} \cdots \mathcal{J}(\omega_2) e^{\mathcal{L}_0(t_2-t_1)} \mathcal{J}(\omega_1) e^{\mathcal{L}_0 t_1} \rho_S(0) \right]$$
$$\partial_t \tilde{\rho}_S(t) = \mathcal{L}_0 \tilde{\rho}_S(t) + \sum_\omega \mathcal{J}(\omega) \tilde{\rho}_S(t).$$

Exercise 4.9: Moment and cumulant generating functions

Consider a probability distribution $p(q)$ and its Fourier transform $M(\chi) = \int đq e^{iq\chi} p(q)$.

Show that the moments $\langle q^n \rangle = \int đq q^n p(q)$ for any $n \in \mathbb{N}$ can be obtained from the moment generating function $M(\chi)$ through

$$\langle q^n \rangle = (-i)^n \frac{\partial^n}{\partial \chi^n} M(\chi) \Big|_{\chi=0}.$$

Show explicitely that the first two cumulants (the mean value and variance) follow from the cumulant generating function $C(\chi) = \ln M(\chi)$ as

$$\kappa_1 \equiv \langle q \rangle = -i \frac{\partial}{\partial \chi} C(\chi) \Big|_{\chi=0}, \quad \kappa_2 \equiv \langle q^2 \rangle - \langle q \rangle^2 = (-i)^2 \frac{\partial^2}{\partial \chi^2} C(\chi) \Big|_{\chi=0}.$$

Solution:

$$\partial_\chi^n M(\chi) = i^n \int đq q^n e^{iq\chi} p(q) \longrightarrow (-i)^n \, \partial_\chi^n M(\chi)\big|_{\chi=0} = \int đq q^n p(q) = \langle q^n \rangle.$$

Since $C(\chi) = \ln M(\chi)$ the first two derivatives are

$$\partial_\chi C(\chi) = \frac{\partial_\chi M(\chi)}{M(\chi)}, \qquad \partial_\chi^2 C(\chi) = \frac{\partial_\chi^2 M(\chi)}{M(\chi)} - \frac{[\partial_\chi M(\chi)]^2}{M^2(\chi)}$$

Noticing that $M(0) = 1$, we have

$$\partial_\chi C(\chi)|_{\chi=0} = i\langle q \rangle, \qquad \partial_\chi^2 C(\chi)\big|_{\chi=0} = i^2 \langle q^2 \rangle - i^2 \langle q \rangle^2$$

$$\kappa_1 \equiv \langle q \rangle = -i \frac{\partial}{\partial \chi} C(\chi) \Big|_{\chi=0}, \quad \kappa_2 \equiv \langle q^2 \rangle - \langle q \rangle^2 = (-i)^2 \frac{\partial^2}{\partial \chi^2} C(\chi) \Big|_{\chi=0}.$$

Exercise 4.10: Heat current from the full counting statistics

The counting field Liouvillian is defined as

$$\mathcal{L}(\chi) = \mathcal{L}_0 + \sum_\omega \mathcal{J}(\omega) e^{-i\hbar\omega\chi},$$

and generates the dynamics of the full counting statistcs through

$$\partial_t \tilde{\rho}_S(\chi, t) = \mathcal{L}(\chi) \tilde{\rho}_S(\chi, t).$$

The corresponding moment generating function is obtained by taking the trace: $M(\chi, t) = \mathrm{Tr}_S \{\tilde{\rho}_S(\chi, t)\}$.

Show that, for the Born-Markov secular master equation describing a system coupled to one bath, the heat current $\dot{Q}(t) = \partial_t \langle q \rangle(t)$ is

$$\dot{Q}(t) = -i\partial_t \, \partial_\chi M(\chi, t)|_{\chi=0} = -\hbar \sum_{\omega\alpha} \omega r_\alpha(\omega) \mathrm{Tr}_S \left\{ S_\alpha^\dagger(\omega) S_\alpha(\omega) \tilde{\rho}_S(t) \right\},$$

and verify that it coincides with $\dot{Q}(t) = \mathrm{Tr}_S \{H_S \mathcal{D} \rho_S(t)\}$.

Solution:
Let's start from the time derivative

$$\mathrm{Tr}_S\left\{\partial_t\tilde{\rho}_S(\chi,t)\right\} = \mathrm{Tr}_S\left\{\mathcal{L}(\chi)\tilde{\rho}_S(\chi,t)\right\}.$$

Since we are interested in the χ-derivative around $\chi = 0$, we can expand the Liouvillian as

$$\mathcal{L}(\chi) \approx \mathcal{L}_0 + \sum_\omega \mathcal{J}(\omega)(1 - i\hbar\omega\chi) = \mathcal{D} - i\hbar\chi\sum_\omega \omega\mathcal{J}(\omega).$$

Notice that the dissipator $\mathcal{D}$ cancels out in the trace because

$$\begin{aligned}\mathrm{Tr}_S\left\{\mathcal{D}\sigma\right\} &= \sum_{\alpha\omega} r_\alpha(\omega)\mathrm{Tr}_S\left\{S_\alpha(\omega)\sigma S_\alpha^\dagger(\omega) - \frac{1}{2}\{S_\alpha^\dagger(\omega)S_\alpha(\omega),\sigma\}\right\}\\ &= \sum_{\alpha\omega} r_\alpha(\omega)\mathrm{Tr}_S\left\{S_\alpha(\omega)^\dagger S_\alpha(\omega)\sigma\left[1-\frac{1}{2}-\frac{1}{2}\right]\right\} = 0\end{aligned}$$

for any σ thanks to the cyclic property of the trace. Then, we are left with

$$\begin{aligned}\dot{Q}(t) &= -i\lim_{\chi\to 0}\frac{1}{\chi}\mathrm{Tr}_S\left\{-i\hbar\chi\sum_\omega \omega\mathcal{J}(\omega)\tilde{\rho}_S(\chi,t)\right\} = -\hbar\mathrm{Tr}_S\left\{\sum_\omega \omega\mathcal{J}(\omega)\tilde{\rho}_S(0,t)\right\}\\ &= -\hbar\sum_{\alpha\omega}\omega r_\alpha(\omega)\mathrm{Tr}_S\left\{S_\alpha^\dagger(\omega)S_\alpha(\omega)\tilde{\rho}_S(t)\right\}.\end{aligned}$$

Remembering that the Forier component $S_\alpha(\omega)$ satisfy the properties demonstrated in Exercise 3.5, most importantly that

$$S_\alpha^\dagger(\omega) = S_\alpha(-\omega), \qquad [S_\alpha(\omega), H_S] = \hbar\omega S_\alpha(\omega) \to [H_S, S_\alpha^\dagger(\omega)] = \hbar\omega S_\alpha^\dagger(\omega).$$

Then, we can use these relation to get rid of the $\hbar\omega$ term as follows:

$$\begin{aligned}\dot{Q}(t) &= -\sum_{\alpha\omega} r_\alpha(\omega)\mathrm{Tr}_S\left\{\hbar\omega S_\alpha^\dagger(\omega)S_\alpha(\omega)\tilde{\rho}_S(t)\right\}\\ &= -\sum_{\alpha\omega} r_\alpha(\omega)\mathrm{Tr}_S\left\{\frac{1}{2}\left([H_S, S_\alpha^\dagger(\omega)]S_\alpha(\omega) + S_\alpha^\dagger(\omega)[S_\alpha(\omega), H_S]\right)\tilde{\rho}_S(t)\right\}\\ &= -\sum_{\alpha\omega}\frac{r_\alpha(\omega)}{2}\mathrm{Tr}_S\left\{\left(H_S S_\alpha^\dagger(\omega)S_\alpha(\omega) + S_\alpha^\dagger(\omega)S_\alpha(\omega)H_S - S_\alpha^\dagger(\omega)H_S S_\alpha(\omega) - S_\alpha^\dagger(\omega)H_S S_\alpha(\omega)\right)\tilde{\rho}_S(t)\right\}\\ &= -\sum_{\alpha\omega}\frac{r_\alpha(\omega)}{2}\mathrm{Tr}_S\left\{H_S\left(\{S_\alpha^\dagger(\omega)S_\alpha(\omega),\tilde{\rho}_S(t)\} - 2S_\alpha(\omega)\tilde{\rho}_S(t)S_\alpha^\dagger(\omega)\right)\right\} = \mathrm{Tr}_S\left\{H_S\mathcal{D}\tilde{\rho}_S(t)\right\}\end{aligned}$$

Exercise 4.11: Fluctuation theorem and symmetries of the moment generating function

Starting from the anti-Fourier transform relating the probability distribution and the moment generating function

$$p_t(\mathbf{q}) = \frac{1}{(2\pi)^n}\int_{-\infty}^{\infty} d\chi_1\cdots\int_{-\infty}^{\infty} d\chi_n e^{-i\mathbf{q}\boldsymbol{\chi}}M(\boldsymbol{\chi},t),$$

prove that

$$\frac{p_t(\mathbf{q})}{p_t(-\mathbf{q})} = \exp\left(\sum_{\nu=1}^n a_\nu q_\nu\right) \qquad\Leftrightarrow\qquad M(\boldsymbol{\chi},t) = M(i\mathbf{a}-\boldsymbol{\chi},t)\quad \forall\boldsymbol{\chi}\in\mathbb{R}^n$$

for $M(\boldsymbol{\chi},t)$ analytic and decaying to zero for $|\chi_\nu|\to\infty$.

Solution:

(⇒) The moment generating function is the Fourier transform, so we have

$$M(\boldsymbol{\chi},t)=\int d\mathbf{q}p_t(\mathbf{q})e^{i\mathbf{q}\boldsymbol{\chi}}=\int d\mathbf{q}p_t(-\mathbf{q})e^{i\mathbf{q}(\boldsymbol{\chi}-i\mathbf{a})}=\int_{-\infty}^{\infty}dq_1\cdots\int_{-\infty}^{\infty}dq_\nu p_t(-\mathbf{q})e^{i\mathbf{q}(\boldsymbol{\chi}-i\mathbf{a})}$$
$$=\int_{-\infty}^{\infty}dq_1\cdots\int_{-\infty}^{\infty}dq_\nu p_t(\mathbf{q})e^{i\mathbf{q}(-\boldsymbol{\chi}+i\mathbf{a})}=\int d\mathbf{q}p_t(\mathbf{q})e^{i\mathbf{q}(-\boldsymbol{\chi}+i\mathbf{a})}=M(i\mathbf{a}-\boldsymbol{\chi},t)$$

(⇐) We can use the analyticity and the asymptotic bechaiour of the moment generating function to change the integration contour in the complex plane and obtain

$$p_t(\mathbf{q})=\frac{1}{(2\pi)^n}\int d\boldsymbol{\chi}e^{-i\mathbf{q}\boldsymbol{\chi}}M(\boldsymbol{\chi},t)=\frac{1}{(2\pi)^n}\int d\boldsymbol{\chi}e^{-i\mathbf{q}\boldsymbol{\chi}}M(i\mathbf{a}-\boldsymbol{\chi},t)$$
$$\overset{\boldsymbol{\xi}=i\mathbf{a}-\boldsymbol{\chi}}{=}\frac{1}{(2\pi)^n}\int d\boldsymbol{\xi}e^{-i\mathbf{q}(i\mathbf{a}-\boldsymbol{\xi})}M(\boldsymbol{\xi},t)=\frac{e^{\mathbf{q}\mathbf{a}}}{(2\pi)^n}\int d\boldsymbol{\xi}e^{i\mathbf{q}\boldsymbol{\xi})}M(\boldsymbol{\xi},t)=e^{\mathbf{q}a}p_t(-q).$$

Exercise 4.12: Symmetry of the counting field Liouvillian

Given the counting field Liouvillian $\mathcal{L}(\boldsymbol{\chi})=\sum_\nu\mathcal{L}_\nu(\chi_\nu)=\sum_\nu(\mathcal{L}_{0\nu}+\sum_\omega\mathcal{J}_\nu(\omega)e^{-i\hbar\omega\chi_\nu})$, where

$$\mathcal{L}_{0\nu}\rho=\sum_{\alpha\omega}\frac{r_{\alpha\nu}(\omega)}{2}\{S^\dagger_{\alpha\nu}(\omega)S_{\alpha\nu}(\omega),\rho\},\quad \mathcal{J}_\nu(\omega)\rho=\sum_\alpha r_{\alpha\nu}(\omega)S_{\alpha\nu}(\omega)\rho S^\dagger_{\alpha\nu}(\omega),$$

prove that

$$\mathcal{L}(\boldsymbol{\chi}-i\boldsymbol{\beta})=\mathcal{L}(\boldsymbol{\chi})^\dagger.$$

Solution:
Remembering that the rates $r_{\alpha\nu}(\omega)$ satisfy local detailed balance

$$\frac{r_{\alpha\nu}(\omega)}{r_{\alpha\nu}(-\omega)}=e^{\beta_\nu\hbar\omega}$$

and that the Fourier components of the interaction satisfy $S_{\alpha\nu}(-\omega)=S^\dagger_{\alpha\nu}(\omega)$ we have

$$\begin{aligned}\mathcal{L}(\boldsymbol{\chi}-i\boldsymbol{\beta})\rho&=\sum_\nu\left(\mathcal{L}_{0\nu}+\sum_\omega\mathcal{J}_\nu(\omega)e^{-i\hbar\omega\chi_\nu-\beta_\nu\hbar\omega}\right)\rho\\&=\sum_\nu\left(\mathcal{L}_{0\nu}\rho+\sum_{\alpha\omega}e^{-i\hbar\omega\chi_\nu}r_{\alpha\nu}(\omega)e^{-\beta_\nu\hbar\omega}S_{\alpha\nu}(\omega)\rho S^\dagger_{\alpha\nu}(\omega)\right)\\&=\sum_{\nu\alpha\omega}\left(\frac{r_{\alpha\nu}(\omega)}{2}\{S^\dagger_{\alpha\nu}(\omega)S_{\alpha\nu}(\omega),\rho\}+e^{-i\hbar\omega\chi_\nu}r_{\alpha\nu}(-\omega)S^\dagger_{\alpha\nu}(-\omega)\rho S_{\alpha\nu}(-\omega)\right)\\&=\sum_{\nu\alpha\omega}\left(\frac{r_{\alpha\nu}(\omega)}{2}\{S^\dagger_{\alpha\nu}(\omega)S_{\alpha\nu}(\omega),\rho\}+e^{i\hbar\omega\chi_\nu}r_{\alpha\nu}(\omega)S^\dagger_{\alpha\nu}(\omega)\rho S_{\alpha\nu}(\omega)\right)=[\mathcal{L}(\boldsymbol{\chi})\rho]^\dagger.\end{aligned}$$

Since $\mathcal{L}(\boldsymbol{\chi}-i\boldsymbol{\beta})\rho=[\mathcal{L}(\boldsymbol{\chi})\rho]^\dagger$ for all density matrices we identify $\mathcal{L}(\boldsymbol{\chi}-i\boldsymbol{\beta})=\mathcal{L}(\chi)^\dagger$

Exercise 4.13: Full counting statistics of single-electron transistor

Consider the single-electron transistor from Exercise 3.33 for $\beta_L=\beta_R\equiv\beta$, for which the dynamics is described by the rate master equation

$$\frac{d}{dt}\begin{pmatrix}p_F(t)\\p_E(t)\end{pmatrix}=\sum_\nu\Gamma_\nu(\epsilon_0)\begin{pmatrix}-[1-f_\nu(\epsilon_0)]&f_\nu(\epsilon_0)\\1-f_\nu(\epsilon_0)&-f_\nu(\epsilon_0)\end{pmatrix}\begin{pmatrix}p_F(t)\\p_E(t)\end{pmatrix}.$$

For simplicity, set $\Gamma_L(\epsilon_0)=\Gamma_R(\epsilon_0)\equiv\Gamma$, $\mu_L=\epsilon_0+V/2$, and $\mu_R=\epsilon_0-V/2$.

We are now interested in counting the number of electron jumps n_ν from bath $\nu=L,R$ into the system. The state of the system conditioned on $\mathbf{n}=(n_L,n_R)$ jumps is denoted by $p_\sigma(t|\mathbf{n})$, with $\sigma=E,F$ denoting the state of the quantum dot (empty or filled). Since the number of electron jumps is discrete, $n_\nu \in \mathbb{Z}$, we define the counting field by

$$\rho_\sigma(\boldsymbol{\chi}, t) = \sum_{\mathbf{n}} e^{i\mathbf{n}\cdot\boldsymbol{\chi}} p_\sigma(t|\mathbf{n}) \quad \Leftrightarrow \quad p_\sigma(t|\mathbf{n}) = \int_{-\pi}^{\pi} \frac{d\chi_L}{2\pi} \int_{-\pi}^{\pi} \frac{d\chi_R}{2\pi} e^{-i\mathbf{n}\cdot\boldsymbol{\chi}} \rho_\sigma(\boldsymbol{\chi}, t),$$

with $\boldsymbol{\chi} = (\chi_L, \chi_R)$.

(i) Deduce that the master equation with the counting fields reads

$$\frac{d}{dt}\begin{pmatrix} p_F(\boldsymbol{\chi}, t) \\ p_E(\boldsymbol{\chi}, t) \end{pmatrix} = \sum_\nu \Gamma \begin{pmatrix} -[1 - f_\nu(\epsilon_0)] & e^{i\chi_\nu} f_\nu(\epsilon_0) \\ e^{-i\chi_\nu}[1 - f_\nu(\epsilon_0)] & -f_\nu(\epsilon_0) \end{pmatrix} \begin{pmatrix} p_F(\boldsymbol{\chi}, t) \\ p_E(\boldsymbol{\chi}, t) \end{pmatrix}.$$

(ii) Compute the two eigenvalues $\lambda_\pm(\boldsymbol{\chi})$ of the rate matrix with the counting fields and confirm that both obey the symmetries

$$\lambda_\pm(\chi_L, \chi_R) = \lambda_\pm(\chi_L - \chi_R, 0), \quad \lambda_\pm(\chi_L, \chi_R) = \lambda_\pm\left(-\chi_L + i\frac{\beta V}{2}, -\chi_R - i\frac{\beta V}{2}\right).$$

Show that the first symmetry imples at steady state the conservation law $n_L + n_R = 0$, while the second one implies the exchange fluctuation theorem $P(\Delta n_L)/P(-\Delta n_L) = e^{-\beta(\mu_L - \mu_R)\Delta n_L}$.

Solution:

(i) From Exercise 3.33 we recall the Born-Markov master equation in the interacting picture:

$$\partial_t \tilde{\rho}_S = \sum_\nu \left(\frac{1 - f_\nu(\epsilon_0)}{\tau_\nu} \left[\tilde{d}\tilde{\rho}_S\tilde{d}^\dagger - \frac{1}{2}\{\tilde{d}^\dagger\tilde{d}, \tilde{\rho}_S\} \right] + \frac{f_\nu(\epsilon_0)}{\tau_\nu} \left[\tilde{d}^\dagger\tilde{\rho}_S\tilde{d} - \frac{1}{2}\{\tilde{d}\tilde{d}^\dagger, \tilde{\rho}_S\} \right] \right)$$

Crucially, we are now interested in counting the particle exchange, so the counting fields Liouvillian becomes

$$\mathcal{L}(\boldsymbol{\chi})\rho = \sum_\nu \left(\mathcal{L}_{0\nu}\rho + \frac{1 - f_\nu}{\tau_\nu} \tilde{d}\rho\tilde{d}^\dagger e^{-i\chi_\nu} + \frac{f_\nu}{\tau_\nu} \tilde{d}^\dagger\rho\tilde{d} e^{i\chi_\nu} \right)$$

from which we can derive the rate master equation with the counting fields by using $\langle E|\rho|E\rangle = p_E$ as well as $\langle E|\tilde{d}\tilde{d}^\dagger|E\rangle = 1$ and analogously for F.

$$\partial_t p_E(\boldsymbol{\chi}, t) = \sum_\nu \left(-\frac{f_\nu}{\tau_\nu} p_E(\boldsymbol{\chi}, t) + \frac{1 - f_\nu}{\tau_\nu} e^{-i\chi_\nu} p_F(\boldsymbol{\chi}, t) \right)$$
$$\partial_t p_F(\boldsymbol{\chi}, t) = \sum_\nu \left(-\frac{1 - f_\nu}{\tau_\nu} p_F(\boldsymbol{\chi}, t) + \frac{f_\nu}{\tau_\nu} e^{i\chi_\nu} p_E(\boldsymbol{\chi}, t) \right)$$

which, after imposing $\Gamma = 1/\tau_\nu$ can be summarized as

$$\frac{d}{dt}\begin{pmatrix} p_F(\boldsymbol{\chi}, t) \\ p_E(\boldsymbol{\chi}, t) \end{pmatrix} = \sum_\nu \Gamma \begin{pmatrix} -[1 - f_\nu(\epsilon_0)] & e^{i\chi_\nu} f_\nu(\epsilon_0) \\ e^{-i\chi_\nu}[1 - f_\nu(\epsilon_0)] & -f_\nu(\epsilon_0) \end{pmatrix} \begin{pmatrix} p_F(\boldsymbol{\chi}, t) \\ p_E(\boldsymbol{\chi}, t) \end{pmatrix}.$$

(ii) We now find the eigenvalues of the rate matrix

$$\begin{aligned}
(f_L + f_R + \lambda)(\lambda + 2 - f_L - f_R) - (e^{i\chi_L} f_L + e^{i\chi_R} f_R)(e^{-i\chi_L}[1 - f_L] + e^{-i\chi_R}[1 - f_R]) = 0 \\
\lambda^2 + 2\lambda + 2(f_L + f_R) - (f_L + f_R)^2 - f_L(1 - f_L) - f_R(1 - f_R) + \\
-e^{i(\chi_R - \chi_L)} f_R[1 - f_L] - e^{i(\chi_L - \chi_R)} f_L[1 - f_R] = 0 \\
\lambda^2 + 2\lambda + \left[f_L(1 - f_R)\left(1 - e^{i(\chi_L - \chi_R)}\right) + f_R(1 - f_L)\left(1 - e^{i(\chi_R - \chi_L)}\right) \right] = 0 \\
\lambda^2 + 2\lambda + C(\chi_L - \chi_R) = 0 \to \lambda_\pm = -1 \pm \sqrt{1 - C(\chi_L - \chi_R)}.
\end{aligned}$$

Notice that the first symmetry is satisfied because the eigenvalues only depend on the difference $\chi_L - \chi_R$.

For the second symmetry, we realize that

$$e^{i(\chi_L-\chi_R)} \to e^{i(-\chi_L+\chi_R)}e^{-\beta V} = e^{i(\chi_R-\chi_L)}\frac{e^{-\beta(\epsilon_0-\mu_R)}}{e^{-\beta(\epsilon_0-\mu_L)}} = e^{i(\chi_R-\chi_L)}\frac{f_R}{1-f_R}\frac{1-f_L}{f_L}.$$

Therefore, applying the transformation to $C(\chi_L-\chi_R)$ leads to

$$C(\chi_L-\chi_R) \to \left[f_L(1-f_R)\left(1-\frac{f_R(1-f_L)}{f_L(1-f_R)}e^{i(\chi_R-\chi_L)}\right)+f_R(1-f_L)\left(1-\frac{f_L(1-f_R)}{f_R(1-f_L)}e^{i(\chi_L-\chi_R)}\right)\right]$$
$$C(\chi_L-\chi_R) \to C(\chi_L-\chi_R)$$

meaning that leaves C, and consequently $\lambda_\pm$, invariant.

The formal solution of the rate master equation with the counting fields is

$$\begin{pmatrix} p_F(\boldsymbol{\chi},t) \\ p_E(\boldsymbol{\chi},t)\end{pmatrix} = e^{At}\begin{pmatrix} p_F(0) \\ p_E(0)\end{pmatrix} = e^{\lambda_+ t}\alpha_+\mathbf{v}_+ + e^{\lambda_- t}\alpha_-\mathbf{v}_-$$

where A is the matrix defining the dynamics, $\mathbf{v}_\pm$ are the eigenvectors relative to the eigenvalues $\lambda_\pm$ and the coefficients $\alpha_\pm$ are determined by the initial condition. Then, also $p_\sigma(\boldsymbol{\chi},t)$ obeys the same symmetries as $\lambda_\pm$. This means that the moment generating function is $M(\boldsymbol{\chi},t) = \mathrm{Tr}_S\{\tilde{\rho}_S(\boldsymbol{\chi},t)\} = p_E(\boldsymbol{\chi},t)+p_F(\boldsymbol{\chi},t)$ is a function of the difference of the counting fields, $M(\chi_L-\chi_R,0,t)$. We now can think of looking at the statistics of n_L+n_R by considering the transformation of variables:

$$\xi = \frac{\chi_L+\chi_R}{2}, \quad \zeta = \chi_L-\chi_R$$

from which follows that the moment generating function does not depend on ξ, which leads to

$$\langle\left(\frac{n_L+n_R}{2}\right)^n\rangle \propto \partial_\xi^n M = 0, \quad n>0.$$

This means that $n_L+n_R=0$.

On the other hand, the second symmetry means that

$$M(\boldsymbol{\chi},t) = M(-\boldsymbol{\chi}+i\beta\boldsymbol{\mu},t).$$

Therefore, by using the result of Exercise 4.11 we have

$$\frac{P(n_L)}{P(-n_L)} = e^{\beta(Vn_L/2-Vn_R/2)} = e^{\beta V n_L} = e^{\beta(\mu_L-\mu_R)n_L}$$

Exercise 4.14: Cavity master equation with one jump operator

Consider the cavity master equation derived in Exercise 3.28. Show that it reduces to

$$\partial_t\rho_S(t) = J\rho_S(t)J^\dagger - \frac{1}{2}\{J^\dagger J,\rho_S(t)\}$$

in the limit $\beta\hbar\omega_c\to\infty$.

Solution:
The cavity master equation is

$$\partial_t\rho_S = -i[\omega_c a^\dagger a,\rho_S] + \frac{1}{\tau_c}\left\{[N_c+1]\left(a\rho_S a^\dagger - \frac{1}{2}\{a^\dagger a,\rho_S(t)\}\right) + N_c\left(a^\dagger\rho_S a - \frac{1}{2}\{aa^\dagger,\rho_S(t)\}\right)\right\}.$$

with $N_c = \frac{1}{e^{\beta\hbar\omega_c}-1} \overset{\beta\hbar\omega\to\infty}{\longrightarrow} 0$ so we are left with

$$\partial_t\rho_S = -i[\omega_c a^\dagger a,\rho_S] + \frac{1}{\tau_c}\left(a\rho_S a^\dagger - \frac{1}{2}\{a^\dagger a,\rho_S(t)\}\right).$$

In the interaction picture this reads

$$\partial_t\tilde{\rho}_S = J\rho_S J^\dagger - \frac{1}{2}\{J^\dagger J,\rho_S\}$$

with $J = \frac{a}{\sqrt{\tau_c}}$ represents the decay to the ground state due to spontaneous emission.

Exercise 4.15: Master equation and quantum measurement process

Consider the average post-measurement state $\rho_S(t+dt) = (\mathcal{M}_0 + \mathcal{M}_1)\rho_S(t)$, with

$$\mathcal{M}_0\rho = \mathcal{J}\rho dt = J\rho J^\dagger dt, \qquad \mathcal{M}_1\rho = \left(1 - \frac{J^\dagger J}{2}dt\right)\rho\left(1 - \frac{J^\dagger J}{2}dt\right)$$

Show that for infinitesimal dt the time evolutions is identical to the prediction of the master equation.

Solution:

$$\rho(t+dt) = (\mathcal{M}_0 + \mathcal{M}_1)\rho(t) = J\rho J^\dagger dt + \rho - \frac{dt}{2}\{J^\dagger J, \rho\} + \mathcal{O}(dt^2)$$

$$\partial_t\rho = J\rho J^\dagger - \frac{1}{2}\{J^\dagger J, \rho\}$$

Interestingly, by considering the Kraus representation of a POVM $\{K_i\}$, the post measument state is

$$\rho^+ = \sum_i \mathcal{M}_i\rho^- = \sum_i K_i\rho^- K_i^\dagger$$

$$\rho^+ - \rho^- = \sum_i \left(K_i\rho^- K_i^\dagger - \frac{1}{2}\{K_i^\dagger K_i, \rho^-\}\right)$$

so when the probability of a measurement becomes infinitesimal, one can cast the above equation as a differential equation.

Exercise 4.16: Master equation and stochastic Schrödinger equation

Given the stochastic Schrödinger equation

$$d\left|\psi(t)\right\rangle = \left[dn(t)\left(\frac{J}{\sqrt{\langle J^\dagger J\rangle_{\psi(t)}}} - 1\right) + \frac{dt}{2}\left(\langle J^\dagger J\rangle_{\psi(t)} - J^\dagger J\right)\right]\left|\psi(t)\right\rangle,$$

with $[dn(t)]^2 = dn(t)$, $\mathbb{E}_{\psi(t)}[dn(t)] = \langle J^\dagger J\rangle_{\psi(t)}dt$ and $\langle X\rangle_{\psi(t)} = \langle\psi(t)|X|\psi(t)\rangle$, consider the density matrix $\sigma = |\psi(t)\rangle\langle\psi(t)|$ and show that

$$d\sigma(t) = dn(t)\left[\frac{J\sigma(t)J^\dagger}{\langle J^\dagger J\rangle_{\sigma(t)}} - \sigma(t)\right] + dt\left[\langle J^\dagger J\rangle_{\sigma(t)}\sigma(t) - \frac{1}{2}\{J^\dagger J, \sigma(t)\}\right]$$

and use it tho derive

$$\rho_S(t) = \mathbb{E}[\sigma(t)],$$

namely that the density matrix obtained from the master equation is the expectation value over the ensemble of quantum jump trajectories generated by the stochastic Schrödinger equation.

Solution:
Since $\sigma = |\psi(t)\rangle\langle\psi(t)|$ we have

$$d\sigma = |d\psi(t)\rangle\langle\psi(t)| + |\psi(t)\rangle\langle d\psi(t)| + |d\psi(t)\rangle\langle d\psi(t)|,$$

where in the last term only the term $[dn(t)]^2 = dn$ contributes at first order in dt at the level of the expectation value. Therefore, we have

$$d\sigma = \left[dn(t)\left(\frac{J}{\sqrt{\langle J^\dagger J\rangle_\sigma}} - 1\right) + \frac{dt}{2}\left(\langle J^\dagger J\rangle_\sigma - J^\dagger J\right)\right]\sigma +$$
$$+ \sigma\left[dn(t)\left(\frac{J^\dagger}{\sqrt{\langle J^\dagger J\rangle_\sigma}} - 1\right) + \frac{dt}{2}\left(\langle J^\dagger J\rangle_\sigma - J^\dagger J\right)\right] + dn(t)\left(\frac{J}{\sqrt{\langle J^\dagger J\rangle_\sigma}} - 1\right)\sigma\left(\frac{J^\dagger}{\sqrt{\langle J^\dagger J\rangle_\sigma}} - 1\right)$$
$$d\sigma = dn\left[\frac{J\sigma J^\dagger}{\langle J^\dagger J\rangle_\sigma} - \sigma\right] + dt\left[\langle J^\dagger J\rangle_\sigma\sigma - \frac{1}{2}\{J^\dagger J, \sigma\}\right].$$

Taking the expectation value of this equation we find

$$\begin{aligned}\mathbb{E}[d\sigma] &= \sum_k \lambda_k(0)\left\{\langle J^\dagger J\rangle_{\sigma_k} dt\left[\frac{J\sigma_k J^\dagger}{\langle J^\dagger J\rangle_{\sigma_k}} - \sigma_k\right] + dt\left[\langle J^\dagger J\rangle_{\sigma_k}\sigma_k - \frac{1}{2}\{J^\dagger J, \sigma_k\}\right]\right\} \\ &= dt\sum_k \lambda_k(0)\left\{J\sigma_k J^\dagger - \frac{1}{2}\{J^\dagger J, \sigma_k\}\right\} \\ d\rho &= dt\left(J\rho J^\dagger - \frac{1}{2}\{J^\dagger J, \rho\}\right)\end{aligned}$$

where we used that the average over the ensemble of quantum jump trajectories acts as

$$\mathbb{E}[\sigma(t)] \approx \sum_k \lambda_k(0)\mathbb{E}_{\psi_k(0)}[\cdots[\mathbb{E}_{\psi_k(N\delta t)}[\sigma]]\cdots] = \sum_k \lambda_k(0)\sigma_k(t)$$

Then, since $\mathbb{E}[\sigma(0)] = \rho$ and they obey the same differential equation they coincide at all times

$$\mathbb{E}[\sigma(t)] = \rho(t).$$

Exercise 4.17: Stochastic Schrödinger equation preserves purity

Show that

$$d\sigma(t) = dn(t)\left[\frac{J\sigma(t)J^\dagger}{\langle J^\dagger J\rangle_{\sigma(t)}} - \sigma(t)\right] + dt\left[\langle J^\dagger J\rangle_{\sigma(t)}\sigma(t) - \frac{1}{2}\{J^\dagger J, \sigma(t)\}\right]$$

preserves the purity of a state.

Solution:
A pure state satisfies $\rho^2 = \rho$. Therefore, let's look at $\sigma(t+dt)^2$ assuming that $\sigma(t)$ is pure:

$$\begin{aligned}\sigma(t+dt)^2 &= \left(\sigma(t) + dn(t)\left[\frac{J\sigma(t)J^\dagger}{\langle J^\dagger J\rangle_{\sigma(t)}} - \sigma(t)\right] + dt\left[\langle J^\dagger J\rangle_{\sigma(t)}\sigma(t) - \frac{1}{2}\{J^\dagger J, \sigma(t)\}\right]\right)^2 \\ &= \sigma(t) + dn\left[\frac{J\sigma(t)J^\dagger}{\langle J^\dagger J\rangle_{\sigma(t)}} - \sigma(t)\right]^2 + dn\left\{\left[\frac{J\sigma(t)J^\dagger}{\langle J^\dagger J\rangle_{\sigma(t)}} - \sigma(t)\right], \sigma\right\} + \\ &\quad + dt\left\{\left[\langle J^\dagger J\rangle_{\sigma(t)}\sigma(t) - \frac{1}{2}\{J^\dagger J, \sigma(t)\}\right], \sigma\right\} + \mathcal{O}(dt^2) \\ &= \sigma + dn\left(\left[\frac{J\sigma J^\dagger}{\langle J^\dagger J\rangle_\sigma}\right]^2 - \sigma\right) + dt\left(2\langle J^\dagger J\rangle_\sigma\sigma - \frac{1}{2}\{J^\dagger J, \sigma\} - \sigma J^\dagger J\sigma\right) \\ &= \sigma(t+dt) + dn\left(\frac{J\sigma J^\dagger J\sigma J^\dagger}{\langle J^\dagger J\rangle_\sigma^2} - \frac{J\sigma J^\dagger}{\langle J^\dagger J\rangle_\sigma}\right) + dt\left(\langle J^\dagger J\rangle_\sigma\sigma - \sigma J^\dagger J\sigma\right).\end{aligned}$$

Crucially, since σ is pure it can be written as $\sigma = |x\rangle\langle x|$, then, one notices that

$$\sigma J^\dagger J\sigma = |x\rangle\langle x| J^\dagger J |x\rangle\langle x| = \langle J^\dagger J\rangle_\sigma\sigma$$

which makes the dn and dt contributions vanish, leaving us with

$$\sigma^2(t) = \sigma(t) \quad \Rightarrow \quad \sigma^2(t+dt) = \sigma(t+dt)$$

which means that, as long as the dynamics starts from a pure state, the state will continue to be pure.

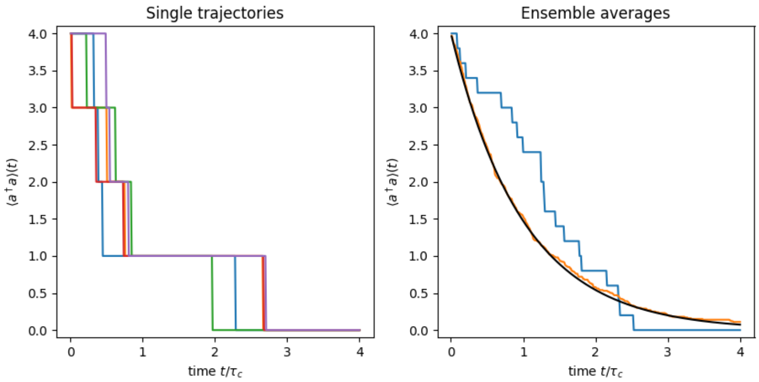


Figure 5: Single trajectories and enseble averages for the stochastic Schrödinger equation of a low-temperature cavity. The initial state was chosen to be $a^\dagger a\,|\psi(0)\rangle = 4\,|\psi(0)\rangle$.

Exercise 4.18: Comparing master equation and stochastic Schrödinger equation

In Exercise 4.14 it was shown that the master equation of an open cavity in the low-temperature and high-frequency regime is determined by one Lindblad operator $J = \sqrt{\gamma} a$ for some rate γ.

Show that the average number of photons in the cavity decays exponentially to zero:

$$\langle a^\dagger a\rangle(t) = e^{-\gamma t}\langle a^\dagger a\rangle(0).$$

Reproduce the behaviour using the stochastic Schrödinger equation.

Solution:
From Exercise 4.14 we read the master equation:

$$\partial_t\tilde{\rho} = J\tilde{\rho}J^\dagger - \frac{1}{2}\{J^\dagger J, \tilde{\rho}\}$$

with $J = \frac{a}{\sqrt{\tau_c}}$. To calculate the average photon number we can start from the derivative

$$\partial_t n(t) = \partial_t \mathrm{Tr}\left\{a^\dagger a\rho\right\} = \mathrm{Tr}\left\{a^\dagger a\left(-\frac{i}{\hbar}[H,\rho] + \mathcal{D}\rho\right)\right\} = -\frac{i}{\hbar}\mathrm{Tr}\left\{[a^\dagger a, H]\rho\right\} + \mathrm{Tr}\left\{a^\dagger a\mathcal{D}\rho\right\} = \mathrm{Tr}\left\{a^\dagger a\mathcal{D}\rho\right\}$$

since the system Hamiltonian is $H = \omega_c a^\dagger a$. Since

$$\mathrm{Tr}\left\{a^\dagger a\mathcal{D}\rho\right\} = \frac{1}{\tau_c}\mathrm{Tr}\left\{a^\dagger a a\rho a^\dagger - a^\dagger a a^\dagger a\rho\right\} = \frac{1}{\tau_c}\mathrm{Tr}\left\{a^\dagger a^\dagger a a\rho - a^\dagger(1 + a^\dagger a)a\rho\right\} = -\frac{1}{\tau_c}\mathrm{Tr}\left\{a^\dagger a\rho\right\} = -\frac{n(t)}{\tau_c},$$

we have the differential equation $\partial_t n(t) = -n(t)/\tau_c$ which is solved by the negative exponential

$$n(t) = e^{-t/\tau_c} n(0).$$

```
import numpy as np
from qutip import *
import matplotlib.pyplot as plt
#######################################################################
N= 5;    # Cut of the Hilbert space
a = destroy(N); # Annihilation operator
ad= create(N);  # Creation operator
n = num(N);     # Number operator
#######################################################################
def evolution_step(J, sigma, dt):
    Jd = J.dag();
    JdJs = Jd*J*sigma;
    sJdJ = sigma*Jd*J;

    sigmaF=sigma;

    avg = JdJs.tr();
    pjump = avg*dt;
    rnd = np.random.random();
    if rnd<pjump:
```

```
        sigmaF = J*sigma*Jd/avg;
    sigmaF+= dt*(avg*sigma - (JdJs+sJdJ)/2);
    return sigmaF/sigmaF.tr()

def evolution_tot(sigma0, Ntot, J, dt):
    nlist = np.zeros(Ntot);
    sigma = evolution_step(J, sigma0, dt)
    for i in range(Ntot):
        nlist[i] = (n*sigma).tr();
        sigma = evolution_step(J, sigma, dt)
    return nlist

def ensemble_avg(iterations, sigma0, Ntot, J, dt):
    Nensemble = np.zeros(Ntot)
    for i in range(iterations):
        Nensemble += evolution_tot(sigma0, Ntot, J, dt)
    return Nensemble/iterations
########################################################################
dt = 0.01;  # time step
tau = 1.;   # cavity relaxation time
Ntot = 4*int(tau/dt)

J = a/np.sqrt(tau);
sigma0 = fock_dm(N, 4); # Initial state

n0 = (n*sigma0).tr();
times = np.linspace(dt, Ntot*dt, Ntot);

plt.subplot(121)
for i in range(5):
    nlist = evolution_tot(sigma0, Ntot, J, dt)
    plt.plot(times, nlist)
plt.title(r"Single trajectories"); plt.ylim([-0.1,4.1])
plt.xlabel(r"time $t/\tau_c$"); plt.ylabel(r"$\langle a^\dagger a \rangle(t)$");

plt.subplot(122)
iterations = [5, 100]
for it in iterations:
    Nensemble = ensemble_avg(it, sigma0, Ntot, J, dt)
    plt.plot(times, Nensemble)
plt.plot(times, n0*np.exp(-times/tau), 'k')
plt.title(r"Ensemble averages"); plt.ylim([-0.1,4.1])
plt.xlabel(r"time $t/\tau_c$"); plt.ylabel(r"$\langle a^\dagger a \rangle(t)$")
########################################################################
plt.show()
```

Exercise 4.19: General stochastic Schrödinger equation

Show that the unraveling of the master equation of the form

$$\partial_t \rho_S(t) = -\frac{i}{\hbar}[H, \rho_S(t)] + \sum_k \left(J_k \rho_S(t) J_k^\dagger - \frac{1}{2}\{J_k^\dagger J_k, \rho_S(t)\} \right),$$

which contains a coherent part $H = H^\dagger$, and multiple jump superoperators $\mathcal{J}_k \rho_S = J_k \rho_S J_k^\dagger$, leads to the stochastic Schrödinger equation

$$d|\psi(t)\rangle = \sum_k \left[dn_k(t) \left(\frac{J_k}{\langle J_k^\dagger J_k \rangle_{\psi(t)}^{1/2}} - 1 \right) + \frac{dt}{2} \left(\langle J_k^\dagger J_k \rangle_{\psi(t)} - J_k^\dagger J_k \right) \right] |\psi(t)\rangle - dt \frac{i}{\hbar} H |\psi(t)\rangle,$$

where the point process is defined by

$$dn_k(t) dn_l(t) = \delta_{kl} dn_k(t), \quad \mathbb{E}_{\psi(t)}[dn_k(t)] = \langle J_k^\dagger J_k \rangle_{\psi(t)} dt.$$

Solution:
Consider a jump detector described by the set $\{\mathcal{M}_0, \mathcal{M}_k\}$, with

$$\mathcal{M}_k \rho = J_k \rho J_k^\dagger dt \to M_k = J_k \sqrt{dt}$$

and $\mathcal{M}_0$ completing the CPTP map through

$$M_0^\dagger M_0 + \sum_k M_k^\dagger M_k = \mathbb{I} \to M_0^\dagger M_0 = \mathbb{I} - dt \sum_k J_k^\dagger J_k \to M_0 = \mathbb{I} - \frac{dt}{2} \sum_k J_k^\dagger J_k$$

such that the detector map is a CPTP map at the first order in dt. At each time step dt, the detector can detect a jump k, meaning $dn_k(t) = 1$, causing the collapse of the way function. Since the probability of seeing the jump k in the time step dt is

$$p_{\text{jump}\, k} = \mathbb{E}[dn_k(t)] = \langle J_k^\dagger J_k \rangle dt$$

for sufficiently small dt at most one jump will happen: $dn_k(t) dn_l(t) = \delta_{kl} dn_l(t)$. If instead no jump k happened, the detector acted through $\mathcal{M}_0$. On top of that, we also have to consider the unitary evolution induced by the Hamiltonian. For the moment, let's write the latter as the superoperator $\mathcal{U}$, such that the state at time $t + dt$ reads

$$|\psi(t+dt)\rangle = \sum_k dn_k \mathcal{U} \frac{J_k |\psi(t)\rangle}{\sqrt{\langle J_k^\dagger J_k \rangle_{\psi(t)}}} + \left(1 - \sum_j dn_j\right) \mathcal{U} \left(\frac{|\psi(t)\rangle - \frac{dt}{2} \sum_k J_k^\dagger J_k |\psi(t)\rangle}{\sqrt{1 - dt \sum_k \langle J_k^\dagger J_k \rangle_{\psi(t)} + \mathcal{O}(dt^2)}} \right)$$

$$|\psi(t+dt)\rangle \approx \sum_k dn_k \mathcal{U} \frac{J_k |\psi(t)\rangle}{\sqrt{\langle J_k^\dagger J_k \rangle_{\psi(t)}}} + \left(1 - \sum_j dn_j\right) \mathcal{U} \left(|\psi(t)\rangle + \frac{dt}{2} \sum_k \left(\langle J_k^\dagger J_k \rangle_{\psi(t)} - J_k^\dagger J_k \right) |\psi(t)\rangle \right)$$

We now consider the Hamiltonian evolution explicitely:

$$\mathcal{U} |\psi\rangle = |\psi\rangle - \frac{i}{\hbar} H |\psi\rangle \, dt$$

and neglect the quadratic terms in dt^2 as wellas the terms $dn_k dt$ because the expectation value of dn_k already scales as dt. Then, the state difference $d|\psi(t)\rangle$ is

$$d|\psi(t)\rangle \approx \sum_k dn_k \left(\frac{J_k |\psi(t)\rangle}{\sqrt{\langle J_k^\dagger J_k \rangle_{\psi(t)}}} - |\psi(t)\rangle \right) + dt \left(\frac{1}{2} \sum_k \left(\langle J_k^\dagger J_k \rangle_{\psi(t)} - J_k^\dagger J_k \right) |\psi(t)\rangle - \frac{i}{\hbar} H |\psi(t)\rangle \right)$$

From this, we can calculate the differential of the density matrix $d\sigma = d[|\psi(t)\rangle\langle\psi(t)|]$

$$\begin{aligned} d\sigma &= \sum_k dn_k \left(\frac{J_k \sigma}{\sqrt{\langle J_k^\dagger J_k \rangle_\sigma}} - \sigma + \frac{\sigma J_k^\dagger}{\sqrt{\langle J_k^\dagger J_k \rangle_\sigma}} - \sigma + \frac{J_k \sigma J_k^\dagger}{\langle J_k^\dagger J_k \rangle_\sigma} + \sigma - \frac{J_k \sigma}{\sqrt{\langle J_k^\dagger J_k \rangle_\sigma}} - \frac{\sigma J_k^\dagger}{\sqrt{\langle J_k^\dagger J_k \rangle_\sigma}} \right) + \\ &\quad + dt \left(\frac{1}{2} \sum_k \left(2 \langle J_k^\dagger J_k \rangle_\sigma \sigma - \{ J_k^\dagger J_k, \sigma \} \right) - \frac{i}{\hbar} [H, \sigma] \right) \\ d\sigma &= \sum_k dn_k \left(\frac{J_k \sigma J_k^\dagger}{\langle J_k^\dagger J_k \rangle_\sigma} - \sigma \right) + dt \left(\sum_k \left(\langle J_k^\dagger J_k \rangle_\sigma \sigma - \frac{1}{2} \{ J_k^\dagger J_k, \sigma \} \right) - \frac{i}{\hbar} [H, \sigma] \right). \end{aligned}$$

We can now take the expectation value over the ensemble of quantum jump trajectories. Crucially, the expectation value over the last jump is done at $\sigma(t)$ fixed. This means that it acts only on dn_k through $\mathbb{E}_{\sigma(t)}[dn_k] = \langle J_k^\dagger J_k \rangle_\sigma dt$, which leads to

$$\begin{aligned} \mathbb{E}[d\sigma] &= \sum_j \lambda_j(0) \left\{ \sum_k \langle J_k^\dagger J_k \rangle_{\sigma_j(t)} dt \left(\frac{J_k \sigma_j(t) J_k^\dagger}{\langle J_k^\dagger J_k \rangle_{\sigma_j(t)}} - \sigma_j(t) \right) + \right. \\ &\quad \left. dt \left(\sum_k \left(\langle J_k^\dagger J_k \rangle_{\sigma_j(t)} \sigma_j(t) - \frac{1}{2} \{ J_k^\dagger J_k, \sigma_j(t) \} \right) - \frac{i}{\hbar} [H, \sigma_j(t)] \right) \right\} \\ d\rho = \mathbb{E}[d\sigma] &= dt \sum_j \lambda_j(0) \left\{ \sum_k \left(J_k \sigma_j(t) J_k^\dagger - \frac{1}{2} \{ J_k^\dagger J_k, \sigma_j(t) \} \right) - \frac{i}{\hbar} [H, \sigma_j(t)] \right\} \\ \partial_t \rho &= -\frac{i}{\hbar} [H, \rho(t)] + \sum_k \left(J_k \rho(t) J_k^\dagger - \frac{1}{2} \{ J_k^\dagger J_k, \rho(t) \} \right), \end{aligned}$$

which is the Markovian master equation.

Exercise 4.20: Coherences do not affect the jump probability

Show that

$$p_{\text{jump}\,\omega}(t) = r_\omega \text{Tr}_S \left\{ S_\omega^\dagger S_\omega \rho_S(t) \right\} dt = r_\omega \text{Tr}_S \left\{ S_\omega^\dagger S_\omega \mathcal{D}_{H_t} \rho_S(t) \right\} dt,$$

where $\mathcal{D}_{H_t}$ is the dephasing operator with respect to the eigenbasis of H_t.

Solution:
From Exercise 3.5 we know that the Fourier components of the coupling are defined by

$$S_\omega = \sum_x \Pi(x) S \Pi(x + \hbar\omega)$$

which means that

$$S_\omega^\dagger S_\omega = \sum_{xy} \Pi(x + \hbar\omega) S^\dagger \Pi(y) \Pi(x) S \Pi(x + \hbar\omega) = \sum_x \Pi(x) S^\dagger S \Pi(x).$$

Then, we can calculate

$$\text{Tr}_S \left\{ S_\omega^\dagger S_\omega \mathcal{D}_H \rho \right\} = \sum_{xk} \text{Tr} \left\{ \Pi(x) S^\dagger S \Pi(x) \Pi(k) \rho \Pi(k) \right\} = \sum_x \text{Tr} \left\{ \Pi(x) S^\dagger S \Pi(x) \rho \right\} = \text{Tr} \left\{ S_\omega^\dagger S_\omega \rho \right\},$$

which leads to the result we were looking for.

Exercise 4.21: Quantum stochastic heat

Starting from the separation of stochastic heat into a classical component and a quantum one,

$$đq = đq_{\text{qu}} + đq_{\text{cl}} = \text{Tr}_S \left\{ H_t [d\sigma(t)] \right\}, \qquad đq_{\text{cl}} = -\sum_\omega \hbar\omega dn_\omega(t),$$

use the stochastic Schrödinger equation from Exercise 4.19 to show that

$$đq_{\text{qu}} \equiv \sum_\omega dn_\omega(t) \text{Tr}_S \left\{ \frac{S_\omega \{H_t, \sigma(t)\} S_\omega^\dagger}{2 \langle S_\omega^\dagger S_\omega \rangle_{\sigma(t)}} - H_t \sigma(t) \right\} + dt \sum_\omega r_\omega \text{Tr}_S \left\{ \langle S_\omega^\dagger S_\omega \rangle_{\sigma(t)} H_t \sigma(t) - H_t S_\omega^\dagger S_\omega \sigma(t) \right\}.$$

Solution:
Let's start with writing down the trace. Notably, the commutator $[H, \sigma]$ entering $d\sigma$ does not contribute to the trace because $\text{Tr}\{A[B,C]\} = \text{Tr}\{[A,B]C\}$ with $A = B = H$ and $C = \sigma$. Then, we are left with

$$\begin{aligned}
\text{Tr}\{H[d\sigma]\} &= \sum_k dn_k(t) \text{Tr} \left\{ \frac{H J_k \sigma J_k^\dagger}{\langle J_k^\dagger J_k \rangle_\sigma} - H\sigma \right\} + dt \sum_k \text{Tr} \left\{ \langle J_k^\dagger J_k \rangle_\sigma H \sigma - \frac{1}{2} H \{J_k^\dagger J_k, \sigma\} \right\} \\
&= \sum_k dn_k(t) \text{Tr} \left\{ \frac{H S_k \sigma S_k^\dagger}{\langle S_k^\dagger S_k \rangle_\sigma} - H\sigma \right\} + dt \sum_k r_k \text{Tr} \left\{ \langle S_k^\dagger S_k \rangle_\sigma H \sigma - \frac{1}{2} H \{S_k^\dagger S_k, \sigma\} \right\}
\end{aligned}$$

where we used $J_k = \sqrt{r_k} S_k$, with S_k being the Fourier components of the coupling Hamiltonians. The latter, according to what we have seen in Exercise 3.5, satisfy

$$[S_\omega, H] = \hbar\omega S_\omega \quad \to \quad -[S_\omega^\dagger, H] = \hbar\omega S_\omega^\dagger$$

which also imples that

$$S_\omega^\dagger S_\omega H = S_\omega^\dagger (\hbar\omega + H) S_\omega = (\hbar\omega + H - \hbar\omega) S_\omega^\dagger S_\omega = H S_\omega^\dagger S_\omega \quad \to \quad [H, S_\omega^\dagger S_\omega] = 0.$$

Let us focus only on the very first term of the trace:

$$\begin{aligned}
\text{Tr} \left\{ \frac{H S_\omega \sigma S_\omega^\dagger}{\langle S_\omega^\dagger S_\omega \rangle_\sigma} \right\} &= \frac{1}{2} \text{Tr} \left\{ \frac{H S_\omega \sigma S_\omega^\dagger}{\langle S_\omega^\dagger S_\omega \rangle_\sigma} + \frac{S_\omega \sigma S_\omega^\dagger H}{\langle S_\omega^\dagger S_\omega \rangle_\sigma} \right\} = \frac{1}{2} \text{Tr} \left\{ \frac{S_\omega (H - \hbar\omega) \sigma S_\omega^\dagger}{\langle S_\omega^\dagger S_\omega \rangle_\sigma} + \frac{S_\omega \sigma (H - \hbar\omega) S_\omega^\dagger}{\langle S_\omega^\dagger S_\omega \rangle_\sigma} \right\} \\
&= \frac{1}{2} \text{Tr} \left\{ \frac{S_\omega \{H, \sigma\} S_\omega^\dagger}{\langle S_\omega^\dagger S_\omega \rangle_\sigma} \right\} - \hbar\omega \text{Tr} \left\{ \frac{S_\omega \sigma S_\omega^\dagger}{\langle S_\omega^\dagger S_\omega \rangle_\sigma} \right\} = \frac{1}{2} \text{Tr} \left\{ \frac{S_\omega \{H, \sigma\} S_\omega^\dagger}{\langle S_\omega^\dagger S_\omega \rangle_\sigma} \right\} - \hbar\omega
\end{aligned}$$

which can be used to identify the classical stochastic heat as

$$đq_{\rm cl} = \sum_\omega dn_\omega {\rm Tr}\left\{\frac{HS_\omega\sigma S_\omega^\dagger}{\langle S_\omega^\dagger S_\omega\rangle_\sigma} - \frac{S_\omega\{H,\sigma\}S_\omega^\dagger}{2\langle S_\omega^\dagger S_\omega\rangle_\sigma}\right\}.$$

Finally, we can extract the quantum stochastic heat from the trace as

$$đq_{\rm qu} = \sum_\omega dn_\omega {\rm Tr}\left\{\frac{S_\omega\{H,\sigma\}S_\omega^\dagger}{2\langle S_\omega^\dagger S_\omega\rangle_\sigma} - H\sigma\right\} + dt\sum_\omega r_\omega {\rm Tr}\left\{\langle S_\omega^\dagger S_\omega\rangle_\sigma H\sigma - HS_\omega^\dagger S_\omega\sigma\right\}$$

where we used $[H, S_\omega^\dagger S_\omega] = 0$ to get rid of the last anticommutator inside the trace.

Exercise 4.22: Quantum stochastic heat vanishes on average

Using the definition of quantum stochastic heat $đq_{\rm qu}$ from Exercise 4.21, show that the ensemble average over the quantum jump trajectories of the quantum stochastic heat vanishes, namely

$$\mathbb{E}[đq_{\rm qu}] = 0.$$

Solution:
Since the expectation values over the very last step of the quantum jump trajectory is done at fixed $\sigma(t)$, it acts nontrivially only of dn_ω through

$$\mathbb{E}_{\sigma(t)}[dn_\omega(t)] = r_\omega\langle S_\omega^\dagger S_\omega\rangle dt.$$

Then, taking the ensemble average over all quantum jump trajectories of the quantum sotchastic heat from Exercise 4.21 we find

$$\begin{aligned}\mathbb{E}[đq_{\rm qu}] &= dt\sum_j\lambda_j\sum_\omega r_\omega{\rm Tr}\left\{S_\omega\frac{\{H,\sigma_j(t)\}}{2}S_\omega^\dagger - \langle S_\omega^\dagger S_\omega\rangle_{\sigma_j(t)}H\sigma_j(t) + \langle S_\omega^\dagger S_\omega\rangle_{\sigma_j(t)}H\sigma_j(t) - HS_\omega^\dagger S_\omega\sigma_j(t)\right\}\\ &= dt\sum_j\lambda_j\sum_\omega r_\omega{\rm Tr}\left\{S_\omega\frac{\{H,\sigma_j(t)\}}{2}S_\omega^\dagger - HS_\omega^\dagger S_\omega\sigma_j(t)\right\} = 0\end{aligned}$$

due to the cyclic property of the trace and the commutation relation $[H, S_\omega^\dagger S_\omega] = 0$.

Exercise 4.23: Concavity of the Shannon entropy

Show that the Shannon entropy $S(p) \equiv -p\ln p - (1-p)\ln(1-p)$ for $p\in[0,1]$ is concave.

Solution:
It is sufficient to show that the second derivative of $S(p)$ is negative in the interval.

$$\partial_p S[p] = -\ln p - 1 + \ln(1-p) + 1 = \ln(1-p) - \ln(p)$$

$$\partial_p^2 S[p] = -\frac{1}{1-p} - \frac{1}{p} < 0 \quad \forall p\in(0,1).$$

Therefore, he Shannon entropy satisfies

$$S(qx + (1-q)y) \geq qS(x) + (1-q)S(y)$$

which means that mixing two probability distributions generates more entropy than the weighted sum of the individual distribution's entropy.

Exercise 4.24: From the integral fluctuation theorem to the 2nd law through Jensen's inequality

Use Jensen's inequality to show that the integral fluctuation theorem $\langle e^{-\sigma}\rangle = 1$ imples the second law $\langle\sigma\rangle \geq 0$.

Solution:
We probably have already used Jensen's inequality to find this result in a previous exercise. Nonetheless, since e^x is convex, we have $e^{px+(1-p)y} \leq pe^x + (1-p)e^y$ which allows us to write

$$1 = \langle e^{-\sigma} \rangle \geq e^{-\langle \sigma \rangle} \quad \rightarrow \quad -\langle \sigma \rangle \leq 0 \quad \rightarrow \quad \langle \sigma \rangle \geq 0.$$

Exercise 4.25: Thermodynamic uncertainty relation for entropy production

Assuming the detailed fluctuation theorem of the form

$$\frac{P(\sigma)}{P(-\sigma)} = e^{\sigma/k_B},$$

and defining

$$Q(\sigma) \equiv (1 + e^{-\sigma/k_B})P(\sigma), \quad \text{for } \sigma \in [0, \infty)$$

show that

$$\Sigma \equiv \langle \sigma \rangle = \left\langle \sigma \tanh\left(\frac{\sigma}{2k_B}\right) \right\rangle_Q, \qquad \langle \sigma^2 \rangle = \langle \sigma^2 \rangle_Q,$$

where $\langle \cdots \rangle$ ($\langle \cdots \rangle_Q$) denotes the average with respect to the probability distirbution P (Q).

Finally, show that

$$\langle \sigma^2 \rangle \geq 2k_B \Sigma.$$

Solution:

$$\langle \sigma \rangle = \int_{-\infty}^{\infty} d\sigma \sigma P(\sigma) = \int_0^{\infty} d\sigma \sigma [P(\sigma) - P(-\sigma)] = \int_0^{\infty} d\sigma \sigma P(\sigma)[1 - e^{-\sigma}] = \int_0^{\infty} d\sigma \sigma Q(\sigma) \tanh\left(\frac{\sigma}{2}\right) = \left\langle \sigma \tanh \frac{\sigma}{2} \right\rangle_Q$$

$$\langle \sigma^2 \rangle = \int_{-\infty}^{\infty} d\sigma \sigma^2 P(\sigma) = \int_0^{\infty} d\sigma \sigma^2 [P(\sigma) + P(-\sigma)] = \int_0^{\infty} d\sigma \sigma^2 Q(\sigma) = \langle \sigma^2 \rangle_Q.$$

The thermodynamic uncertainty relation stems from

$$\langle \sigma^2 \rangle = \langle \sigma^2 \rangle_Q = \langle 4 \frac{\sigma}{2} \frac{\sigma}{2} \rangle_Q \geq 2 \langle \sigma \tanh \frac{\sigma}{2} \rangle_Q = 2\Sigma$$

were we used $x \geq \tanh x$ for $x \geq 0$.

Exercise 4.26: Equivalence between fluctuation theorems

Recall the exchange fluctuation theorem (see Exercise 4.7)

$$\frac{P(\Delta \boldsymbol{\epsilon}, \Delta \mathbf{n})}{P_{\text{tr}}(-\Delta \boldsymbol{\epsilon}, -\Delta \mathbf{n})} = \exp\left[\sum_\nu \beta_\nu (\Delta \epsilon_\nu - \mu_\nu \Delta n_\nu)\right]$$

and define the stochastic entropy production $\sigma \equiv k_B \sum_\nu \beta_\nu (\Delta \epsilon_\nu - \mu_\mu \Delta n_\nu)$.

Which measurement results define the trajectory γ? Show that the fluctuation theorem

$$e^{\sigma(\gamma)/k_B} = \frac{p(\gamma)}{p(\gamma^\dagger)},$$

where $p(\gamma)$ is the probability of observing the trajectory γ and $\gamma^\dagger$ is the conjugate ("time-reversed") trajectory, is identical to the exchange fluctuation theorem.

Verify that the fluctuation theorem in the form

$$\frac{P(\sigma)}{P(-\sigma)} = e^{\sigma/k_B}$$

holds.

Solution:
Defining the trajectory $\gamma = (x_i, x_f)$ where $x = (\boldsymbol{\epsilon}, \mathbf{n})$ is the vector storing the outcomes of the measurements of energy and particle numbers of each bath. Then, from the exchange fluctuation theorem we have

$$\begin{aligned} P(\Delta\boldsymbol{\epsilon}, \Delta\mathbf{n})e^{-\sigma} &= e^{-\sigma}\sum_\gamma p(\gamma)\delta(\Delta\boldsymbol{\epsilon} - [\boldsymbol{\epsilon}_f - \boldsymbol{\epsilon}_i]) = \sum_\gamma e^{-\sigma(\gamma)}p(\gamma)\delta(\Delta\boldsymbol{\epsilon} - [\boldsymbol{\epsilon}_f - \boldsymbol{\epsilon}_i]) \\ &= \sum_\gamma p(\gamma^\dagger)\delta(-\Delta\boldsymbol{\epsilon} - [\boldsymbol{\epsilon}_i - \boldsymbol{\epsilon}_f])\delta(-\Delta\mathbf{n} - [\mathbf{n}_i - \mathbf{n}_f]) = P_{\mathrm{tr}}(-\Delta\boldsymbol{\epsilon}, -\Delta\mathbf{n}) \\ \Rightarrow e^{-\sigma(\gamma)}p(\gamma) = p(\gamma^\dagger). \end{aligned}$$

Then, the probability $P(\sigma)$ satisfies

$$P(\sigma) = \sum_\gamma p(\gamma)\delta[\sigma - \sigma(\gamma)] = \sum_\gamma p(\gamma^\dagger)\delta[\sigma - \sigma(\gamma^\dagger)] = \sum_\gamma p(\gamma)e^{-\sigma(\gamma)}\delta[\sigma + \sigma(\gamma)] = e^\sigma P(-\sigma).$$

Exercise 4.27: Anti-symmetric functionals of stochastic trajectories

Starting from the setup of the previous exercise, Exercise 4.26, show that the change of energy $\Delta\epsilon_\nu$ or particle number Δn_ν of bath ν, as well as any linear combination of them is a functional $\phi(\gamma)$ of the stochastic trajectory γ satisfying

$$\phi(\gamma^\dagger) = -\phi(\gamma),$$

namely they are anti-symmetric under time-reversal.

Solution:
We have seen in Exercise 4.26 that the stochastic trajectory is $\gamma = (x_i, x_f)$ with x representing the outcomes of the energy and particle measurements of each bath, namely $x = (\boldsymbol{\epsilon}, \mathbf{n})$. Since $\gamma^\dagger = (x_f, x_i)$, we have

$$\Delta\boldsymbol{\epsilon}(\gamma) = \boldsymbol{\epsilon}_f - \boldsymbol{\epsilon}_i = -\Delta\boldsymbol{\epsilon}(\gamma^\dagger), \qquad \Delta\mathbf{n}(\gamma) = \mathbf{n}_f - \mathbf{n}_i = -\Delta\mathbf{n}(\gamma^\dagger).$$

Therefore, every $\phi(\gamma) = \boldsymbol{\alpha}\cdot\Delta\boldsymbol{\epsilon}(\gamma) + \boldsymbol{\beta}\cdot\Delta\mathbf{n}(\gamma)$ is antisymmetric under time-reversal:

$$\phi(\gamma) = -\phi(\gamma^\dagger).$$

Exercise 4.28: Thermodynamic uncertainty relation for current-type observables

Let ϕ be an observable anti-symmetric under time-reversal and $P(\sigma, \phi)$ be the joint distribution of observing the entropy production σ and the observable ϕ, which satisfies the detailed fluctuation theorem

$$\frac{P(\sigma, \phi)}{P(-\sigma, -\phi)} = e^{\sigma/k_B}.$$

Analogously to Exercise 4.25, we introduce the probability distribution

$$Q(\sigma, \phi) = (1 + e^{\sigma/k_B})P(\sigma, \phi) \qquad \text{for } \sigma \in [0, \infty]$$

and denote as $\langle\cdots\rangle$ ($\langle\cdots\rangle_Q$) the averages with respect to P (Q). Show that

$$\langle\phi\rangle = \left\langle \phi \tanh\left(\frac{\sigma}{2k_B}\right)\right\rangle_Q, \qquad \langle\phi^2\rangle = \langle\phi^2\rangle_Q.$$

Use Cauchy-Schwarz inequality to prove

$$\langle\phi\rangle^2 \le \langle\phi^2\rangle_Q \left\langle \tanh^2\left(\frac{\sigma}{2k_B}\right)\right\rangle_Q$$

and finally prove the inequality

$$\frac{\mathrm{Var}(\phi)}{\langle\phi\rangle^2} \ge \frac{2}{e^{\Sigma/k_B} - 1}.$$

Solution:

$$\begin{aligned}\langle\phi\rangle &= \int_{-\infty}^{\infty} d\sigma \int d\phi \phi P(\sigma,\phi) = \int_{0}^{\infty} d\sigma \int d\phi \phi [P(\sigma,\phi)+P(-\sigma,\phi)] = \int_{0}^{\infty} d\sigma \int d\phi \phi [P(\sigma,\phi)-P(-\sigma,-\phi)] \\ &= \int_{0}^{\infty} d\sigma \int d\phi \phi P(\sigma,\phi)(1-e^{-\sigma}) = \langle \phi \tanh \frac{\sigma}{2}\rangle_Q \\ \langle\phi^2\rangle &= \int_{-\infty}^{\infty} d\sigma \int d\phi \phi^2 P(\sigma,\phi) = \int_{0}^{\infty} d\sigma \int d\phi \phi^2 [P(\sigma,\phi)+P(-\sigma,\phi)] = \int_{0}^{\infty} d\sigma \int d\phi \phi^2 [P(\sigma,\phi)+P(-\sigma,-\phi)] \\ &= \langle\phi^2\rangle_Q.\end{aligned}$$

Cauchy-Schwarz says that, given a scalar product $(\cdot,\cdot)$ then $(u,v)^2 \le |u|^2|v|^2\, \forall u,v$. Let's denote $(f,g) = \langle f(\phi,\sigma)g(\phi,\sigma)\rangle_Q$ for all f,g real functions. Clearly, $(\cdot,\cdot)$ is symmetric, bilinear and positive definite: $\langle f^2(\phi,\sigma)\rangle_Q \ge 0$, with equality if and only if $f=0$ almost everywhere. Then, we can apply Cauchy-Schwarz with the functions $f(\phi,\sigma)=\phi$ and $g(\phi,\sigma)=\tanh\frac{\sigma}{2}$:

$$\langle\phi\rangle^2 = \langle\phi\tanh\frac{\sigma}{2}\rangle_Q^2 \le \langle\phi^2\rangle_Q \langle\tanh^2\frac{\sigma}{2}\rangle_Q = \langle\phi^2\rangle\langle\tanh^2\frac{\sigma}{2}\rangle_Q.$$

Notice that the hyperbolic tangent $\tanh x$ is concave for $x \ge 0$, which allows us to write

$$\tanh^2 x = \tanh x \tanh x + (1-\tanh x)\tanh(0) \le \tanh(x\tanh x)$$

which means that

$$\langle\tanh^2\frac{\sigma}{2}\rangle_Q \le \langle\tanh\left(\frac{\sigma}{2}\tanh\frac{\sigma}{2}\right)\rangle_Q \le \tanh\left\langle\frac{\sigma}{2}\tanh\frac{\sigma}{2}\right\rangle_Q = \tanh\frac{\Sigma}{2}$$

where we used once more that $\tanh x$ is concave for $x\ge 0$ in the last inequality. Then, we have

$$\langle\phi\rangle^2 \le \langle\phi^2\rangle\tanh\frac{\Sigma}{2} \Rightarrow \frac{\mathrm{Var}(\phi)}{\langle\phi\rangle^2} \ge \frac{1}{\tanh\frac{\Sigma}{2}} - 1 = \frac{2}{e^{\Sigma}-1}.$$

Notably, if $\Sigma \ll 1$ the thermodynamic uncertainty relation can be approximated as

$$\frac{\mathrm{Var}(\phi)}{\langle\phi\rangle^2} \ge \frac{2}{\Sigma}.$$

Exercise 4.29: Thermodynamic uncertainty relation in the single-electron transistor

In the context of Exercise 4.13, use the cumulant generating function in the long time limit to verify the thermodynamic uncertainty relation with the observable ϕ corresponding to the number of electrons n flowing from left to right at steady state.

Show that the thermodynamic uncertainty relation

$$\frac{\mathrm{Var}(\phi)}{\langle\phi\rangle^2} \ge \frac{2k_B}{\Sigma}$$

can be expressed as

$$\frac{\mathrm{Var}(I)}{I^2} \ge \frac{2k_B}{\dot{\Sigma}},$$

where $I = \langle n\rangle(t)/t$ is the current, $\mathrm{Var}(I) = [\langle n^2\rangle(t) - \langle n\rangle^2(t)]/t$ is the current variance and $\dot{\Sigma}$ is the entropy production rate, all evaluated at steady state.

Solution:

In Exercise 4.13 we calculated the eigenvalues of the rate equation with the counting fields, obtaining

$$\frac{\lambda_\pm}{\Gamma} = -1 \pm \sqrt{1-F(\chi_L-\chi_R)}, \quad F(\chi_L-\chi_R) = f_L(1-f_R)\left(1-e^{i(\chi_L-\chi_R)}\right) + f_R(1-f_L)\left(1-e^{i(\chi_R-\chi_L)}\right).$$

These eigenvaues enter the cumulant generating function $C(\boldsymbol{\chi},t) = \ln\mathrm{Tr}\{\tilde{\rho}(\boldsymbol{\chi},t)\}$ through the time-evolution $\tilde{\rho}(\boldsymbol{\chi},t) = e^{\mathcal{L}(\chi)t}\rho(0)$. In particular, at large times the eigenvalue with the largest real part will dominate over the others, such that the scaled cumulant generating function becomes

$$S(\boldsymbol{\chi}) = \lim_{t\to\infty} \frac{C(\boldsymbol{\chi}, t)}{t} = \lambda_+.$$

Then, since $F(0) = 0$ and

$$\partial_\chi F = -if_L(1-f_R)e^{i\chi} + if_R(1-f_L)e^{-i\chi} \rightarrow \partial_\chi F(0) = -i(f_L - f_R)$$

$$\partial_\chi^2 F = f_L(1-f_R)e^{i\chi} + f_R(1-f_L)e^{-i\chi} \rightarrow \partial_\chi^2 F(0) = f_L(1-f_R) + f_R(1-f_L)$$

we can calculate the moments of the number of particles n leaving the left contact through the cumulant generating function. In particular, the current is

$$I = \lim_{t\to\infty} \frac{\langle n\rangle(t)}{t} = -i\partial_{\chi_L} S(\boldsymbol{\chi})|_{\boldsymbol{\chi}=0} = -i\Gamma \left.\frac{1}{2}\frac{-\partial_\chi F(\chi_L - \chi_R)}{\sqrt{1 - F(\chi_L - \chi_R)}}\right|_{\boldsymbol{\chi}=0} = \frac{\Gamma}{2}(f_L - f_R)$$

and its variance is

$$\mathrm{Var}(I) = \lim_{t\to\infty} \frac{\langle \Delta^2 n\rangle(t)}{t} = (-i)^2\partial^2_{\chi_L} S(\boldsymbol{\chi})|_{\boldsymbol{\chi}=0} = -\Gamma\left(\frac{1}{2}\frac{-\partial^2_\chi F(\chi_L - \chi_R)}{\sqrt{1 - F(\chi_L - \chi_R)}} - \frac{1}{4}\frac{(-\partial_\chi F(\chi_L - \chi_R))^2}{(1 - F(\chi_L - \chi_R))^{3/2}}\right)_{\boldsymbol{\chi}=0}$$
$$= \frac{\Gamma}{2}\left(f_L(1-f_R) + f_R(1-f_L) - \frac{1}{2}(f_L - f_R)^2\right).$$

Since we have both average current and current variance, the missing ingredient for the thermodynamic uncertainty relation is the entropy production. Notably, since the tunneling electrons have all the same energy ϵ, we are in the strong coupling regime, and the entropy production can be written as

$$\Sigma = [\beta_R(\epsilon - \mu_R) - \beta_L(\epsilon - \mu_L)]I.$$

To write the thermodynamic uncerainty relation for the current is sufficient to introduce the positive and large time t in the inequality, and use the definitions of current, current variance and entropy prodution rate.
Then, the thermodynamic uncertainty relation becomes

$$\frac{f_L(1-f_R) + f_R(1-f_L)}{(f_L - f_R)^2} - \frac{1}{2} \geq \frac{2}{(f_L - f_R)\log\left(\frac{f_L}{1-f_L}\frac{1-f_R}{f_R}\right)}$$

that we verify numerically.

```
import numpy as np
import matplotlib.pyplot as plt
########################################################################
n = 300;
a = 0.001;
x = np.linspace(a, 1-a, n);
y = np.linspace(a, 1-a, n);

out = np.zeros([n,n]);

for i in range(n):
    X = x[i]
    for j in range(n):
        Y = y[j]
        entr = (X-Y)*np.log(X*(1-Y)/(Y*(1-X)));
        out[i, j] = ((X*(1-Y)+ Y*(1-X))-.5*(X-Y)**2)/(X-Y)**2 - 2/entr
        if out[i, j]<0:
            print(out[i, j])

X, Y = np.meshgrid(x, y)
plt.pcolormesh(X, Y, out, cmap="RdBu");
plt.colorbar()
plt.xlabel("$f_L$");plt.ylabel("$f_R$");
########################################################################
plt.show()
```

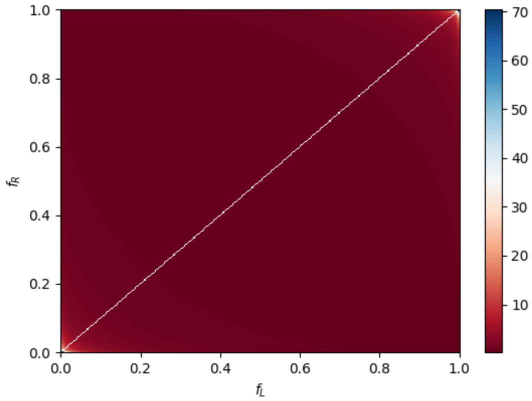


Figure 6: Thermodynamic uncertainty relation for the single electron transistor.

Exercise 4.30: Time-reversal anti-symmetry of stochastic work and chemical work

Show that the stochastic work introduced in the two-point measurement scheme, namely

$$w = \epsilon_\tau - \epsilon_0$$

the work done being the difference in internal energy of the system, is anti-symmetric under time reversal $w(\gamma^\dagger) = -w(\gamma)$.

Show that the chemical work, defined through

$$\dot{W}_{\text{chem}}(t) \equiv -\sum_\nu \mu_\nu d_t N_\nu(t)$$

is also anti-symmetric under time reversal.

Solution:
In the time-reversed two-point measurement scheme the work done is $w = \epsilon_0 - \epsilon_\tau$ because we firs do the measurement at time τ and then we follow $\gamma^\dagger$ to finally measure the system at $t = 0$. Therefore, $w(\gamma^\dagger) = -w(\gamma)$.
From integration, the chemical work reads

$$W_{\text{chem}}(\tau) = -\sum_\nu \mu_\nu \Delta N_\nu(\tau).$$

Now, the time-reversed process starts with the bats having $N_\nu(\tau)$ particles and ends with them having $N_\nu(0)$ particles, therefore also the chemical work is anti-symmetric under time reversal.

Exercise 4.31: Rank inequality

Prove that

$$\text{rank}(\rho_{SB}) \leq \text{rank}(\rho_S)\text{rank}(\rho_B)$$

by using the Schmidt decomposition, namely that one can always write $|\psi\rangle = \sum_i c_i |i\rangle_A \otimes |i\rangle_B$ for some orthonormal set of vetors $\{|i\rangle_{A/B}\} \in \mathcal{H}_{A/B}$ and some *positive, real-valued* coefficients c_i.

Solution:
Let

$$\rho_{SB} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$$

be the eigendecomposition of the joint state. Using the schmidt decomposition on each eigenvector, we have

$$\rho_{SB} = \sum_{ij\alpha} p_\alpha c_{i\alpha} c_{j\alpha} |i_\alpha i_\alpha\rangle\langle j_\alpha j_\alpha| \,.$$

Taking the partial trace we have

$$\rho_B = \mathrm{Tr}_S\{\rho_{SB}\} = \sum_{ij\alpha} p_\alpha c_{i\alpha} c_{j\alpha} \mathrm{Tr}_S\{|i_\alpha\rangle\langle j_\alpha|_S\} |i_\alpha\rangle\langle j_\alpha|_B = \sum_{i\alpha} p_\alpha c_{i\alpha}^2 |i_\alpha\rangle\langle i_\alpha|_B .$$

This means that the support of ρ_B is $\mathrm{supp}(\rho_B) = \mathrm{Span}(\{|i_\alpha\rangle\langle i_\alpha|_B\}_{i\alpha})$, which means that

$$\mathrm{supp}(\rho_S \otimes \rho_B) = \mathrm{Span}(\{|i_\alpha j_\beta\rangle\langle i_\alpha j_\beta|\}_{ij\alpha\beta})$$

while

$$\mathrm{supp}(\rho_{SB}) = \mathrm{Span}(\{|\psi_\alpha\rangle\langle\psi_\alpha|\}_\alpha) = \mathrm{Span}(\{|i_\alpha i_\alpha\rangle\langle i_\alpha i_\alpha|\}_{i\alpha})$$

which means that

$$\mathrm{supp}(\rho_{SB}) \subseteq \mathrm{supp}(\rho_S \otimes \rho_B) = \mathrm{supp}(\rho_S) \otimes \mathrm{supp}(\rho_B)$$

Since the dimension of the support equals the rank, we finally have

$$\mathrm{rank}(\rho_{SB}) \leq \mathrm{rank}(\rho_S)\mathrm{rank}(\rho_B).$$

Exercise 4.32: Local pure state ⇒ separable global state

Show that $\mathrm{Tr}_E\{\rho_{SE}\} = |\psi\rangle\langle\psi|_S$ for some $|\psi\rangle_S$ imples $\rho_{SE} = |\psi\rangle\langle\psi|_S \otimes \rho_E$ for any ρ_{SE}.

Solution:
Let

$$\rho_{SE} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$$

be the eigendecomposition of the global state. Using the Schmidt decomposition on each eigenvector we have

$$|\psi_\alpha\rangle = \sum_i c_{i\alpha} |i_\alpha i_\alpha\rangle ,$$

and the global state becomes

$$\rho_{SE} = \sum_{\alpha ij} p_\alpha c_{i\alpha} c_{j\alpha} |i_\alpha i_\alpha\rangle\langle j_\alpha j_\alpha| .$$

Taking the partial trace leads to

$$\rho_S = \sum_{\alpha i} p_\alpha c_{i\alpha}^2 |i_\alpha\rangle\langle i_\alpha|_S \stackrel{!}{=} |\psi\rangle\langle\psi|_S .$$

To satisfy the purity condition we need $c_{i\alpha} = \delta_{ix_\alpha}$ for one x_α and $|x_\alpha\rangle_S = |\psi\rangle_S$ for all x_α. Then, going back to the Schmidt decomposed global state we find

$$\rho_{SE} = \sum_{\alpha x_\alpha} p_\alpha |\psi\rangle\langle\psi|_S \otimes |x_\alpha\rangle\langle x_\alpha|_E = |\psi\rangle\langle\psi|_S \otimes \rho_E$$

with $\rho_E = \sum_\alpha p_\alpha |x_\alpha\rangle\langle x_\alpha|_E$. Note that since the environment vectors $|x_\alpha\rangle_E$ need not be all equal, the environment's local state is generally mixed.

Exercise 4.33: Impossibility of projective measurements with a mixed ancilla

Show that, for an initially mixed ancilla state, an ideal projective measurement, namely

$$\rho_S'(x) = \frac{\Pi_S(x)\rho_S\Pi_S(x)}{p(x)} = \frac{\mathrm{Tr}_A\left\{|x\rangle\langle x|_A V\rho_S \otimes \rho_A V^\dagger\right\}}{p(x)}$$

becomes impossible.

Show that

$$\mathrm{rank}[\rho_S]\mathrm{rank}[\rho_A] \leq \mathrm{rank}[\rho_S']\mathrm{rank}[\rho_A']$$

where $\rho_{S/A}$ ($\rho'_{S/A}$) denotes the marginal state of the system/ancilla before (after) the interaction.

Solution:
Taking a mixed ρ_A we find

$$\mathrm{Tr}_A\left\{|x\rangle\langle x|_A\, V\rho_S\otimes\sum_\alpha p_\alpha\,|\psi_\alpha\rangle\langle\psi_\alpha|_A\, V^\dagger\right\}=\sum_\alpha M_{\alpha x}\rho_S M^\dagger_{\alpha x}$$

with

$$M_{\alpha x}=\sqrt{p_\alpha}\,\langle x|V|\psi_\alpha\rangle_A\,.$$

Thse operators define the POVM associated with the measurement. Now, for the measurement on S to be projective, we need

$$\sum_{\alpha\beta} M_{\beta x}M_{\alpha x}\rho_S M^\dagger_{\alpha x}M^\dagger_{\beta x}$$

which is generally satisfied if $M_{\alpha x}M_{\beta x}=M_{\alpha x}\delta_{\alpha\beta}$, namely the operators $\{M_{\alpha x}\}_\alpha$ are a set of mutually exclusive projectors. However, for this to happen one needsto have only one possible α ($p_\alpha=1$) which means that the initial ancilla state has to be pure.
Using the resut of Exercise 4.31 we have

$$\mathrm{rank}[\rho_S]\mathrm{rank}[\rho_A]=\mathrm{rank}[\rho_S\otimes\rho_A]=\mathrm{rank}[\rho_{SA}(0)]=\mathrm{rank}[\rho_{SA}(t)]\leq\mathrm{rank}[\rho'_S\otimes\rho'_A]=\mathrm{rank}[\rho'_S]\mathrm{rank}[\rho'_A].$$

with

$$\rho'_S=\sum_x\mathrm{Tr}_A\left\{|x\rangle\langle x|_A\,V\rho_S\otimes\rho_A V^\dagger\right\}=\sum_{\alpha x}M_{\alpha x}\rho_S M^\dagger_{\alpha x}$$

and analogously for ρ'_A. Note that the marginal state coincide with the local state because $\sum_x|x\rangle\langle x|_A=\mathbb{I}_A$.

5 Operational Quantum Stochastic Thermodynamics

Exercise 5.1: Classicality of the two-point measurement scheme

Consider the two-point measurement scheme, in which the two-point probability is

$$p(x_\tau, x_0) = \text{Tr}\left\{\Pi(x_\tau)U(\tau,0)\Pi(x_0)\rho\Pi(x_0)U^\dagger(\tau,0)\right\}.$$

Show that, independent of the initial state, it satisfies

$$\sum_{x_\tau} p(x_\tau, x_0) = p(\not{x}_\tau, x_0).$$

Then, show that by choosing the initial state to be $\rho = \sum_{x_0} \mu(x_0)\Pi(x_0)$, it also satisfies

$$\sum_{x_0} p(x_\tau, x_0) = p(x_\tau, \not{x}_0),$$

thereby completing the Kolmogorov consistency condition.

Solution:
Using the linearity of the trace we can bring the sum over x_τ inside. There, using the completeness of the projector set, namely $\sum_{x_\tau} \Pi(x_\tau) = \mathbb{I}$ we find

$$\sum_{x_\tau} p(x_\tau, x_0) = \text{Tr}\left\{U(\tau,0)\Pi(x_0)\rho\Pi(x_0)U^\dagger(\tau,0)\right\} = \text{Tr}\left\{\Pi(x_0)\rho\right\} = p(\not{x}_\tau, x_0),$$

where we used the cyclic property of the trace combined with the unitarity of $U(\tau,0)$ $[U(\tau,0)U^\dagger(\tau,0) = \mathbb{I}]$ and the projector property $\Pi^2(x_0) = \Pi(x_0)$.
Again, we use the linearity of the trace to brin the summation inside. Now, we use the structure of the initial state to simplify notably the equation and leaving only one projector $\Pi(x_0)$ since $\Pi(x)\Pi(y) = \delta_{xy}\Pi(x)$

$$\begin{aligned}
\sum_{x_0} p(x_\tau, x_0) &= \text{Tr}\left\{\Pi(x_\tau)U(\tau,0)\left(\sum_{x_0 y}\mu_y\Pi(x_0)\Pi(y)\Pi(x_0)\right)U^\dagger(\tau,0)\right\} \\
&= \text{Tr}\left\{\Pi(x_\tau)U(\tau,0)\left(\sum_{y}\mu_y\Pi(y)\right)U^\dagger(\tau,0)\right\} = \text{Tr}\left\{\Pi(x_\tau)U(\tau,0)\rho(0)U^\dagger(\tau,0)\right\} \\
&= \text{Tr}\left\{\Pi(x_\tau)\rho(\tau)\right\} = p(x_\tau, \not{x}_0).
\end{aligned}$$

Exercise 5.2: Two-point measurement scheme with degeneracies

Consider an isolated system with Hamiltonian $H(\lambda_t)$ containing degeneracies. In particular, let $|\epsilon_t, g_t\rangle$ denote an eigenstate of $H(\lambda_t)$ with eigenvalue ϵ_t and g_t labels eigenvectors in the corresponding degenerate subspace.
Show that

$$M_{\text{TPMS}}(w) = \sum_{\epsilon_\tau g_\tau, \epsilon_0 g_0} \delta[w - (\epsilon_\tau - \epsilon_0)] |\langle\epsilon_\tau, g_\tau|U(\tau,0)|\epsilon_0, g_0\rangle|^2 |\epsilon_0, g_0\rangle\langle\epsilon_0, g_0|$$

is normalized and positive, and therefore constitues a POVM.
Show that $\text{Tr}\{M_{\text{TPMS}}(w)\rho(0)\}$ coincides with the work probability distribution from the two-point measurement approach if the initial state obeys $\langle\epsilon_0, g_0|\rho(0)|\epsilon_0, h_0\rangle \sim \delta_{g_0 h_0}$.

Solution:
I will drop the subscript for simplicity. By introducing the eigendecomposition of the state $\rho = \sum_\alpha p_\alpha |\alpha\rangle\langle\alpha|$ we have

$$\begin{aligned}
\text{Tr}\{M(w)\rho\} &= \sum_{\epsilon_\tau g_\tau, \epsilon_0 g_0} \delta[w - (\epsilon_\tau - \epsilon_0)] \langle\epsilon_\tau, g_\tau|U(\tau,0)|\epsilon_0, g_0\rangle|^2 \langle\epsilon_0 g_0|\rho|\epsilon_0 g_0\rangle = \\
&= \sum_{\epsilon_\tau g_\tau, \epsilon_0 g_0, \alpha} \delta[w - (\epsilon_\tau - \epsilon_0)] p_\alpha \langle\epsilon_\tau, g_\tau|U(\tau,0)|\epsilon_0, g_0\rangle|^2 |\langle\epsilon_0 g_0|\alpha\rangle|^2 \geq 0
\end{aligned}$$

where each term multiplying the delta distribution is non-negative. Then, integrating over w wee have

$$\int dw \mathrm{Tr}\left\{M(w)\rho\right\} = \sum_{\epsilon_\tau g_\tau, \epsilon_0 g_0} |\langle \epsilon_\tau, g_\tau|U(\tau,0)|\epsilon_0, g_0\rangle|^2 \langle \epsilon_0 g_0|\rho|\epsilon_0 g_0\rangle =$$

$$= \sum_{\epsilon_0 g_0} \langle \epsilon_0, g_0| U^\dagger \left(\sum_{\epsilon_\tau g_\tau} |\epsilon_\tau, g_\tau\rangle \langle \epsilon_\tau, g_\tau|\right) U |\epsilon_0, g_0\rangle \langle \epsilon_0 g_0|\rho|\epsilon_0 g_0\rangle = \sum_{\epsilon_0 g_0} \langle \epsilon_0 g_0|\rho|\epsilon_0 g_0\rangle = 1$$

$$\int dw \mathrm{Tr}\left\{M(w)\rho\right\} = \mathrm{Tr}\left\{\rho\right\} \quad \forall\rho \quad \Rightarrow \quad \int dw M(w) = \mathbb{I}.$$

The probability of observing the work $\Delta\epsilon = \epsilon_\tau - \epsilon_0$ is

$$\begin{aligned} P(w) &= \sum_{\epsilon_\tau \epsilon_0} \delta(w - \Delta\epsilon) \mathrm{Tr}\left\{\Pi(\epsilon_\tau) U \Pi(\epsilon_0) \rho \Pi(\epsilon_0) U^\dagger\right\} \\ &= \sum_{\epsilon_\tau z} \sum_{\epsilon_0 x y} \delta(w - \Delta\epsilon) \mathrm{Tr}\left\{|\epsilon_\tau z\rangle\langle\epsilon_\tau z| U |\epsilon_0 x\rangle\langle\epsilon_0 x| \rho |\epsilon_0 y\rangle\langle\epsilon_0 y| U^\dagger\right\} \\ &= \sum_{\epsilon_\tau z} \sum_{\epsilon_0 x} \delta(w - \Delta\epsilon) \mathrm{Tr}\left\{|\epsilon_\tau z\rangle\langle\epsilon_\tau z| U |\epsilon_0 x\rangle\langle\epsilon_0 x| \rho |\epsilon_0 x\rangle\langle\epsilon_0 x| U^\dagger\right\} = \mathrm{Tr}\left\{M(w)\rho\right\} \end{aligned}$$

where we used that $\langle \epsilon_0 x|\rho|\epsilon_0 y\rangle \sim \delta_{xy}$ to get rid of of the summing index y.

Exercise 5.3: Implementing a one-time measurement to reproduce the two-time measurement

Consider the following protocol applied to the system and ancilla, the former being described by the Hamiltonian $H(\lambda_t)$, while the letter has negligible Hamiltonian but is described with the position and momentum operators X, P. Consider the initial state $\rho_S \otimes |x=0\rangle\langle x=0|$. The protocol reads as follows

1. Apply $U_0 = e^{-iH(\lambda_0)\otimes P/\hbar}$
2. Let S evolve through $H(\lambda_t)$, which generates the unitary $U(\tau, 0)$
3. Apply $U_\tau = e^{-iH(\lambda_\tau)\otimes P/\hbar}$
4. Measure $|x\rangle\langle x|_A$.

Show that, for any initial state ρ_S, the probability of obtaining outcome $x = w$ coincides with

$$p_{\mathrm{TPMS}}(w) = \sum_{\epsilon_\tau, \epsilon_0} \delta[w - (\epsilon_\tau - \epsilon_0)] |\langle \epsilon_\tau|U(\tau,0)|\epsilon_0\rangle|^2 \langle \epsilon_0|\rho_S|\epsilon_0\rangle .$$

Solution:
Remembering that $[X, P] = i\hbar$, we notice that

$$XP^n = (i\hbar + PX)P^{n-1} = i\hbar P^{n-1} + P(i\hbar + PX)P^{n-2} = 2i\hbar P^{n-1} + P^2 X P^{n-2} = ni\hbar P^{n-1} + P^n X$$

which means that

$$Xe^{i\alpha P} = X\sum_n \frac{(i\alpha)^n P^n}{n!} = \sum_n \frac{(i\alpha)^n [ni\hbar P^{n-1} + P^n X]}{n!} = e^{i\alpha P}[X - \hbar\alpha] \Rightarrow e^{i\alpha P}|x\rangle = |x - \hbar\alpha\rangle$$

The probability of observing the outcome x at the end of the protocol is

$$\mathrm{Tr}\left\{|x\rangle\langle x| U_\tau U U_0 \rho \otimes |0\rangle\langle 0| U_0^\dagger U^\dagger U_\tau^\dagger\right\} = \sum_{\epsilon_\tau} \langle \epsilon_\tau x|U_\tau U U_0 \rho \otimes |0\rangle\langle 0| U_0^\dagger U^\dagger U_\tau^\dagger|\epsilon_\tau x\rangle .$$

The unitary $U_\tau^\dagger$ acts as

$$e^{iH(\lambda_\tau)\otimes P/\hbar}|\epsilon_\tau, x\rangle = e^{i\epsilon_\tau \otimes P/\hbar}|\epsilon_\tau, x\rangle = |\epsilon_\tau, x - \epsilon_\tau\rangle .$$

Introducing the identities $\sum_{\epsilon_0 y} |\epsilon_0, y\rangle\langle\epsilon_0, y|$ we have

$$\begin{aligned}
p(x) &= \sum_{\epsilon_\tau} \sum_{\epsilon_0 \varepsilon_0 y z} \langle\epsilon_\tau, x-\epsilon_\tau| \, UU_0 \, |\epsilon_0 y\rangle\langle\epsilon_0 y| \, \rho \otimes |0\rangle\langle 0| \, |\varepsilon_0 z\rangle\langle\varepsilon_0 z| \, U_0^\dagger U^\dagger \, |\epsilon_\tau, x-\epsilon_\tau\rangle \\
&= \sum_{\epsilon_\tau} \sum_{\epsilon_0 \varepsilon_0} \langle\epsilon_\tau, x-\epsilon_\tau| \, UU_0 \, |\epsilon_0, 0\rangle \, \langle\epsilon_0|\rho|\varepsilon_0\rangle \, \langle\varepsilon_0, 0| \, U_0^\dagger U^\dagger \, |\epsilon_\tau, x-\epsilon_\tau\rangle \\
&= \sum_{\epsilon_\tau} \sum_{\epsilon_0 \varepsilon_0} \langle\epsilon_\tau, x-\epsilon_\tau| \, U \, |\epsilon_0, \epsilon_0\rangle \, \langle\epsilon_0|\rho|\varepsilon_0\rangle \, \langle\varepsilon_0, \varepsilon_0| \, U^\dagger \, |\epsilon_\tau, x-\epsilon_\tau\rangle \\
&= \sum_{\epsilon_\tau} \sum_{\epsilon_0 \varepsilon_0} \langle\epsilon_\tau| \, U \, |\epsilon_0\rangle \, \langle x-\epsilon_\tau|\epsilon_0\rangle \, \langle\epsilon_0|\rho|\varepsilon_0\rangle \, \langle\varepsilon_0|x-\epsilon_\tau\rangle \, \langle\varepsilon_0| \, U^\dagger \, |\epsilon_\tau\rangle \\
&= \sum_{\epsilon_\tau \epsilon_0} \delta[x-(\epsilon_\tau-\epsilon_0)] |\langle\epsilon_\tau| \, U \, |\epsilon_0\rangle|^2 \, \langle\epsilon_0|\rho|\epsilon_0\rangle = p_{\mathrm{TPMS}}(x)
\end{aligned}$$

in the last step we used that $|\langle x|y\rangle|^2 = \delta(x-y)$ to get rid of the sum over ε_0.

Exercise 5.4: Lemma for No-Go theorem: identically 0 operator

Consider an arbitrary non-negative operator $A \geq 0$. Show that if $\langle n|A|n\rangle = 0$ for all elements of some basis set $\{|n\rangle\}$, then $A = 0$ identically.

Solution:
Since A is non-negative, $A + \epsilon\mathbb{I} > 0, \quad \forall\epsilon > 0$. Then, the bilinear product

$$(\phi, \psi) = \langle\phi|A + \epsilon\mathbb{I}|\psi\rangle$$

defines a scalar product: $(\phi, \psi) = (\psi, \phi)^*$, $(\phi, \phi) \geq 0$ with equality only for $\phi = 0$. We can then use the Cauchy-Schwarz inequality, namely

$$|(\phi, \psi)|^2 \leq (\phi, \phi)(\psi, \psi)$$

choosing $\phi = |n\rangle$ and $\psi = |m\rangle$. This leads to

$$|\langle m|A + \epsilon\mathbb{I}|n\rangle|^2 \leq \langle m|A + \epsilon\mathbb{I}|m\rangle \, \langle n|A + \epsilon\mathbb{I}|n\rangle \, .$$

Taking ϵ to be vanishingly small, we have

$$|\langle m|A|n\rangle|^2 \leq \langle m|A|m\rangle \, \langle n|A|n\rangle \, .$$

Then, if $\langle n|A|n\rangle = 0 \quad \forall n$ then also $\langle m|A|n\rangle = 0 \quad \forall m, n$. Therefore, $A = 0$.

Exercise 5.5: Zero measurement work

Consider the following implementation of an ideal projective measurement of the observable $R_S = \sum_{r=1}^n \lambda(r)\Pi_S(r)$ based on the introduction of the auxiliary ideal memory M. Initially, the system and memory are in the state $\rho_{SM}^{(0)} = \rho_S^{(0)} \otimes |1\rangle\langle 1|_M$ and evolve through the unitary

$$U_{SM} = \sum_{r=1}^n \Pi_S(r) \otimes \sum_s |r+s-1\rangle\langle s|_M$$

with $r+s-1$ understood to be modulo n. After the unitary, the state is $\rho_{SM}^{(1)} \equiv \mathcal{U}_{SM}\rho_{SM}^{(0)} \equiv U_{SM}\rho_{SM}^{(0)}U_{SM}^\dagger$ and has marginal state $\rho_S^{(1)} \equiv \sum_r \mathcal{P}(r)\rho_S^{(0)} \equiv \Pi_S(r)\rho_S^{(0)}\Pi_S(r)$. After measuring the memory and obtaining outcome r the post-selected state is

$$\rho_{SM}^{(2)}(r) \equiv \frac{1}{p(r)}\mathcal{P}_S(r)\rho_S^{(0)} \otimes |r\rangle\langle r|_M$$

and the average post-measurement state is $\rho_{SM}^{(2)} \equiv \sum_r p(r)\rho_{SM}^{(2)}(r)$.

Neglecting the internal energy of the memory (which is ideal), the interal energy and the stochastic internal energy of the system are

$$U_j \equiv \mathrm{Tr}_S\left\{H_S\rho_S^{(j)}\right\}, \qquad\qquad u_2(r) \equiv \mathrm{Tr}_S\left\{H_S\rho_S^{(2)}(r)\right\}.$$

respectively. In particular, we split the stochastic energy as

$$\Delta u_{20}(r) \equiv u_2(r) - U_0 = \Delta u_{21}(r) + \Delta U_{10},$$

with $\Delta u_{21}(r) \equiv u_2(r) - U_1$ and $\Delta U_{10} = U_1 - U_0$.

Show that, if $[R_S, H_S] = 0$, then

$$\Delta U_{20} \equiv \sum_r p(r)\Delta u_{20}(r) = 0.$$

Solution:
Noticing that if $[R_S, H_S] = 0$ then the two operators share eigenspaces, specifically

$$[H,R] = 0 \to \sum_r [H, \lambda_r \Pi_r] = 0 \to \sum_r \lambda_r (H\Pi_r - \Pi_r H) = 0 \to \sum_r \lambda_r \Pi_x H \Pi_r - \lambda_x \Pi_x H = 0$$
$$\to (\lambda_y - \lambda_x)\Pi_x H \Pi_y = 0 \quad \forall x, y \Rightarrow \Pi_x H \Pi_y = \delta_{xy}\Pi_x H \Pi_x \to H = \sum_x \Pi_x H \Pi_x$$
$$\to [H, \Pi_x] = 0.$$

$$U_2 = \sum_r p(r)u_2(r) = \mathrm{Tr}_S \left\{ H_S \sum_r p(r)\rho_S^{(2)}(r) \right\} = \mathrm{Tr}_S \left\{ H_S \sum_r \mathcal{P}(r)\rho_S^{(0)} \right\} = \sum_r \mathrm{Tr}_S \left\{ H_S \Pi_r \rho_S^{(0)} \Pi_r \right\}$$
$$= \sum_r \mathrm{Tr}_S \left\{ \Pi_r H_S \rho_S^{(0)} \right\} = \mathrm{Tr}_S \left\{ H_S \rho_S^{(0)} \right\} = U_0$$

which means that $\Delta U_{20} = 0$.

Exercise 5.6: Second law for a quantum measurement

Starting from the setup of Exercise 5.5, we define the conditional entropy

$$s_2(r) \equiv -k_B \ln p(r) + k_B S[\rho_S^{(2)}(r)].$$

Show that

$$S_2 - S_0 \geq 0, \qquad S_2 = \sum_r p(r)s_2(r).$$

For a measurement of a rank-1 observable, show that the second law is equivalent to

$$S_{\mathrm{Sh}}(\mathbf{p}) \geq S[\rho_S^{(0)}]$$

with $\mathbf{p}$ being the vector probability of $p(r)$ and the equality is reached if and only if $[R_S, \rho_S^{(0)}] = 0$.

Solution:
Since $\rho_S^{(2)}(r) = \frac{1}{p_r}\Pi_r \rho_S^{(0)} \Pi_r$ the average of $s_2(r)$ reads

$$S_2 = \sum_r p_r s_2(r) = S(\mathbf{p}) - \sum_r \mathrm{Tr}\left\{ \Pi_r \rho_S^{(0)} \Pi_r \left(\ln \Pi_r \rho_S^{(0)} \Pi_r - \ln p_r \right) \right\} = S(\mathbf{p}) + \sum_r p_r S[\rho_S^{(2)}(r)].$$

We can now use the following inequalities on convex combinations and on set of projectors $\rho_n = P_n \rho P_n / \lambda_n$, $\lambda_n = \mathrm{Tr}\{\mathcal{P}_n \rho\}$:

$$S[\rho] \leq S\left[\sum_n \lambda_n \rho_n \right] \leq \sum_n \lambda_n S[\rho_n] + S(\boldsymbol{\lambda})$$

we obtain

$$S_2 \geq S\left[\sum_r p_r \rho_S^{(2)}(r) \right] = S\left[\sum_r p_r \frac{\Pi_r \rho_S^{(0)} \Pi_r}{p_r} \right] \geq S[\rho_S^{(0)}] = S_0$$

which is the second law $S_2 - S_0 \geq 0$.
If we have a rank-1 obersable then all the projectors have rank 1 and the post-selected states $\rho_S^{(2)}(r)$ also have rank 1, i.e. they are pure states. This means that S_2 reduces to $S_2 = S(\mathbf{p})$, such that the second law becomes $S(\mathbf{p}) - S_0 \geq 0$.

If $[R_S, \rho_S^{(0)}] = 0$ then the two share the same eigenspaces. In particular, they are diagonal in the same basis. This allows us to identify the probability of observing outcome r with $\rho_{rr} = \langle r|\rho_S^{(0)}|r\rangle = \langle r|\sum_s p_s |s\rangle\langle s| |r\rangle = p_r$. Therefore, the entropies $S(\mathbf{p})$ and S_0 coincide. On the other hand, generally the probbaility of observing outcome r would be $p_r = \sum_\alpha q_\alpha |\langle\alpha|r\rangle|^2$, with $\rho_S^{(0)} = \sum_\alpha q_\alpha |\alpha\rangle\langle\alpha|$. Consider now the relative entropy between initial and (averaged) final state

$$D[\rho^{(0)}|\rho^{(2)}] = \sum_\alpha q_\alpha \ln q_\alpha - \sum_{r\alpha} q_\alpha |\langle\alpha|r\rangle|^2 \ln p_r = S(\mathbf{p}) - S(\mathbf{q}) = 0$$

which is zero by hypothesis. However, we know from Klein's inequality that

$$D[\rho|\sigma] \geq 0, \qquad \text{with} \quad D[\rho|\sigma] = 0 \Leftrightarrow \rho = \sigma$$

therefore, the initial state and the averaged final state must coincide (up to reshuffling of the basis). This means that $\rho_S^{(0)}$ and $\rho_S^{(2)}$ are diagonal in the same basis, which is the eigenbasis of R_S, meaning that $[R_S, \rho_S^{(0)}] = 0$.

Exercise 5.7: Entropy production in a general control operation

Consider a general control operation in which, first, the system and the ancilla (SA) are evolved through $\mathcal{U}_{SA}$. Then, a projective measurement on A is implemented with an ideam memory M in such a way that AM evolves with $\mathcal{U}_{AM}$. Only then, the memory is observed.

Defining the stochastic entropy as

$$s_3(r) = -k_B \ln p(r) + k_B S[\rho_{SA}^{(3)}(r)],$$

find an example where $s_3(r) - S_0 < 0$, with S_0 being the initial entropy, for some r, but $S_3 - S_0 \geq 0$.

Solution:
Consider the following averaged post-measurement state

$$\rho_{SAM}^{(3)} = p\,|\psi\rangle\langle\psi|_{SA} \otimes |0\rangle\langle 0|_M + (1-p)\sigma_{SA} \otimes |1\rangle\langle 1|_M$$

that crucially yields a pure state on SA when the outcome of the measurement is 0. Indeed, the stochastic entropy for $r = 0$ is

$$s_3(0) = -\ln p.$$

Consider now the simplest possible case: Before the measurement the state is simply

$$\rho_{SAM}^{(2)} = \rho_{SAM}^{(3)}.$$

This has entropy

$$S_2 = S(\mathbf{p}) + (1-p)S[\sigma_{SA}] = S_1 = S_0,$$

and we can write the difference

$$s_3(0) - S_0 = -\ln p + p\ln p + (1-p)\ln(1-p) - (1-p)S[\sigma_{SA}] = (1-p)\left[-S[\sigma_{SA}] + \ln\frac{1-p}{p}\right].$$

Since $(1-p) \geq 0$ we see that to have a negative stochastic entropy production we need

$$e^{-S[\sigma]}(1-p) < p \to p > \frac{1}{1+e^{S[\sigma]}}$$

Exercise 5.8: Repeated interactions in operational stochastic thermodynamics: idle ancillae

Consider the framework of repeated interactions, where the system S interacts with a stream of auxiliary ancillae $A \equiv A(0)A(1)\cdots A(n)$ to produce the control operations ($\mathcal{C}$) between the dynamical evolutions ($\mathcal{E}$) of S. This means that the conditional non-normalized state is

$$\tilde{\rho}_S(t|\mathbf{r}_n) = \mathcal{C}_n(r_n|\mathbf{r}_{n-1})\mathcal{E}_{n,n-1}(\mathbf{r}_{n-1})\cdots\mathcal{C}_1(r_1|r_0)\mathcal{E}_{1,0}(r_0)\mathcal{C}_0(r_0)\rho_S(0),$$

with
$$\mathcal{C}_n(r_n|\mathbf{r}_{n-1})\rho_S^{(0)} = \mathrm{Tr}_{SA(n)}\left\{\mathcal{P}_{A(n)}(r_n)\mathcal{U}_{SA(n)}(\mathbf{r}_{n-1})\left[\rho_S^{(0)}\otimes\rho_{A(n)}^{(0)}(\mathbf{r}_{n-1})\right]\right\}.$$
The Hamiltonian of system and ancillae is
$$H_{SA}[\lambda_t(\mathbf{r}_n)] = H_S[\lambda_t(\mathbf{r}_n)] + \sum_{j=0}^{n} H_{A(j)}$$
and allows to define the stochastic internal energy as
$$u_{SA}(\mathbf{r}_n,t) \equiv \mathrm{Tr}_{SA}\left\{H_{SA}[\lambda_t(\mathbf{r}_n)]\rho_{SA}(t|\mathbf{r}_n)\right\} = u_S(\mathbf{r}_n,t) + \sum_{j=0}^{n} u_{A(j)}(\mathbf{r}_n,t).$$

Show that the ancillae stochastic energy does not change in the time between two control operations.

Solution:
Between (but excluding) two consecutive control operations, $t_n < t_{n+1}$, the system evolves according to the dynamical map $\mathcal{E}_{n+1,n}(\mathbf{r}_n,t)$ such that the state is
$$\rho_{SA}(t|\mathbf{r}_n) = \mathcal{E}_{n+1,n}(\mathbf{r}_n,t)\rho_{SA}(t_n|\mathbf{r}_n)$$
such that the stochastic internal energy of the ancillae at time t is
$$u_A(\mathbf{r}_n,t) = \mathrm{Tr}_{SA}\left\{H_A\mathcal{E}_{n+1,n}(\mathbf{r}_n,t)\rho_{SA}(t_n|\mathbf{r}_n)\right\}$$
Crucially, H_A and $\mathcal{E}_{n+1,n}(\mathbf{r}_n,t)$ commute because they act on different Hilbert spaces. Furthermore, introducing the Kraus decomposition of the dynamical map $\mathcal{E}_{n+1,n}(\mathbf{r}_n,t)\rho_{SA}(t_n|\mathbf{r}_n) = \sum_i K_i\rho_{SA}(t_n|\mathbf{r}_n)K_i^\dagger$ with $\sum_i K_i^\dagger K_i = \mathbb{I}_S$ Kraus operators generally depending on both t and $\mathbf{r}_n$, we have
$$\begin{aligned} u_A(\mathbf{r}_n,t) &= \mathrm{Tr}_{SA}\left\{H_A\mathcal{E}_{n+1,n}(\mathbf{r}_n,t)\rho_{SA}(t_n|\mathbf{r}_n)\right\} = \sum_i \mathrm{Tr}_{SA}\left\{H_A K_i\rho_{SA}(t_n|\mathbf{r}_n)K_i^\dagger\right\} \\ &= \sum_i \mathrm{Tr}_{SA}\left\{K_i^\dagger K_i H_A\rho_{SA}(t_n|\mathbf{r}_n)K_i^\dagger\right\} = \mathrm{Tr}_{SA}\left\{H_A\rho_{SA}(t_n|\mathbf{r}_n)\right\} = u_A(r_n,t_n^+). \end{aligned}$$

Exercise 5.9: Repeated interactions in operational stochastic thermodynamics: Monty Hall style

In the framework of repeated interaction for operational stochastic thermodyncamis, introduced in Exercise 5.8, construct an example with two ancillae $A(0), A(1)$, where the internal energy of $A(0)$ changes after receiving result r_1.

Show that this is *not* a quantum effect in general.

Solution:
Let's assume that after the control operation with the 0-th ancilla the SA state is
$$\rho_{SA} = \left(\frac{|00\rangle\langle 00| + |11\rangle\langle 11|}{2}\right)_{SA(0)} \otimes |0\rangle\langle 0|_{A(1)}$$
which is classically correlated state that has internal energy of $A(0)$ equal to $\epsilon/2$ (taking $H_{A(0)} = \epsilon\,|1\rangle\langle 1|$ as Hamiltonian). Let's consider the trivial dynamical map $\mathcal{E}_{1,0} = \mathbb{I}$ and the control-flip unitary between S and $A(1)$
$$U\,|00\rangle = |00\rangle\,, \qquad U\,|10\rangle = |01\rangle\,.$$
Notice how also this operation is classical since it can be done with a permutation. After this unitary evolution we have
$$\left(\frac{|000\rangle\langle 000| + |011\rangle\langle 011|}{2}\right)$$
we now measure $A(1)$ which leads to the outcomes
$$\frac{|000\rangle\langle 000|}{2}, \qquad \frac{|011\rangle\langle 011|}{2}.$$

Notice that, if the outcome of the measurement is 0, then the post-selected state has internal energy of $A(0)$ equal to 0, whereas if the outcome is 1, the internal energy of $A(0)$ is ϵ.
This is basically the classical "collapse of the wave function": once more information is gathered, we update the state and change the probabilities accordingly, just like in the Monty Hall problem.

Exercise 5.10: Repeated interactions in operational stochastic thermodynamics: 1st law

In the framework of repeated interactions in operational stochastic thermodynamics, introduced in Exercise 5.8, consider the change in energy due to the control operation, namely

$$\Delta u_{SA}^{\mathrm{ctrl}}(\mathbf{r}_n) \equiv \lim_{\epsilon\to 0^+} [u_{SA}(\mathbf{r}_n, t_n+\epsilon) - u_{SA}(\mathbf{r}_n, t_n-\epsilon)] = \Delta u^{\mathrm{meas}}(\mathbf{r}_n) + w^{\mathrm{ctrl}}(\mathbf{r}_{n-1})$$

where $w^{\mathrm{ctrl}}(\mathbf{r}_{n-1})$ is the change in energy due to the unitary evolution $\mathcal{U}_{SA(n)}$ calculated *before* the projective measurement on the ancilla, whereas $\Delta u^{\mathrm{meas}}(\mathbf{r}_n)$ is the change in energy between before and after the ancilla's measurement.

In particular, we separate

$$\Delta u^{\mathrm{meas}}(\mathbf{r}_n) = q_S^{\mathrm{meas}}(\mathbf{r}_n) + w_A^{\mathrm{meas}}(\mathbf{r}_n)$$

with

$$q_S^{\mathrm{meas}}(\mathbf{r}_n) \equiv \mathrm{Tr}_S\left\{H_S[\lambda_n(\mathbf{r}_{n-1})]\left[\rho_S^{(2)}(\mathbf{r}_n) - \rho_S^{(1)}(\mathbf{r}_{n-1})\right]\right\}, \qquad w_A^{\mathrm{meas}}(\mathbf{r}_n) \equiv \mathrm{Tr}_A\left\{H_A\left[\rho_A^{(2)}(\mathbf{r}_n) - \rho_A^{(1)}(\mathbf{r}_{n-1})\right]\right\},$$

where

$$\rho_{SA(n)}^{(1)}(\mathbf{r}_{n-1}) \equiv \mathcal{U}_{SA(n)}(\mathbf{r}_{n-1})\left[\rho_S^{(0)}(\mathbf{r}_{n-1}) \otimes \rho_A^{(0)}(\mathbf{r}_{n-1})\right], \qquad \rho_{SA(n)}^{(2)}(\mathbf{r}_n) = \frac{\mathcal{P}_{A(n)}(r_n)\rho_{SA(n)}^{(1)}(\mathbf{r}_{n-1})}{p(r_n|\mathbf{r}_{n-1})}$$

are the states immediately after the unitary evolution and the projective ($[\Pi_{A(n)}(r_n), H_{A(n)}] = 0$) measurement, respectively.

Show that

$$\sum_{r_n} p(r_n|\mathbf{r}_{n-1}) q_S^{\mathrm{meas}}(\mathbf{r}_n) = 0, \qquad \sum_{r_n} p(r_n|\mathbf{r}_{n-1}) w_A^{\mathrm{meas}}(\mathbf{r}_n) = 0.$$

Solution:
We can tackle the sums directly:

$$\begin{aligned}
\sum_{r_n} p(r_n|\mathbf{r}_{n-1}) q_S^{\mathrm{meas}}(\mathbf{r}_n) &= \mathrm{Tr}_S\left\{H_S\left[\sum_{r_n} p(r_n|\mathbf{r}_{n-1})\rho_S^{(2)}(\mathbf{r}_n) - \rho_S^{(1)}(\mathbf{r}_{n-1})\right]\right\} \\
&= \mathrm{Tr}_S\left\{H_S\left[\sum_{r_n} \mathrm{Tr}_A\left\{\mathcal{P}_{A(n)}(r_n)\rho_{SA}^{(1)}(\mathbf{r}_{n-1})\right\} - \rho_S^{(1)}(\mathbf{r}_{n-1})\right]\right\} \\
&= \mathrm{Tr}_S\left\{H_S\left[\mathrm{Tr}_A\left\{\rho_{SA}^{(1)}(\mathbf{r}_{n-1})\right\} - \rho_S^{(1)}(\mathbf{r}_{n-1})\right]\right\} = 0
\end{aligned}$$

$$\begin{aligned}
\sum_{r_n} p(r_n|\mathbf{r}_{n-1}) w_A^{\mathrm{meas}}(\mathbf{r}_n) &= \mathrm{Tr}_A\left\{H_A\left[\sum_{r_n} p(r_n|\mathbf{r}_{n-1})\rho_A^{(2)}(\mathbf{r}_n) - \rho_A^{(1)}(\mathbf{r}_{n-1})\right]\right\} \\
&= \mathrm{Tr}_A\left\{H_A\left[\sum_{r_n} \mathrm{Tr}_S\left\{\mathcal{P}_{A(n)}(r_n)\rho_{SA}^{(1)}(\mathbf{r}_{n-1})\right\} - \rho_A^{(1)}(\mathbf{r}_{n-1})\right]\right\} \\
&= \mathrm{Tr}_A\left\{H_A\left[\mathrm{Tr}_S\left\{\rho_{SA}^{(1)}(\mathbf{r}_{n-1})\right\} - \rho_A^{(1)}(\mathbf{r}_{n-1})\right]\right\} = 0
\end{aligned}$$

Exercise 5.11: Repeated interactions in operational stochastic thermodynamics: 2nd law

In the framework of repeated interactions in operational stochastic thermodynamics, introduced in Exercise 5.8, consider the change in entropy in absence of control operations, namely in the time interval $(t_{n-1}+\epsilon, t_n-\epsilon)$.

The stochastic entropy production in such an interval is

$$\sigma^{(n)}(\mathbf{r}_{n-1}) = k_B \left\{ S[\rho_{SA}^{(0)}(\mathbf{r}_{n-1})] - S[\rho_{SA}^{(2)}(\mathbf{r}_{n-1})] \right\} - \frac{q^{(n)}(\mathbf{r}_{n-1})}{T},$$

where $\rho_{SA}^{(2)}(\mathbf{r}_{n-1})$ is the initial state obtained after the starting control operation, and $S[\rho_{SA}^{(0)}(\mathbf{r}_{n-1})]$ is the final state, obtained through the dynamical map $\mathcal{E}_{n,n-1}(\mathbf{r}_{n-1})$ as

$$\rho_{SA}^{(0)}(\mathbf{r}_{n-1}) = [\mathcal{E}_{n,n-1}(\mathbf{r}_{n-1}) \otimes \mathcal{I}_A] \rho_{SA}^{(2)}(\mathbf{r}_{n-1}),$$

and the stochastic heat $q^{(n)}(\mathbf{r}_{n-1})$ is the one exchanged during the dynamical map with the bath, namely

$$q^{(n)}(\mathbf{r}_{n-1}) = \int_{t_{n-1}}^{t_n} dt \mathrm{Tr}_S \left\{ H_S[\lambda_t(\mathbf{r}_{n-1})] \partial_t \rho_S(t|\mathbf{r}_{n-1}) \right\}.$$

Show that

$$\sigma^{(n)}(\mathbf{r}_{n-1}) \geq 0$$

Solution:
First of all, we would like to separate the entropies on the joint states ρ_{SA} into the entropies of the marginal states, therefore we make use of the mutual information

$$I_{S:A}[\rho_{SA}] = S[\rho_S] + S[\rho_A] - S[\rho_{SA}]$$

which allows us to write

$$\sigma^{(n)}(\mathbf{r}_{n-1}) = k_B \left\{ \Delta S_S + \Delta S_A + I_{S:A}[\rho_{SA}^{(2)}(\mathbf{r}_{n-1})] - I_{S:A}[\rho_{SA}^{(0)}(\mathbf{r}_{n-1})] \right\} - \frac{q^{(n)}(\mathbf{r}_{n-1})}{T}.$$

Crucially, the marginal state of the ancilla does not change. In fact, by introducing the Kraus decomposition K_i of the dynamical map $\mathcal{E}_{n,n-1}$ we have

$$\begin{aligned} \mathrm{Tr}_A \left\{ X_A \rho_A^{(0)} \right\} &= \mathrm{Tr}_{SA} \left\{ X_A [\mathcal{E} \otimes \mathcal{I}_A] \rho_{SA}^{(2)} \right\} = \sum_i \mathrm{Tr}_{SA} \left\{ X_A K_i \rho_{SA}^{(2)} K_i^\dagger \right\} = \sum_i \mathrm{Tr}_{SA} \left\{ K_i^\dagger K_i X_A \rho_{SA}^{(2)} \right\} \\ &= \mathrm{Tr}_{SA} \left\{ X_A \rho_{SA}^{(2)} \right\} = \mathrm{Tr}_A \left\{ X_A \rho_A^{(2)} \right\} \quad \forall X_A \quad \Rightarrow \quad \rho_A^{(0)} = \rho_A^{(2)}. \end{aligned}$$

This means that $\Delta S_A = S[\rho_A^{(0)}] - S[\rho_A^{(2)}] = 0$.
Additionally, we can apply the second law to the system-bath exchange, see Exercise 3.10: Calling $\Sigma = \Delta S_S - \frac{q}{T}$ we have

$$\partial_t \Sigma = -\mathrm{Tr} \left\{ \partial_t \rho_S \ln \rho_S \right\} - \frac{\mathrm{Tr} \left\{ H_S(\lambda_t) \partial_t \rho_S \right\}}{T} = - \left. \frac{\partial}{\partial t} \right|_{\lambda_t} D[\rho_S | \pi(\lambda_t)]$$

Using that the thermal state is a fixed point of the dynamics (for sufficiently small times such that the driving protocol does not matter), $\mathcal{E}(dt)\pi(\lambda_t) = \pi(\lambda_t)$ and the monotonicity of the relative entropy, namely $D[\mathcal{E}\rho|\mathcal{E}\sigma] \leq D[\rho|\sigma]$ we find

$$\partial_t \Sigma = \lim_{dt \to 0} \frac{D[\rho_S(t)|\pi(\lambda_t)] - D[\mathcal{E}(dt)\rho_S(t)|\mathcal{E}(dt)\pi(\lambda_t)]}{dt} \geq 0$$

which also imples $\Sigma \geq 0$. Then, the stochastic entropy production satisfies

$$\sigma^{(n)}(\mathbf{r}_{n-1}) \geq k_B \left\{ I_{S:A}[\rho_{SA}^{(2)}(\mathbf{r}_{n-1})] - I_{S:A}[\rho_{SA}^{(0)}(\mathbf{r}_{n-1})] \right\}.$$

Finally, noticing that the mutual information can be written in terms of a relative entropy as

$$I_{S:A}[\rho_{SA}] = S[\rho_S] + S[\rho_A] - S[\rho_{SA}] = D[\rho_{SA}|\rho_S \otimes \rho_A]$$

the lower bound of the stochastic entropy production reads

$$k_B \left\{ D[\rho_{SA}^{(2)}|\rho_S^{(2)} \otimes \rho_A^2] - D[\rho_{SA}^{(0)}|\rho_S^{(0)} \otimes \rho_A^0] \right\}$$

Since we already discussed how $\rho_A^{(2)} = \rho_A^{(0)}$ we can write this difference of relative entropies as

$$k_B \left\{ D[\rho_{SA}^{(2)}|\rho_S^{(2)} \otimes \rho_A^2] - D[(\mathcal{E} \otimes \mathcal{I}_A)\rho_{SA}^{(2)}|(\mathcal{E} \otimes \mathcal{I}_A)\rho_S^{(2)} \otimes \rho_A^2] \right\} \geq 0$$

which is positive by virtue of the relative entropy monotonicity. This means that the stochastic entropy production without control operations is positive:

$$\sigma^{(n)}(\mathbf{r}_{n-1}) \geq 0.$$

Exercise 5.12: Repeated interactions in operational stochastic thermodynamics: no measurements

Verify that the framework of repeated interactions in operational stochastic thermodynamics, introduced in Exercise 5.8 satisfies the following statements:

(i) If one does not perform any ancilla measurement, it reduces to the repeated interaction framework.

(ii) If one does not perform any control operations, it reduces to the standard quantum thermodynamics framework based on the Born-Markov-secular equation.

Solution:

(i) If one does not perform any ancilla measurement, namely $\mathcal{P}_{A(n)} = \mathcal{I}_{A_n}$, the map of the joint system+ancillae state after n interactions reads

$$\rho(t) = \mathcal{E}_{t,n}\mathcal{U}_{SA(n)}\cdots\mathcal{U}_{SA(1)}\mathcal{E}_{1,0}\rho(0).$$

As expected, we notice that heat and work associated with the measurement vanish (see Exercise 5.10) because $\rho_{SA}^{(2)} = \rho_{SA}^{(1)}$. This means that the energy difference in the control operation is all work:

$$\Delta u_{SA}^{\text{ctrl}} = W^{\text{ctrl}}(t).$$

(ii) If one does not perform any control operations, we can set all unitaries $\mathcal{U}_{SA} = \mathcal{I}_{SA}$ as well, so the state evolution simply becomes

$$\rho(t) = \mathcal{E}_{t,0}\rho(0)$$

which is the formalism of the BMS master equation, in which $\mathcal{E}_{t,0} = \mathcal{T}e^{\int_0^t \mathcal{L}(s)ds}$.

Exercise 5.13: Stochastic entropy production with continuous measurements

Consider the framework of repeated interactions in operational stochastic thermodynamics, introduced in Exercise 5.8, in which the measurements happen very frequently (at each time step δt), such that one can approximate the dynamical maps as

$$\mathcal{E}(t+\delta t, t) \approx \mathcal{I}_S + \delta t\mathcal{L}(\lambda_t),$$

which we take to be independent of the previous measurement results. Furthermore, we consider the classical case in which the system Hamiltonians at different times commute, such that we can write the eigendecomposition $H_S(\lambda_t) = \sum_r \epsilon(r, \lambda_t)\,|r\rangle\langle r|$, and the measurement is done on the energy eigenbasis, such that the control operation reads

$$\mathcal{C}_n(r_n)\rho_S^{(0)}(\mathbf{r}_{n-1}) = |r_n\rangle\langle r_n|\,\rho_S^{(0)}(\mathbf{r}_{n-1})\,|r_n\rangle\langle r_n|\,.$$

From the definition of stochastic entropy production in the repeated interactions in operational stochazstic thermodynamics,

$$\sigma^{(n]}(\mathbf{r}_n) = \sigma^{(n)}(\mathbf{r}_{n-1}) + \sigma^{\text{ctrl}}(\mathbf{r}_n)$$

where

$$\sigma^{(n)}(\mathbf{r}_{n-1}) = \Delta s_{SA}^{(n)}(\mathbf{r}_{n-1}) - \frac{q^{(n)}(\mathbf{r}_{n-1})}{T}, \qquad \sigma^{\text{ctrl}}(\mathbf{r}_n) = \Delta s_{SA}^{\text{ctrl}}(\mathbf{r}_n) - \frac{q_S^{\text{meas}}(\mathbf{r}_n)}{T},$$

show that

$$\Delta s_S^{(n]}(\mathbf{r}_n) = -k_B \ln(r_n|\mathbf{r}_{n-1}) = -k_B \ln p(s_n|s_{n-1}).$$

Solution:
The heat exchanged during the dynamical map is

$$q^{(n)}(\mathbf{r}_{n-1}) = \int_{(n-1)\delta t}^{n\delta t} dt\text{Tr}\left\{H_S(\lambda_t)\partial_t\rho_S(t)\right\} \approx \int_{(n-1)\delta t}^{n\delta t} dt\text{Tr}\left\{H_S(\lambda_t)\mathcal{L}(\lambda_{t-\delta t})\rho_S(t-\delta t)\right\} \approx \delta t\text{Tr}\left\{H_S(\lambda_n)\mathcal{L}(\lambda_{n-1})\rho_S(t_{n-1})\right\}.$$

Notice that, since $\rho_S(t_{n-1})$ is the state right after the measurement, we have $\rho_S(t_{n-1}) = |r_{n-1}\rangle\langle r_{n-1}|$.

Instead, the heat exchanged during the measurement is

$$\begin{aligned} q_S^{\text{meas}}(\mathbf{r}_n) &= \text{Tr}\left\{H_S(\lambda_n)\left(|r_n\rangle\langle r_n| - [\mathcal{I}_S + \delta t \mathcal{L}(\lambda_{n-1})]\,|r_{n-1}\rangle\langle r_{n-1}|\right)\right\} \\ &= \epsilon(r_n, \lambda_t) - \epsilon(r_{n-1}, \lambda_t) - \delta t \text{Tr}\left\{H_S(\lambda_n)\mathcal{L}(\lambda_{n-1})\,|r_{n-1}\rangle\langle r_{n-1}|\right\}. \end{aligned}$$

Noticing that

$$\Delta s_{SA}^{(n)}(\mathbf{r}_{n-1}) = S[\rho_{SA}^{(0)}(t_n)] - S[\rho_{SA}^{(2)}(t_{n-1})], \quad \Delta s_{SA}^{\text{ctrl}}(\mathbf{r}_n) = -\ln p(r_n|\mathbf{r}_{n-1}) + S[\rho_{SA}^{(2)}(t_n)] - S[\rho_{SA}^{(1)}(t_n)],$$

using that the control operation is implemented through a unitary transformation, and therefore does not change the entropy, their sum yields

$$\Delta s_{SA}^{(n)}(\mathbf{r}_{n-1}) + \Delta s_{SA}^{\text{ctrl}}(\mathbf{r}_n) = -\ln p(r_n|\mathbf{r}_{n-1}) + S[\rho_{SA}^{(2)}(t_n)] - S[\rho_{SA}^{(2)}(t_{n-1})].$$

Crucially, $\rho_S^{(2)}(t_n) = |r_n\rangle\langle r_n| \Rightarrow \rho_{SA}^{(2)}(t_n) = |r_n\rangle\langle r_n|_S \otimes \rho_A(t_n)$. Furthermore, if we consider the implementation of the control operation $\mathcal{C}_n(\mathbf{r}_n)$ to be done through a projective measurement on the ancilla, also $\rho_A(t_n)$ will be pure. This means that $S[\rho_{SA}^{(2)}(t_n)] = S[\rho_{SA}^{(2)}(t_{n-1})] = 0$ and we can write the entropy production as

$$\sigma^{(n]} = -\ln p(r_n|\mathbf{r}_{n-1}) - \frac{\epsilon(r_n, \lambda_t) - \epsilon(r_{n-1}, \lambda_t)}{T}.$$

Here, the conditional probability $p(r_n|\mathbf{r}_{n-1})$ is given by the norm of $\mathcal{C}_n(r_n)\rho_S^{(0)}(\mathbf{r}_{n-1})$. In particular, we find that

$$p(r_n|\mathbf{r}_{n-1}) = \langle r_n|\rho_S^{(0)}(\mathbf{r}_{n-1})|r_n\rangle = \langle r_n|\,|r_{n-1}\rangle\langle r_{n-1}| + \delta t \mathcal{L}(\lambda_t)[|r_{n-1}\rangle\langle r_{n-1}|]|r_n\rangle$$

depends only on the current outcome r_n and the immediately preceding outcome r_{n-1}, meaning that the probability distribution satisfies the Markov property

$$p(r_n|\mathbf{r}_{n-1}) = p(r_n|r_{n-1}).$$

Then, the average entropy production in one time interval δt reads

$$đ\Sigma^{(n]} = \sum_{r_{n-1}} p(r_{n-1}) S[p(r_n|r_{n-1})] - \frac{đQ_S^{(n]}}{T}.$$

Exercise 5.14: Faulty Maxwell's demon

In the framework of repeated interaction for operational stochastic thermodynamics, consider the case in which the ancillae are used to implement the arbitrary channels $\mathcal{C}_k(r_k|\mathbf{r}_{k-1})$ on the system S through projective, rank-1 measurements $\mathcal{P}_{A(n)}(r_n)$ on the ancillae, which act as a memory.

Furthermore, assume the ancillae to be energy-degenerate. However, unlike an ideal memory, consider the case in which the initial ancilla state is mixed and show that the amount of extractable work is reduced.

Solution:
We can write the initial state as

$$\rho_{SA}(0) = \rho_S(0) \bigotimes_{i=0}^{n} \rho_{A(i)}(0)$$

where all ρ_x are arbitrary.
The final state, i.e. the state after n measurements, is

$$\rho_{SA}(t|\mathbf{r}_n) = \rho_S(t|\mathbf{r}_n) \bigotimes_{i=0}^{n} |r_i\rangle\langle r_i|_{A(i)}$$

because all the measurements on the ancillae collapse their state into a pure state.
Notice that the ancillae encode the outcomes of the measurements, and therefore there is an entropy associated with this information storage.
In particular, the final stochastic entropy reads

$$s_{SA}(\mathbf{r}_n, t) = -\ln p(\mathbf{r}_n) + S[\rho_S(t|\mathbf{r}_n)]$$

while the initial entropy is

$$s_{SA}(0) = S[\rho_S(0)] + \sum_{i=0}^{n} S[\rho_{A(i)}(0)].$$

Thus, the average second law becomes

$$\Sigma(t) = S[p(\mathbf{r}_n)] + \sum_{\mathbf{r}_n} p(\mathbf{r}_n) S[\rho_S(t|\mathbf{r}_n)]] - S[\rho_S(0)] - \sum_{i=0}^{n} S[\rho_{A(i)}(0)] - \frac{Q(t)}{T} \geq 0$$

If the final S state coincides with the initial one, the entropy difference in average second law cancels out, as well as the internal energy difference in the first law, which then becomes

$$\Delta U_S(t) = 0 = W(t) + Q(t)$$

allowing us to write

$$T\left(S[p(\mathbf{r}_n)] - \sum_{i=0}^{n} S[\rho_{A(i)}(0)]\right) \geq -W(t).$$

This shows that the maximum extracted work is reduced by the amount of work needed to reset the memory. Notice that one could also have assumed the ancillae to be entangled, leading to the ancillae state $\rho_A(0)$, without changing the the result:

$$T\left(S[p(\mathbf{r}_n)] - S[\rho_A(0)]\right) \geq -W(t).$$

Notably, if the state $\rho_A(0)$ is pure, then we recover the ideal memory case. In fact, if the ancillae state is pure, one can implement a unitary transformation on the ancillae to map the initial pure state into the desired "zero" state of the memory without requiring any cost (unitaries do not change entropy and it does not change the energy of the degenerate memory).

Exercise 5.15: Demon in the single-electron transistor:

Consider the single-electron transistor introduced in Exercise 3.33, described by the classical rate equation

$$\frac{d}{dt}\begin{pmatrix} p_F(t) \\ p_E(t) \end{pmatrix} = \sum_{\nu} \Gamma_\nu(\epsilon_0) \begin{pmatrix} -[1 - f_\nu(\epsilon_0)] & f_\nu(\epsilon_0) \\ 1 - f_\nu(\epsilon_0) & -f_\nu(\epsilon_0) \end{pmatrix} \begin{pmatrix} p_F(t) \\ p_E(t) \end{pmatrix}.$$

Set $\mu_L = \epsilon_0 + eV/2$, $\mu_R = \epsilon_0 - eV/2$ with $eV > 0$, such that electrons would have the tendency to travel from left to right, and define $\alpha \equiv \beta eV/2$.s

Consider the possibility of changing the tunnelling constants Γ_ν between the values $0, \Gamma_0 > 0$ instantaneously.

At time $t = 0$, take the dot to be filled and the rates to be $(\Gamma_L, \Gamma_R) = (\Gamma_0, 0)$ and consider the following feedback loop:

(1) Wait for time τ.

(2) Measure the occupation r of the dot:

- If $r = 0$: set the tunneling constants to $(\Gamma_L, \Gamma_R) = (0, \Gamma_0)$;
- If $r = 1$: set the tunneling constants to $(\Gamma_L, \Gamma_R) = (\Gamma_0, 0)$;

(3) Go to step (1).

Show that, for any finite α and sufficiently large n, this control protocol transports electrons from the right to the left *against* the voltage bias.

Solution:
Notice that, right after the measurement and feedback, the dot is either:

- Filled and connected *only* to the left bath.
- Empty and connected *only* to the right bath.

Therefore, as long as the electron can tunnel from the dot to the left bath, and electrons can tunnel from the right bath to the dot, we will have particle transfer from right to left. This condition can be stated as

$$1 - f_L \neq 0 \qquad f_R \neq 0$$

which in this case, since $f_L = \frac{1}{1+e^{-\alpha}} = 1 - f_R$ means that $\alpha \neq \infty$.

Exercise 5.16: Demon in the single-electron transistor: electron jumps

Consider the setting of the feedback control on the single-electron transistor introduced in Exercise 5.15. Find a relation between the measurement outcomes $\mathbf{r}_n$ and the number of electrons transfered from right to left.

Solution:

The measurement outcomes is a boolean vector starting with 1 (assuming that a measurement also happened at $t = 0$), e.g

$$\mathbf{r}_n = (1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 1, 1, 1, 1, \cdots).$$

Crucially, when the outcomes switch from $1 \to 0$ it means that an electron tunneled from the dot into the left bath, whereas when the outcomes switch from $0 \to 1$ it means that an electron tunneled from the right bath into the dot. Therefore, the total number of switches s gives the number of net electron jumps (i.e. electron jumps that are actually detected by the measurement scheme). Furthermore, since the values can only switch from $0 \to 1$ or from $1 \to 0$ and the system starts with $r_0 = 1$, we have that $s(1 \to 0) - s(0 \to 1) \in \{0, 1\}$: is s is even, then $s(1 \to 0) = s(0 \to 1)$, if s is odd then $s(1 \to 0) = s(0 \to 1) + 1$.

Exercise 5.17: Demon in the single-electron transistor: entropy

Consider the setting of the feedback control on the single-electron transistor introduced in Exercise 5.15, but now assume that the waiting time τ is much larger than $1/\Gamma_0$, such that we can approximate the dot state at the measurement times $n\tau$ with the corresponding steady state.

Show that

$$S[p(\mathbf{r}_n)] = n S_{\text{Sh}}(\pi_{0|L}, \pi_{1|L}),$$

where $\pi_{0|L} = 1 - \pi_{1|L} = \frac{1}{e^{\alpha}+1}$.

Solution:
Given the symmetric choice of voltage bias, we have

$$f_L = \frac{1}{1 + e^{-\alpha}} = 1 - f_R.$$

Additionally, if the dot is in contact with the left bath, the next measurement will give as outcomes

- $r = 1$ with probability f_L;
- $r = 0$ with probability $1 - f_L$.

Instead, if the dot is in contact with the right bath, the next measurement will give as outcomes

- $r = 1$ with probability $f_R = 1 - f_L$;
- $r = 0$ with probability $1 - f_R = f_L$.

Now, consider a sequence of outcomes $\mathbf{r}_n$ ($n \geq 1$) and let's also write the vector $\boldsymbol{\nu}$ with components chosen between L, R that indicate what probability distribution is used to determine the outcome of the measurement. Notice that we have the 4 possibilities for the pair (r_i, ν_i), which lead to the probabilities of observing r_i

$$(1, L) \to f_L, \quad (0, L) \to f_R, \quad (1, R) \to f_R, \quad (0, R) \to f_L$$

we can now write the two vectors and the corresponding probabilities in a "stack", for example

$$\begin{pmatrix} 1 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \\ L & L & L & R & R & L & L & L & R & L \\ f_L & f_L & f_R & f_L & f_R & f_L & f_L & f_R & f_R & f_L \end{pmatrix}$$

where we can notice how $\boldsymbol{\nu}$ lags one step behind $\mathbf{r}_n$. This makes it so that the number of f_R appeating is equal to the number of switches s. In fact, one can see the number of switches as the logical operation $\mathbf{r}_n \dot{\vee} \tilde{\mathbf{r}}_n$ where $\tilde{\mathbf{r}}_n$ is the boolean vector with coordinates $\tilde{r}_1 = 1, \tilde{r}_i = r_{i-1}$ for $i = 2, \cdots, n$. This logical operation is exactly what we are doing here with the stacking of $\mathbf{r}_n$ and $\boldsymbol{\nu}_n$.
Therefore, the probability of seeing a precise sequence with s switches is

$$p(\mathbf{r}_n) = f_L^{n-s} f_R^s$$

Notice that this is actually independent of the specific sequence $\mathbf{r}_n$ but only depends on the number of switches s. We can therefore look at the number of sequences $\mathbf{r}_n$ with s switches. Crucially, a switch *cannot* be in any position: in fact, we require switches to be separated by at least one digit, i.e. there cannot be more than one swith in a single position, and we cannot end with a switch. Introducing the generalized switch-outcome sequence with elements from the set $\{r_1, \cdots, r_n, s_1, \cdot, s_s\}$ we construct all possible sequences by looking at the composites $x_i = s_i r_i$, which allows us to satisfy both conditions. Then, we need all possible sequences from the set $\{x_1, \cdots, x_s, r_{s+1}, \cdots, r_n\}$ which are given by the binomial coefficient $\frac{n!}{(n-s)!s!}$ because we can shuffle the indeces of both x and r without changing the outcome.
We can now calculate the entropy of the probability distribution $p(\mathbf{r}_n)$:

$$S(p(\mathbf{r}_n)) = -\sum_s \sum_{\mathbf{r}_n \in S_s} p(\mathbf{r}_n) \ln p(\mathbf{r}_n) = -\sum_s \frac{n!}{(n-s)!s!} f_L^{n-s} f_R^s \left((n-s) \ln f_L + s \ln f_R\right).$$

Using that

$$\sum_{k=0}^{n} \frac{n!}{(n-k)!k!} k x^{n-k} y^k = ny \sum_{k=1}^{n} \frac{(n-1)!}{[n-1-(k-1)]!(k-1)!} x^{n-1-(k-1)} y^{k-1} = ny(x+y)^{n-1}$$

using $f_L = 1 - f_R$, we find

$$S(p(\mathbf{r}_n)) = nS(f_L, 1 - f_L).$$

Exercise 5.18: Implementing arbitary unitaries

Consider the system-ancilla interaction

$$V_{SA}(\lambda_t) = \sum_j V_{SA(j)}(\lambda_t), \quad V_{SA(j)}(\lambda_t) = i\hbar\delta(t - t_j) \ln(U_{SA(j)}).$$

Show that $V_{SA(j)}(\lambda_t)$ is Hermitian and verify that it implements the desired unitary operator $U_{SA(j)}$ at time t_j.

I think there is an error in the book concerning the definition of $V_{SA(j)}$. Here I changed it to something that makes more sense to me: I moved the imaginary unit i outside the log.

Solution:
Any unitary operator U can be written in terms of an Hermitian operator K as

$$U = e^{iK}$$

Then, the interaction with the j-th ancilla reads

$$V_{SA(j)}(\lambda_t) = i\hbar\delta(t - t_j) \ln(e^{iK}) = -\hbar K \delta(t - t_j) = -\hbar K^\dagger \delta(t - t_j) = V^\dagger_{SA(j)}(\lambda_t).$$

The unitary induced by the interaction is

$$U = \mathcal{T} \exp\left[-\frac{i}{\hbar} \int_{t_0}^{t_1} dt V_{SA(j)}(\lambda_t)\right] = \exp\left[iK\right]$$

because the δ distribution selects only one time, thereby making the time-ordered exponential rather simple.

Exercise 5.19: Implementing arbitrary control operations

Conside the ancilla-memory interaction

$$H_{AM}(\lambda_t) = \sum_j V_{A(j)M(j)}(\lambda_t), \quad V_{A(j)M(j)}(\lambda_t) = i\hbar\delta(t - t_j^+)\ln(U_{A(j)M(j)})$$

with $t_j^+ = t_j + \epsilon$ immediately after t_j. After tracing out the memory, the action of $V_{A(j)M(j)}(\lambda_t)$ implements the CPTP map $\sum_{r_j} \mathcal{P}_{A(j)}(r_j)$, describing the average effect of the measurement on the ancilla.

Same comment as the previous Exercise: I changed the definition of the interaction Hamiltonian moving the imaginary unit i outside the log.

Show that this description, combined with the one discussed in Exercise 5.18 implements a set of control operations $C_j = \sum_{r_j} C_j(r_j)$ at times t_j.

Solution:
We have seen in Exercise 5.18 that the interaction Hamiltonian of the given structure generates the desired unitary transformation. Now, we can look at the marginal of S after this last CPTP map:

$$\rho_S^{(2)} = \mathrm{Tr}_{AM}\left\{\mathcal{U}_{AM}\rho_{SAM}^{(1)}\right\} = \sum_{r_j}\mathrm{Tr}_A\left\{\mathcal{P}_{A(j)}(r_j)\rho_{SA}^{(1)}\right\} = \sum_{r_j}\mathrm{Tr}_A\left\{\mathcal{P}_{A(j)}(r_j)\mathcal{U}_{SA}\rho_{SA}^{(0)}\right\} = \sum_{r_j} C_j(r_j)\rho_S^{(0)}.$$

Exercise 5.20: Implementing feedback control

Consider a system S coupled to a bath B, and an ancilla A. Furthermore, the ancilla is coupled to a preparation apparatus P, which is used to set the initial ancilla state, and a memory M. The interactions between S and A, and A and M were studied in Exercise 5.18 and Exercise 5.19. Here, we consider a quickly dephasing memory M, such that its state is

$$\rho_M(t) = \sum_{\mathbf{r}_n} p(\mathbf{r}_n, t)\,|\mathbf{r}_n\rangle\langle\mathbf{r}_n|_M \quad \forall t,$$

and introduce feedback control by considering the Hamiltonian

$$H_{SBPAM}(\lambda_t) = \sum_{\mathbf{r}_n} H_{SBPA}[\lambda_t(\mathbf{r}_n)] \otimes |\mathbf{r}_n\rangle\langle\mathbf{r}_n|_M + H_{AM}(\lambda_t).$$

Show that the unitary time evolution after the n-th control operation at t_n is

$$\rho_{SBPAM}(t) = \sum_{\mathbf{r}_n} U_{SBPA}(\mathbf{r}_n)\tilde{\rho}_{SBPA}(t_n|\mathbf{r}_n)U_{SBPA}^\dagger(\mathbf{r}_n) \otimes |\mathbf{r}_n\rangle\langle\mathbf{r}_n|_M\,,$$

where

$$U_{SBPAM}(t) = \mathcal{T}\exp\left[-\frac{i}{\hbar}\int_{t_n}^t H_{SBPA}[\lambda_s(\mathbf{r}_n)]ds\right].$$

Solution:
The generic global state can be written as

$$\rho_{SBPAM}(t) = \sum_{\mathbf{r}_n} \tilde{\rho}_{SBPA}(t|\mathbf{r}_n) \otimes |\mathbf{r}_n\rangle\langle\mathbf{r}_n|_M$$

So, the evolution from time t_n to time t is given by the unitary evolution

$$\rho_{SBPAM}(t) = \mathcal{U}\rho_{SBPAM}(t_n).$$

Crucially, as seen in Exercise 5.19, the ancilla-memory interaction $H_{AM}(\lambda_t)$ only acts at $t = t_n + \epsilon$, $\epsilon \to 0$ to implement a control operation. Therefore, in the time interval (t_n, t), $H_{AM} = 0$. Then, the evolution is fully determined by $H_{SBPA}[\lambda_t(\mathbf{r}_n)] \otimes |\mathbf{r}_n\rangle\langle\mathbf{r}_n|_M$. Crucially, these components commute thanks to the projectors on the memory Hilbert space, and allow us to write

$$\rho_{SBPAM}(t) = \sum_{\mathbf{r}_n}\mathcal{U}_{\mathbf{r}_n}(t,t_n)\tilde{\rho}_{SBPA}(t_n|\mathbf{r}_n)\otimes|\mathbf{r}_n\rangle\langle\mathbf{r}_n|_M = \sum_{\mathbf{r}_n} U_{\mathbf{r}_n}(t,t_n)\tilde{\rho}_{SBPA}(t_n|\mathbf{r}_n)\otimes|\mathbf{r}_n\rangle\langle\mathbf{r}_n|_M\, U_{\mathbf{r}_n}^\dagger(t,t_n)$$

with

$$U_{\mathbf{r}_n}(t,t_n) = \mathcal{T}\exp\left[-\frac{i}{\hbar}\int_{t_n}^t ds H_{SBPA}[\lambda_s(\mathbf{r}_n)]ds\right].$$

Exercise 5.21: From autonomous process tensor to quantum Markov process with feedback

Starting from the setup of Exercise 5.20, show that

$$\tilde{\rho}(t|\mathbf{r}_n) = \mathrm{Tr}_{BPA}\left\{\langle \mathbf{r}_n|\rho_{SBPAM}(t)|\mathbf{r}_n\rangle\right\} = \mathfrak{T}[\mathbf{C}_{n:0}(\mathbf{r}_n)]$$

reduces to

$$\tilde{\rho}(t|\mathbf{r}_n) = \mathcal{C}_n(r_n|\mathbf{r}_{n-1})\mathcal{E}_{n,n-1}(\mathbf{r}_{n-1})\cdots\mathcal{C}_1(r_1|r_0)\mathcal{E}_{1,0}(r_0)\mathcal{C}_0(r_0)\rho_S(0)$$

if the dynamics is Markovian and we consider only classical feedback control, i. e. conditional on the measurement results $\mathbf{r}_n$.

Verify that is equivalent to the general strategy to generate the process tensor $\mathfrak{T}[\mathbf{C}_{n:0}(\mathbf{r}_n)]$.

Solution:
Using the decomposition on the memory eigenstates discussed in Exercise 5.20, we have

$$\tilde{\rho}_S(t|\mathbf{r}_n) = \mathrm{Tr}_{BPA}\left\{\langle \mathbf{r}_n|\rho_{SBPAM}(t)|\mathbf{r}_n\rangle\right\} = \mathrm{Tr}_{BPA}\left\{U_{\mathbf{r}_n}(t,t_n)\tilde{\rho}_{SBPA}(t_n|\mathbf{r}_n)U^{\dagger}_{\mathbf{r}_n}(t,t_n)\right\}.$$

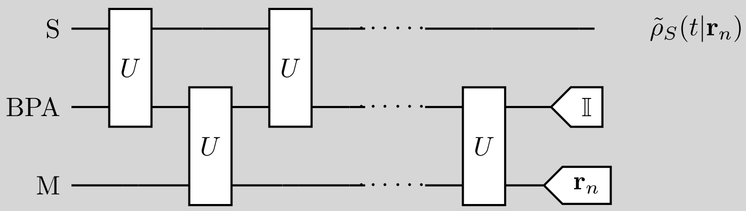
Here, we make use of the Markovian property of the dynamics, which allows us to split the total evolution into different segments. Indeed, a quantum dynamics $\mathfrak{E}_{t_2,t_1}$ is Markovian if $\mathfrak{E}_{t_2,x}\mathfrak{E}_{x,t_1}\ \forall x$. In particular, here we use it to split the total channel $\mathfrak{E}_{t,0}$ into the dynamical evolutions $\mathcal{E}_{t_{n+1},t_n}$ and the control operations $\mathcal{C}$. Then, using the the feedback operations implemented through the maps $\mathcal{E}$ are conditional on $\mathbf{r}_n$ we find

$$\tilde{\rho}_S(t|\mathbf{r}_n) = \mathrm{Tr}_{BPA}\left\{\langle \mathbf{r}_n|\rho_{SBPAM}(t)|\mathbf{r}_n\rangle\right\} = \mathcal{E}_{t,t_n}(\mathbf{r}_n)\tilde{\rho}_S(t_n|\mathbf{r}_n) = \mathcal{E}_{t,t_n}(\mathbf{r}_n)\mathcal{C}(r_n|\mathbf{r}_{n-1})\tilde{\rho}_S(t_n|\mathbf{r}_{n-1})$$

which leads to

$$\tilde{\rho}(t_n|\mathbf{r}_n) = \mathcal{C}_n(r_n|\mathbf{r}_{n-1})\mathcal{E}_{n,n-1}(\mathbf{r}_{n-1})\cdots\mathcal{C}_1(r_1|r_0)\mathcal{E}_{1,0}(r_0)\mathcal{C}_0(r_0)\rho_S(0).$$

Notice that by implementing all control and feedback operations with unitaries by means of the unitary dilation map. This means that we are starting from a larger Hilbert space, made of the system of interested S, a bath B, and ancillae PAM, and then focus on S by taking the partial trace. Notably, by grouping together BPA, we can sketch the implementation of the process tensor as



which is the most general way to implement a process tensor.

Exercise 5.22: Hamiltonian of mean force of tripartite system

Consider a tripartite system XYB with Hamiltonian $H_X + H_Y + H_B + V_{XB}$.

Show that the Hamiltonian of mean force H^*_{XY} for XY can be written as $H^*_X + H_Y$.

Consider the case $S' = SAM$, with S coupled to a bath B, and the ideal memory with H_M negligible weakly coupled to a bath B'. Deduce

$$H^*_{S'}(\lambda_t) = \sum_{\mathbf{r}_n}\{H^*_S[\lambda_t(\mathbf{r}_n)] + H_A(\mathbf{r}_n)\} \otimes |\mathbf{r}_n\rangle\langle\mathbf{r}_n|_M$$

Solution:
The Hamiltonian of mean force of a system S in contact with a bath B is defined through

$$\pi^*_S = \mathrm{Tr}_B\left\{\pi_{SB}\right\} \equiv \frac{e^{-\beta H^*_S}}{\mathcal{Z}^*_S}, \quad \mathcal{Z}^*_S \equiv \frac{\mathcal{Z}_{SB}}{\mathcal{Z}_B}$$

and when applied to the considered tripartite system we find

$$\pi^*_{XY} = \pi_Y \pi^*_X \to H^*_{XY} = H^*_X + H_Y,$$

by using $\pi_{XYB} = e^{-\beta H_{XYB}}/\mathcal{Z}_{XYB} = e^{-\beta H_Y} e^{-\beta H_{XB}}/(\mathcal{Z}_Y \mathcal{Z}_{XB})$.
In the system-ancilla-memory case we can split $X = S$, $Y = AM$ because only the system S is (possibly) strongly coupled to the bath B. Furthermore, the SAM Hamiltonian implements feedback controls, as discussed in Exercise 5.20, so we can write the Hamiltonian of mean force as

$$H^*_{SAM} = \sum_{\mathbf{r}_n} (H^*_S[\lambda_t(\mathbf{r}_n)] + H_A[\lambda_t(\mathbf{r}_n)]) \otimes |\mathbf{r}_n\rangle\langle\mathbf{r}_n|_M$$

which holds during the dynamical evolutions of the system. During the control operations the Hamiltonian must also include the ancilla-memory interaction.

Exercise 5.23: Entropy production in strongly coupled tripartite system

Consider the supersystem $S' = SAM$ coupled to the baths B (strongly) and B' (weakly) such that the initial state is

$$\rho_{SBAMB'} = \pi_{SB} \otimes \rho_A(0) \otimes \rho_M(0) \otimes \pi_{B'}$$

with $\rho_{A/M}(0)$ pure and $\pi_{SB/B'}$ thermal states at temperature T.

Using the Hamiltonian of mean force, one can define the strong coupling internal energy and entropy on S' as

$$U^*_{S'}(t) = \mathrm{Tr}_{S'}\left\{\rho_{S'}(t)\left(H^*_{S'}(\lambda_t) + \beta\partial_\beta H^*_{S'}(\lambda_t)\right)\right\}$$
$$S^*_{S'}(t) = \mathrm{Tr}_{S'}\left\{\rho_{S'}(t)\left(-\ln\rho_{S'}(t) + \beta^2\partial_\beta H^*_{S'}(\lambda_t)\right)\right\}$$

one can write the first and second laws of thermodynamics as

$$\Delta U^*_{S'}(t) = Q^*(t) + W(t), \qquad \Sigma^* = \Delta S^*_{S'}(t) - \frac{Q^*(t)}{T},$$

where the work is the one done in the global unitary transformation.

Show that the strong coupling entropy production can also be written as

$$\Sigma^* = D[\rho_{S'BB'}(t)|\pi_{S'B}(\lambda_t) \otimes \pi_{B'}] - D[\rho_{S'}(t)|\pi^*_{S'}(\lambda_t)]$$

and use it to prove that $\Sigma^* \geq 0$.

Solution:
This is analogous to Exercise 3.20, but let's do the derivation anyway.
First, remember that the Hamiltonian of mean force is defined through the relations

$$\pi^*_{S'} = \mathrm{Tr}_{BB'}\{\pi_{S'BB'}\} \equiv \frac{e^{-\beta H^*_{S'}}}{\mathcal{Z}^*_{S'}}, \quad \mathcal{Z}^*_{S'} \equiv \frac{\mathcal{Z}_{S'BB'}}{\mathcal{Z}_{BB'}}.$$

In this case the baths are not coupled together, so $\mathcal{Z}_{BB'} = \mathcal{Z}_B\mathcal{Z}_{B'}$. Additionally, we remind here that the total work is

$$W(t) = \mathrm{Tr}\{H_{S'BB'}(\lambda_t)\rho_{S'BB'}(t) - H_{S'BB'}(\lambda_0)\rho_{S'BB'}(0)\}$$

and that the equilibrium free energy is $\mathcal{F} = -T\ln\mathcal{Z} = \mathcal{U} - T\mathcal{S}$, while the nonequilibrium free energy is $F = U - TS$.
Now, we procede working on the difference between the relative entropies. In the following I will specify

the time dependence *only* for $t=0$, and will use the notation $X_{S'BB'} \equiv X$.

$$\begin{aligned} D[\rho|\pi_{S'B}\otimes\pi_{B'}] - D[\rho_{S'}|\pi^*_{S'}] &= -S[\rho] + \mathrm{Tr}\{\rho\beta H\} + \ln\mathcal{Z} + S[\rho_{S'}] - \mathrm{Tr}\{\rho_{S'}\beta H^*_{S'}\} - \ln\mathcal{Z}^*_{S'} \\ &= -S[\rho(0)] + \ln(\mathcal{Z}_B\mathcal{Z}_{B'}) + S[\rho_{S'}] + \beta\mathrm{Tr}\{\rho H\} - \beta\mathrm{Tr}\{\rho_{S'}H^*_{S'}\} \\ &= -S[\rho(0)] + \ln\mathcal{Z}_B + \mathcal{S}_{B'} - \beta\mathcal{U}_{B'} + S[\rho_{S'}] + \beta\mathrm{Tr}\{\rho H\} - \beta\mathrm{Tr}\{\rho_{S'}H^*_{S'}\} \\ &= -\mathcal{S}_{S'B}(0) + \ln\mathcal{Z}_B - \beta\mathcal{U}_{B'} + S[\rho_{S'}] + \beta\mathrm{Tr}\{\rho H\} - \beta\mathrm{Tr}\{\rho_{S'}H^*_{S'}\} \\ &= \beta[\mathcal{F}_{SB}(0) - \mathcal{U}_{SB}(0)] + \ln\mathcal{Z}_B - \beta\mathcal{U}_{B'} + S[\rho_{S'}] + \beta\mathrm{Tr}\{\rho H\} - \beta\mathrm{Tr}\{\rho_{S'}H^*_{S'}\} \\ &= \beta\mathcal{F}_{S'B}(0) + \ln\mathcal{Z}_B + S[\rho_{S'}] + \beta W - \beta\mathrm{Tr}\{\rho_{S'}H^*_{S'}\} \\ &= \beta\mathcal{F}^*_{S'}(0) + \beta[\Delta U^*_{S'} - Q^*] - \beta F^*_{S'} \\ &= \Delta S^*_{S'} - \beta Q^* \end{aligned}$$

Now, using the monotonicity of the relative entropy under partial trace, namely $D[\rho_{AB}|\sigma_{AB}] \geq D[\rho_A|\sigma_A]$ we have

$$D[\rho|\pi_{S'BB'}] \geq D[\mathrm{Tr}\{BB'\}\rho|\mathrm{Tr}_{BB'}\{\pi_{S'BB'}\}] = D[\rho_{S'}|\pi^*_{S'}]$$

which proves $\Sigma^* \geq 0$.

Exercise 5.24: Average system energy conservation in control operations

Consider the system-bath-ancilla-memory supersystem introduced in Exercise 5.20.

Show that

$$\sum_{\mathbf{r}_n}\sum_{k=0}^{n}\mathrm{Tr}\left\{H_S(\lambda_k)\left[p(\mathbf{r}_n,t_k^+)\rho_S^{(2)}(t_k|\mathbf{r}_n) - p(\mathbf{r}_n;t_k^-)\rho_S^{(1)}(t_k|\mathbf{r}_n)\right]\right\} = 0.$$

Solution:
Remembering that $\rho^{(2)}(t_k) = \mathcal{U}_{A(k)M(k)}\rho^{(1)}(t_k)$ and that

$$\rho_{SAM} = \sum_{\mathbf{r}_n}\tilde{\rho}_{SA}(t|\mathbf{r}_n)\otimes|\mathbf{r}_n\rangle\langle\mathbf{r}_n|_M\,,$$

with $p(\mathbf{r}_n,t) = \mathrm{Tr}\{\tilde{\rho}_{SA}(t|\mathbf{r}_n)\}$ we can sum over all outcomes $\mathbf{r}_n$ first, obtaining

$$\sum_{k=0}^{n}\mathrm{Tr}_{SAM}\left\{H_S(\lambda_k)\left[\mathcal{U}_{A(k)M(k)}\rho^{(1)}_{SAM}(t_k) - \rho^{(1)}_{SAM}(t_k)\right]\right\}$$

focusing on only one element in the sum, we can use the cyclic property of the trace combined with the unitarity of $U_{A(k)M(k)}$, and the fact that $[H_S(\lambda_k), U_{A(k)M(k)}] = 0$ as they act on different Hilbert spaces to get

$$\mathrm{Tr}\{H_S[\mathcal{U}_{AM}\rho - \rho]\} = \mathrm{Tr}\left\{H_S\left(U_{AM}\rho^{(1)}U^\dagger_{AM} - \rho\right)\right\} = 0$$

which imples the desired equality.

Exercise 5.25: Ramsey interferometry

Consider an atom interacting with three cavities, R_1, C, and R_2 before reaching the detector D, according to the following steps:

(1) In the first Ramsey cavity R_1, a $\pi/2$ microwave pulse is implemented, which induces the transformations $|g\rangle \to |+\rangle$ and $|e\rangle \to -|-\rangle$, with $|\pm\rangle = (|g\rangle \pm |e\rangle)/\sqrt{2}$, on the atom.

(2) Afterwards, if the cavity C is in a Fock state with n photons, the dispersive interaction with the atom implements the phase-shift $|e\rangle \to e^{-i\Phi_0 n}|e\rangle$ with Φ_0 the phase shift per photon. Importantly, *only* the excited state experiences a phase shift.

(3) Finally, the atom interacts with the second Ramsey cavity R_2, which implements a phase-shifted $\pi/2$ pulse such that

$$|g\rangle \to \frac{|g\rangle + e^{i\phi_r}|e\rangle}{\sqrt{2}}, \quad |e\rangle \to \frac{-e^{-i\phi_r}|g\rangle + |e\rangle}{\sqrt{2}},$$

with ϕ_r adjustable phase of the Ramsey interferometer.

(4) In the end, the arom is detected in D by ionization to an electric field. Since the gound and excited states of the atom have different ionazation energies, the detection of a resulting electron implements a projective measurement in the basis $\{|g\rangle, |e\rangle\}$.

Provided that the atoms are prepared in the ground state, show that the probability of detecting the atom in $|g\rangle$ or $|e\rangle$ is

$$p_s(g|n) = \frac{1}{2}\left[1 - \cos(\Phi_0 n + \phi_r)\right], \quad p_s(e|n) = \frac{1}{2}\left[1 + \cos(\Phi_0 n + \phi_r)\right],$$

which depends on the number of photons n

Solution:
Let's follow the state of the atom:

After (0) $|g\rangle$

After (1) $|+\rangle = \frac{|g\rangle + |e\rangle}{\sqrt{2}}$

After (2) $\frac{|g\rangle + e^{-i\Phi_0 n}|e\rangle}{\sqrt{2}}$

After (3) $\frac{1}{2}\left(|g\rangle + e^{i\phi_r}|e\rangle + e^{-i\Phi_0 n}\left[-e^{-i\phi_r}|g\rangle + |e\rangle\right]\right) = \frac{1}{2}\left(\left[1 - e^{-i\Phi_0 n - i\phi_r}\right]|g\rangle + \left[e^{i\phi_r} + e^{-i\Phi_0 n}\right]|e\rangle\right)$

Then, we can calculate the probability of being in the gorund state

$$p_s(g|n) = |\langle 0|\psi_3\rangle|^2 = \frac{1}{4}\left|1 - e^{-i\Phi_0 n - i\phi_r}\right|^2 = \frac{1}{2}[1 - \cos(\Phi_0 n + \phi_r)] = 1 - p_s(e|n).$$

Exercise 5.26: Controlled evolution of uncorrelated cavity

Consider the setting of Exercise 3.30, where a cavity evolving according to the Born-Markov secular master equation interacts with a stream of atoms. Assuming that the time τ between two consecutive atoms is much smaller than the cavity relaxation time τ_c, i. e. $\tau \ll \tau_c$, the free dynamics of the cavity can be approximated as

$$\mathcal{E}_{n+1,n} = e^{\mathcal{L}_0 \tau} \approx \mathcal{I} + \mathcal{L}_0 \tau,$$

and assuming that the interaction time t_{int} between cavity and atom is also much smaller than τ_c, i.e. $t{-}\text{int} \ll \tau_c$, we can approximate the interaction with an instantaneous unitary.

Consider the case in which, after having interacted with the cavity, the atoms are measured in a Ramsey interferometer, as described in Exercise 5.25. Furthermore, assume that initially the cavity contains no coherences in the Fock basis, such that its state can be described by the classical vector $\mathbf{P}(0)$ containing the probabilities $P_n(0)$ of having n photons inside the cavity.

Using the evolution matrix $E_{nm} \equiv \langle n|\mathcal{I} + \mathcal{L}_0\tau|m\rangle$ and the measurement matrix $M_{nm}(r) \equiv \delta_{nm} p_s(r|n)$, derive

$$\tilde{\mathbf{P}}(t_n|\mathbf{r}_n) = M(r_n)E \cdots M(r_1)EM(r_0)\mathbf{P}(0).$$

Solution:
When an atom passes through the cavity and its state is measured, the outcomes $r = 0, 1$ happen with probability $p_s(r|n)$, where n is the number of photons in the cavity. Since the cavity starts diagonal in the Fock basis, and both measurements and dynamical evolution do not introduce coherences, $p_s(r|n)$ is well defined and the measurement outcome induces an update on the cavity state:

$$\tilde{P}'_n = p_s(r|n)P_n$$

where $\tilde{P}'_n$ is the non-normalized state immediately after the measurement. This can also be written with the matrix $M_{nm}(r) = \delta_{nm} p_s(r|m)$ as $\tilde{\mathbf{P}}' = M\mathbf{P}$. Then, the cavity evolves through the Lindbladian $\mathcal{L}_0$ according to the channel $\mathcal{I} + \mathcal{L}_0\tau$. Since we are restricted to the diagonal elements, we use the matrix E_{nm} to write the dynamical evolution as

$$\tilde{P}'' = E\tilde{P}'.$$

Chaining these two processes over and over we obtain the non-normalized probability vector conditioned on n previous measurement outcomes:

$$\tilde{\mathbf{P}}(t_n|\mathbf{r}_n) = M(r_n)E \cdots M(r_1)EM(r_0)\mathbf{P}(0),$$

as desired.

Exercise 5.27: Conditional atom-cavity probability

Using the Jaynes-Cummings Haimltonian, see Exercise 3.1, to describe the atom-cavity interaction of the setup introduced in Exercise 5.26, calculate the conditional probability $p(r,n|r',n')$ of detecting the atom state r and n photons in the cavity given that the arom was prepared in r' and the cavity had n' photons.

For the emitter case, $r'=e$, consider the interaction time $t_e=\pi/(2g\sqrt{n_T})$, and show that the conditional probability is

$$p_e(r,n|n')=\delta_{n+r-1,n'}\sin^2\left(\frac{\pi}{2}\frac{\sqrt{n+r}}{\sqrt{n_T}}+\frac{\pi}{2}r\right).$$

For the absorber case, $r'=a$, consider the interaction time $t_a=\pi/(2g\sqrt{n_T+1})$, and show that the conditional probability is

$$p_a(r,n|n')=\delta_{n+r,n'}\cos^2\left(\frac{\pi}{2}\frac{\sqrt{n+r}}{\sqrt{n_T+1}}+\frac{\pi}{2}r\right).$$

Solution:

From Exercise 3.1 we know that the unitary evolution associated with the Jaynes-Cummings Hamiltonian can be written as

$$\tilde{U}(t)=\cos(tg\sqrt{N+1})\,|e\rangle\langle e|+\cos(tg\sqrt{N})\,|g\rangle\langle g|-i\left(\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}}a\,|e\rangle\langle g|+a^\dagger\frac{\sin(tg\sqrt{N+1})}{\sqrt{N+1}}\,|g\rangle\langle e|\right).$$

with $N=a^\dagger a$ being the photon number operator of the cavity.

Now, suppose that the cavity is initially in the Fock state with m photons. Remembering that $a\,|m\rangle=\sqrt{m}\,|m-1\rangle\,, a^\dagger\,|m\rangle=\sqrt{m+1}\,|m+1\rangle$ we can write

$$\begin{aligned}\tilde{U}(t)\,|m\rangle=&\cos(tg\sqrt{m+1})\,|e\rangle\langle e|\otimes|m\rangle+\cos(tg\sqrt{m})\,|g\rangle\langle g|\otimes|m\rangle+\\&-i\left(\sin(tg\sqrt{m})\,|e\rangle\langle g|\otimes|m-1\rangle+\sin(tg\sqrt{m+1})\,|g\rangle\langle e|\otimes|m+1\rangle\right).\end{aligned}$$

In the first line we have the phase shift similar to what happens in the Ramsey interferometer, see Exercise 5.25, whereas in the second line the terms describe the absorption or emission of a photon by the atom.

Now, let also suppose that the atom is initially in the excited state $|e\rangle$. This corresponds to the emitter case, so let the interaction time be $t_e=\pi/(2g\sqrt{n_T})$. Then, the evolved atom-cavity state is

$$\tilde{U}(t)\,|e,m\rangle=\cos\left(\frac{\pi}{2}\frac{\sqrt{m+1}}{\sqrt{n_T}}\right)|e,m\rangle-i\sin\left(\frac{\pi}{2}\frac{\sqrt{m+1}}{\sqrt{n_T}}\right)|g,m+1\rangle\,.$$

From this we can calculate the probability of observing the state $|r,n\rangle$ using the Born rule $|\langle r,n|\tilde{U}(t)|e,m\rangle|$:

$$p(e,m)=\cos^2\left(\frac{\pi}{2}\frac{\sqrt{m+1}}{\sqrt{n_T}}\right),\quad p(g,m+1)=\sin^2\left(\frac{\pi}{2}\frac{\sqrt{m+1}}{\sqrt{n_T}}\right)$$

with $p(r,n)=0$ if $n\neq m,m+1$. This can be written in a compact form as

$$p_e(r,n|m)=\delta_{n+r-1,m}\sin^2\left(\frac{\pi}{2}\frac{\sqrt{m+1}}{\sqrt{n_T}}+\frac{\pi}{2}r\right).$$

Similarly, let's look at the case in which the atom is initially in the ground state $|g\rangle$. This corresponds to the absorber case, so let the interaction time be $t_a=\pi/(2g\sqrt{n_T+1})$. Then, the evolved atom-cavity state is

$$\tilde{U}(t)\,|g,m\rangle=\cos\left(\frac{\pi}{2}\frac{\sqrt{m}}{\sqrt{n_T+1}}\right)|g,m\rangle-i\sin\left(\frac{\pi}{2}\frac{\sqrt{m}}{\sqrt{n_T+1}}\right)|e,m-1\rangle\,,$$

which leads to the probabilities

$$p(g,m)=\cos^2\left(\frac{\pi}{2}\frac{\sqrt{m}}{\sqrt{n_T+1}}\right),\quad p(e,m-1)=\sin^2\left(\frac{\pi}{2}\frac{\sqrt{m}}{\sqrt{n_T+1}}\right)$$

and $p(r,n)=0$ if $n\neq m,m-1$. As for the previous case, we write these in the compact form

$$p_a(r,n|m)=\delta_{n+r,m}\cos^2\left(\frac{\pi}{2}\frac{\sqrt{m}}{\sqrt{n_T+1}}+\frac{\pi}{2}r\right).$$

A Concepts from Information Theory

Exercise A.1: Positivity of the total information

The total information is defined as

$$I_{\rm tot}(\rho_{1\cdots N}) \equiv \sum_{i=1}^{N} S[\rho_i] - S[\rho_{1\cdots N}].$$

Show that

$$\begin{aligned} I_{\rm tot}(\rho_{1\cdots N}) &= D(\rho_{1\cdots N}|\rho_1 \otimes \cdots \otimes \rho_N) \\ &= I_{1:2} + I_{12:3} + \cdots + I_{1\cdots N-1:N} \end{aligned}$$

where $I_{X:Y}$ denotes the mutual information between X and Y.

Solution:
Dropping the subscript $1\cdots N$, we write explicitely the relative entropy

$$D(\rho|\rho_1 \otimes \cdots \otimes \rho_N) = -S[\rho] + S[\rho_1] + \cdots + S[\rho_N] = I_{\rm tot}(\rho) \geq 0.$$

Additionally, we notice that the sum of mutual informations contains terms that cancel out:

$$I_{1:2} + I_{12:3} = S(\rho_1) + S(\rho_2) - S(\rho_{12}) + S(\rho_{12}) + S(\rho_3) - S(\rho_{123}) = S(\rho_1) + S(\rho_2) + S(\rho_3) - S(\rho_{123}),$$

and so on, which proves the last equality.

Exercise A.2: Projective measurements increase the average post-measurement entropy

Show that projective measurements increase the von Neumann entropy of the *average* post-measurement state.

Solution:
We can derive this from the monotonicity of the relative entropy: Consider a POVM $\{P_n\}$ such that $\sum_n P_n^2 = \mathbb{I}$, and let the "dephasing" operation be

$$\mathcal{D}_{\mathcal{P}}\rho = \sum_n P_n \rho P_n.$$

Notice that $\mathcal{D}_{\mathcal{P}}\mathbb{I} = \mathbb{I}$. Then, the relative entropy between a state ρ and the completely mized state is

$$D(\rho|\mathbb{I}/d) = -S[\rho] + \ln d \geq D(\mathcal{D}_{\mathcal{P}}\rho|\mathbb{I}/d) = -S[\mathcal{D}_{\mathcal{P}}\rho] + \ln d.$$

From which we conclude that

$$S[\mathcal{D}_{\mathcal{P}}\rho] \geq S[\rho].$$

Exercise A.3: Monotonicity of the relative entropy

Consider two arbitrary bipartite states ρ_{AB} and σ_{AB} and show that

$$D(\mathcal{C}\rho|\mathcal{C}\sigma) \leq D(\rho|\sigma) \quad \forall \mathcal{C}, \rho, \sigma \quad \Rightarrow \quad D(\rho_A|\sigma_A) \leq D(\rho_{AB}|\sigma_{AB})$$

Then, prove the other direction:

$$D(\rho_A|\sigma_A) \leq D(\rho_{AB}|\sigma_{AB}) \quad \Rightarrow \quad D(\mathcal{C}\rho|\mathcal{C}\sigma) \leq D(\rho|\sigma) \forall \quad \mathcal{C}, \rho, \sigma.$$

Solution:

($\Rightarrow$) Consider the channel $\mathcal{C} : \mathcal{H}_A \otimes \mathcal{H}_B \to \mathcal{H}_A$ acting as $\mathcal{C}\rho_{AB} = {\rm Tr}_B\{\rho_{AB}\}$. This is a valid channel, and applying it to two arbitrary ρ_{AB}, σ_{AB} we have

$$D(\rho_A|\sigma_A) = D(\mathcal{C}\rho_{AB}|\mathcal{C}\sigma_{AB}) \leq D(\rho_{AB}|\sigma_{AB}).$$

($\Leftarrow$) Any channel $\mathcal{C}$ can be seen as the leftover action of a unitary transformation acting on a larger space:

$$\mathcal{C}\rho = \mathrm{Tr}_E \left\{ U\rho \otimes |0\rangle\langle 0|_E \, U^\dagger \right\} = \mathrm{Tr}_E \left\{ \rho_{AE} \right\}.$$

Then,

$$D(\mathcal{C}\rho|\mathcal{C}\sigma) = D(\mathrm{Tr}_E \{\rho_{AE}\} |\mathrm{Tr}_E \{\sigma_{AE}\}) \leq D(\rho_{AE}|\sigma_{AE}) = D(\rho \otimes |0\rangle\langle 0|_E \, |\sigma \otimes |0\rangle\langle 0|_E)$$

Since the initial system-environment state is decorrelated and the environment is prepared in a pure state we have

$$D(\rho \otimes |0\rangle\langle 0|_E \, |\sigma \otimes |0\rangle\langle 0|_E) = \mathrm{Tr} \left\{ \rho(\ln \rho - \ln \sigma) \right\} = D(\rho|\sigma).$$

B Superoperators

Exercise B.1: Frobenius scalar product

Consider the vectorization

$$\rho \leftrightarrow |\rho\rangle\rangle = \sum_{kl} \rho_{kl} \, |kl\rangle\rangle = \sum_{kl} \rho_{kl} \, |k\rangle \otimes |l\rangle^* = \sum_{kl} \rho_{kl} \, |k\rangle\langle l| \, .$$

Show that the Frobenius scalar product $(\rho|\sigma) \equiv \mathrm{Tr}\left\{\rho^\dagger \sigma\right\}$ is equal to the scalar product of the vectorized matrices, namely

$$(\rho|\sigma) = \langle\langle \rho|\sigma\rangle\rangle \, .$$

Introducing the vector $|I\rangle\rangle \equiv \sum_k |k\rangle \otimes |k\rangle^*$, show that $|I\rangle\rangle$ is the vectorization if the identity matrix I. Show also that the trace can be written in superoperator space as $\langle\langle I|A\rangle\rangle = \mathrm{Tr}\{A\}$ for any arbitrary matrix A.

Solution:
Starting from the scalar product of the vectorized states we have

$$\langle\langle \rho|\sigma\rangle\rangle = \sum_{kl} \rho^*_{kl} \sigma_{kl} = \sum_{kl} \rho^\dagger_{lk} \sigma_{kl} = \sum_{l} (\rho^\dagger \sigma)_{ll} = \mathrm{Tr}\left\{\rho^\dagger \sigma\right\} = (\rho|\sigma)$$

which proves the correspondence with the Frobenius scalar product.
Writing the identity as a vector we have

$$I = \sum_{lk} \delta_{lk} \, |k\rangle\langle l| = \sum_k |k\rangle\langle k| = \sum_k |kk\rangle\rangle$$

and the scalar product with the vectorization of any A is

$$\langle\langle I|A\rangle\rangle = \sum_k A_{kk} = \mathrm{Tr}\{A\} \, .$$

Exercise B.2: Matrix representation of unitary evolution

Consider the superoperator emerging from the time evolution of an isolated system, $\mathcal{U}\rho \equiv U\rho U^\dagger$ for some unitary U. The matrix representation of $\mathcal{U}$ is given by $\mathcal{U} = U \otimes U^*$.

Show that $\hat{\mathcal{U}}$ is unitary: $\hat{\mathcal{U}} \cdot \hat{\mathcal{U}}^\dagger = \hat{\mathcal{U}}^\dagger \cdot \hat{\mathcal{U}} = \hat{\mathcal{I}}$, where $\hat{\mathcal{I}} = \mathbb{I} \otimes \mathbb{I}$ is the identity matrix in superoperator space.

On the other hand, the map $\mathcal{U}\rho \equiv U\rho U^\dagger$ is completely positive. Show that this does *not* imply that the matrix $\hat{\mathcal{U}}$ is positive.

Solution:
The matrix representation is indeed unitary:

$$\hat{\mathcal{U}} \cdot \hat{\mathcal{U}}^\dagger = (U \otimes U^*)(U^\dagger \otimes U^T) = UU^\dagger \otimes (UU^\dagger)^* = \mathcal{I}.$$

To show that is not necessarily positive, it is sufficient to provide an example: Let

$$U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Notice that we choose a matrix x which is *not* a quantum state. Then, the scalar product

$$\langle\langle x|\hat{\mathcal{U}}|x\rangle\rangle = \mathrm{Tr}\left\{x^\dagger U x U^\dagger\right\} = \mathrm{Tr}\{UxUx\} = \mathrm{Tr}\left\{\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}^2\right\} = \mathrm{Tr}\{-\mathbb{I}\} = -2$$

which means that the matrix $\hat{\mathcal{U}}$ is not positive.

Exercise B.3: Properties of the Choi matrix

Show that, if $\mathcal{A}$ is trace-preserving, the trace of the Choi matrix, $\hat{\mathcal{A}} \equiv \sum_{ij} \mathcal{A}(|i\rangle\langle j|) \otimes |i\rangle\langle j|$, is $\mathrm{Tr}\left\{\hat{\mathcal{A}}\right\} = d$, where $d = \dim \mathcal{H}_1$.

Show that the Choi matrix of a unitary time evolution map $\mathcal{U}\rho = U\rho U^\dagger$ is no longer unitary.

Solution:
The trace of the Choi matrix is

$$\mathrm{Tr}\left\{\hat{\mathcal{A}}\right\} = \sum_{ijkl} \langle kl|\mathcal{A}(|i\rangle\langle j|) \otimes |i\rangle\langle j|\,|kl\rangle = \sum_{ki} \langle k|\mathcal{A}(|i\rangle\langle i|)|k\rangle = \sum_{i} \mathrm{Tr}\left\{\mathcal{A}(|i\rangle\langle i|)\right\} = d$$

where in the last step we used the trace-preserving property of $\mathcal{A}$.
Now let's look at the unitary case:

$$\hat{\mathcal{U}}\hat{\mathcal{U}}^\dagger = \sum_{ijkl} U\,|i\rangle\langle j|\,U^\dagger U\,|k\rangle\langle l|\,U^\dagger \otimes |i\rangle\langle j|\,|k\rangle\langle l| = \sum_{ijl} U\,|i\rangle\langle l|\,U^\dagger \otimes |i\rangle\langle l| = \dim(\mathcal{H}_1)\hat{\mathcal{U}} \neq \mathcal{I}$$

Exercise B.4: Tedious equivalence between representations of the process tensor

Show that (note that in the book some $'$ are missing)

$$\mathrm{Tr}_B\left\{\mathcal{C}_2\mathcal{U}_1\mathcal{C}_1\mathcal{U}_0\mathcal{C}_0\rho(0)\right\} = \mathrm{Tr}_{S_2S_1'S_1S_0'S_0}\Bigg\{\mathbb{I}_{S_2'} \otimes \sum_{\text{Latin}}\sum_{\text{Greek}} \mathcal{U}^{\epsilon\alpha_1,\epsilon\beta_1}_{a_2a_1',b_2b_1'}\mathcal{U}^{\alpha_1\alpha_0,\beta_1\beta_0}_{a_1a_0',b_1b_0'}\,\rho^{\alpha_0,\beta_0}_{a_0,b_0}\,|a_2a_1'a_1a_0'a_0\rangle\langle b_2b_1'b_1b_0'b_0|$$
$$\times \sum_{\text{Latin}} \mathcal{C}_{\bar{a}_2'\bar{a}_2,\bar{b}_2'\bar{b}_2}\mathcal{C}_{\bar{a}_1'\bar{a}_1,\bar{b}_1'\bar{b}_1}\mathcal{C}_{\bar{a}_0'\bar{a}_0,\bar{b}_0'\bar{b}_0}\,|\bar{a}_2'\bar{a}_2\bar{a}_1'\bar{a}_1\bar{a}_0'\bar{a}_0\rangle\langle\bar{b}_2'\bar{b}_2\bar{b}_1'\bar{b}_1\bar{b}_0'\bar{b}_0|\Bigg\}$$

is identical to

$$\mathfrak{T}[\mathcal{C}(r_n),\cdots,\mathcal{C}(r_0)] = \mathsf{C}_{S_n',S_n} * \cdots * \mathsf{C}_{S_0',S_0} * \mathrm{Tr}_{B_n}\left\{\mathsf{U}_{S_nB_n,S_{n-1}'B_{n-1}} * \cdots * \mathsf{U}_{S_1B_1,S_0'B_0}\,\rho_{S_0B_0}\right\}$$

when we use the Choi representation of the superoperators $\mathcal{U} \leftrightarrow \mathsf{U}$, $\mathcal{C} \leftrightarrow \mathsf{C}$.

Solution:
Given that the first equation is a general representation of the process tensor, and the second is the representation of the process tensor using the Choi matrices and the link product $*$, it is conceptually straightforward to understand why the latter is found from the former.
To show it concretely, let's start from the control operations. In the Choi representation

$$\mathsf{C}_{S_2',S_2} * \mathsf{C}_{S_1',S_1} * \mathsf{C}_{S_0',S_0} = \mathsf{C}_{S_2',S_2} \otimes \mathsf{C}_{S_1',S_1} \otimes \mathsf{C}_{S_0',S_0}$$

because they do not share any Hilbert space. Then, using the explicit matrix representation,

$$\mathsf{C}_{S',S} = \sum_{ij} \mathcal{C}(|i\rangle\langle j|_S) \otimes |i\rangle\langle j|_{S'} = \sum_{ij\alpha\beta} \mathcal{C}_{i\alpha,j\beta}\,|\alpha\rangle\langle\beta|_S \otimes |i\rangle\langle j|_{S'}\,,$$

we find the second part of the first equation, namely

$$\sum_{\text{Latin}} \mathcal{C}_{\bar{a}_2'\bar{a}_2,\bar{b}_2'\bar{b}_2}\mathcal{C}_{\bar{a}_1'\bar{a}_1,\bar{b}_1'\bar{b}_1}\mathcal{C}_{\bar{a}_0'\bar{a}_0,\bar{b}_0'\bar{b}_0}\,|\bar{a}_2'\bar{a}_2\bar{a}_1'\bar{a}_1\bar{a}_0'\bar{a}_0\rangle\langle\bar{b}_2'\bar{b}_2\bar{b}_1'\bar{b}_1\bar{b}_0'\bar{b}_0|\,.$$

Similarly, the link product of the Choi represented unitaries which written explicitely reads

$$\mathsf{U}_{S_1B_1,S_0'B_0} = \sum \mathcal{U}(|a_0\alpha_0\rangle\langle b_0\beta_0|_{S_0'B_0}) \otimes |a_0\alpha_0\rangle\langle b_0\beta_0|_{S_1B_1} = \sum \mathcal{U}^{a_1\alpha_1,b_1\beta_1}_{a_0\alpha_0,b_0\beta_0}\,|a_1\alpha_1\rangle\langle b_1\beta_1|_{S_0'B_0} \otimes |a_0\alpha_0\rangle\langle b_0\beta_0|_{S_1B_1}$$

corresponds to the first part of the first equality, namely

$$\sum_{\text{Latin}}\sum_{\text{Greek}} \mathcal{U}^{\epsilon\alpha_1,\epsilon\beta_1}_{a_2a_1',b_2b_1'}\mathcal{U}^{\alpha_1\alpha_0,\beta_1\beta_0}_{a_1a_0',b_1b_0'}\,\rho^{\alpha_0,\beta_0}_{a_0,b_0}\,|a_2a_1'a_1a_0'a_0\rangle\langle b_2b_1'b_1b_0'b_0|\,.$$

Indeed, since two consecurive unitaries only share one bath Hilbert space, we can use the associative property to focus on the link product of two consecutive unitaries:

$$\mathsf{B}_{21} * \mathsf{A}_{10} = \mathrm{Tr}_1\left\{(\mathbb{I}_2 \otimes \mathsf{A}_{10}^{T_1})(\mathsf{B}_{21} \otimes \mathbb{I}_0)\right\}$$

$$\mathsf{U}_1 * \mathsf{U}_0 = \mathrm{Tr}_{B_1}\left\{\sum \mathcal{U}^{a_2\alpha_2,b_2\beta_2}_{a_1'\bar{\alpha}_1,b_1'\bar{\beta}_1}\mathcal{U}^{a_1\alpha_1,b_1\beta_1}_{a_0'\alpha_0,b_0'\beta_0}\left((|a_1\alpha_1\rangle\langle b_1\beta_1|)^{T_{B_1}} \otimes |a_0'\alpha_0\rangle\langle b_0'\beta_0|\right)\left(|a_2\alpha_2\rangle\langle b_2\beta_2| \otimes |a_1'\bar{\alpha}_1\rangle\langle b_1'\bar{\beta}_1|\right)\right\}$$

Since the trace only acts on B_1 we have to calculate

$$\mathrm{Tr}_{B_1}\left\{(|\alpha_1\rangle\langle\beta_1|)^T\,|\bar{\alpha}_1\rangle\langle\bar{\beta}_1|\right\} = \langle\bar{\beta}_1|(|\alpha_1\rangle\langle\beta_1|)^T|\bar{\alpha}_1\rangle = \delta_{\beta_1\bar{\beta}_1}\delta_{\alpha_1\bar{\alpha}_1}$$

where we used the basis representation of $\{|\alpha\rangle\}$. Then, the link product becomes

$$\mathsf{U}_1 * \mathsf{U}_0 = \sum \mathcal{U}^{a_2\alpha_2,b_2\beta_2}_{a_1'\alpha_1,b_1'\beta_1}\mathcal{U}^{a_1\alpha_1,b_1\beta_1}_{a_0'\alpha_0,b_0'\beta_0}\,|a_2\alpha_2a_1'a_1a_0'\alpha_0\rangle\langle b_2\beta_2b_1'b_1b_0'\beta_0|\,,$$

with the summation carried over the indices appearing in the ketbra. Notice how this link product removed the B_1 space from the ketbra. Indeed, repreating this procedure for $\mathsf{U}_1 * \mathsf{U}_0 * \rho_0$ one finds that also the bath B_0 gets traced out. Therefore, tracing out also the final bath B_2 one recovers

$$\sum_{\text{Latin}}\sum_{\text{Greek}}\mathcal{U}^{\epsilon\alpha_1,\epsilon\beta_1}_{a_2a_1',b_2b_1'}\mathcal{U}^{\alpha_1\alpha_0,\beta_1\beta_0}_{a_1a_0',b_1b_0'}\,\rho^{\alpha_0,\beta_0}_{a_0,b_0}\,|a_2a_1'a_1a_0'a_0\rangle\langle b_2b_1'b_1b_0'b_0|\,.$$

Then, we recognize the link product between the control operations and the unitary evolutions

$$\mathsf{C}(\mathbf{r}_n) * \mathrm{Tr}_{B_2}\{\mathsf{U}\cdots\mathsf{U}\rho\}\,.$$

Exercise B.5: Choi matrix of a quantum Markov process

Derive

$$\mathsf{T} = \mathrm{Tr}_{B_2}\left\{\mathsf{U}_{S_nB_n,S_{n-1}'B_{n-1}} * \cdots * \mathsf{U}_{S_1B_1,S_0'B_0}\rho_{S_0B_0}\right\} \cong \mathrm{Tr}_B\left\{\mathcal{U}_1\mathcal{S}_{SA_1}\mathcal{U}_0\mathcal{S}_{SA_0}\rho_{SB}(0)\otimes\psi_0^+\otimes\psi_1^+\right\},$$

where the swap superoperator is defined through

$$\mathcal{S}_{S,A_j}(\rho_S\otimes\psi_j^+) = \mathcal{S}_{S,A_j}\sum\rho_{ab}\,|aa_j'a_j'\rangle\langle bb_j'b_j'| \equiv \sum\rho_{ab}\,|a_j'aa_j'\rangle\langle b_j'bb_j'|\,.$$

Show that the Choi matrix corresponding to a quantum Markov process is isomorphic to $\mathcal{E}(t_n,t_{n-1})\otimes\cdots\otimes\mathcal{E}(t_1,0)\otimes\rho_S(0)$, namely a many-body state where correlations only exist between a preparation and its subsequent measurement, or, alternatively, between an output state S_{j-1}' and an input state S_j.

Solution:
Starting fromthe right hand side, let's work it out step by step:

- After the first swap and unitary we have

  $$\sum\rho^{a_0\alpha_0}_{b_0\beta_0}\mathcal{U}_0\left(|a_0'\alpha_0\rangle\langle b_0'\beta_0|\right)\otimes|a_0a_0'\rangle\langle b_0b_0'|\otimes|a_1'a_1'\rangle\langle b_1'b_1'|$$

  which becomes

  $$\sum\rho^{a_0\alpha_0}_{b_0\beta_0}\mathcal{U}^{a_1\alpha_1,b_1\beta_1}_{a_0'\alpha_0,b_0'\beta_0}\,|a_1\alpha_1\rangle\langle b_1\beta_1|\otimes|a_0a_0'\rangle\langle b_0b_0'|\otimes|a_1'a_1'\rangle\langle b_1'b_1'|$$

  once we introduce the matrix representation of $\mathcal{U}$.
- Applying the second swap we have

  $$\sum\rho^{a_0\alpha_0}_{b_0\beta_0}\mathcal{U}^{a_1\alpha_1,b_1\beta_1}_{a_0'\alpha_0,b_0'\beta_0}\,|a_1'\alpha_1\rangle\langle b_1'\beta_1|\otimes|a_0a_0'\rangle\langle b_0b_0'|\otimes|a_1a_1'\rangle\langle b_1b_1'|$$

- Applying the second unitary we have

  $$\sum\rho^{a_0\alpha_0}_{b_0\beta_0}\mathcal{U}^{a_1\alpha_1,b_1\beta_1}_{a_0'\alpha_0,b_0'\beta_0}\mathcal{U}^{a_1'\alpha_1,b_1'\beta_1}_{a_2\alpha_2,b_2\beta_2}\,|a_2\alpha_2\rangle\langle b_2\beta_2|\otimes|a_0a_0'\rangle\langle b_0b_0'|\otimes|a_1a_1'\rangle\langle b_1b_1'|$$

- Taking the trace over the bath ensures $\alpha_2=\beta_2=\epsilon$ and leaves us with

  $$\sum\rho^{a_0\alpha_0}_{b_0\beta_0}\mathcal{U}^{a_1\alpha_1,b_1\beta_1}_{a_0'\alpha_0,b_0'\beta_0}\mathcal{U}^{a_1'\alpha_1,b_1'\beta_1}_{a_2\epsilon,b_2\epsilon}\,|a_2a_0a_0'a_1a_1'\rangle\langle b_2b_0b_0'b_1b_1'|\,,$$

  which coincides (up to reordering of the Hilbert spaces) with the unitary part of Exercise B.4, where we showed that it corresponds to

  $$\mathrm{Tr}_{B_2}\{\mathsf{U}*\cdots*\mathsf{U}\rho\}\,.$$

Using this result we can look at the Choi matrix T for a quantum Markovian process:

$$\mathsf{T} \cong \mathrm{Tr}_B \left\{ \mathcal{U}_n \mathcal{S}_n \cdots \mathcal{U}_0 \mathcal{S}_0 \rho_{SB} \otimes \psi^+ \otimes \cdots \otimes \psi^+ \right\} = \mathcal{E}_{n,n-1} \mathcal{S}_n \cdots \mathcal{E}_{1,0} \mathcal{S}_0 \rho_S \otimes \psi^+ \otimes \cdots \otimes \psi^+$$

where we used the Markovianity to split the unitary processes into the composition of channels. Then, since the swap operators make the channels act on the maximally entangled ψ^+ we have

$$\mathsf{T} \cong \rho_S \otimes \mathcal{E}_{1,0} \psi^+ \otimes \cdots \otimes \mathcal{E}_{n,n-1} \psi^+.$$

C Time-Reversal Symmetry

Exercise C.1: Time-reversal symmetry with even Hamiltonian

Assume that the Hamiltonian obeys the symmetry $H(q,p) = H(-q,p)$, and consider the time-reversal operator $\Theta'(q,p) \equiv (-q,p)$, and define the reversed dynamics via $H_{\Theta'}(q,p) \equiv H(q,p)$.

Show that these transformations also lead to the notion of time-reversal symmetry.

Solution:

Let $(\tilde{q}_0, \tilde{p}_0) \equiv \Theta'(q_{dt}, p_{dt}) = (-q_{dt}, p_{dt})$ Their evolution according to the reversed dynamics is

$$\begin{aligned}
\tilde{q}_{dt} &= \tilde{q}_0 + dt \left.\frac{\partial H}{\partial p}\right|_{(\tilde{q}_0,\tilde{p}_0)}, \quad & \tilde{p}_{dt} &= \tilde{p}_0 - dt \left.\frac{\partial H}{\partial q}\right|_{(\tilde{q}_0,\tilde{p}_0)} \\
\tilde{q}_{dt} &= -q_{dt} + dt \left.\frac{\partial H}{\partial p}\right|_{(-q_{dt},\tilde{p}_{dt})}, \quad & \tilde{p}_{dt} &= p_{dt} - dt \left.\frac{\partial H}{\partial q}\right|_{(-q_{dt},p_{dt})} \\
\tilde{q}_{dt} &= -q_{dt} + dt \left.\frac{\partial H}{\partial p}\right|_{(q_{dt},\tilde{p}_{dt})}, \quad & \tilde{p}_{dt} &= p_{dt} + dt \left.\frac{\partial H}{\partial q}\right|_{(q_{dt},p_{dt})} \\
\tilde{q}_{dt} &= -q_{dt} + dt \left.\frac{\partial H}{\partial p}\right|_{(q_0,\tilde{p}_0)}, \quad & \tilde{p}_{dt} &= p_{dt} + dt \left.\frac{\partial H}{\partial q}\right|_{(q_0,p_0)} \\
q_{dt} &= -\tilde{q}_{dt} + dt \left.\frac{\partial H}{\partial p}\right|_{(q_0,\tilde{p}_0)}, \quad & p_{dt} &= \tilde{p}_{dt} - dt \left.\frac{\partial H}{\partial q}\right|_{(q_0,p_0)}
\end{aligned}$$

by choosing $(\tilde{q}_{dt}, \tilde{p}_{dt}) = (-q_0, p_0) = \Theta'(q_0, p_0)$ we recover the forward Hamilton equation of motion. Therefore, while (q,p) evolve forward from $t=0$ to $t=\tau$, the time-reversed $(\tilde{q},\tilde{p})$ evolve backwards from (q_τ, p_τ) to (q_0, p_0).

Exercise C.2: Time-reversed master equation

Consider a master equation $d_t\mathbf{p}(t) = R\mathbf{p}(t)$ described by a time-independent rate matrix R. The solution of the dynamics is given by the transition matrix e^{Rt}. Thus, the dynamics is *invertible* as we can associate to each final state $\mathbf{p}(t)$ a unique initial state $\mathbf{p}(0) = e^{-Rt}\mathbf{p}(t)$.

One could choose the time-reversal operation $\Theta = \mathbb{I}$ and postulate that the time-reversed dynamics obeys the 'master equation' $d_t\mathbf{p}(t) = -R\mathbf{p}(t)$. However, this does not satisfy the requirements of time-reversal symmetry. What is wrong with the time-reversed master equation?

Solution:
The time-reversed master equation leads to

$$d_t\mathbf{p}(t) = -R\mathbf{p}(t) \to \mathbf{p}(t+dt) = \mathbf{p}(t) - dtR\mathbf{p}(t).$$

Remembering that R is a rate matrix, we know that its spectrum is non-positive: $\lambda_j \leq 0$. If all $\lambda_j = 0$ then nothing happens to the probability distribution and the time-reversal operation is fine. However, if there exists one eigenvalue $\lambda_j < 0$, we can use it to generate non-physical states. In fact, calling v_0 an eigenvector with $\lambda_0 = 0$ eigenvalue, and v_j the eigenvector corresponding to $\lambda_j < 0$, we can choose as initial state $\mathbf{p}(0) = v_0 + \alpha_j v_j$, finding

$$\mathbf{p}(t) = v_0 + \alpha_j e^{-\lambda_j t} v_j.$$

Crucially, $-\lambda_j t > 0$, meaning that the state will be dominated by the unphysical v_j, which contains negative entries.

Exercise C.3: Anti-unitarity and anti-linearity

Show that anti-unitarity, i.e. $\langle\Theta\psi|\Theta\phi\rangle = \langle\phi|\psi\rangle$, imples anti-linearity, i.e. $\Theta i = -i\Theta$.

Solution:

Using the anti-linearity property we find

$$\langle\Theta\psi|\Theta i\phi\rangle = -i\langle\phi|\psi\rangle = -i\langle\Theta\psi|\Theta\phi\rangle \longrightarrow \langle\Theta\psi|\left(|\Theta i\phi\rangle + i|\Theta\phi\rangle\right) = 0, \quad \forall\psi,\phi$$

Assuming that $|\Theta\phi\rangle$ spans the whole Hilbert space, we can then conclude that

$$\Theta i = -i\Theta.$$

Exercise C.4: Trace of time-reversed operator

Show that, given Θ anti-unitary, $\mathrm{Tr}\left\{\Theta O\Theta^{-1}\right\} = \mathrm{Tr}\left\{O\right\}^* = \mathrm{Tr}\left\{O^\dagger\right\}$ for any operator O.

Solution:
First of all, notice that Θ^{-1} is anti-unitary as well. Indeed, by choosing $\psi = \Theta^{-1}\alpha, \psi = \Theta^{-1}\beta$ we have

$$\langle\Theta\psi|\Theta\phi\rangle = \langle\alpha|\beta\rangle = \langle\phi|\psi\rangle = \langle\Theta^{-1}\beta|\Theta^{-1}\alpha\rangle.$$

Moving on to the trace we have

$$\mathrm{Tr}\left\{\Theta O\Theta^{-1}\right\} = \sum_k \langle k|\Theta O\Theta^{-1}|k\rangle.$$

Introducing two identity decompositions before and after the operator O and writing $|k\rangle = \Theta|l\rangle$ we find

$$\mathrm{Tr}\left\{\Theta O\Theta^{-1}\right\} = \sum_{ijl}\langle\Theta l|\Theta i\rangle\langle i|O|j\rangle\langle j|\Theta^{-1}|\Theta l\rangle = \sum_{ij}\langle ij\rangle\langle j|O^\dagger|i\rangle = \sum_i\langle i|O^\dagger|i\rangle = \mathrm{Tr}\left\{O^\dagger\right\}.$$

Exercise C.5: Spectrum of time-reversed observable

Show for any observable O that the time-reversed observable $\Theta O\Theta^{-1}$ is also an observable, i.e. it is Hermitian.
Show for any observable O that $\Theta O\Theta^{-1}$ has the same spectrum as O.

Solution:
Since O is hermitian we denote with $|\psi_k\rangle$ its eigenvectors with eigenvalues $\lambda_k \in \mathbb{R}$. Calling $|\phi_k\rangle = \Theta|\psi_k\rangle$, we have

$$\Theta O\Theta^{-1}|\phi_k\rangle = \Theta O|\psi_k\rangle = \Theta\lambda_k|\psi_k\rangle = \lambda_k\Theta|\psi_k\rangle$$

which means that $|\phi_k\rangle$ is eigenvector of $\Theta O\Theta^{-1}$ with eigenvalues $\lambda_k \in \mathbb{R}$. This also means that O and $\Theta O\Theta^{-1}$ have the same spectrum.

Exercise C.6: Real matrix representation of the Hamiltonian

Show that any Hamiltonian that obeys $[\Theta, H] = 0$ for an anti-unitary operator Θ with $\Theta^2 = \mathbb{I}$ can be given a real matrix representation without knowing the eigenbasis.

Solution:
Notice that the commutation relation allows us to write

$$\langle\Theta i|\Theta Hj\rangle = \langle j|H|i\rangle = \langle\Theta i|H|\Theta j\rangle$$

Therefore, the eigenvectors satisfy $|\Theta i\rangle = |i\rangle$ we have

$$\langle i|H|j\rangle = \langle j|H|i\rangle$$

which means that all elements of H in the given basis are real numbers.
Therefore, we need to construct such a basis.
Take any vector $|\psi\rangle$. The (non-normalized) vector $|\phi\rangle = |\psi\rangle + \Theta|\psi\rangle$ satisfies

$$\Theta|\phi\rangle = |\phi\rangle$$

thanks to $\Theta^2 = \mathbb{I}$.
Now, we can provide a protocol to generate a Θ invariant basis:

- Take a vector $|0\rangle$ and construct $|\tilde{\phi}_0\rangle = |0\rangle + \Theta|0\rangle$. If $|\tilde{\phi}_0\rangle = 0$, meaning that $\Theta|0\rangle = -|0\rangle$, take instead the state $i|0\rangle$, which yields $|\tilde{\phi}_0\rangle = i|0\rangle - i\Theta|0\rangle = 2i|0\rangle \neq 0$.
- Normalize the vector $|\phi_0\rangle = \frac{|\tilde{\phi}_0\rangle}{\sqrt{\langle\tilde{\phi}_0|\tilde{\phi}_0\rangle}}$, which is always possible because we excluded the case $|\tilde{\phi}_0\rangle = 0$ in the previous step.
- Choose a new vector $|1\rangle$ and make it orthogonal to $|\phi_0\rangle$:

$$|1\rangle \to N\left(|1\rangle - \langle\phi_0|1\rangle|\phi_0\rangle\right)$$

with N normalization constant.
- Construct $|\tilde{\phi}_1\rangle \neq 0$ as done in the first step. Notice that

$$\langle\phi_0|\tilde{\phi}_1\rangle = \langle\phi_0|1\rangle + \langle\Theta\phi_0|\Theta 1\rangle = \langle\phi_0|1\rangle + \langle 1|\phi_0\rangle = 0$$

by construction, meaning that the newly constructed normalized vector $|\phi_1\rangle$ is already orthogonal to $|\phi_0\rangle$.
- Keep going until the set $\{|\phi_i\rangle\}$ spans the entire Hilbert space.

Exercise C.7: Time-reversal and local detailed balance

Consider first two observables $X = \sum_x x\Pi(x)$ and $Y = \sum_y y\Pi(y)$ and their time-reversal $\Theta X\Theta^{-1} = \sum_x x\Pi_\Theta(x)$ and $\Theta Y\Theta^{-1} = \sum_y y\Pi_\Theta(y)$. Show the validity of the following identity:

$$\mathrm{Tr}\left\{\Pi(y)U(t,0)\Pi(x)U^\dagger(t,0)\right\} = \mathrm{Tr}\left\{\Pi_\Theta(x)U_\Theta(t,0)\Pi_\Theta(y)U_\Theta^\dagger(t,0)\right\}.$$

The rate to jump from a coarse-grained state x' to x under the assumption of time-scale separation reads

$$R_{x,x'} = \frac{1}{\delta t}\frac{1}{V_{E,x'}}\mathrm{Tr}\left\{\Pi(E,x)U(\delta t)\Pi(E,x')U^\dagger(\delta t)\right\}$$

with $V_{E,x'} = \mathrm{Tr}\left\{\Pi(E,x')\right\}$. We now consider the time-reversed process. The rate to jump from a time-reversed coarse-grained state x_Θ to x'_Θ under the assumption of time-scale separation becomes

$$R^\Theta_{x'_\Theta,x_\Theta} = \frac{1}{\delta t}\frac{1}{V_{E,x}}\mathrm{Tr}\left\{\Pi_\Theta(E,x')U_\Theta(\delta t)\Pi_\Theta(E,x)U_\Theta^\dagger(\delta t)\right\}.$$

Note that the number of microstates remains unchanged by the time-reversal operator: $V_{E,x_\Theta} = \mathrm{Tr}\left\{\Theta\Pi(E,x)\Theta^{-1}\right\} = \mathrm{Tr}\left\{\Pi(E,x)\right\}^* = V_{E,x}$.

Show that

$$\frac{R_{x,x'}}{R^\Theta_{x'_\Theta,x_\Theta}} = \frac{V_{E,x}}{V_{E,x'}}$$

Solution:
Starting from the trace we get

$$\mathrm{Tr}\left\{\Pi_y U\Pi_x U^\dagger\right\} = \sum_k \langle k|\Theta^{-1}\Pi_{\Theta,y}U_\Theta\Pi_{\Theta,x}U_\Theta^\dagger\Theta|k\rangle = \sum_{ijk}\langle k|\Theta^{-1}|i\rangle\langle i|\Pi_{\Theta,y}U_\Theta\Pi_{\Theta,x}U_\Theta^\dagger|j\rangle\langle j|\Theta|k\rangle.$$

Using $|k\rangle = |\Theta^{-1}l\rangle$ the trace becomes

$$\sum_{ij}\langle\Theta^{-1}j|\Theta^{-1}i\rangle\langle i|\Pi_{\Theta,y}U_\Theta\Pi_{\Theta,x}U_\Theta^\dagger|j\rangle = \sum_{ij}\langle i|j\rangle\langle j|U_\Theta\Pi_{\Theta,y}U_\Theta^\dagger\Pi_{\Theta,x}|i\rangle = \mathrm{Tr}\left\{\Pi_{\Theta,x}U_\Theta\Pi_{\Theta,y}U_\Theta^\dagger\right\}$$

as desired.
By applying the result just proven we find

$$\frac{R_{x,x'}}{R^\Theta_{x'_\Theta,x_\Theta}} = \frac{V_{E,x}}{V_{E,x'}}$$

immediately.