Quantum Thermodynamics

Applications and examples

Landauer's principle

Landauer's principle connects thermodynamics and information. Consider a system S with a density matrix ρ_S. Recall that it's von Neumann entropy is defined as

$$S(\rho_S) = -\mathrm{tr}\,(\rho_S \ln \rho_S) \tag{1}$$

and measures the lack of information we have about S.

Indeed, suppose S is of dimension d. Then we can define the information about S as

$$I(\rho_S) = \ln d - S(\rho_S) \tag{2}$$

If the system is in a pure state, $\rho_S = |\psi\rangle\langle\psi|$ then $S(\rho_S) = 0$ and our information is maximal, $I = \ln d$. Instead, if the system is in the maximally mixed state

$$\pi_S = \frac{I_d}{d} \tag{3}$$

then $S(\pi_S) = \ln d$ and $I = 0$.

We have also shown before that (2) may be written as

$$\boxed{I(\rho_S) = S(\rho_S \| \pi_S)} \qquad (4)$$

where

$$S(\rho \| \sigma) = \mathrm{tr}\{\rho \ln \rho - \rho \ln \sigma\} \qquad (5)$$

Eq (4) has a really cool interpretation: "The information about S is the distance between ρ_S and the state for which we have no information at all (π_S)"

Suppose now that we wish to extract some information about S. Landauer showed that extracting information always has a fundamental energy cost. Thus, information is physical! It is a resource, like heat and work.

Here we will follow the more modern approach of Reeb and Wolf in 1306.4352. We consider a system S prepared in an arbitrary state ρ_S. We then put this system in contact with an environment E, with Hamiltonian H_E and prepared in a thermal state

$$\rho_E = \frac{e^{-\beta H_E}}{Z_E} \tag{6}$$

We then put the two to interact via an arbitrary interaction Hamiltonian. The state of the system at some late time will then have the form

$$\rho_{SE}' = U(\rho_S \otimes \rho_E)U^\dagger \tag{7}$$

for some unitary U. This state will in general not be separable (S and E become entangled due to the interaction).

Consider now the following quantity

$$\Sigma = I'(S:E) + S(\rho_E' \| \rho_E) \tag{8}$$

where $\rho_E' = \mathrm{tr}_S\, \rho_{SE}'$ is the reduced density matrix of E after the interaction and

$$I'(S:E) = S(\rho_S') + S(\rho_E') - S(\rho_{SE}') \tag{9}$$

is the mutual information between S and E, which measures the amount of correlations developed between S and E.

We have already shown in a previous set of notes that both $S(\rho\|\sigma) \geq 0$ and $I(S:E) \geq 0$. Thus, clearly, $\Sigma \geq 0$.

Now we use the fact that unitaries do not change the entropy

$$S(U\rho U^{\dagger}) = S(\rho) \tag{10}$$

This implies that

$$S(\rho_{SE}') = S(\rho_S \otimes \rho_E) = S(\rho_S) + S(\rho_E) \tag{11}$$

Eq (8) then becomes

$$\Sigma = S(\rho_S') + S(\rho_E') - S(\rho_S) - S(\rho_E) + S(\rho_E'\|\rho_E) \tag{12}$$

Let us now focus on the "E" terms. From (5) we may write

$$\begin{aligned} S(\rho_E'\|\rho_E) &= \mathrm{tr}\{\rho_E' \ln \rho_E' - \rho_E' \ln \rho_E\} \\ &= -S(\rho_E') - \mathrm{tr}\{\rho_E' \ln \rho_E\} \end{aligned} \tag{13}$$

The term $S(\rho_E')$ cancels in (12), leaving us with

$$\Sigma = S(\rho_S') - S(\rho_S) - S(\rho_E) - \mathrm{tr}\{\rho_E' \ln \rho_E\} \tag{14}$$

But now we use the fact that ρ_E is thermal, Eq (6), to write

$$-S(\rho_E) - \mathrm{tr}\{\rho_E' \ln\rho_E\} = \mathrm{tr}\{(\rho_E - \rho_E')\ln\rho_E\}$$

$$= -\beta\,\mathrm{tr}\{(\rho_E - \rho_E')H_E\} - \ln Z_E \underbrace{\mathrm{tr}\{\rho_E - \rho_E'\}}_{0}$$

$$= \beta\left(\langle H_E\rangle' - \langle H_E\rangle\right)$$

$$= \beta\,\Delta Q \qquad (15)$$

where ΔQ is the heat which entered the bath

$$\Delta Q_E = \langle H_E\rangle' - \langle H_E\rangle \qquad (16)$$

Finally, in Eq (14) we write

$$S(\rho_S') - S(\rho_S) = I(\rho_S) - I(\rho_S') = -\Delta I_S \qquad (17)$$

where ΔI_S is the change in the information of the system.

We then finally arrive at

$$\boxed{\Sigma = \beta\,\Delta Q_E - \Delta I_S \geq 0} \qquad (18)$$

this is Landauer's principle

Landauer's principle provides a bound on the heat required to extract some information. Let's try to clarify the signs of each term:

$$\text{Extract information about } S: \quad \Delta I_S > 0 \qquad (\Delta S_S < 0) \tag{19}$$

(learn something)

Thus we see from (18) that for $\Delta I_S > 0$

$$\beta \Delta Q_E \geq \Delta I_S \tag{20}$$

Moreover

$$\Delta Q_E > 0: \text{ the bath heats up} \tag{21}$$

Hence, in order to learn something about the system, the bath has to heat up

As an example, take a qubit which is prepared in the maximally mixed state

$$\pi = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{22}$$

We know absolutely nothing about this qubit. But suppose we wish to learn in which pure state it is. In this case $\Delta I_S = \ln 2$. Thus, the minimum amount of energy that the bath has to absorb to learn in which state the qubit is in, is

$$\boxed{\Delta Q_E \geq T \ln 2} \tag{23}$$

Entropy production

The quantity Σ in (18) is called the entropy production.
This is a historical name. But the point is that it quantifies the irreversibility of a process.

Suppose that the system-bath interaction can be considered a thermal operation, so that

$$\Delta Q_E = - \Delta U_S \tag{24}$$

where

$$\Delta U_S = \langle H_S \rangle' - \langle H_S \rangle \tag{25}$$

is the change in energy of the system. Then Eq (18) becomes

$$\Sigma = - \beta \Delta U_S + \Delta S_S \tag{26}$$

where I wrote $\Delta I_S = - \Delta S_S$. We now recognize here the non-equilibrium free energy

$$F(\rho_S) = U(\rho_S) - T S(\rho_S) \tag{27}$$

Thus

$$\boxed{\Sigma = - \beta \Delta F}$$

Since $\Sigma \geq 0$ we conclude that $\Delta F \leq 0$. In a thermal operation the free energy always goes down. Or, putting it differently, equilibrium is the state of smallest free energy.

Instead, suppose that some work is also performed in the system. Then, according to the first law,

$$\Delta U_S = \Delta Q_S + \langle W \rangle$$

where $\langle W \rangle$ is the total (average) work done on S. Then

$$\Delta Q_E = -\Delta Q_S = -\Delta U_S - \langle W \rangle$$

so that Eq (18) becomes instead

$$\Sigma = -\beta \Delta U_S + \Delta S_S + \beta \langle W \rangle$$

or

$$\boxed{\Sigma = \beta\left(\langle W \rangle - \Delta F\right)} \qquad (19)$$

We have already seen this guy before when we talked about fluctuation theorems.

Recall that the Crooks fluctuation theorem read

$$\frac{P_F(W)}{P_B(-W)} = e^{\beta(W-\Delta F)} \qquad (20)$$

and the Jarzynski equality read

$$\langle e^{-\beta(W-\Delta F)} \rangle = 1 \qquad (21)$$

We can now reinterpret these as fluctuations of entropy production, instead of work. That is, we define a stochastic entropy production

$$\sigma = \beta(W-\Delta F) \qquad (22)$$

which is such that

$$\langle \sigma \rangle = \Sigma = \text{Eq } (19) \qquad (23)$$

Then (20) and (21) are recast as

$$\frac{P_F(\sigma)}{P_F(-\sigma)} = e^{\sigma} \qquad (24)$$

$$\langle e^{-\sigma} \rangle = 1 \qquad (25)$$

We believe that this is how fluctuation theorems should be interpreted: as <u>fundamental</u> <u>symmetries</u> <u>of</u> <u>the</u> <u>entropy</u> <u>production</u>.

Example : heat exchange between two qubits

Now let's work out some examples with qubits. We start by considering the heat exchange between two qubits

$$H_A = \frac{\Omega}{2}\sigma_z^A \qquad H_B = \frac{\Omega}{2}\sigma_z^B \tag{26}$$

They are each prepared in equilibrium at different temperatures

$$\rho_0 = \frac{e^{-\beta_A H_A}}{Z_A} \otimes \frac{e^{-\beta_B H_B}}{Z_B} \tag{27}$$

It is convenient to write

$$\frac{e^{-\beta_A H_A}}{Z_A} = \begin{pmatrix} \frac{1}{e^{\beta_A \Omega}+1} & \\ & \frac{e^{\beta_A \Omega_A}}{e^{\beta_A \Omega_A}+1} \end{pmatrix} = \begin{pmatrix} f_A & 0 \\ 0 & 1-f_A \end{pmatrix} \tag{28}$$

where f_A is the Fermi-Dirac distribution

$$f_A = \frac{1}{e^{\beta_A \Omega}+1} \tag{29}$$

and similarly for B. We also use the notation, when convenient

$$\bar{f}_A = 1 - f_A \tag{30}$$

Then

$$\rho_0 = \mathrm{diag}(f_A f_B, f_A \bar{f}_B, \bar{f}_A f_B, \bar{f}_A \bar{f}_B)$$

$$= f_A f_B |00\rangle\langle 00| + f_A \bar{f}_B |01\rangle\langle 01| + \bar{f}_A f_B |10\rangle\langle 10| + \bar{f}_A \bar{f}_B |11\rangle\langle 11| \quad (31)$$

Next we put the qubits to interact with a potential

$$V = g(\sigma_+^A \sigma_-^B + \sigma_-^A \sigma_+^B) \quad (32)$$

this is a thermal operation (conserves energy)

$$[H_A + H_B, V] = 0 \quad (33)$$

Thus, $H = H_A + H_B + V$ can be separated as

$$e^{-iHt} = e^{-iVt} e^{-i(H_A + H_B)t}$$

But $H_A + H_B$ is diagonal so

$$\rho_{AB}(t) = e^{-iHt} \rho_0 e^{iHt} = e^{-iVt} \underbrace{e^{-i(H_A + H_B)t} \rho_0 e^{i(H_A+H_B)t}}_{\rho_0} e^{iVt}$$

Thus

$$\rho_{AB}(t) = e^{-iVt} \rho_0 e^{iVt} \quad (34)$$

Next you may use Mathematica to check that

$$e^{-iVt} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(gt) & -i\sin(gt) & 0 \\ 0 & i\sin(gt) & \cos(gt) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{35}$$

Thus

$$\begin{aligned} \rho_{AB}(t) = {} & f_A f_B |00\rangle\langle 00| + \bar{f}_A \bar{f}_B |11\rangle\langle 11| + \\ & + \left\{ f_A \bar{f}_B \cos^2(gt) + \bar{f}_A f_B \sin^2(gt) \right\} |01\rangle\langle 01| \\ & + \left\{ \bar{f}_A f_B \cos^2(gt) + f_A \bar{f}_B \sin^2(gt) \right\} |10\rangle\langle 10| \\ & + \frac{i}{2} \left(f_A \bar{f}_B - \bar{f}_A f_B \right) \sin(2gt) |01\rangle\langle 10| \\ & - \frac{i}{2} \left(f_A \bar{f}_B - f_A \bar{f}_B \right) \sin(2gt) |10\rangle\langle 01| \end{aligned} \tag{36}$$

The reduced density matrices are

$$\begin{aligned} \rho_A(t) = {} & \mathrm{tr}_B\, \rho_{AB}(t) \\ = {} & f_A f_B |0\rangle\langle 0| + \bar{f}_A \bar{f}_B |1\rangle\langle 1| \\ & + \left\{ f_A \bar{f}_B \cos^2(gt) + \bar{f}_A f_B \sin^2(gt) \right\} |0\rangle\langle 0| \\ & + \left\{ \bar{f}_A f_B \cos^2(gt) + f_A \bar{f}_B \sin^2(gt) \right\} |1\rangle\langle 1| \end{aligned}$$

If we simplify things a bit, we get

$$\rho_A(t) = \frac{1}{2}\left\{ f_A + f_B + (f_A - f_B)\cos(2gt)\right\} |0\rangle\langle 0| + \frac{1}{2}\left\{ \bar{f}_A + \bar{f}_B + (\bar{f}_A - \bar{f}_B)\cos(2gt)\right\} |1\rangle\langle 1| \tag{37}$$

which is quite symmetric. Stop a second also to check the consistency of this result.

It is now easy to compute

$$\langle H_A\rangle_0 = \mathrm{tr}\{H_A \rho_0\} = \frac{\Omega}{2}(2f_A - 1) \tag{38}$$

and

$$\langle H_A\rangle_t = \frac{\Omega}{2}\left\{ f_A + f_B - 1 + (f_A - f_B)\cos(2gt)\right\} \tag{39}$$

Thus

$$\boxed{\langle Q\rangle = \langle H_A\rangle_t - \langle H_A\rangle_0 = \Omega(f_B - f_A)\sin^2(gt)} \tag{40}$$

I will leave for you to check that this equal to $\langle H_B\rangle_0 - \langle H_B\rangle_t$.

Now let's construct the distribution of heat. Recall that

$$\mathcal{P}(Q) = \sum_{\substack{m, n \\ \mu, \nu}} \delta\left[Q - (E_n^A - E_m^A)\right] p(n\nu|m\mu)\, P_m^A\, P_\mu^B \tag{41}$$

Here m, n are the quantum numbers of A and μ, ν are those of B.

$$P_m^A : \quad P_0^A = f_A, \qquad P_1^A = \bar{f}_A$$

$$P_\mu^A : \quad P_0^B = f_B, \qquad P_1^B = \bar{f}_B$$

and

$$p(n\nu|m\mu) = |\langle n\nu|U|m\mu\rangle|^2$$

where U is given in (35).

What are the allowed values of Q?

$$E_0^A = \frac{\Omega}{2} \qquad E_1^A = -\frac{\Omega}{2}$$

$$|0\rangle_A \to |1\rangle_A \; : \; Q = -\frac{\Omega}{2} - \frac{\Omega}{2} = -\Omega$$

$$|1\rangle_A \to |0\rangle_A \; : \; Q = \frac{\Omega}{2} + \frac{\Omega}{2} = \Omega \tag{42}$$

$$\left.\begin{matrix} |0\rangle_A \to |0\rangle_A \\ \text{or} \\ |1\rangle_A \to |1\rangle_A \end{matrix}\right. \; : \; Q = 0$$

Thus

$$\mathcal{P}(Q=\Omega) = \sum_{\mu\nu} p(0\nu|1\mu)\, P_1^A P_\mu^B$$

$$= p(0,0|1,0)\, P_1^A P_0^B + p(0,0|1,1)\, P_1^A P_1^B$$

$$+ p(0,1|1,0)\, P_1^A P_0^B + p(0,1|1,1)\, P_1^A P_1^B$$

But looking at (35) we see that we are only left with

$$\mathcal{P}(Q=\Omega) = p(0,1|1,0)\, P_1^A P_0^B = \sin^2(gt)\, \bar{f}_A f_B \tag{43}$$

This makes sense: the only way for A to undergo a transition from $|1\rangle_A \to |0\rangle_A$ is if B undergoes a transition from $|0\rangle_B \to |1\rangle_B$. This prob. depends on f_B, which is the prob. that B is initially in $|0\rangle_B$ and on $\bar{f}_A$, which is the prob. that A is initially in $|1\rangle_A$.

We can now by symmetry figure out that

$$\mathcal{P}(Q=-\Omega) = \sin^2(gt)\, f_A \bar{f}_B \tag{44}$$

The last one, $\mathcal{P}(Q=0)$, is easy to determine because the 3 must add to 1.

$$\mathcal{P}(Q=0) = 1 - \mathcal{P}(Q=\Omega) - \mathcal{P}(Q=-\Omega) \tag{45}$$

Thus, to summarize

$$\boxed{\begin{aligned} P(Q=\Omega) &= \sin^2(gt)\, \bar{f}_A f_B &&:= P_+ \\ P(Q=-\Omega) &= \sin^2(gt)\, f_A \bar{f}_B &&:= P_- \\ P(Q=0) &= 1 - \sin^2(gt)\,(\bar{f}_A f_B + f_A \bar{f}_B) &&:= P_0 \end{aligned}} \tag{46}$$

The average heat is

$$\begin{aligned} \langle Q \rangle &= \Omega\, P(Q=\Omega) + (-\Omega)\, P(Q=-\Omega) + 0\, P(Q=0) \\ &= \Omega \sin^2(gt)\,(\bar{f}_A f_B - f_A \bar{f}_B) \\ &= \Omega \sin^2(gt)\,(f_B - f_A) \end{aligned} \tag{47}$$

which is exactly Eq (40).

We can now also check the fluctuation theorem

$$\frac{P(Q=\Omega)}{P(Q=-\Omega)} = \frac{(1-f_A)}{f_A} \frac{f_B}{1-f_B} \tag{48}$$

But

$$\left.\begin{aligned} f_A &= \frac{1}{e^{\beta_A \Omega}+1} \\ 1-f_A &= \frac{e^{\beta_A \Omega}}{e^{\beta_A \Omega}+1} \end{aligned}\right\} \quad \frac{1-f_A}{f_A} = e^{\beta_A \Omega} \tag{49}$$

Thus

$$\frac{P(Q = \Omega)}{P(Q = -\Omega)} = e^{(\beta_A - \beta_B)\Omega} = e^{\Delta\beta\,\Omega} \qquad (50)$$

which is the fluctuation theorem

$$\frac{P(Q)}{P(-Q)} = e^{\Delta\beta\, Q} \qquad (51)$$

Finally, we check the Jarzynski equality. But once we have (50), verifying it is trivial

$$\langle e^{-\Delta\beta Q} \rangle = \underbrace{e^{-\Delta\beta\Omega} P(Q = \Omega)}_{e^{\Delta\beta\Omega} P(Q=-\Omega)} + e^{-\Delta\beta(-\Omega)} \underbrace{P(Q = -\Omega)}_{e^{-\Delta\beta\Omega} P(Q = \Omega)} + e^{0} P(Q = 0)$$

$$= P(Q = \Omega) + P(Q = -\Omega) + P(Q = 0)$$

$$= 1$$

$$\therefore \quad \langle e^{-\Delta\beta Q} \rangle = 1 \qquad (52)$$

which is what we wanted to check :)