Simulating the non-equilibrium thermodynamics of quantum dots
Stationary State - single-level quantum dot in contact with two reservoirs

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1 Single level quantum dot in contact with two reservoirs

Here we have a completely different setup. The dot who's state now has a fixed energy ε, is in contact with two different thermal baths. The reservoirs are set such that the temperature of the one in the right T_r is higher than the one in the left T_l.

The dot-reservoir interactions have are characterised by the time-independent rates

$$W_{12} = \sum_{\nu=l,r} W_{12}^{\nu} = \sum_{\nu=1,2} a_{\nu} f_{\nu} \tag{1}$$

$$W_{21} = \sum_{\nu=l,r} W_{21}^{\nu} = \sum_{\nu=1,2} a_{\nu} \left(1 - f_{\nu}\right) \tag{2}$$

where f_{ν} is the fermi distribution and a_{ν} is a constant taking into account tunneling factors between the reservoirs and the dot.
The form of the rates can be found by quantum mechanical theory, but here we can see that they have an intuitive form.
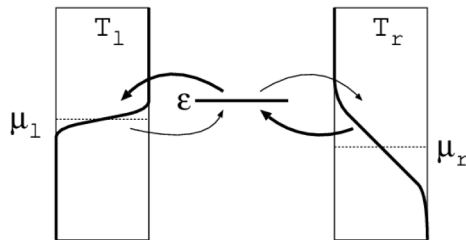

Figure 1: Stationary state sketch [1]

The rate to go up the state from a reservoir is proportional to the fermi distribution of the reservoir, which gives the probability distribution of finding an electron that has a particular energy in that reservoir, in this case that has the needed energy to enter the dot's state. In the same way the rate to go down a state due to a reservoir is proportional to $1 - f_\nu$, the complementary of the fermi distribution which gives the probability distribution of finding an empty whole in the reservoir for the electron.

In the section of stochastic thermodynamics, we defined the probability current $J(t) = W_{12}p_2(t) - W_{21}p_1(t)$. Setting

$$J = J^{ss} = 0 \iff W_{21}p_1^{ss} = W_{12}p_2^{ss} \tag{3}$$

using the two-states master equation, we find the stationary distributions

$$\begin{cases} p_1^{ss} = \frac{W_{12}}{W_{21}+W_{12}} = \frac{a_1 f_1 + a_2 f_2}{a_1 + a_2} \\ p_2^{ss} = \frac{W_{21}}{W_{21}+W_{12}} = \frac{a_1(1-f_1) + a_2(1-f_2)}{a_1 + a_2} \end{cases} \tag{4}$$

where p_1^{ss} is the stationary probability for the dot being full and p_2^{ss} is the stationary probability for the dot being empty

The probability currents for the reservoir ν is given by

$$I_\nu = W_{12}^\nu p_2 - W_{21}^\nu p_1 \tag{5}$$

hence, by rewriting (5) using (4), in the stationary regime we have

$$I_r = \alpha(f_r - f_l) \tag{6}$$
$$I_l = -I_r = \alpha(f_l - f_r) \tag{7}$$

with $\alpha = \frac{a_r a_l}{a_r + a_l}$

The heat rate from the reservoir r is given by

$$\dot{Q}_r = (I_{r,\varepsilon} - \mu_r I_{r,m}) \tag{8}$$

where $I_{r,\varepsilon}$ is the energy current from the reservoir r and $I_{r,m}$ is the matter current from the reservoir r. However, because we are in a stationary state, the only way to give energy to the dot is to put an electron in the dots level, we hence have a proportionality between the energy current and the matter current where the proportionality constant is the energy of the dots level ε. Hence

$$I_{r,\varepsilon} = \varepsilon I_{r.m} = I_r$$

from which

$$\dot{Q}_r = (\varepsilon - \mu_r)I_r = \alpha \left(\beta^\nu\right)^{-1} x_r(f_r - f_l) > 0 \tag{9}$$

due to the conditions we set on the dots temperatures, $f_r > f_l$

The chemical work rate corresponds to the net flux of matter from one reservoir to the other

$$\dot{w}_{chem} = \sum_{\nu=r,l} I_{\nu,m}\mu_\nu = (\mu_r - \mu_l)I_r = \alpha T_r \left(x_r - (1-\eta_c)x_l\right)(f_r - f_l) \quad (10)$$

where $\eta_c = 1 - \frac{T_l}{t_r}$ is the Carnot efficiency

Having the expressions for the right heat rate $\dot{Q}_r$ and the work rate $\dot{w} = \dot{w}_{chem}$, we can write the expression for the efficiency of the machine

$$\eta = \frac{Q_r}{w} = \frac{\dot{Q}_r}{\dot{w}} = 1 - (1-\eta_c)\frac{x_l}{x_r} \quad (11)$$

Having the expression of the efficiency and the work in terms of the effective energies x_ν, we could imagine finding the values for the effective energies for which the extraction of work is maximum and hence finding the efficiency at maximum power, which it's what is done in the article [1]

Concerning the entropy production rate $\dot{S}_i$

$$\dot{S}_i = \sum_\nu (W_{12}^\nu p_2^{ss} - W_{21}^\nu p_1^{ss})\left[\ln\left(\frac{W_{12}^\nu}{W_{21}^\nu}\right) + \ln\left(\frac{p_2^{ss}}{p_1^{ss}}\right)\right] = F_m J_m + F_e J_e \quad (12)$$

with $J_m = -I_r$ and $J_e = -\varepsilon I_r$ being the matter and energy flux with their corresponding thermodynamic forces $F_m = \frac{\mu_l}{t_l} - \frac{\mu_r}{T_r}$ and $F_e = \frac{1}{T_r} - \frac{1}{T_l}$.
As expected, we see that the entropy production rate has a component of matter flux and component of energy flux $\Rightarrow$ in a stationary state heat an matter gets dissipated $\Rightarrow$ we have heat dissipation plus current production by dissipation. Forthermore

$$\dot{S}_i = F_m J_m + F_e J_e = \alpha(x_l - x_r)(f_r - f_l) \quad (13)$$

which is always positive due to he fact that $f_r > f_l \iff x_l > x_r$ or $f_r < f_l \iff x_l < x_r$.
From Eq (13) we also notice that in these conditions, the equality of the temperatures of the of the two reservoirs is not a necessary condition to achieve equilibrium, what is important here is that the two effective energies are equal

$$x_l = x_r \implies \dot{S}_i = 0$$

Infact, if the reservoirs electronic distributions is the same for the two reservoirs, equilibrium is reached, and in the case of the fermi-disribution, this is achieved when $\mu_r T_r = \mu_l T_l$

1.1 Trajectory quantities and simulation results

To simulate the dynamics we need to take in to account the sorting of the rates. In principle, because

$$f_i < 1 \; \forall i \Longrightarrow f_i > f_j \iff 1 - f_i < 1 - f_j$$

only two sorting cases can occur, that we identify by checking for which reservoir the quantity $\mu_i T_i$ is bigger. In this case, the physical intuition already tells us the order.
Because the rates are time-independent, these variables stay constant through all the simulation and hence we don't have to do any check on them.

For the thermodynamic quantities we can just apply the formulation given in the previous file being careful to treat them differently than the occupation probability as explained in section of the Gillespie algorithm.

Figure 2 represents the results of the simulation of the out of equilibrium regime 2a and the equilibrium regime 2b. In all the graphs the dashed plots are the theoretical values and for all plots a part from the top one, the blue and red color are used to identify respectively quantities for the left and right reservoir. The top plot represent the occupation probability and we can see that in both cases it satisfies the expected values. The big oscillations come from meaning from non-equally spaced trajectory jumps, but they anyway enter the relatively small confidence interval set.
I recall that in the middle and bottom graphs, the quantity are not ensemble averages, their "evolution" is calculated from a single trajectory as explained in the section of the Gillespie algorithm in the file **Introduction˙to˙stochastic-Thermodynamics˙and˙simulations**. This kind of approximation works because the process is markovian.
The middle plot represent the heat rate from the two reservoirs. In the out of equilibrium regime 2a we see that as expected the heat rate from one reservoir is at each time opposite an equal in modulus to the other reservoir and we see that the heat rate from the right reservoir is the positive one. Infant in mean value, the heat should exit from the right reservoir and enter in the left one. Concerning the equilibrium regime 2b we see that the quantities go relatively fast to zero as expected.
The bottom graph represents the currents from the two reservoirs and the entropy production rate. The currents follow the exact behavior of the heat rate, which is correct because they are the ones that cause the heat rates. The entropy production rate (green line) follows the behaviour of the right current I_r which is also correct because its the one that characterises the dissipated flow that establish to try to equilibrate the temperatures.

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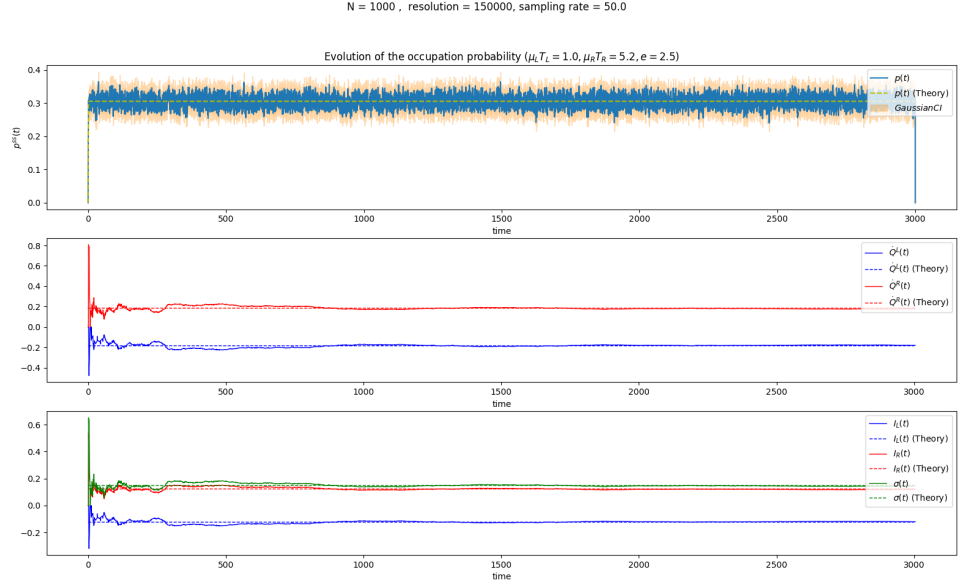
(a) out of equilibrium regime
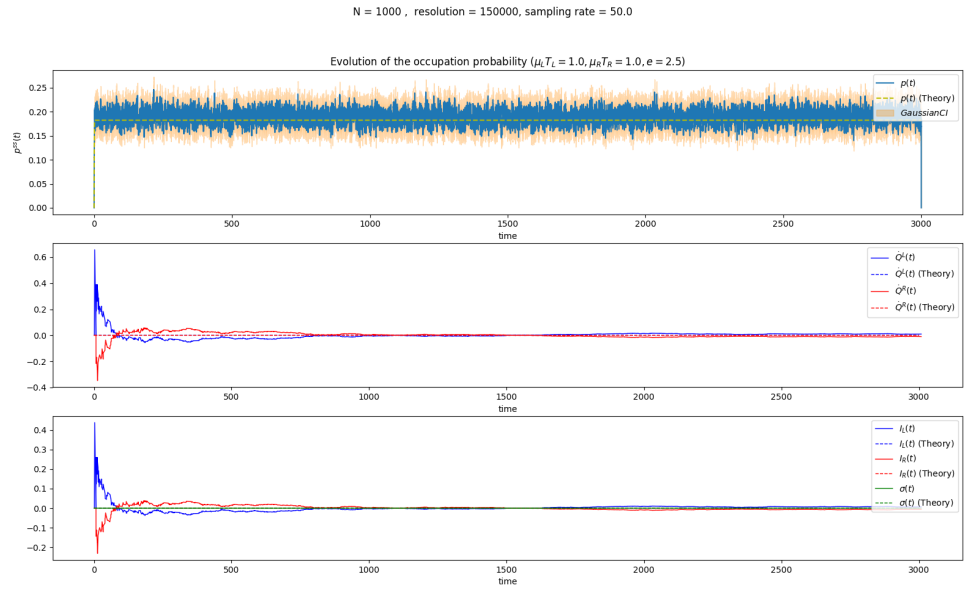
(b) equilibrium regime

Figure 2: Stationary state single level quantum dot in contact with two reservoirs

References

[1] Massimiliano Esposito, Katja Lindenberg, and Christian Van den Broeck. "Thermoelectric efficiency at maximum power in a quantum dot". In: *EPL (Europhysics Letters)* 85.6 (2009), p. 60010.