Simulating the nonequilibrium thermodynamics of quantum dots
Driven regime

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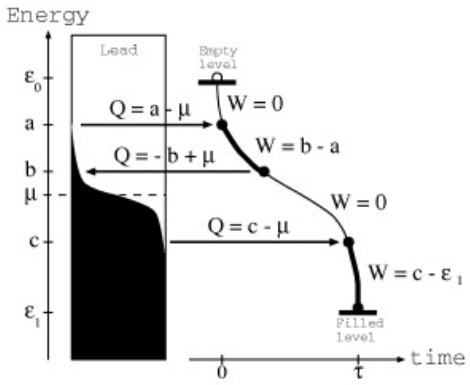


Figure 1: driven single-level quantum dot in contact with a bath sketch [**esposito2010finite**]

1 Driven single-level quantum dot in contact with a bath

In the first case we deal with a driven single level quantum dot in contact with a bath whose electronic population is governed by the fermi-dirac distribution. The bath has a constant chemical potential μ and a temperature T.

We define the time-dependent energy of the dot as $\varepsilon(t)$ and an effective energy $x(t) = \varepsilon(t) - \mu$ and the population probability as $p(t)$.
The dot-reservoir relation is characterised by the rates

$$W_{12}(t) = \frac{C}{e^{\beta x(t)} + 1} \tag{1}$$

$$W_{21}(t) = \frac{C}{e^{-\beta x(t)} + 1} \tag{2}$$

where C is a constant that takes into account tunneling factors between the dot and the reservoir.
We vary the energy of the dots level during a time τ and we search for the protocol of changing the energy of the level that extracts the maximum amount of work from the system [resp. injects the minimum amount of work in the system].

Using the mater equation describing the evolution of the dot population, with $p(t) = p_1(t)$ and $p_2(t) = 1 - p(t)$ we get

$$\dot{p}(t) = -p(t)\left(W_{12}(t) + W_{21}(t)\right) + W_{21}(t) \tag{3}$$

and substituting the rates (1) and (2)

$$\dot{p}(t) = C\left(-p(t) + \frac{1}{e^{\beta x(t)} + 1}\right) \tag{4}$$

with the dot initially in equilibrium with the bath

$$p(0) = \frac{C}{e^{\beta x(0)} + 1}$$

The differential equation (4) is not solvable due to the time-dependence of the energy term.

The thermodynamic quantities are given by

$$\dot{w} = \dot{\varepsilon}(t)p(t) \Longrightarrow w = \int_0^\tau \dot{\varepsilon}(t)p(t)dt \tag{5}$$

$$\dot{Q} = x(t)\dot{p}(t) \Longrightarrow Q = \int_0^\tau x(t)\dot{p}(t)dt \tag{6}$$

$$\Delta E = w + Q = x(\tau)p(\tau) - x(0)p(0) \tag{7}$$

In the article, the optimisation of the work is done with respect to the occupation probability to then get back the corresponding protocol $\varepsilon(t)$. The injected work is minimised by minimizing the total energy ΔE and hence by maximising the heat Q for a given value of $p(\tau)$

setting $C = 1$ and solving for $x(t)$ in (4), we get

$$\dot{Q} = x(t)\dot{p}(t) = \frac{1}{\beta} \ln \left[\frac{1}{\dot{p}(t) + p(t)} - 1 \right] \dot{p}(t)$$

hance

$$Q = \int_0^\tau \mathcal{L}(p, \dot{(p)}, t)dt$$

where $\mathcal{L}(p, \dot{(p)}, t) = \frac{1}{\beta} \ln \left[\frac{1}{\dot{p}(t)+p(t)} - 1 \right] \dot{p}(t)$ is the Lagrangian.
From Euler-Lagrange we know that $\mathcal{L} - \dot{p}\frac{\delta \mathcal{L}}{\delta \dot{p}} = cost \equiv K$, from which we find

$$\frac{\dot{p}^2}{(p + \dot{p})(1 - p - \dot{p})} = K \iff \dot{p} = \frac{K(1-2p) \mp \sqrt{K^2 + 4Kp(1-p)}}{2(1+K)} \tag{8}$$

solving by separation of variable

$$t = F(p) - F(p(0))$$

where $F(p)$ is a complicated form that can't be inverted analytically. However, in the high temperature regime of $\varepsilon(t) << K_B T$, $F(p)$ reduces to a form that enables to solve for the optimal protocol in the high temperature regime [**esposito2010finite**]

$$x(t) = x(0) \pm \sqrt{K}(t+1) \tag{9}$$

where

$$K = \frac{1}{4}\left(\frac{x(\tau) - x(0)}{\tau + 2}\right)^2$$

We see that the optimal protocol (9) has two solutions

$$x_+ = x(0) + \sqrt{K}(t+1) \tag{10}$$

$$x_- = x(0) - \sqrt{K}(t+1) \tag{11}$$

x_+ corresponding to the "upward process" in which we increase the energy of the level and we work on the dot.
x_- corresponding to the "downward process" in which we decrease the energy of the level and we extract work from the the dot.

1.1 Trajectory quantities and simulation results

To simulate the trajectories we use the method from the section of the algorithms in the file **Introduction˙to˙Stochastic-Thermodynamics˙and˙simulations** and for the the trajectory thermodynamic quantities, the equation are given in the section of trajectory level description. We could also understand the thermodynamic quantities by looking at the Figure 1 taken from the article [**esposito2010finite**].

Figure 2 represents the results of the simulation using the optimal protocol. The top graph represents the occupation probability (blue line) as function of time with the dashed line that represents one single trajectory population. We can see that both protocols satisfy the intuition of having an high population probability when the energy is low and a low occupation probability when the energy is high.
The middle graph represents the ensemble work rate (blue line) and the ensemble heat rate (red line). We see that as expected the upward protocol 2a has at at each time a positive mean work rate,

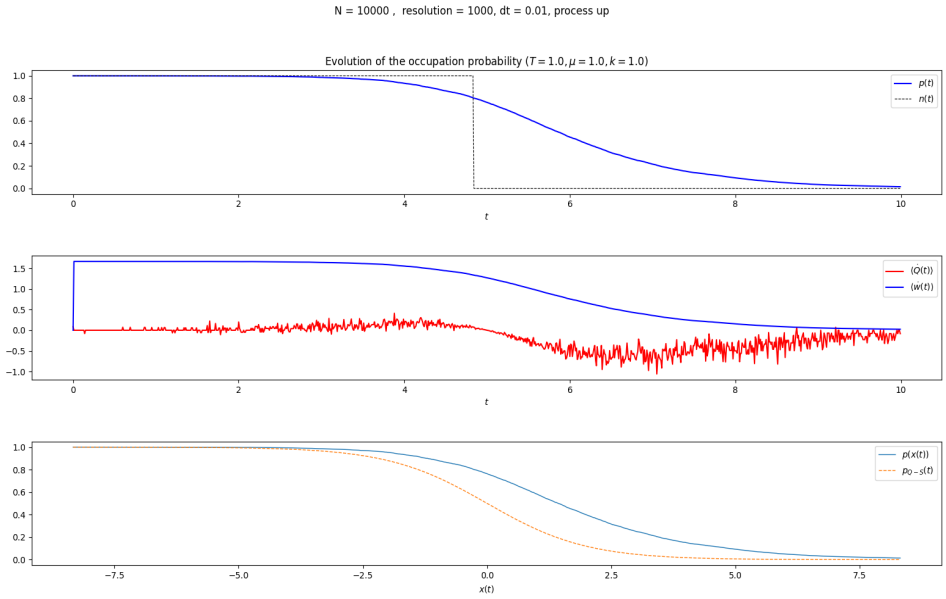
$$\dot{w}(t) = \frac{dw}{dt} > 0 \Rightarrow dw > 0 \text{ since } dt > 0$$

and since $w = \sum_i dw(t_i)$

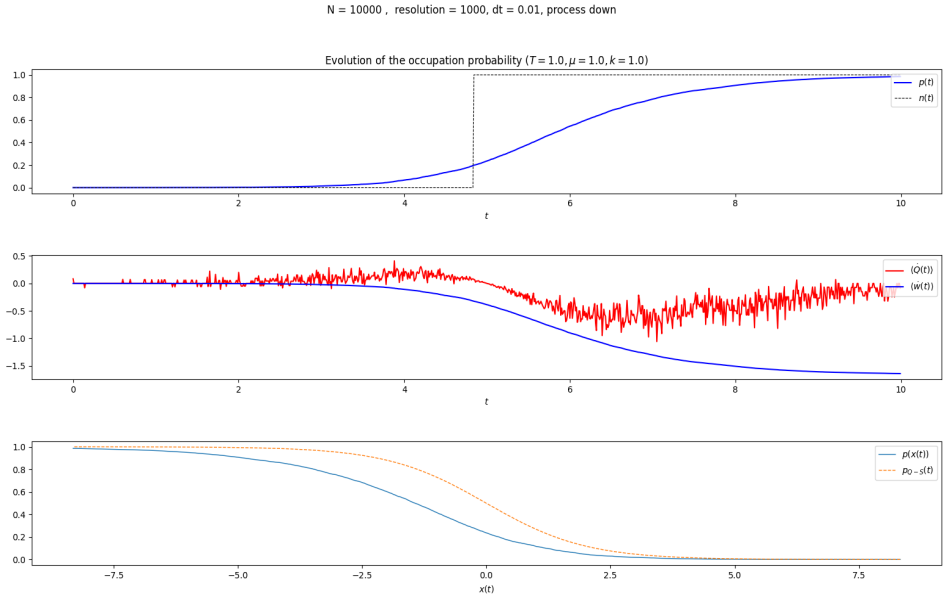
$$dw(t_i) > 0 \forall i \Rightarrow w > 0$$

hence the total ensemble work is positive and hence we are doing work on the system.
In the same way, we see that he downward protocol 2b has a negative ensemble work rate at each time, hence negative work ensemble work contribution at each time, and hence the total mean work is negative $\Longrightarrow$ we are extracting work on from the system.

Lastly, in the bottom graph I plotted the occupation probability as a function of the energy to see how far I was from a quasi-static transformation - the Fermi-Dirac distribution (dashed orange line). It's interesting to compare it with the ensemble heat rate of the middle graphs: when we have the stronger deviations from the equilibrium distribution, is where we have stronger oscillations and stronger deviations of the heat rate to zero. The oscillations becomes then smaller and also the heat contribution approaches zero when we approach back the equilibrium distribution.



(a) upward optimal protocol (10) - work done on the system



(b) downward optimal protocol (11) - work extracted from the system

Figure 2: Optimal protocols