We consider below a system which is driven through the application of an external time-dependent control parameter $\lambda(\tau)$. The following Langevin equation describes the driven overdamped motion of a single degree of freedom x in a 1D potential $V(x,\lambda)$,

$$\dot{x}(\tau) = -\mu \frac{\partial V(x,\lambda(\tau))}{\partial x} + \xi(\tau), \tag{1}$$

where $\xi(\tau)$ is a Gaussian white noise such that $\langle \xi(\tau) \rangle = 0$ and $\langle \xi(\tau)\xi(\tau') \rangle = 2\mu k_B T \delta(\tau-\tau')$. For the sake of simplicity, one set $\mu = k_B T = 1$.

Initially, the system is in equilibrium in the potential $V(x,\lambda_0)$, and we choose $\lambda_0 = 0$. During the interval $0 \leq \tau \leq t$, the control parameter is varied from λ_0 at the initial time to $\lambda_f \neq 0$ at the final time $\tau = t$. Below, we are particularly interested in the optimal protocol $\lambda^*(\tau)$ which minimizes the mean work for an imposed finite duration t of the process.

1. Write the expression of the work for an arbitrary potential which corresponds to a realization of this process. Explain why the work is in fact a stochastic variable, and give the expression of the mean work.

   In the following, we assume that the potential is harmonic of the form

   $$V(x,\tau) = \frac{1}{2}\left(x - \lambda(\tau)\right)^2. \tag{2}$$

   Let us first consider two simple cases where : (i) the control parameter is varied infinitely slowly, corresponding to the quasi-static limit when $t \to \infty$ and (ii) the control parameter is varied very fast, corresponding to the limit $t \to 0$.

2. For both cases, obtain the expression of the mean work $\langle W \rangle$ and the variation of free energy ΔF. Why can one say that the results are compatible with the second law of thermodynamics.
3. Let us now return to the general problem of determining the optimal the control parameter $\lambda(\tau)$ which optimizes the mean work in a fixed given time t. To progress, introduce the variable $u(t) = \langle x(t) \rangle$ and obtain an evolution equation for this variable using the Langevin equation.
4. With the equation obtained above, write the mean work in terms of only $u(t)$ and its derivatives. This mean work should have the form of a sum of a boundary term plus an integral of the form $\int_0^t d\tau \dot{u}^2$, where the dot means the time derivative.
5. In order to optimize the mean work, one should solve the Euler-Lagrange equations associated with the mean work obtained above. In the present case, the Euler-Lagrange equation is very simple $\ddot{u} = 0$. What is the solution of this equation compatible with the boundary conditions ?
6. Minimize the mean work for fixed λ_f and t, and deduce from this that the optimal protocol has the form

   $$\lambda^*(\tau) = \lambda_f \frac{1+\tau}{2+t}. \tag{3}$$

7. Deduce from the above, the expression of the optimal mean work. The result should have a compact simple form. Verify that the results obtained in question 2 for cases (i) and (ii) are recovered when $t \to \infty$ and $t \to 0$ respectively.
8. The optimal protocol differs from the simple linear protocol $\lambda(\tau) = \lambda_f \tau / t$. Verify that the mean work associated with that protocol is not optimal in the sense that

$$W^{lin} = (\lambda_f^2/t)^2(t + e^{-t} - 1) > W^*, \tag{4}$$

where W^* is the optimal mean work found previously.

Références

[1] Schmiedl, Tim and Seifert, Phys. Rev. Lett. **98** (2007), 108301