

Optimal driving protocols for nano-sized devices and their dependence on couplings to reservoirs

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Abstract. The development of efficient artificial nanodevices poses challenges which are of fundamental and technological nature. Recent progress has been made in the context of finite-time thermodynamics. A central question in finite-time thermodynamics is to identify the optimal procedure to extract the greatest amount of work from a system operating under well-defined constraints. For externally controlled small systems, the optimal driving protocol maximizes the mean work spend in a finite-time transition between two given system states under the constraints of given initial and final energy values, and a fixed total operation time. For simplicity we consider an externally controlled single level system, which is embedded in a thermal environment and coupled to a particle reservoir. The optimal protocols are calculated from a master equation approach for different system-reservoir couplings. For open systems, the system-reservoir couplings are shown to have a striking influence on the optimal driving setup. We point out that the optimal protocols have discontinuous jumps at the initial and final times. Finally, this work provides a first attempt to extend these calculations to larger system sizes.

1. Introduction

A good theoretical understanding of the optimal control of energy conversion processes is a prerequisite for tailoring efficient artificial nanodevices for specific needs. Typical examples are soft and biomatter systems, such as Brownian or molecular motors, organic photovoltaic solar cells and quantum dots. With minimization of the system size thermal fluctuations become relevant and the non-equilibrium behavior of such systems depends strongly on the driving forces and the changes of one system state to another, which are inherently finite in time. Thus, thermodynamic processes take place in finite time and the thermodynamic quantities like heat and work are now random but still fulfill a stochastic energy balance. In these systems it is useful to introduce microscopic heat and work quantities as random variables whose averages lead to the common thermodynamic quantities. Averages over functions of these microscopic heat and work quantities yield generalized fluctuation theorems (for reviews, see [1], and references therein). A common feature of many artificial nano-sized devices, where fluctuation theorems can be applied, is that those are mostly driven by time-varying external fields (often called as protocol) or electrochemical potential differences.

Of particular importance of this class of non-equilibrium systems is to identify the optimal procedure to extract the greatest amount of work from the device operating under given constraints [2]. Only a few studies so far have addressed the problem of identifying the optimal protocol that yields the minimum amount of work done on the system, which is required to drive a nano-scale system from one equilibrium state to another in finite time [2, 3, 4, 5]. Note that



this formulation is in reverse to the quest for the optimal protocol that provides the greatest amount of work from the artificial device. Whether on a continuous (Langevin equation) or a discrete (master equation) state space, a surprising result of all these studies is that the optimal protocol exhibits sudden jumps at the beginning and at the end of the thermodynamic process, while in between the optimal protocol varies smoothly. It can be argued that the initial jump in the optimal protocol is an immediate jump from equilibrium to a stationary state and the final jump allows a slower driving of the system at earlier times.

Here, we address a similar question on optimal driving setups. The focus of this work is on the couplings of the system to reservoirs, which have a strong influence on the specific form of the optimal protocol. To keep the analysis conceptual simple, we consider as working medium a single level system driven by a time-dependent protocol. We apply an optimization procedure based on a variational analysis. This allows us to get an analytic expression of the optimal protocol with respect to different system-reservoir couplings.

2. Model

We consider a single level system as working medium of an artificial nanodevice, in contact with a particle reservoir at temperature T , which is characterized by the chemical potential μ . The site energy $\varepsilon(t)$ is assumed to be time-dependent, which can be modified between an initial value ε_0 and a final value ε_1 by an external agent according to a given protocol. In what follows, it is convenient to introduce the energy difference $\epsilon(t) = \varepsilon(t) - \mu(t)$. The population of the single level at time t is characterized by the occupation probability $p(t)$. The system dynamics is modeled by a master equation approach with time-dependent rates $w_1(t)$ and $w_2(t)$ [6, 7, 8, 9, 10] accounting for the time evolution of the occupation probability $p(t)$,

$$\dot{p} = -w_1(t)p(t) - w_2(t)(1 - p(t)). \quad (1)$$

We assume that these transition rates obey detailed balance at each time instant.

Due to the time-varying of the site energy $\epsilon(t)$, positive or negative energy flows into the system. From the thermodynamic point of view the time derivative of the internal energy $E(t) = \epsilon(t)p(t)$ is the sum of a work flow $\dot{W} = \dot{\epsilon}(t)p(t)$ and a heat flow $\dot{Q} = \epsilon(t)\dot{p}(t)$. During the process time τ the energy change obeys the statistical mechanics formulation of the first law of thermodynamics, $\Delta E(\tau) = Q(\tau) + W(\tau)$, where $\Delta E(\tau) = \int_0^\tau dt \dot{E}(t) = E(\tau) - E(0) \equiv \epsilon(\tau)p(\tau) - \epsilon(0)p(0)$ with $\epsilon(0) = \epsilon_0$ and $\epsilon(\tau) = \epsilon_1$. The occupation probability of the equilibrium state at the beginning is $p(0) = [e^{\beta\epsilon_0} + 1]^{-1}$ with $\beta = 1/k_B T$. Accordingly, we have $W = \int_0^\tau dt \dot{\epsilon}(t)p(t)$ and $Q = \int_0^\tau dt \epsilon(t)\dot{p}(t)$. Both work W and heat Q can be interpreted as functionals of the occupation probability and thus depend, in particular, on the realized transition path. If $W(t) < 0$, the work $-W(t)$ is done by the system on the environment.

The details of the system-reservoir coupling determine decisive the exchange of particles between the reservoir and the system [11]. This is reflected in the form of the transition rates. In order to proceed, we need to specify these transition rates consistent with the detailed balance condition. In a quantum dot coupled to a metal lead, the rates $w_1(t)$ and $w_2(t)$ are Glauber (Fermi) rates [4], i. e., $w_1(t) = C[e^{-\beta\epsilon(t)} + 1]^{-1}$ and $w_2(t) = C[e^{\beta\epsilon(t)} + 1]^{-1}$. C is the inverse of a characteristic time scale involve in the exchange of particles between the reservoir and the system. We adopt here symmetric rates $w_1(t) = Ce^{\beta\epsilon(t)/2}$ and $w_2(t) = Ce^{-\beta\epsilon(t)/2}$. Symmetric transition rates are widely used in biomatter or ionic systems [12, 8].

3. Calculation of optimal driving protocols

In order to calculate the optimal driving protocol $\epsilon(t)$ which minimizes the work for the given constraints ϵ_0 , ϵ_1 , $p(0)$, and τ , we apply the proposed procedure given in Reference [4]. To minimize $W = \Delta E - Q$ we have to minimize ΔE and maximize Q simultaneously. Since ΔE

depends only on $p(\tau)$, we need to maximize the heat Q . The essential steps of this procedure are: (i) find the protocol that gives the maximum heat Q for a given value of $p(\tau)$ and (ii) conduct the optimization with respect to the final state $p(\tau)$. To this end we rewrite the heat as $Q = \int_0^\tau dt L(p, \dot{p})$ with $L(p, \dot{p}) = \epsilon(t)\dot{p}$, because $\epsilon(t)$ can be expressed as function of $p(t)$ and $\dot{p}(t)$. A variational analysis $\delta \int L dt = 0$ leads to the Euler-Lagrange equation $L - \dot{p} \frac{\partial L}{\partial \dot{p}} \equiv -\dot{p}^2 \frac{\partial \epsilon}{\partial \dot{p}} = \tilde{K}$. Here \tilde{K} is the constant of integration. For symmetric rates the Euler-Lagrange equation reads

$$\pm \frac{2(\dot{p}/C)^2}{\sqrt{(\dot{p}/C)^2 + 4p(1-p)}} = K, \quad (2)$$

where $K = \tilde{K}\beta/C$. Equation (2) is a quartic equation with respect to \dot{p} , which has two real (physical) solutions $\dot{p}/C = \pm \frac{1}{4} \sqrt{2K^2 + 2\sqrt{K^4 + 64K^2p(1-p)}}$ and two imaginary solutions. From these two first-order differential equations one can calculate $p(\tau)$ for given $p(0)$ and τ via

$$C\tau = \pm \int_{p(0)}^{p(\tau)} \frac{dp}{\frac{1}{4} \sqrt{2K^2 + 2\sqrt{K^4 + 64K^2p(1-p)}}} \quad (3)$$

as function of K . Subsequently, $p(\tau)|_K$ can be used to maximize the heat Q with respect to K by performing the integration

$$\beta Q|_K = \int_{p(0)}^{p(\tau)} dp \ln \left[\frac{A(p, K) + B(p, K)}{16p^2} \pm \frac{\sqrt{2K^2 D(p, K) + 2A(p, K)B(p, K)}}{16p^2} \right], \quad (4)$$

where $A(p, K) = K^2 + 16p(1-p)$, $B(p, K) = \sqrt{K^4 + 64K^2p(1-p)}$, and $D(p, K) = K^2 + 48p(1-p)$. Here, the K -dependent protocol ϵ can be rewritten with respect to p . Finally, we are able to optimize the work $W|_K = \Delta E|_K - Q|_K = \epsilon_1 p(\tau)|_K - \epsilon_0 p(0) - Q|_K$ with respect to K .

4. Results and discussion

In the calculation discussed below, the following choice of parameters was used: $C = 1$, $\beta = 1$, $\epsilon_0 = 10$, and $\epsilon_1 = 0$. Let us first take a closer look at the optimal protocol for symmetric rates as function of the processing time t for different values of K . To this end we calculate Equation (4) with the upper sign (+) by using Equation (3) with the lower sign (-) for downward processes. In this case, work is done by the system on the environment. Figure 1(a) shows both the optimal protocol (black solid line) and three non-optimal protocols as function of the processing time t . We can clearly identify jumps of the protocol at the beginning and at the end of the process. As seen in Figure 1(b), an initially almost empty systems is populated with particles with increasing time. The protocol controls how fast this single level can be occupied. Figure 2 shows the optimal protocol for fast ($\tau = 1$) and slow ($\tau = 10$) processes. We observe that the associated value of K_{opt} is larger for fast processes than for slow processes.

Thus, to understand the meaning of the parameter K , we square equation (2). By using evolution equation (1) with symmetric rates we arrive, after sorting with respect to p , at a quartic equation, which has two real and two complex conjugated roots. The two real roots read

$$p(t) = \frac{1}{e^{\beta\epsilon} + 1} \left(1 + \frac{K}{4} e^{\beta\epsilon/2} \tanh(\beta\epsilon/2) \pm \sqrt{\frac{K^2}{8} e^{\beta\epsilon} \tanh^2(\beta\epsilon/2) + \frac{K}{2} \frac{e^{\beta\epsilon}}{\cosh(\beta\epsilon/2)}} \right). \quad (5)$$

Equation (5) expresses the occupation probability as function of the protocol ϵ and K . If we assume a different system-reservoir coupling, say Fermi rates, the form of $p(t)$ [4] is quit different from those given in Equation (5). This emphasizes that the nature of the system-reservoir coupling has a striking influence on the optimal driving setup.

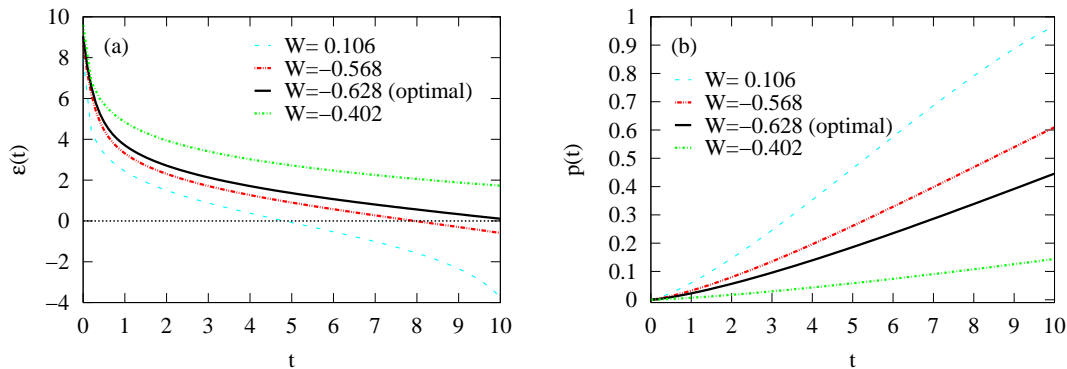


Figure 1. System properties for the case, in which the energy level is lowered from $\epsilon_0 = 10$ to $\epsilon_1 = 0$ as function of time t starting from $t_0 = 0$ until $t_1 = 10$; (a) protocol and (b) occupation probability. An optimal protocol (black solid line) can be identified with minimum cumulated work $W = -0.628$ for $K_{\text{opt}} = 0.0059$ and the total available time $\tau = t_1 - t_0 = 10$.

If $K = 0$, $p(t)$ is the equilibrium distribution of a single level system. This implies that $K = 0$ coincides with a quasistatic process control. Consequently, the parameter K quantifies how far the system differs from the quasistatic limit.

In order to extend these investigations to large systems, we consider the simplest case, in which a system with N sites and energies $\epsilon_l(t)$ interacts with a particle reservoir at temperature T . Particles can only enter or leave each level and we assume that no transitions between site l and site k take place. Thus, the internal energy of the system is given by an additive principle, $E(t) = \sum_l \epsilon_l(t)p_l(t)$, and the time-derivative of $E(t)$ yields $\dot{W} + \dot{Q}$ with $\dot{W} = \sum_l \dot{W}_l = \sum_l \dot{\epsilon}_l(t)p_l(t)$ and $\dot{Q} = \sum_l \dot{Q}_l = \sum_l \epsilon_l(t)\dot{p}(t)$. In this special case the application of the variational analysis presented in Section 3 is straightforward in order to get the optimal setup of large systems.

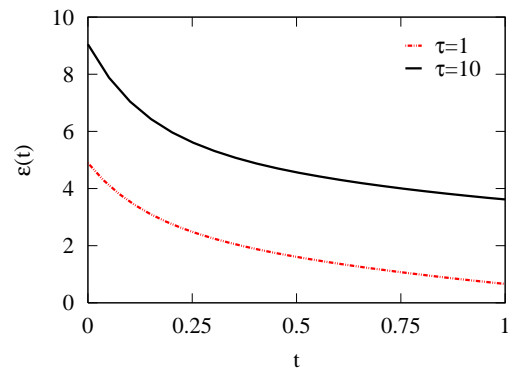


Figure 2. The optimal protocol for $\tau = 1$ ($K_{\text{opt}} = 0.17$) and $\tau = 10$ ($K_{\text{opt}} = 0.0059$) as function of time t .

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