Finite-time thermodynamics for a single-level quantum dot

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Abstract – We investigate the finite-time thermodynamics of a single-level fermion system interacting with a particle reservoir. The optimal protocol to extract the maximum work from the system when moving the single energy level between an initial higher value and a final lower value in a finite time is calculated from a quantum master equation. The calculation also yields the optimal protocol to raise the energy level with the expenditure of the least amount of work on the system. The optimal protocol displays discontinuous jumps at the initial and final times.

Introduction. – The search for the least work-intensive protocols for the extraction or insertion of energy into or out of a thermal system has been a major research topic since the inception of the laws of thermodynamics. While the regime of quasi-static transformations, which is described by close-to-equilibrium thermodynamics, is well understood, many questions remain unsolved when dealing with problems far from equilibrium. A first question of particular interest deals with thermodynamic processes taking place in a finite time. This issue has been the object of detailed investigations in the context of finite-time thermodynamics (FTT) [1]. Other developments are related to recent progress in nanotechnology and cellular biology, where small systems far from equilibrium are subject to large thermal fluctuations. Deviations from average behavior, even rare events, play a significant role in their behavior. During the past decade, major progress has been achieved toward understanding and describing the role of fluctuations in such small non-equilibrium systems. The fluctuation theorem [2,3], the Jarzynski equality [4], Crook's theorem [5], and the formulation of stochastic thermodynamics [6] provide a novel framework to tackle the role of fluctuations in entropy production and dissipative work far from equilibrium. In addition, exact expressions for the irreversible entropy production have also been derived [7–10]. A third frontline of research deals with quantum mechanical behavior in FTT. As the size of a system is reduced to the nanometer scale, quantum mechanical properties such as discreteness, quantum coherence, quantum statistics, and quantum correlations (entanglement) must be taken into account. We cite in particular the thermodynamics of quantum information processing [11,12], the related quantum heat engines [11,13,14], and quantum entanglement as a source of canonical typicality [15].

One of central questions addressed in FTT is to identify the optimal procedure to extract the greatest amount of work from a device operating under given constraints, or, in reverse, to cause a device to operate under such constraints with the minimum injection of work. According to the convention in which $\mathcal{W}$ is the work done *on* the system, maximum work extracted or minimum work injected both correspond to the minimum $\mathcal{W}$. The question is thus that of identifying the protocol that involves the minimum amount of work done on the system. For example, Schmiedl and Seifert [16] considered the optimal protocol to relocate a Brownian particle using a laser tweezer. They found that the optimal variation of the laser intensity which minimizes the work done on the system exhibits sudden jumps. Such singularities in the optimal protocol may seem surprising, but in fact they turn out to be generic [17–20].
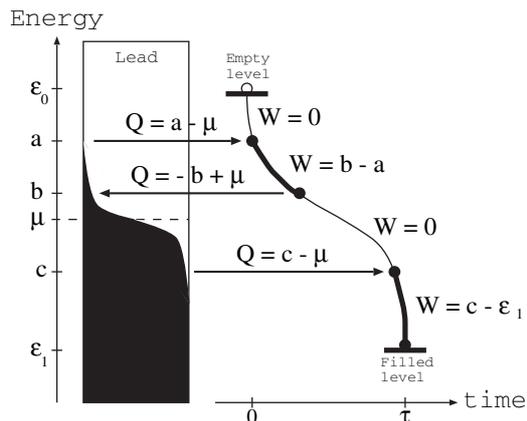
Fig. 1: The model: a single-level quantum dot interacts with a metallic lead. The level is initially at ε_0 in thermal equilibrium but is lowered to ε_1 in a finite time τ according to a given protocol $\varepsilon(t)$. We depict a typical trajectory for such a process along which heat is exchanged and work is extracted. Work and heat are obtained by averaging over all possible trajectories associated with this process.

In the present letter we address a similar question for a simple quantum process. We consider a single-level quantum system interacting with a particle reservoir. By raising or lowering the energy ε of this level, we can inject work ($\mathcal{W} > 0$) or extract work ($\mathcal{W} < 0$). The time dependence of the protocol $\varepsilon(t)$ can be controlled externally. Our aim is to find an optimal protocol, one that minimizes the work done on the system, under the constraints of given initial and final values ε_0 and ε_1, and a fixed total operation time τ. We will specifically consider a quantum dot coupled to a metal lead, the latter playing the role of a fermion particle reservoir. The detailed analysis of time-dependent phenomena in open quantum systems is extremely complicated. In order to obtain exact analytical and numerical results, we restrict ourselves to a simple model based on a quantum master equation. We thus neglect quantum coherency and entanglement between the system and the reservoir, but take into account the discreteness of the level and the proper Fermi-Dirac statistics.

The model. – We consider a single-level quantum dot interacting with a metallic lead, as illustrated in fig. 1. The other levels of the dot are assumed to be sufficiently far away from the Fermi level of the lead to be neglected. We also assume that the electrons thermalize instantaneously to temperature T upon tunneling to the reservoir. In order to describe the basic mechanism to produce heat and work, we assume that the energy of the level is varied in time, $\varepsilon(t)$, and that the chemical potential of the lead remains fixed. Upon varying the energy of the level, a certain amount of (positive or negative) energy flows into the system in the form of heat and work. If the level is and remains occupied by an electron while it is lowered (raised), work is extracted from (injected into) the system, $\mathcal{W} < 0$ ($\mathcal{W} > 0$). If the level remains empty while its energy

is changed, neither work nor heat are produced. When the empty (filled) level at energy $\varepsilon(t)$ is filled (emptied) by an electron, an amount of heat $\mathcal{Q} = \varepsilon - \mu$ ($\mathcal{Q} = -\varepsilon + \mu$) enters the system. The amount of heat and work corresponding to a given protocol is a statistical average of the heat and work produced along all the possible histories of charge and discharge of the level during the protocol. Our goal is to find an optimal way of varying the energy level, the so-called optimal protocol, such that a maximum amount of work $-\mathcal{W}$ is extracted from the system or a minimum amount of work $\mathcal{W}$ is injected.

Dynamics. We describe the time evolution of the quantum state using a master equation for the occupation probability $p(t)$,

$$\dot{p}(t) = -\omega_1(t)p(t) + \omega_2(t)[1 - p(t)], \tag{1}$$

where the ω_i are transition rates [21,22]. In the wide-band approximation, these rates are given by

$$\omega_1 = \frac{C}{e^{-\beta[\varepsilon(t) - \mu(t)]} + 1}, \tag{2a}$$

$$\omega_2 = \frac{C}{e^{+\beta[\varepsilon(t) - \mu(t)]} + 1}, \tag{2b}$$

where C is a constant describing the system-reservoir coupling strength in the weak-coupling regime where level broadening can be neglected. We set the Planck and Boltzmann constants to unity ($\hbar = 1$ and $k = 1$). Therefore C^{-1} determines the characteristic time between successive electron transfers (tunneling events) and will be taken as our unit of time. Noting that formally raising the energy level is in fact equivalent to lowering the chemical potential, we introduce an effective energy $\epsilon(t) \equiv \varepsilon(t) - \mu(t)$ measured in units of C. The master equation (1) thus reduces to the simple form

$$\dot{p}(t) = -p(t) + \frac{1}{e^{\epsilon(t)/T} + 1}. \tag{3}$$

The system is initially assumed to be in thermal equilibrium,

$$p(0) = \frac{1}{e^{\epsilon_0/T} + 1}. \tag{4}$$

The protocol is defined by the change of $\epsilon(t)$ from ϵ_0 to ϵ_1 in a time τ.

Thermodynamics. We next turn to the thermodynamic description of the model. We use the convention that heat entering the system is (like work) positive. The internal energy of the system at time t is

$$E(t) = U(t) - \mu N(t) = \epsilon(t)p(t), \tag{5}$$

where

$$U(t) = \varepsilon(t)p(t), \quad N(t) = p(t). \tag{6}$$

The rate of change in the internal energy, $\dot{E}$, is the sum of two parts, namely, a work flux $\dot{\mathcal{W}}$ and a heat flux $\dot{\mathcal{Q}}$,

$$\dot{\mathcal{W}} \equiv \dot{\epsilon}p = \dot{\varepsilon}p - \dot{\mu}p, \tag{7a}$$

$$\dot{\mathcal{Q}} \equiv \epsilon\dot{p} = \varepsilon\dot{p} - \mu\dot{p}. \tag{7b}$$

Note that the particle exchange contributes to the heat flux (last term in eq. (7b)). When the energy level is below the Fermi level, the direction of heat flow is opposite to the direction of tunneling.

The net total work and net total heat during the process of duration τ are obtained as functionals of the occupation probability,

$$\mathcal{W}[p(\cdot)] = \int_0^\tau \dot{\epsilon}(t)p(t)\mathrm{d}t, \tag{8a}$$

$$\mathcal{Q}[p(\cdot)] = \int_0^\tau \epsilon(t)\dot{p}(t)\mathrm{d}t. \tag{8b}$$

The resulting total net change in the internal energy is given by the First Law of thermodynamics,

$$\Delta E = p(\tau)\epsilon_1 - p(0)\epsilon_0 = \mathcal{W}[p(\cdot)] + \mathcal{Q}[p(\cdot)]. \tag{9}$$

While work and heat depend on the path of $p(t)$, ΔE depends only on the final probability $p(\tau)$ and the given constraints ϵ_0, ϵ_1 and $p(0)$.

Minimizing work. – We first consider the case of arbitrary temperature and subsequently focus on the high-temperature regime for analytic tractability.

General approach. Our aim is to find an optimal protocol $\epsilon(t)$ which minimizes the work $\mathcal{W}$. From the First Law of the thermodynamics, eq. (9), the work can be written as a functional of $p(t)$,

$$\mathcal{W}[p(\cdot)] = \Delta E - \mathcal{Q}[p(\cdot)]. \tag{10}$$

However, performing a variational analysis directly with respect to $\epsilon(t)$ is complicated due to expected discontinuities. Instead, we optimize the work with respect to $p(t)$ which by definition is always differentiable, and identify the corresponding optimal $\epsilon(t)$ from it. To do so, we need to minimize ΔE and maximize $\mathcal{Q}$ simultaneously. However, from eq. (9) we see that ΔE depends only on the final probability $p(\tau)$. Hence, we can first identify the protocol leading to maximum heat $\mathcal{Q}$ for a given value of $p(\tau)$, and in a second step we perform the optimization with respect to the final state $p(\tau)$.

To find the protocol that maximizes the heat, we express $\epsilon(t)$ in terms of $p(t)$ and $\dot{p}(t)$ and rewrite eq. (8b) as

$$\mathcal{Q}[p(\cdot)] = \int_0^\tau \mathcal{L}(p, \dot{p})\mathrm{d}t, \tag{11}$$

where

$$\mathcal{L} \equiv T \ln\left[\frac{1}{p(t) + \dot{p}(t)} - 1\right]\dot{p}(t). \tag{12}$$

The extremum is found via the standard Euler-Lagrange method, leading, after integration, to

$$\mathcal{L} - \dot{p}\frac{\partial \mathcal{L}}{\partial \dot{p}} = \frac{\dot{p}^2}{(p + \dot{p})(1 - p - \dot{p})} = K. \tag{13}$$

Here K is the constant of integration. Before turning to the solution of this differential equation, we show that it

implies a discontinuity in the protocol $\epsilon(t)$. Eliminating $\dot{p}$ in eq. (13) by using the master equation (3), the resulting quadratic equation for $p(t)$ leads to the relation

$$p(t) = \frac{1}{e^{\epsilon(t)/T} + 1}\left[1 \pm e^{\epsilon(t)/2T}\sqrt{K}\right]. \tag{14}$$

If one determines the value of the integration constant K from the initial condition $p(0)$ assuming $\lim_{t\to 0}\epsilon(t) = \epsilon(0)$, this relation implies that $K = 0$, *i.e.*, that $p(t)$ is the equilibrium distribution associated with the instantaneous value of the energy. However, except in the case of an infinitely slow quasi-static process one expects that $p(t)$ *will* deviate from thermal equilibrium, that is, that in general $K > 0$. This apparent inconsistency indicates that $\lim_{t\to 0}\epsilon(t) \neq \epsilon(0)$. In other words, there must be a sudden jump from ϵ_0 to $\epsilon(0^+)$. By comparing eq. (4) to eq. (14) at $t = 0$, we find the magnitude of the jump,

$$\epsilon(0^+) - \epsilon_0 = \pm 2T\,\mathrm{arcsinh}\left[\sqrt{K}\cosh[\epsilon_0/2T]\right]. \tag{15}$$

Equation (14) also indicates that when $K > 0$ there are two possibilities. The plus sign in $\pm$ leads to an occupation probability $p(t)$ that is larger than that of thermal equilibrium, and corresponds to the scenario of moving to a higher energy $\epsilon_1 \geqslant \epsilon_0$. We refer to these as upward processes. For downward processes, the lower sign should be used. Henceforth it should thus be understood that the upper (lower) sign has to be considered when processes are upward (downward), respectively.

Proceeding with the discussion of eq. (13), we solve the quadratic equation for $\dot{p}$, leading to

$$\dot{p} = \frac{K(1 - 2p) \mp \sqrt{K^2 + 4Kp(1-p)}}{2(1 + K)}. \tag{16}$$

This equation can be solved by separation of the variables t and p, leading to the following explicit result:

$$t = \int_{p(0)}^{p(t)} \frac{1}{\dot{p}}\mathrm{d}p = F[p(t)] - F[p(0)], \tag{17}$$

with

$$F(p) = -\alpha_\pm \pm \frac{1}{\sqrt{K}}\arctan\left[\frac{1 - 2p}{\sqrt{K + 4p(1-p)}}\right]$$
$$\pm \frac{1}{2}\ln\left[\frac{K + 2p + \sqrt{K^2 + 4Kp(1-p)}}{2 + K - 2p + \sqrt{K^2 + 4Kp(1-p)}}\right], \tag{18}$$

where $\alpha_+ = \ln p$ and $\alpha_- = \ln(1-p)$. We note that $F(p)$ is not exactly the primitive of the integrand in (17) due to cancellation of some terms in the definite integral.

While in general we will need to proceed with a numerical inversion for the resulting transcendental equation, an analytically tractable approximation is discussed later for

the high-temperature case. Having thus obtained the optimal $p(t)$ for a given K, we insert this expression in eq. (8b) to obtain the corresponding heat,

$$
\begin{aligned}
\mathcal{Q} &= \int_0^\tau \epsilon(t)\dot{p}\mathrm{d}t = \int_{p(0)}^{p(\tau)} \epsilon(p)\mathrm{d}p \\
&= T \int_{p(0)}^{p(\tau)} \mathrm{d}p \ln\left[\frac{K + 2p - 2p^2 \pm \sqrt{K^2 + 4Kp(1-p)}}{2p^2}\right] \\
&= T\left(G[p(\tau)] - G[p(0)]\right),
\end{aligned}
\tag{19}
$$

where

$$
\begin{aligned}
G(p) &= p\ln\left[\frac{K + 2(1-p)p \pm \sqrt{K^2 + 4Kp(1-p)}}{2p^2}\right] \\
&\quad -\tilde{\alpha}_\pm \mp \sqrt{K}\arcsin\left[\frac{1-2p}{\sqrt{K+1}}\right] \\
&\quad \mp \ln\left[2 + K - 2p + \sqrt{K^2 + 4Kp(1-p)}\right],
\end{aligned}
\tag{20}
$$

where $\tilde{\alpha}_+ = 0$ and $\tilde{\alpha}_- = 2\ln(1-p)$. Finally, we need to optimize the resulting work, given in eq. (10), with respect to $p(\tau)$, as explained earlier. Since $p(\tau)$ is uniquely determined by K, it suffices to numerically optimize the expression with respect to K.

The high-temperature regime. The mathematical expressions for the general minimization presented in the previous subsection are rather complicated. However, the functions (18) and (20) simplify in the high-temperature limit, allowing us to find the optimal protocol and its properties in full analytical detail. The high-temperature limit is defined in terms of the physical parameters by the condition $\epsilon(t) \ll T$. In terms of our original variables it means that $\varepsilon(t) - \mu(t) \ll kT$.

We introduce $\eta(t)$:

$$
p(t) = \frac{1}{2} - \frac{\eta(t)}{4},
\tag{21}
$$

which has the meaning of an effective energy level divided by kT in the high-temperature regime and is implicitly defined via eq. (14).

Next, we consider eqs. (18) and (20) as functions of η. Since $\epsilon(t) \ll T$, we only keep the lowest-order terms. Noting from eq. (13) that $\sqrt{K}$ is of order ϵ/T, we find that eqs. (14), (18) and (20) simplify as follows:

$$
\epsilon(t)/T = \eta(t) \pm 2\sqrt{K},
\tag{22}
$$

$$
F(\eta(t)) = \pm \frac{\eta(t)}{2\sqrt{K}},
\tag{23}
$$

$$
G(\eta(t)) = \mp\frac{1}{2}\sqrt{K}\eta(t) - \frac{1}{8}\eta^2(t).
\tag{24}
$$

Solving eq. (17), we find $\eta(t) = (\epsilon_0 \pm 2\sqrt{K}t)/T$ and hence the optimal protocol reads

$$
\epsilon(t) = \epsilon_0 \pm 2\sqrt{K}(t+1).
\tag{25}
$$

The work is minimum for

$$
K = \frac{1}{4\,T^2}\left(\frac{\epsilon_1 - \epsilon_0}{\tau + 2}\right)^2.
\tag{26}
$$

The optimal work and associated heat thus become

$$
\mathcal{W} = \frac{(\epsilon_1 - \epsilon_0)[8T - 4\epsilon_0 + \tau(4T - \epsilon_1 - \epsilon_0)]}{8T(\tau + 2)},
\tag{27a}
$$

$$
\mathcal{Q} = \frac{\tau(\epsilon_0^2 - \epsilon_1^2)}{8\,T(\tau + 2)}.
\tag{27b}
$$

From eq. (25) we find that the initial and final energy jumps are given by $\pm 2\sqrt{K}$. The size of the jumps increases as the deviation from the quasi-static limit (measured by K) increases. In between the jumps, the optimal protocol raises/lowers the level linearly with time (but we stress that this linear dependence only applies to the high-temperature regime). Here for the case with the symmetry $\epsilon_0 = -\epsilon_1$ there is no net heat flow. In this case all the work is converted into internal energy.

Results. – In this section we present numerical results for the optimal protocol. First we consider the situation where the energy level is raised from $\epsilon_0 = -10T$ to $\epsilon_1 = 10T$ during a total available time $\tau = 10$. This is the situation in which work is done on the quantum dot. The chosen parameter values guarantee that the initial energy level is well below, and the final level well above, the Fermi level. The top panel in fig. 2 shows the optimal protocol. We also include two non-optimal protocols, that is, ones corresponding to non-optimal values of K. The middle and bottom panels show the corresponding occupation probabilities and heat current. When the initial jump is "too small" (dot-dashed lines), the level stays mostly below the Fermi level and thus the system receives heat from the reservoir. While this favors the reduction of work, there is not enough time for electrons, being below the Fermi level most of the time, to tunnel, thus costing a large amount of work when raising the electrons during the final jump. On the other hand, when the initial jump is too large (dashed line), the electrons quickly escape and thus almost no work is required at the final jump. However, the rapid tunneling induces a large heat current to the reservoir, increasing the work during the process. The optimal protocol (solid line) guarantees that the level is most likely empty before the final jump, with only a small outbound heat current. Note that heat initially flows into the system, compensating for part of the outgoing heat after $\epsilon(t)$ crosses the Fermi level.

Figure 3 shows downward processes where the energy level is lowered from $\epsilon_0 = 10T$ to $\epsilon_1 = -10T$ over the same period of time $\tau = 10$. In this scenario, work is extracted from the quantum dot. Three different cases parallel to the upward cases of fig. 2 are illustrated.

Next, we reduce the time of operation. Figure 4 compares optimal protocols for slow ($\tau = 10$), intermediate
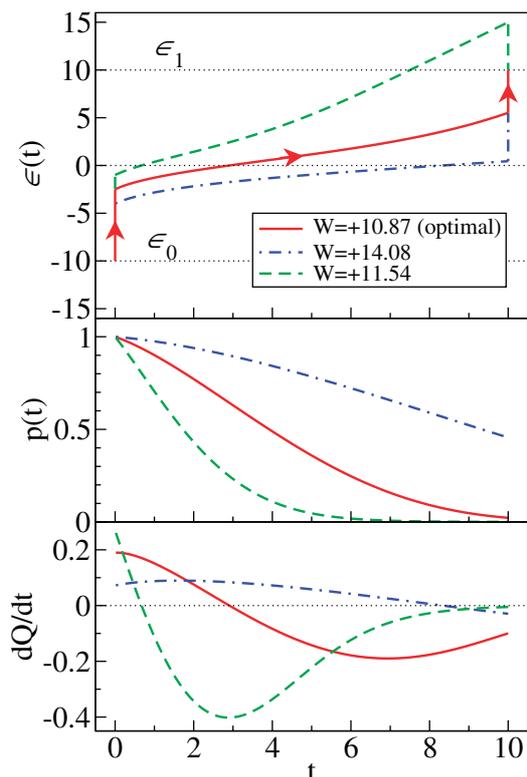
Fig. 2: (Color online) Protocol (top), occupation probability (middle), and heat flux (bottom). The energy level is raised from $\epsilon_0 = -10T$ to $\epsilon_1 = 10T$ during time $\tau = 10$. The red solid lines indicate optimal protocol with minimum work $W = 10.87T$. A protocol with a large initial jump (green dashed lines) and another protocol with a small initial jump (blue dot-dashed lines) result in higher work $W = 16.79T$ and $W = 11.16T$, respectively.
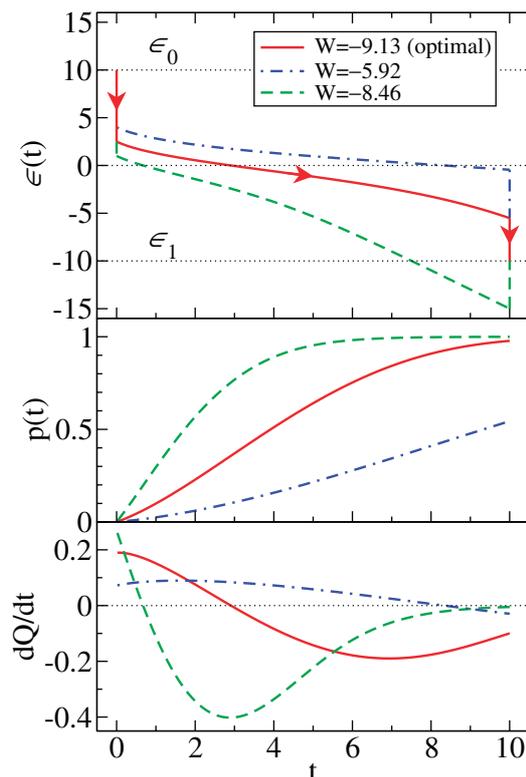
Fig. 3: (Color online) Protocol (top), occupation probability (middle), and heat flux (bottom). The energy level is lowered from $\epsilon_0 = 10T$ to $\epsilon_1 = -10T$ during time $\tau = 10$. The red solid lines indicate optimal protocol with minimum work $W = -9.13T$. A protocol with a large initial jump (green dashed lines) and another protocol with a small initial jump (blue dot-dashed lines) result in higher work $W = -8.58T$ and $W = -5.92T$, respectively.

($\tau = 1$) and fast ($\tau = 0.1$) processes of work extraction from the quantum dot. As τ decreases, the initial and final jumps become larger. When the electrons have almost no time to tunnel into the system, the optimal protocol becomes nearly a jump-stay-jump process.

Finally, fig. 5 shows the optimal protocols for work extraction at various temperatures. As temperature is increased, the optimal protocol becomes symmetric with respect to the Fermi level, in good agreement with the high-temperature approximation, eq. (25).

Discussion. – Discontinuities in the protocol that minimizes the work on a device operating under given constraints may seem to be surprising. However, a simple argument explains the initial and final jumps in the optimal protocols, starting from an analysis of the low-temperature case. The key points to keep in mind are: i) moving an empty level requires no work, ii) tunneling at the Fermi level carries no heat, and iii) the direction of heat flow changes at the Fermi level. Consider an upward process at $T = 0$. Since tunneling is not possible below the Fermi level, the same amount of work is required to raise the level to the Fermi level regardless of the
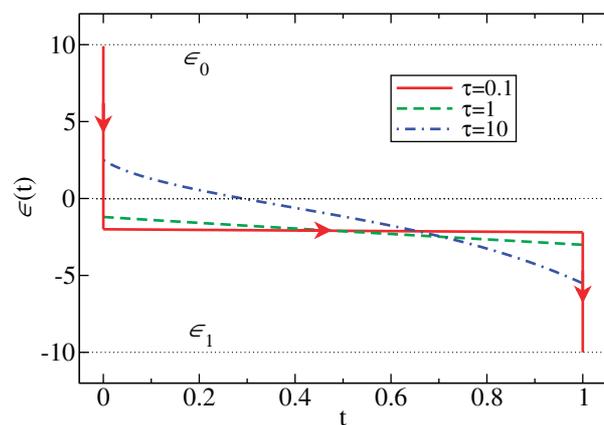

Fig. 4: (Color online) The optimal protocols for three different processing times, $\tau = 0.1$ (solid line), $\tau = 1$ (dashed line), and $\tau = 10$ (dash-dotted line). The energy level is lowered from $\epsilon_0 = 10T$ to $\epsilon_1 = -10T$ during time τ.

protocol. Hence, the instantaneous jump to the Fermi level is preferred since it leaves maximum time for electrons to subsequently tunnel out. After the jump, it is clear that the optimal protocol must keep the level just above the
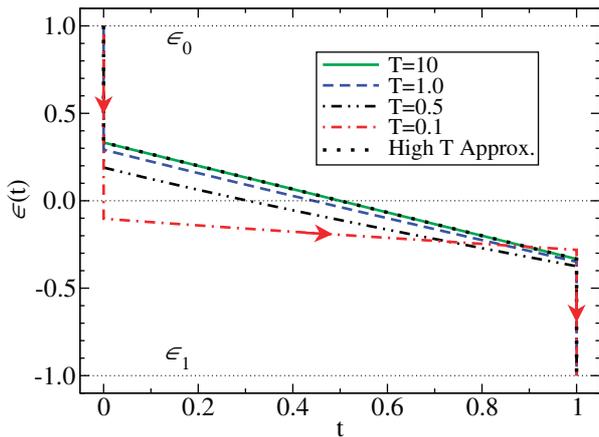
Fig. 5: (Color online) The optimal protocols for four different temperatures, $T = 10$ (green solid line), $T = 1$ (blue dashed line), $T = 0.5$ (black dash–double-dotted line), and $T = 0.1$ (red dash-dotted line). The energy level is lowered from $\epsilon_0 = 1$ to $\epsilon_1 = -1$.

Fermi level until the final time. In this way, heat transfer to the reservoir is avoided. During this period no work is done, and the population in the energy level is reduced to close to zero without heat transfer. At the end, the level jumps up to its final value with almost no work.

When the temperature is finite, tunneling is possible even below the Fermi level. Note that heat flux is inward into the system when the electrons tunnel out below the Fermi level, which helps reduce the work. On the other hand, the tunneling rate is small, which increases the work at a later time. The optimal protocol now includes an initial jump to a level slightly below the Fermi level. At this stage, heat flows into the system. Next, the energy level moves slowly above the Fermi level. As electrons tunnel out, heat flows to the reservoir, which compensates the initial heat gain. At the high-temperature limit, the loss and gain of the heat are exactly balanced and no net heat flows to the reservoir during the process. All results shown in the previous section are consistent with this argument.

We close with a critical discussion concerning the discontinuities in the optimal protocol. The jumps have been derived using a master equation, which is valid only on a coarse grained time scale. Furthermore, we know from the time-energy uncertainty principle that an instantaneous jump in energy level would redistribute electrons over all energy levels, *i.e.*, the single-level model cannot hold in this strict jump limit. Therefore, the discontinuities in the optimal protocols identified here should be interpreted as rapid but continuous changes of the energy level. The corresponding typical time δt must be much shorter than the tunneling time ($\delta t \ll C^{-1}$). On the other hand, the single-level model will remain valid

only when $\delta t \gg 1/\Delta \omega$, where $\Delta \omega$ is the gap between the energy levels inside the dot. Even if the chemical potential is changed, we have assumed that the reservoir remains in thermal equilibrium. Hence, δt must also be longer than the relaxation time of the reservoir. These conditions can be satisfied if the tunneling rate C is small, which is also a requirement for the validity of the master equation itself.

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