Minimal dissipation in processes far from equilibrium

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A central goal of thermodynamics is to identify optimal processes during which the least amount of energy is dissipated into the environment. Generally, even for simple systems, such as the parametric harmonic oscillator, optimal control strategies are mathematically involved, and contain peculiar and counter-intuitive features. We show that optimal driving protocols determined by means of linear response theory exhibit the same step and δ-peak like structures that were previously found from solving the full optimal control problem. However, our method is significantly less involved, since only a minimum of a quadratic form has to be determined. In addition, our findings suggest that optimal protocols from linear response theory are applicable far outside their actual range of validity.

For infinitely slow processes the maximally usable work is given by the change of availability or exergy [1, 2]. All real processes operate in finite-time, and thus they are accompanied by dissipation into the envrionment. For instance, for isothermal processes the amount of energy that is irretrievably lost is quantified by the irreversible work, $W_{\text{irr}} = W - \Delta F$ [3]. One of the central goals of modern thermodynamics is to develop methods to minimize W_{irr}, i.e., to identify *optimal processes* during which the least amount of energy is wasted.

One of the first approaches was developed in finite-time thermodynamics [4–6]. Here, the irreversible entropy production is calculated from a heuristic expansion of the thermodynamic entropy around its value in equilibrium. The leading order of the expansion can then be used as the definition of the thermodynamic length [5]. This length measures how far from equilibrium a system operates [7–9] and it allows, e.g., to measure the arrow of time [10]. It also has been shown that the thermodynamic length induces a Riemannian geometry. Therefore optimal processes can be found as geodesics on the thermodynamic manifold [11–18], and the irreversible entropy production can be written as a quadratic form of the susceptibility matrix [12, 19, 20].

The downside of this approach is its limited range of validity since it is inherently a linear response theory [21–24]. More detailed insight and general results can be obtained by means of stochastic thermodynamics [25–27]. In particular, the theorems of Jarzynski [28] and Crooks [29] motivated to analyze stochastic properties of thermodynamic work, rather than to focus on its average value. In stochastic thermodynamics a system is described microscopically, e.g. by a Langevin equation. Thermodynamic quantities like work, heat, or entropy are then associated with single realizations, or single trajectories of the process under study. From this approach optimal driving protocols can then be studied explicitely, which showed some rather unexpected features, such as jump and delta-peak-like protocols [30–34]. These "ragged" driving protocols appear to be in stark contrast to the very smooth functions commonly used in free energy estimation [35].

A disadvantage of the microscopic approach is that only relatively few problems can be solved analytically. Thus, for general situations advanced and computationally expensive tools from Optimal Control Theory need to be employed [36]. The natural question arises, whether and how well results from a phenomenological approach based on linear response theory carry over to systems that are driven far from thermal equilibrium.

The purpose of the present analysis is twofold: In a previous work [22] we found that for slowly driven processes the resulting irreversible work for optimal protocols from exact microscopic dynamics and linear response become identical. In the following, we will demonstrate convergence of the driving protocols by numerically solving the optimal control problem. However, we will also find that the jump and delta-peak-like features [30–32] are not present in the regime of slow driving. Therefore, we developed a novel approach to find optimal driving protocols of the linear-response quadratic form in the regime of weak but fast driving. As a main result we will show the appearance of jumps and delta-peak-like features. Our findings suggest that optimal protocols from linear response theory might perform remarkably well far outside their actual range of validity.

Preliminaries. We consider a system with Hamiltonian $H(\lambda)$ weakly coupled to a heat bath. Initially, system and heat bath are in thermal equilibrium for a fixed value $\lambda = \lambda_0$. An external observer then varies λ in finite time τ using a certain protocol $g(t)$ such that $\lambda(t) = \lambda_0 + \delta\lambda\, g(t)$, with $g(0) = 0$ and $g(\tau) = 1$. This allows us to characterize the processes under consideration by their strength $\delta\lambda/\lambda_0$ and their speed τ_R/τ, where τ_R is a typical relaxation time. The corresponding "phase" diagram is depicted in Fig. 1.

As a 0th class we categorize processes that are induced by weak, $\delta\lambda/\lambda_0 \ll 1$, and slow, $\tau_R/\tau \ll 1$, perturbation; class 1 refers to weak, but not necessarily slow driving, whereas class 2 consists of slowly varying processes [22]. Finally, a 3rd class refers to any other driving, which is neither slow nor weak.

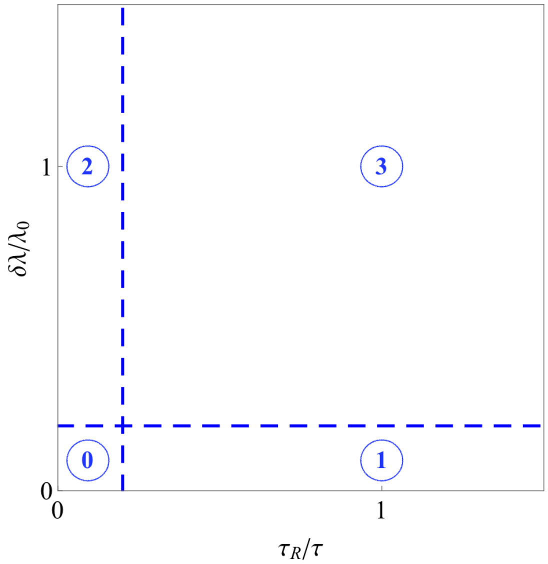

FIG. 1. (color online) **Illustration of the four classes of processes:** class 0, slow and weak perturbation; class 1, conventional linear response theory; class 2, slowly varying processes; class 3, arbitrary driving far from thermal equilibrium.

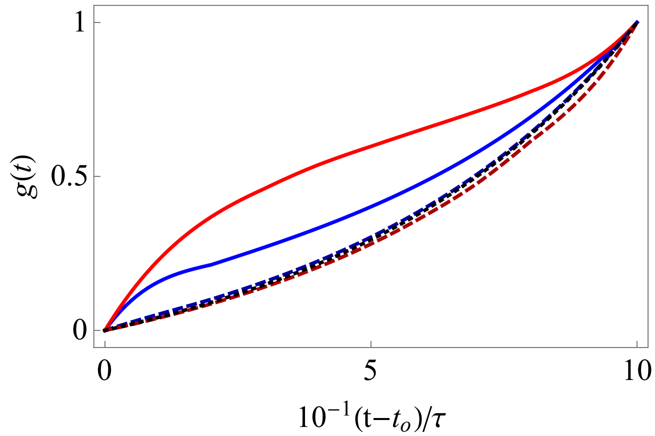

FIG. 2. (color online) **Optimal driving in class 3:** Optimal driving protocols for the time dependent harmonic oscillator (2) with $\lambda_0 = 1$ and $\delta\lambda = 3$. Blue lines correspond to overdamped dynamics (5) with $\tau = 1$ (blue, lower solid line) and $\tau = 10$ (blue, dashed line), and red lines are found for underdamped dynamics (6) with $\gamma = 1$, $\tau = 1$ (red, upper solid line) and $\tau = 10$ (red, dashed line). The analytical protocol (7) for slowly varying processes (black, dotted line) coincides to very good approximation with slow ($\tau = 10$) processes for any damping.

Class 3: A case for optimal control theory. Since our main interest is to asses how well optimal protocols from approximate theories perform far from thermal equilibrium, we begin the analysis with class 3. For such driving, optimal protocols can be determined by means of Optimal Control Theory [36, 37].

Consider a physical system whose state is fully described by a vector $\boldsymbol{x}_t$. The components of $\boldsymbol{x}_t$ could be the real, physical microstate, a point in phase space, the state of a qubit [38], or a collection of macroscopic variables as, for instance, voltage, current, volume, pressure, etc. The evolution of $\boldsymbol{x}_t$ for times $0 \leq t \leq \tau$ is described by a first order differential equation, the so-called *state equation*,

$$\dot{\boldsymbol{x}}_t = \boldsymbol{f}\left(\boldsymbol{x}_t, \boldsymbol{\lambda}_t\right) \quad \text{and} \quad \boldsymbol{x}_{t=0} = \boldsymbol{x}_0\,, \tag{1}$$

where the vector $\boldsymbol{\lambda}_t$ is a collection of external control parameters, or simply the control.

The task is, then, to find the particular $\boldsymbol{\lambda}_t^*$ such that a *performance measure*, or *cost functional* is minimized. In other words, to find the *optimal control* $\boldsymbol{\lambda}_t^*$ we have to minimize the cost functional $\mathcal{J}\left[\boldsymbol{x}_t, \boldsymbol{\lambda}_t\right]$ under the condition that $\boldsymbol{x}_t$ evolves under the state equation (1). In the present context, $\mathcal{J}\left[\boldsymbol{x}_t, \boldsymbol{\lambda}_t\right]$ can be naturally identified with the irreversible work W_{irr}.

Note that generally not all controls $\boldsymbol{\lambda}_t$ are *physically allowed* or *admissible*. In particular, we will see in the following example that, if we restrict ourselves to continuous protocols with fixed initial and finals values, no jump or delta peculiarities are found.

To illustrate the application of optimal control theory and as a fully solvable case study we consider the time-dependent harmonic oscillator with Hamiltonian

$$H(t) = \frac{p^2}{2} + \lambda_t \frac{q^2}{2} \tag{2}$$

where we set the mass $m = 1$. For this system exact optimal driving protocols have been derived analytically for overdamped dynamics [30], numerically in the underdamped regime [31], and analytically for slowly varying processes by means of linear response theory [22]. In either case the irreversible work can be written as

$$W_{\mathrm{irr}} = \frac{1}{2}\int_0^\tau \mathrm{d}t\, \dot{\lambda}_t\, \overline{q^2} + \frac{1}{2}\ln\left(\frac{\lambda_0}{\lambda_0 + \delta\lambda}\right), \tag{3}$$

where we set $\beta = 1$. Thus, we choose as a *performance measure*

$$\mathcal{J}[q, \lambda_t] = \int_0^\tau \mathrm{d}t\, \dot{\lambda}_t\, \overline{q^2}\,. \tag{4}$$

In the case of overdamped dynamics the *state equation* reads [30]

$$\partial_t\, \overline{q^2} = -2\lambda_t\, \overline{q^2} + 2\,, \tag{5}$$

whereas we have in the underdamped regime [31]

$$\begin{aligned} \partial_t\, \overline{q^2} &= 2\,\overline{qp} \\ \partial_t\, \overline{p^2} &= -2\lambda_t\, \overline{qp} - 2\gamma\, \overline{p^2} + 2\gamma \\ \partial_t\, \overline{qp} &= \overline{p^2} - \lambda_t\, \overline{q^2} - \gamma\, \overline{qp}\,. \end{aligned} \tag{6}$$

The latter performance measure (4) together with the state equation, Eq. (5) or Eq. (6) respectively, allow us to formulated Pontryagin's extremum principle [36]. Optimal protocols are then numerically found by a modified algorithm of steepest decent [38], where we restrict ourselves to continuous protocols with $g(0) = 0$ and $g(\tau) = 1$.

In Fig. 2 we plot the results from optimal control theory together with the analytically obtained optimal protocol for slowly varying processes [22],

$$g^*(t) = -\frac{\lambda_0}{\delta\lambda} + \frac{1}{A((t/\tau) + B)^4} \tag{7}$$

where A and B are free constants to be determined by the boundary conditions $g^*(0) = 0$ and $g^*(\tau) = 1$. We observe that for *slow* processes, i.e., long switching times τ the protocols obtained from the full dynamics are in very good agreement with the result from linear response theory (7). For faster driving, i.e., short switching times τ, the optimal protocols significantly differ [39].

As a first main result, we find that numerically exact solutions from optimal control theory converge to the optimal protocols from linear response theory by taking the appropriate limits. Note, however, that a judicious choice of boundary conditions, $g^*(0) = 0$ and $g^*(\tau) = 1$, and restricting the admissible protocols to continuous functions suppressed jump and delta-peak features. The remainder of this analysis is dedicated to finding exactly these features from linear response theory, which illustrates that phenomenological tools can be powerful also far outside their range of validity.

Optimal driving from class 1. To describe the work performed along processes lying in class 1 (see Fig. 1), we demand that $|\delta\lambda\, g(t)/\lambda_0| \ll 1$ for $0 \le t \le \tau$. This allows for a linear response treatment of the average work W_{irr} whose expression reads [23]

$$\begin{aligned} W_{\mathrm{irr}} &\equiv W - \Delta F \\ &= \frac{(\delta\lambda)^2}{2} \int_0^1 ds \int_0^1 ds'\, \Psi_0[\tau(s-s')]\, \dot{g}(s)\, \dot{g}(s')\,, \end{aligned} \tag{8}$$

where $\dot{g}(s)$ and $\dot{g}(s')$ denote the derivatives with respect to $s \equiv t/\tau$ and $s' \equiv t'/\tau$, and $\Psi_0(t) = \beta\left(\langle \partial_\lambda H(0)\partial_\lambda H(t)\rangle - \langle \partial_\lambda H(0)\rangle^2\right)$ is the *relaxation* function [22, 40] with $\beta = (k_B T)^{-1}$ and $\langle\cdot\rangle$ denoting an average with the canonical distribution.

As explained in Ref. [22], the relaxation function is the phenomenological input of the Hamiltonian-based linear response theory since its fully microscopic derivation requires the solution of classical or quantum equations of motion of the system plus heat bath. Hence it is at the same time the weak and strong point of our linear response approach since, on the one hand, it excludes the possibility of an exact treatment of a specific system and, on the other hand, it allows for system-independent conclusions from the qualitative behavior of $\Psi_0(t)$.

The phenomenological modeling of the relaxation function provides the possibility of finding optimal protocols of (8) not only for one or two examples but for *classes* of systems. At the same time, we still want to keep track of the influence of a specific system in our results. As shown in Ref. [22], this can be done through a self-consistent modeling that matches a given *ansatz* of $\Psi_0(t)$ with its Hamiltonian requirements.

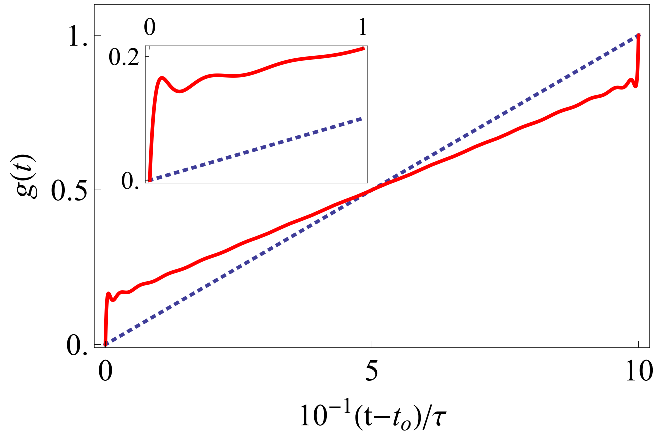

FIG. 3. (color online) **Optimal protocol for overdamped dynamics:** Optimal protocol (red solid line) that minimizes Eq. (8) using a truncated expansion of $g(s)$ with 35 modes and the relaxation function $\Psi_0(0)\, e^{-\alpha|t|}$. The switching time was chosen to be five times bigger than the relaxation time $\tau_R = \int_0^\infty dt\, \Psi_0(t)/\Psi_0(0)$. Blue dotted line corresponds to the linear protocols $g(s) = s$. **Inset:** short time behavior of the optimal protocol showing a smooth version of a "step".

Figures 3 and 4 show optimal protocols obtained from Eq. (8) using two models for the relaxation function, namely, the *over*damped $\Psi_0(t) = \Psi_0(0)\, e^{-\alpha|t|}$, and the *under*damped $\Psi_0(t) = \Psi_0(0)\, e^{-\alpha|t|}\left[\cos(\omega t + (\alpha/\omega)\sin(\omega|t|)\right]$. The nomenclature we use clearly refers to the corresponding regimes of Brownian motion under an external harmonic potential. Nevertheless, they are very good models for several different relaxation phenomena such as dieletric polarization.

To obtain the optimal protocols we note that Eq. (8) is a quadratic form in the $\dot{g}(s)$. Therefore, we expand the functions $g(s)$ in a series of Chebyshev polynomials in the interval $[0, 1]$ (for more details see Suppl. Mater. [41]). The series is then truncated and therefore regularized (to deal with the common problems of finite order expansions) using well-known methods [42]. Inserting the finite order expansions in Eq. (8), the double integrals can be solved analytically and the parity of the Chebyshev polynomials and of $\Psi_0(t)$ (the relaxation function satisfies $\Psi_0(-t) = \Psi_0(t)$; see Refs. [22, 23]) help to verify that many of them are zero. Consequently, expression (8) becomes a finite quadratic form whose extremum is obtained from the numerical solution of a linear system of equations. The unknown variables of this system are the coefficients of the finite order expansion of the $g(s)$ subjected to the boundary conditions $g(0) = 0$ and $g(1) = 1$. The results clearly show smooth versions of the same features (steps

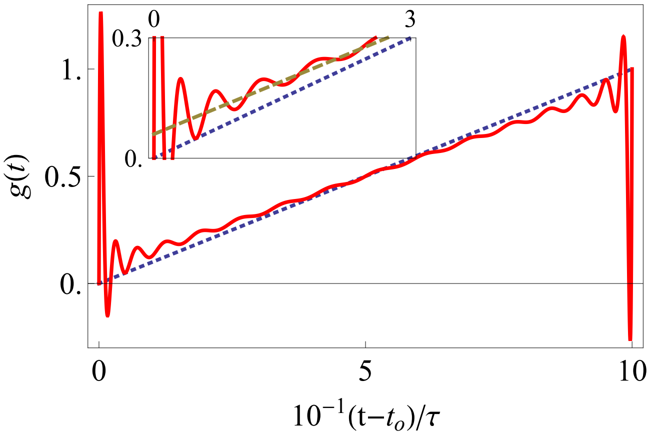

FIG. 4. (color online) **Optimal protocol for underdamped dynamics:** Optimal protocol (red solid line) that minimizes Eq. (8) using a truncated expansion of $g(s)$ with 35 modes and the relaxation function $\Psi_0(0)\, e^{-\alpha|t|}\, [\cos(\omega t + (\alpha/\omega)\sin(\omega|t|)]$. The switching time was chosen to be five times bigger than the relaxation time $\tau_R = \int_0^\infty dt\, \Psi_0(t)/\Psi_0(0)$. Blue dotted line corresponds to the linear protocol $g(s) = s$. **Inset:** short time behavior showing that after the peak, the optimal protocol also presents a smooth step since it oscillates around a linear protocol (green dashed line) whose inclination is lower than one.

and peaks) obtained in Refs. [30, 31] for a driven Brownian particle trapped in a harmonic potential in overdamped and underdamped regimes. As mentioned above, exact optimal protocols are determined by solving Eqs. (5) and (6), respectively.

It is remarkable that our linear response optimization leads to the same counterintuitive features which were originally attributed to far from equilibrium driving. As the process gets faster (i.e., τ approaches τ_R), such features become even sharper (see Fig. S1 in Suppl. Mater. [41]). In addition, for a fixed switching time τ, the steps and peaks also get sharper as we increase the number of polynomials in the finite order expansion of $g(t)$ (see Fig. S2 in Suppl. Mater. [41]). This suggests that the optimal linear response process can get arbitrarily close to the singular features of the exact result of Ref. [31].

A natural question to ask then is how well do the linear response optimal paths perform in the nonequilibrium region. To test this, we have solved numerically Eqs. (6) since we need $\overline{q^2}(t)$ to obtain $W_{\rm irr}$ (see Eq. (3)). We were not able to go beyond an expansion of $g(s)$ with 17 modes due to a numerical instability caused by high-frequency oscillations. Hence our preliminary results about performance show that, for fixed $\tau = 5\tau_R$ and for $\delta\lambda/\lambda_0$ ranging from 1 to 2.7, the linear response optimal paths are roughly 1% to 5% better than a linear protocol (although it sometimes performs worse since $W_{\rm irr}$ seems to have a non-monotonic dependence with $\delta\lambda/\lambda_0$ for the linear protocol). However, our optimal protocols are always 6% to 14% better than the $C_2(t)$ protocol proposed by Watanabe and Reinhardt (see Eq. (5) in Ref. [35]).

Concluding remarks. In the present analysis we found that although a lot of work has been done to find optimal linear response processes in class 2, namely, slowly-varying optimal processes, those lying in class 1 are much closer to what happens in the fully nonequilibrium regime. Hence they should be a better choice as seeds of optimal control procedures far from equilibrium. Our results also show that, despite of sharing the same underlying theory, the linear response approaches for the irreversible work in classes 1 and 2 are qualitatively different and only match when $\delta\lambda/\lambda_0$ and τ_R/τ are both much smaller than 1.

The relaxation functions we have analyzed here can describe the relaxation of several physical phenomena. Thus, our results also state that the peculiar features found in Refs. [30, 31] are indeed very general and are not restricted just to driven Brownian motion. Our approach also allows the analysis of optimal protocols for different kinds of relaxation dynamics (see Fig. S3 in Suppl. Mater. for results considering a relaxation function decaying algebraically). A preliminary analysis in this direction suggests that what happens at the boundaries of the optimal protocols depends strongly on the short time behavior of the relaxation function (which is linear for overdamped dynamics and quadratic for the underdamped one). It is possible to show that the sum rules of linear response theory [43] (which can be used to turn the phenomenological relaxation functions compatible with the underlying Hamitonian dynamics [22]) demand a quadratic behavior for short times.

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Supplemental Material: Minimal dissipation in processes far from equilibrium

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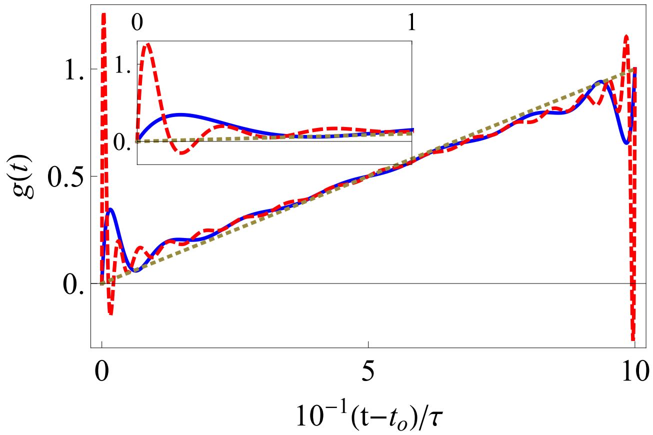

FIG. 1. (Color Online) Optimal protocols that minimize Eq. (1) using a truncated expansion of $g(s)$ with 17 modes (blue solid line) and 35 modes (red dashed line) and the relaxation function $\Psi(0)\, e^{-\alpha|t|}\,[\cos(\omega t) + (\alpha/\omega)\sin(\omega|t|)]$. The switching time was chosen to be five times bigger than the relaxation time $\tau_R = \int_0^\infty dt\, \Psi_0(t)/\Psi_0(0)$. The green dotted line corresponds to the linear protocol $g(s) = s$.

In the regime of weak but fast driving, the linear response expression for the irreversible work is given by the following functional [1]

$$W_{\rm irr} \equiv W - \Delta F = \frac{(\delta\lambda)^2}{2}\int_0^1 ds \int_0^1 ds'\, \Psi_0(\tau(s-s'))\dot{g}(s)\dot{g}(s')\,, \tag{1}$$

where $\Psi_0(t) = \beta\left(\langle \partial_\lambda H(0)\partial_\lambda H(t)\rangle - \langle \partial_\lambda H(0)\rangle^2\right)$ is the relaxation function [2, 3], $\langle\cdot\rangle$ denotes an equilibrium average taken with a canonical distribution parametrized with $\beta = (k_B T)^{-1}$, T being the temperature of the heat bath, and H is the Hamiltonian of the system. The functions $\dot{g}(s)$ and $\dot{g}(s')$ denote the derivatives of the protocol $g(s)$ with respect to $s \equiv t/\tau$ and $s' \equiv t'/\tau$.

In order to find the optimal protocols that minimize Eq. (1) for a τ, we expand $\dot{g}(s)$ in terms of Chebyshev polynomials in the interval $[0,1]$ following Ref. [4]

$$\dot{g}(s) = \sum_{n=1}^{N} a_n\, g(N,n)\, T_n(2s-1)\,, \tag{2}$$

where

$$g(x,y) = \frac{1}{x+1}\left[(x-y+1)\cos\left(\frac{\pi y}{x+1}\right) + \sin\left(\frac{\pi y}{x+1}\right)\cot\left(\frac{\pi}{x+1}\right)\right] \tag{3}$$

is a factor that regularizes the truncated series with finite N terms (see Sec.II.C of Ref. [4]). The Chebyshev polynomials have the nice property of being odd or even with respect to the transformation $s \to 1-s$. Inserting expansion (2) into (1), we obtain a multidimensional finite quadratic form in terms of the coefficients a_n

$$W_{\rm irr}\left((\delta\lambda)^2\Psi_0(0)/2\right)^{-1} = \sum_{n,l} A_{nl}\, a_n a_l\,, \tag{4}$$

whose minimum we would like to find for the following boundary conditions $g(0) = 0$ and $g(1) = 1$. The matrix elements A_{nl} are given by

$$A_{nl} = \int_0^1 ds \int_0^1 ds' \tilde{\Psi}(\tau(s-s'))\, g(N,n)g(N,l)\, T_n(2s-1)T_l(2s'-1)\,, \tag{5}$$

where we have defined $\tilde{\Psi}(t) = \Psi_0(t)/\Psi_0(0)$. It can be easily shown that the parity of the T_n combined with $\tilde{\Psi}(-t) = \tilde{\Psi}(t)$ leads to $A_{nl} = 0$ every time n is even and l is odd. Besides, $A_{nl} = A_{ln}$ and hence many of the A_{nl} are zero.

Depending on the function $\tilde{\Psi}(t)$, the integrals above can be performed analytically. Once the A_{nl} are known, the minimization problem comes down to solving a linear system of equations coming from the extremum condition (first derivative of (4) equals to zero) plus the two additional constraints $g(0) = 0$ and $g(1) = 1$. For all the examples we

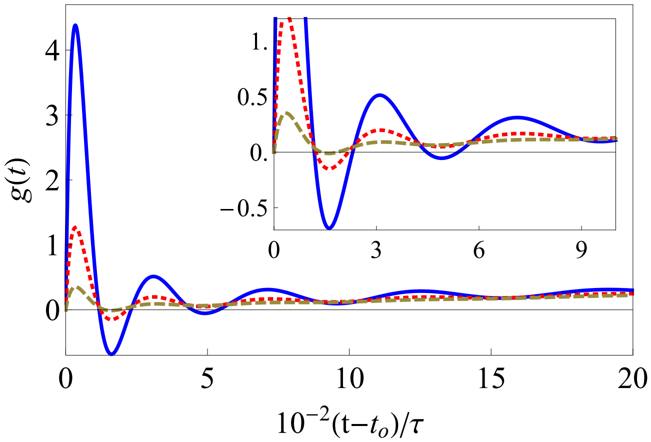

FIG. 2. (Color Online) Optimal protocols that minimize Eq. (1) using a truncated expansion of $g(s)$ with 35 modes and the relaxation function $\Psi_0(0)\, e^{-\alpha|t|}\, [\cos(\omega t) + (\alpha/\omega)\sin(\omega|t|)]$. The ratio $(\tau_R/\tau)^{-1}$ was chosen to be 2.5 (blue solid line), 5 (red dotted line) and 10 (green dashed line).

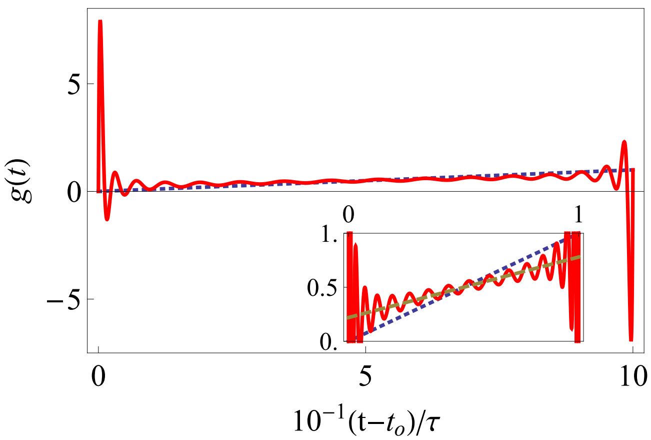

FIG. 3. (Color Online) Optimal protocol (red solid line) that minimizes Eq. (1) for the relaxation function $\Psi_0(0)e^{-\alpha|t|}(1+\alpha|t|/2)^2$ using a truncated expansion of $g(s)$ with 35 modes and $(\tau_R/\tau)^{-1} = 5$. The blue dotted line corresponds to $g(s) = s$. Inset: the optimal protocol oscillates around a linear function $f(s) = a\, s + b$ with $a < 1$.

present here, this linear systems was solved numerically. Figure 1 shows an example of how the optimal protocol we have obtained depends on the number of modes N for a given value of τ and considering underdamped dynamics. As we increase the number of polynomials in our expansion (2), the especial features at the boundaries of the protocol become sharper. Additionally, for a fixed N, Fig. 2 shows that these features also become sharper and sharper as the ratio τ_R/τ increases, i.e., as the protocol gets faster.

Our approach provides means of testing different kinds of relaxation behavior and therefore investigate whether the unexpected features we observe in the optimal protocols are universal. Figure 3 shows that even the monotonic exponential decay given by $e^{-\alpha|t|}(1+\alpha|t|/2)^2$ leads to very pronounced peaks and “steps” since, apart from the boundaries, the protocol oscillates around a linear function $f(s) = a\, s + b$ with $a < 1$. Figure 4 shows an example of optimal protocol for a non-exponential decay of the relaxation function. Very pronounced peaks are also present in this case and persist for much slower processes.

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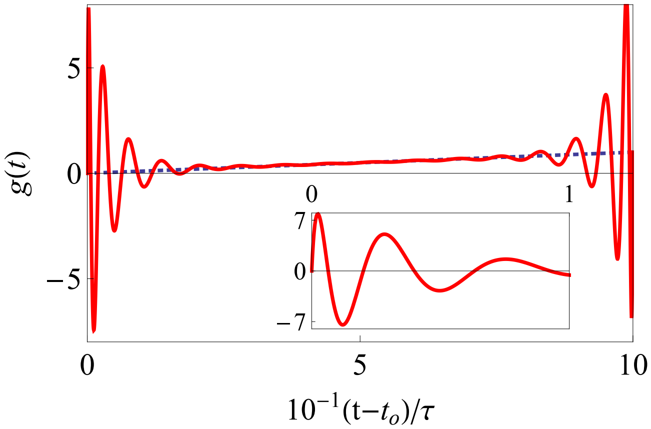

FIG. 4. (Color Online) Optimal protocol (red solid line) that minimizes Eq. (1) using a truncated expansion of $g(s)$ with 35 modes, $(\tau_R/\tau)^{-1} = 80$ and the relaxation function $\Psi_0(0)\, J_0(\alpha s)$, where $J_0(x)$ is the Bessel function of first kind. The blue dotted line corresponds to the linear protocol $g(s) = s$.

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