Shortcuts to adiabaticity from linear response theory

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Shortcuts to adiabaticity from linear response theory

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A shortcut to adiabaticity is a finite-time process that produces the same final state as would result from infinitely slow driving. We show that such shortcuts can be found for weak perturbations from linear response theory. With the help of phenomenological response functions a simple expression for the excess work is found – quantifying the nonequilibrium excitations. For two specific examples, the quantum parametric oscillator and the spin-1/2 in a time-dependent magnetic field, we show that finite-time zeros of the excess work indicate the existence of shortcuts. Finally, we propose a degenerate family of protocols, which facilitate shortcuts to adiabaticity for specific and very short driving times.

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I. INTRODUCTION

Thermodynamics is a phenomenological theory to describe the transformation of heat into work. However, only quasistatic, i.e., infinitely slow processes are fully describable by means of conventional thermodynamics [1]. For all realistic, finite-time – *nonequilibrium* – processes the second law of thermodynamics constitutes merely an *inequality*, expressing that some portion of the energy or entropy is irreversibly lost into nonequilibrium excitations. For isothermal processes, this "loss" is quantified by the excess work $\langle W_{\mathrm{ex}} \rangle$, which is the difference between the total nonequilibrium work $\langle W \rangle$ and the work performed during a quasistatic – *equilibrium* – process $\langle W_{\mathrm{qs}} \rangle$, $\langle W_{\mathrm{ex}} \rangle = \langle W \rangle - \langle W_{\mathrm{qs}} \rangle$. For macroscopic, open systems $\langle W_{\mathrm{qs}} \rangle$ is simply given by the free energy difference ΔF. However, the identification of the equilibrium work, $\langle W_{\mathrm{qs}} \rangle$, with the free energy difference, ΔF, is only true for open systems. For isolated systems the minimal work is not given by the free energy difference and $\langle W_{\mathrm{qs}} \rangle$ has to be analyzed carefully [2]. In addition, for quantum systems the situation is particularly involved as quantum work is not an observable in the usual sense, as there is no hermitian operator, whose eigenvalues are given by the classical work values [3–7].

Nevertheless, finding "optimal" quantum processes, for which only the minimal amount of $\langle W_{\mathrm{ex}} \rangle$ is lost into nonequilibrium excitations is of fundamental importance. Consequently, a lot of theoretical and experimental research has been dedicated to the design of so-called shortcuts to adiabaticity, i.e., finite-time processes with suppressed nonequilibrium excitations [8]. To this end a variety of techniques has been proposed: the use of dynamical invariants [9], the inversion of scaling laws [10], the fast-forward technique [11, 12], and transitionless quantum driving [13–16]. All methods have in common that practical implementations are rather involved as the full dynamics has to be solved to determine the shortcut. Therefore, more recent research efforts have been focusing on identifying optimal protocols from optimal control theory [17, 18], from properties of the quantum work statistics [19], or "environment" assisted methods [20].

The present analysis is dedicated to finding shortcuts to adiabaticity from a phenomenological approach – linear response theory. For classical systems it has been recently shown that there exist finite-time processes with zero excess work [21]. In this paradigm $\langle W_{\mathrm{ex}} \rangle$ is fully determined by the phenomenological response of the system to an external perturbation [22, 23]. Thus, we neither have to solve the dynamics [13–16] nor do we have to determine the quantum work statistics [19] to minimize $\langle W_{\mathrm{ex}} \rangle$. In the following, we will extend our previous findings [21, 23] to the quantum domain. To this end, we will consider a thermally isolated quantum system under weak perturbation and derive a linear response expression for $\langle W_{\mathrm{ex}} \rangle$. After establishing the general theory we will turn to analytically solvable and pedagogically elucidating examples, namely the parametric harmonic oscillator and the spin-1/2 in a time-dependent magnetic field. This will allow us to study the range of validity of the linear response approach by comparing our novel findings with the exact results from the full quantum work statistics [24, 25]. We will show that the protocols with zero excess work from linear response theory, indeed, facilitate transitionless quantum driving for weak perturbations. Finally, we will propose a family of degenerate protocols, which facilitates shortcuts to adiabaticity for arbitrarily fast driving.

II. QUANTUM WORK FROM LINEAR RESPONSE THEORY

We begin by generalizing the previous classical treatment of the excess work, $\langle W_{\mathrm{ex}} \rangle$, [21] to the quantum domain. Imagine a quantum system with time-dependent

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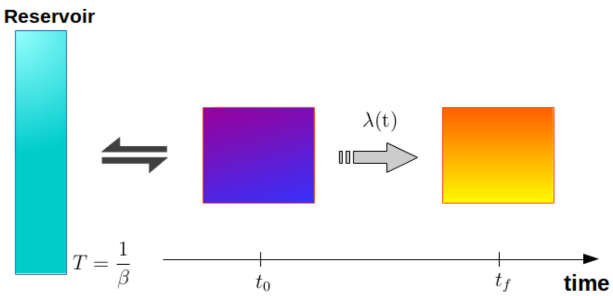

FIG. 1. (color online) Sketch of the thermodynamic processes under study. At $t = t_0$ the system is prepared in equilibrium with inverse temperature β, before the system is decoupled from the environment and controlled externally from $t = t_0 + 0^+$ until a final time t_f.

Hamiltonian H_t, which is prepared initially in a thermal equilibrium state, $\rho_0 = \exp(-\beta H_0)/Z_0$, where Z_0 is the partition function, $Z_0 = \mathrm{tr}\left\{\exp\left(-\beta H_0\right)\right\}$. At $t = t_0 + 0^+$ the system is decoupled from the environment, and the Hamiltonian is varied according to some protocol λ_t with $H_t \equiv H(\lambda_t)$. Such a processes is sketched in Fig. 1.

The external control parameter λ_t is written as

$$\lambda_t \equiv \lambda_0 + \delta\lambda \; g(t), \tag{1}$$

where λ_t starts in an initial value λ_0, $\delta\lambda$ is the amplitude and $g(t)$ obeys: $g(t_0) = 0$ and $g(t_f) = 1$. Thus, λ_t varies from λ_0 to $\lambda_f = \lambda_0 + \delta\lambda$.

For small systems work is a fluctuating quantity [26] and for a specific protocol $g(t)$ the average work reads

$$\langle W \rangle = \int_{t_0}^{t_f} \mathrm{d}t \, \dot{\lambda}_t \, \langle \partial_\lambda H \rangle \,, \tag{2}$$

where the angular brackets denote an average over many realizations of the same process and the dot denotes a derivative with respect to time.

We will now evaluate the general expression for the average work (2) by means of linear response theory. To this end, we expand the Hamiltonian up to linear order in the amplitude $\delta\lambda$,

$$H(\lambda_t) = H(\lambda_0) + \delta\lambda \, g(t) \, \partial_\lambda H + \mathcal{O}(\delta\lambda^2) \,. \tag{3}$$

Substituting Eq. (3) into Eq. (2) and identifying $\partial_\lambda H$ as the generalized force [21, 23, 27, 28] it can be shown [21] that the average work (2) becomes,

$$\begin{aligned} \langle W \rangle = \delta\lambda \, \langle \partial_\lambda H \rangle_{\rho_0} - \frac{(\delta\lambda)^2}{2} \Psi(0) \\ - (\delta\lambda)^2 \int_{t_0}^{t_f} \mathrm{d}t \, \partial_t g \int_0^{t-t_0} \mathrm{d}s \, \Psi(s) \, \partial_s g(t-s) \end{aligned} \tag{4}$$

where $\Psi(t)$ is the relaxation function [27, 28].

Until Eq. (4) the present treatment is identical to the classical case [21]. However, in the quantum case the relaxation function $\Psi(t)$ is determined by the quantum response function $\phi(t)$, $\phi(t) = -\dot{\Psi}(t)$, with [27, 28]

$$\phi(t) = \frac{1}{i\hbar} \, \mathrm{tr}\left\{\rho_0 \left[A_0, \, A_t\right]\right\} , \tag{5}$$

where $A = \partial_\lambda H$ is the generalized force. To avoid clutter in the formulas we introduced in Eq. (5) the notation $A(t) \equiv A_t$.

In complete analogy to the classical case [21], the first two terms of Eq (4) are independent of the specific protocol $g(t)$ and we identify the quasistatic, equilibrium work as

$$\langle W_{\mathrm{qs}} \rangle = \delta\lambda \, \langle \partial_\lambda H \rangle_{\rho_0} - \frac{(\delta\lambda)^2}{2} \Psi(0) \,. \tag{6}$$

In the remainder of this analysis we will analyze the excess work,

$$\langle W_{\mathrm{ex}} \rangle = -(\delta\lambda)^2 \int_{t_0}^{t_f} \mathrm{d}t \, \partial_t g \int_0^{t-t_0} \mathrm{d}s \, \Psi(s) \, \partial_s g(t-s) \tag{7}$$

for two analytically solvable examples. We will show that whenever this thermodynamic quantity vanishes in finite time, the quantum adiabatic invariant is conserved and therefore the system can be driven through a shortcut to adiabaticity.

Generally, it is easy to see that if the adiabatic theorem is fulfilled, no transitions between eigenstates occur, and therefore the excess work. $\langle W_{\mathrm{ex}} \rangle$, has to vanish. However, the reverse is not necessarily true. Even if the excess work vanishes, one could imagine a process during which some transitions between eigenstates do occur, however in such a way that their energetic contribution "cancels out". In the following, we will analyze this issue with the help of two fully analytically solvable examples – the parametric harmonic oscillator and a spin-1/2 particle in a magnetic field. We will find that at least within the range of validity of linear response theory such "canceling" transition do not occur as for a "shortcut" not only the excess work vanishes, but also the adiabatic invariant is (approximately) conserved. For classical systems a similar analysis was developed in Ref. [21].

III. PARAMETRIC HARMONIC OSCILLATOR

We consider the time-dependent Hamiltonian

$$H(\lambda_t) = \frac{p^2}{2} + \frac{1}{2} \, \lambda_t \, x^2 \tag{8}$$

where x and p are the coordinate and momentum operators, respectively. This system can be solved analytically [24, 25] for specific protocols λ_t that drive the system from an initial to final value of λ, as illustrated in Fig. 2. To simplify notation we further set $t_0 = 0$ and $t_f = \tau$.

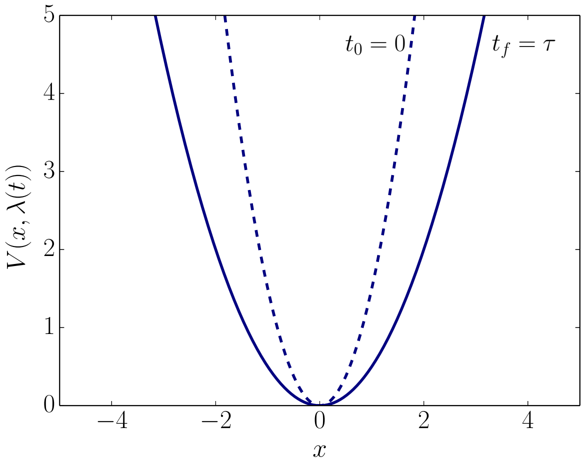

FIG. 2. (color online) Parametric harmonic oscillator (8) with λ_0 (dashed line) at time $t = t_0$ and λ_f (solid line) at $t = \tau$.

A. Linear response approach

The response function (5) is obtained by solving Heisenberg's equations of motion for fixed, initial value of λ. Hence, we obtain after a few simple lines

$$\phi(t) = \frac{\hbar}{\lambda_0} \coth\left(\frac{\beta\hbar\sqrt{\lambda_0}}{2}\right) \sin(2\sqrt{\lambda_0}\,t)\,. \tag{9}$$

It is interesting to note that the system's response is oscillatory. Consequently, we have the "relaxation" function

$$\Psi(t) = \frac{\hbar}{2\lambda_0\sqrt{\lambda_0}} \coth\left(\frac{\beta\hbar\sqrt{\lambda_0}}{2}\right) \cos(2\sqrt{\lambda_0}\,t)\,. \tag{10}$$

Generally, relaxation functions describe how a system relaxes towards an equilibrium state. However, since the present system has only a single degree of freedom and it is thermally isolated, the "relaxation" function exhibits non-decreasing oscillations.

For the sake of simplicity we further assume that the stiffness varies linearly with time,

$$\lambda_t = \lambda_0 + \delta\lambda\, t/\tau\,, \tag{11}$$

for which we obtain

$$\langle W_{\mathrm{ex}}\rangle = \left(\frac{\delta\lambda}{\sqrt{\lambda_0}}\right)^2 \frac{\hbar\sqrt{\lambda_0}}{4} \coth\left(\frac{\beta\hbar\sqrt{\lambda_0}}{2}\right) \frac{\sin^2(\sqrt{\lambda_0}\,\tau)}{\lambda_0\,\tau^2}\,. \tag{12}$$

Equation (12) constitutes our first main result. In complete analogy to the classical case [21] the excess work vanishes for all zeros of the sine function, i.e., for all $\tau = n\pi/\sqrt{\lambda_0}$ with n being an integer. In the classical case these "special" driving times have been attributed to a conservation of the adiabatic invariant during the finite-time process [21].

In the next subsection we will further analyze this observation, and show that the minima of $\langle W_{\mathrm{ex}}\rangle$ (12), indeed, identify shortcuts to adiabaticity.

B. Exact solution

The parametric harmonic oscillator (8) has been extensively studied, since it can be solved analytically [24, 25, 29, 30] for specific driving protocols and it describes quantum thermodynamic experiments in cold ion traps [31–33]. The time-dependent mean energy can be written as [25, 34],

$$\langle H_\tau\rangle = \frac{\hbar\sqrt{\lambda_f}}{2}\, Q^* \coth\left(\frac{\beta\hbar\sqrt{\lambda_0}}{2}\right)\,, \tag{13}$$

where Q^* is a measure of adiabaticity [24, 25, 29]. This measure is fully determined by two special solutions, X_t and Y_t, of the force-free equation of motion [29],

$$\ddot{x}_t + \lambda_t\, x_t = 0\,. \tag{14}$$

We have,

$$Q^* = \frac{1}{2\sqrt{\lambda_0\lambda_f}}\left[\lambda_0\left(\lambda_f\, X_\tau^2 + \dot{X}_\tau^2\right) + \left(\lambda_f\, Y_\tau^2 + \dot{Y}_\tau^2\right)\right]\,. \tag{15}$$

with $X_0 = 0$, $\dot{X}_0 = 1$ and $Y_0 = 1$, $\dot{Y}_0 = 0$. [29]. Note that these initial conditions for X_t and Y_t are chosen for the sole sake of simplifying the mathematical treatment [29]. For the quantum harmonic oscillator the time-dependent action $S = E(t)/\omega(t)$ is conserved if [25]

$$\frac{\dot{X}_t^2 + \lambda_t\, X_t^2}{\sqrt{\lambda_t}} = \frac{1}{\sqrt{\lambda_0}} \quad \text{and} \quad \frac{\dot{Y}_t^2 + \lambda_t\, Y_t^2}{\sqrt{\lambda_t}} = \sqrt{\lambda_0}\,. \tag{16}$$

Thus, it is easy to see that $Q^* \geq 1$, where the equality holds for quasistatic processes. Accordingly, the exact expression for the excess work reads,

$$\left\langle W_{\mathrm{ex}}^{\mathrm{exact}}\right\rangle = \frac{\hbar\sqrt{\lambda_0 + \delta\lambda}}{2} \coth\left(\frac{\beta\hbar\sqrt{\lambda_0}}{2}\right) (Q^* - 1)\,. \tag{17}$$

Note that Q^* depends only implicitly on the protocol λ_t through the solutions of Eq. (14). Therefore, it is ad hoc not clear whether the exact excess work (17) exhibits the same zeros as the expression from linear response theory (12) for the linear protocol (11).

To gain insight and to build intuition we plot the measure of adiabaticity Q^* (15) for the linear protocol in Fig. 3 for various strengths of the perturbation $\delta\lambda$. We observe that generally $Q^* - 1$ exhibits oscillations, but no zeros as a function of τ. For weak driving, however, $\delta\lambda/\lambda_0 \ll 1$, where we expect linear response theory to hold, the minima of $Q^* - 1$ get infinitely close to zero. In Fig. 4 we compare the excess work from linear response theory (12) with the behavior of $Q^* - 1$ for weak driving. We observe very good agreement between the result from linear response theory (12) and $Q^* - 1$.

It has also been shown that for $Q^* = 1$ the quantum adiabatic theorem is fulfilled, i.e., for such processes there are no transitions between different energy eigenstates [29]. Thus, we conclude that the zeros of the excess

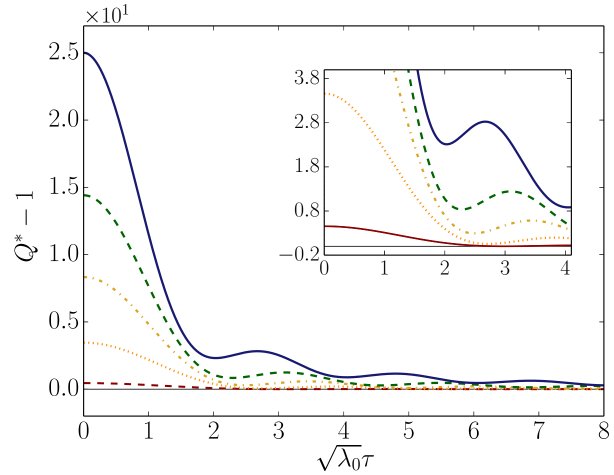

FIG. 3. (color online) Measure of adiabaticity Q^* (17) as a function of the switching time for the linear protocol, $g(t) = t/\tau$, and $\lambda_f = 2.0$ (blue, solid line), $\lambda_f = 1.7$ (green dashed line), $\lambda_f = 1.5$ (yellow, dot-dashed line), $\lambda_f = 1.3$ (orange, dash-dot line) and $\lambda_f = 1.1$ (red, dotted line), and $\lambda_0 = 1.0$.

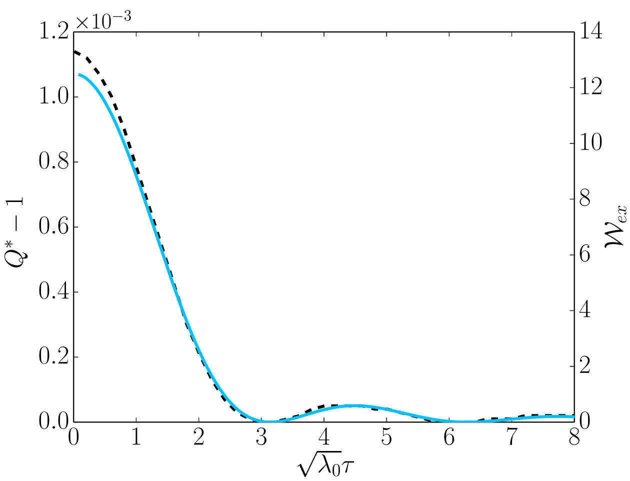

FIG. 4. (color online) Excess work from linear response theory (12) (blue solid line) together with Q^*-1 (black dashed line) as a function of τ for the linear protocol (11) and $\delta\lambda = 0.1$. The symbol $\mathcal{W}_{ex}$ denotes $\langle W_{ex}\rangle$ measured in units of $\left(\delta\lambda/\sqrt{\lambda_0}\right)^2\left(\hbar\sqrt{\lambda_0}\right)\coth\left(\beta\hbar\sqrt{\lambda_0}/2\right)/4$.

work, indeed, identify finite driving times for which transitionless quantum driving is facilitated – shortcuts to adiabaticity from linear response theory.

C. Range of validity of linear response theory

Linear response theory can be understood as a phenomenological theory of weak perturbations [27]. Thus, the numerical and qualitative agreement between exact (17) and approximate (12) results cannot be considered satisfactory. To deepen the insight into the approximations we will now derive Eq. (12) from the exact expression (17) without having to rely on phenomenology.

To this end, we expand the exact expression (17) in powers of $\delta\lambda$ up to second order. Note that Q^* depends implicitly on the protocol λ_t and we write $Q^*(\delta\lambda)$. We have,

$$\begin{aligned}\left\langle W_{\mathrm{exc}}^{\mathrm{exact}}\right\rangle \simeq \frac{\hbar}{2}\coth\left(\frac{\beta\hbar\sqrt{\lambda_0}}{2}\right)\Bigg[\delta\lambda\,\sqrt{\lambda_0}\,\partial_\lambda Q^*(0)\\ +\frac{\delta\lambda^2}{2\sqrt{\lambda_0}}\left(\partial_\lambda Q^*(0)+\lambda_0\,\partial_\lambda^2 Q^*(0)\right)+\mathcal{O}(\delta\lambda^3)\Bigg],\end{aligned}\tag{18}$$

where we used $Q^*(0) = 1$. We now have to show that there exist approximate solutions $\mathcal{X}_t$ and $\mathcal{Y}_t$ of the equation of motion (14) such that Eq. (18) reduces to the linear response expression (12) with $\mathcal{X}_t$ and $\mathcal{Y}_t$ replacing X_t and Y_t in Eq. (15)

Comparing Eqs. (12) and (18) we conclude that $\mathcal{X}_t$ and $\mathcal{Y}_t$ have to fulfill,

$$\partial_\lambda Q^*(0) = 0 \quad \text{and} \quad \partial_\lambda^2 Q^*(0) = \frac{\sin^2\left(\lambda_0\tau\right)}{\lambda_0^3\tau^2}\,. \tag{19}$$

Additionally we know that $\mathcal{X}_t$ and $\mathcal{Y}_t$ have to obey $\dot{\mathcal{X}}_t\mathcal{Y}_t - \mathcal{X}_t\dot{\mathcal{Y}}_t = 1$ [29]. The latter condition is nothing else but an expression of the commutation relation between position and momentum [29]. For $\delta\lambda = 0$ the solution of Eq. (14) is given by sine and cosine function [29]. Hence, we make the ansatz,

$$\begin{aligned}\mathcal{X}_t &= \frac{1}{\sqrt{\lambda_0}}\sin\left(\sqrt{\lambda_0}t\right)+\delta\lambda\,\mathcal{F}_t+\mathcal{O}(\delta\lambda^2)\\ \mathcal{Y}_t &= \cos\left(\sqrt{\lambda_0}t\right)+\delta\lambda\,\mathcal{G}_t+\mathcal{O}(\delta\lambda^2)\,,\end{aligned}\tag{20}$$

where $\mathcal{F}_t$ and $\mathcal{G}_t$ are two time-dependent function determined by the conditions (19).

It is then a tedious but straightforward exercise to show that

$$\mathcal{F}_t = \frac{t^2+4a\lambda_0\tau}{4\lambda_0\tau}\cos\left(\sqrt{\lambda_0}t\right)-\frac{t-4b\lambda_0\tau}{4\lambda_0\sqrt{\lambda_0}\tau}\sin\left(\sqrt{\lambda_0}t\right)\tag{21}$$

and

$$\begin{aligned}\mathcal{G}_t = &-\frac{t^2+4a\lambda_0\tau}{4\lambda_0\tau}\cos\left(\sqrt{\lambda_0}t\right)\\ &+\frac{t^2\lambda_0-4c\lambda_0\tau-1}{4\lambda_0\sqrt{\lambda_0}\tau}\sin\left(\sqrt{\lambda_0}t\right).\end{aligned}\tag{22}$$

The three constants a, b, and c are determined by the boundary conditions, $\mathcal{F}_0 = a$, $\dot{\mathcal{F}}_0 = b$ and $\mathcal{G}_0 = -b$ and $\dot{\mathcal{G}}_0 = c$ [35]. The expressions of $\mathcal{F}$ and $\mathcal{G}$ are rather lengthy and can be found in Appendix A.

The solutions (20) together with Eqs. (21) and (22) are the approximate solutions of the Eq. (14), for which the exact expression for the excess work (17) reduces to

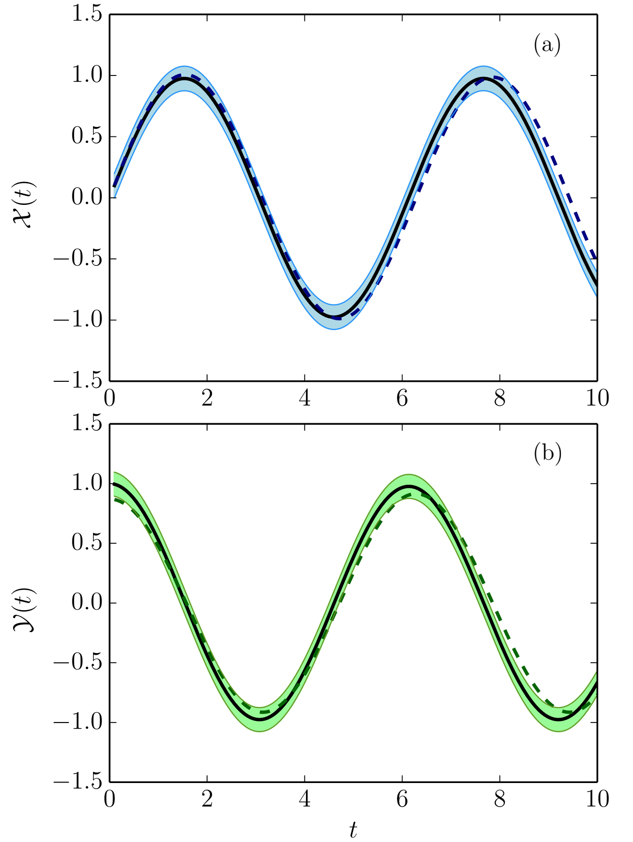

FIG. 5. (color online) (a) Exact solution X_t (solid line) and approximate solution $\mathcal{X}_t$ (20) for $\delta\lambda = 0.1$ (dashed line). (b) Exact solution Y_t (solid line) and approximate solution $\mathcal{Y}_t$ (20) for $\delta\lambda = 0.1$ (dashed line). Shaded area signifies a $\delta\lambda$-environment around the exact results.

the result from linear response theory (12). In Fig. 5 we plot the approximate solutions (20) together with exact solutions of (14). We observe that $\mathcal{X}_t$ and $\mathcal{Y}_t$ are within a $\delta\lambda$-environment around the exact results as one would intuitively expect by construction.

In conclusion, we have shown that results from linear response theory can also be obtained from expanding the exact solutions for weak driving. Thus, the linear response expressions can not only be considered to be qualitatively and phenomenologically true, but also quantitatively exact.

D. Optimal protocols – shortcuts to adiabaticity

In an analogous classical treatment it has been shown that not only the linear parameterization (11) can lead to zero excess work. Rather, there is a degenerate family of optimal protocols [21, 36], for which nonequilibrium excitations are suppressed. This family is given by,

$$g(t) = t/\tau + \alpha\ \sin\left(\kappa\pi\, t/\tau\right)\,, \tag{23}$$

where κ is an integer and α any arbitrary real number.

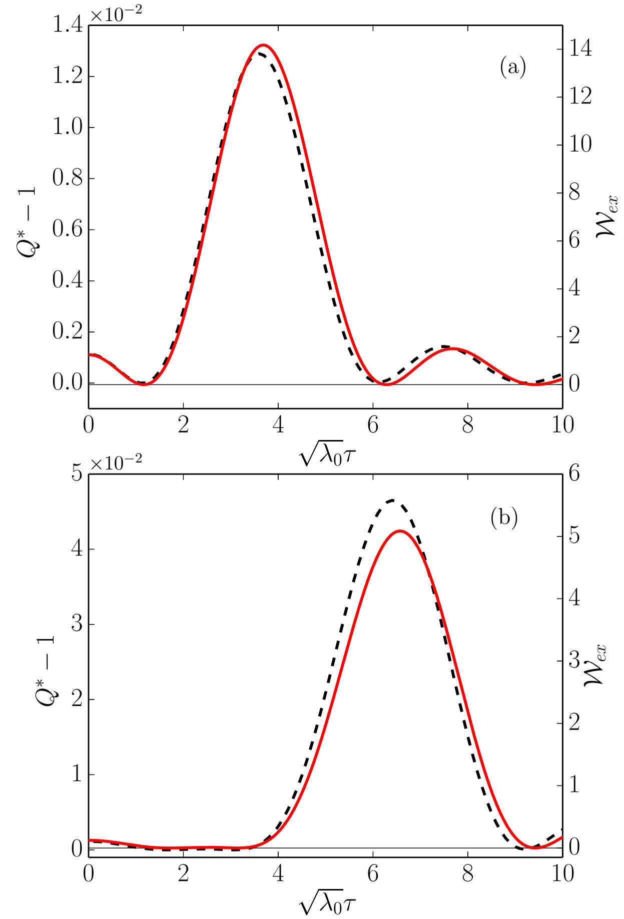

FIG. 6. (color online) Excess work (12) (black, dashed line) and normalized adiabatic parameter $Q^* - 1$ (red, solid line) as a function of the switching time for the optimal protocols (23) with $\alpha = 1$, $\kappa = 2$ (a), and $\alpha = 1$, $\kappa = 4$ (b). The symbol $\mathcal{W}_{ex}$ denotes $\langle W_{ex}\rangle$ measured in units of $\left(\delta\lambda/\sqrt{\lambda_0}\right)^2 (\hbar\sqrt{\lambda_0}) \coth\left(\beta\hbar\sqrt{\lambda_0}/2\right)/4$

The quantum excess work (12) merely differs in the prefactor from the classical expression

$$\langle W_{\mathrm{ex}}\rangle\Big|_{\hbar\beta\sqrt{\lambda_0}\ll 1} = \left(\frac{\delta\lambda}{\sqrt{\lambda_0}}\right)^2 \frac{1}{2\beta}\,\frac{\sin^2(\sqrt{\lambda_0}\,\tau)}{\lambda_0\,\tau^2}\,, \tag{24}$$

which is obtained in the limit $\hbar\beta\sqrt{\lambda_0} \ll 1$. Thus, the degenerate class (23) constitutes a family of shortcuts to adiabaticity for the quantum harmonic oscillator under weak driving. Figure 6 illustrates $\langle W_{\mathrm{ex}}\rangle$ (12) together with $Q^* - 1$ for two members of the family (23). It has been shown [21] that the shortcut to adiabaticity is obtained for $\sqrt{\lambda_0}\tau = n\pi$, n integer, and

$$\sqrt{\lambda_0}\tau = \frac{(\kappa\pi/2)}{(1+\kappa\pi\alpha)^{1/2}}\,. \tag{25}$$

Finally, it is worth emphasizing that such shortcuts to adiabaticity can be obtained for arbitrarily short switching times by choosing α appropriately [21].

IV. SPIN-1/2 IN A TIME-DEPENDENT MAGNETIC FIELD

Our second example is a spin-1/2 in a time-dependent magnetic field subjected to the constraint $|\mathbf{B}(t)| = B_0 =$ constant. Its Hamiltonian reads

$$H(t) = -\frac{\hbar\gamma}{2}\,\boldsymbol{\sigma}\cdot\mathbf{B}(t)\,, \tag{26}$$

where $\boldsymbol{\sigma}$ denotes the Pauli matrices. Due to the above mentioned constraint on $\mathbf{B}(t)$, it is more convenient to choose the following parameterization

$$\mathbf{B}(t) = B_0\begin{pmatrix}\sin[\varphi(t)]\cos[\theta(t)]\\ \sin[\varphi(t)]\sin[\theta(t)]\\ \cos[\varphi(t)]\end{pmatrix}. \tag{27}$$

Hence, the time-dependence of the set of allowed processes parameterized by the angles $\varphi(t)$ and $\theta(t)$ is, in analogy to Eq. (1), expressed as

$$\varphi(t) = \varphi_0 + \delta\varphi\, g_\varphi(t)\,, \tag{28a}$$

$$\theta(t) = \theta_0 + \delta\theta\, g_\theta(t) \tag{28b}$$

where the boundary conditions $g_{\varphi,\theta}(0) = 0$ and $g_{\varphi,\theta}(\tau) = 1$ must hold.

Linear response theory provides a good description of $\langle W_{ex}\rangle$ as long as $\delta\varphi$ and $\delta\theta$ are sufficiently small. In this regime, one can easily show that the angle $\theta(t)$ plays no role and the thermodynamic work (7) depends on the nonequilibrium of $\partial_\varphi H$ only. Thus, the response function is given by Eq. (5) with $A_t = \partial_\varphi H(t)$ and it is straightforward to obtain

$$\phi(t) = \frac{\hbar}{2}\,(\gamma B_0)^2\tanh\left(\frac{\beta\hbar\gamma B_0}{2}\right)\sin(\gamma B_0 t)\,, \tag{29}$$

from which, using again $\phi(t) = -\dot{\Psi}(t)$, we have the relaxation function

$$\Psi(t) = \frac{\hbar\omega_0}{2}\tanh\left(\frac{\beta\hbar\omega_0}{2}\right)\cos(\omega_0 t)\,, \tag{30}$$

where we defined $\omega_0 \equiv \gamma B_0$.

The time-dependence of the relaxation functions (10) and (30) have the same functional form. Therefore, the excess work performed by an external agent while driving the spin-1/2 will behave exactly the same as in the parametric harmonic oscillator. For instance, the protocols given by (23) also constitute a family of optimal protocols for the present system. Nevertheless, the values of $\omega_0\tau$ for which the excess work vanishes are a bit different from those in Fig. (4) due to the absence of the factor 2 in $\cos(\omega_0 t)$ of Eq. (30). The linear protocol generates zeros for $\omega_0\tau = n\,2\pi$.

A. Quantum adiabatic invariant

Analogously to Sec. III, we will now verify that quantum adiabatic invariant is conserved for spin-1/2 particles driven by Eq. (23). To this end, we analyze the time evolution of the coefficients $c_+(t)$ and $c_-(t)$ appearing in the expansion

$$|\psi(t)\rangle = \sum_{n=+,-} c_n(t)\exp\left(-\frac{i}{\hbar}\int_0^t \mathrm{d}t'\,E_n(t')\right)|n;t\rangle\,, \tag{31}$$

of an arbitrary state $|\psi(t)\rangle$. We denote by $E_n(t)$ and $|n;t\rangle$ the instantaneous eigenvalues and eigenstates of (26). The quantum adiabatic invariant is then conserved in finite time if, after starting with $c_+(0) = 1$ and $c_-(0) = 0$ at the beginning of a certain protocol $g_\varphi(t)$, we obtain $c_+(\tau) = c_+(0)$ and $c_-(\tau) = c_-(0)$.

The equations of motion for $c_{+,-}(t)$ are easily derived following standard procedures [37–39]. For the parame-

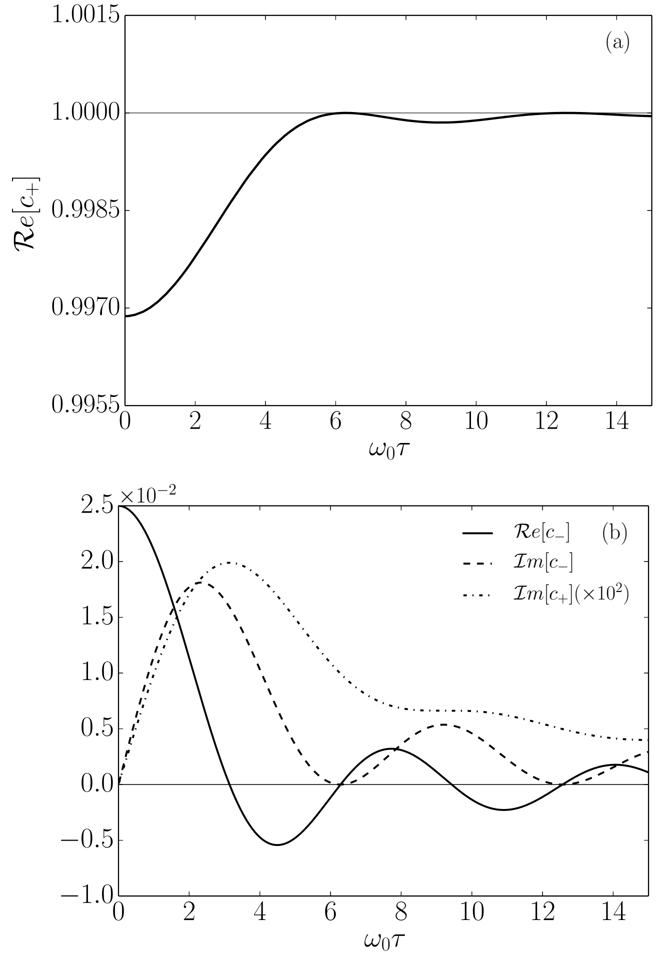

FIG. 7. Time evolution of the real and imaginary parts of the coefficients $c_+(t)$ and $c_-(t)$ given by Eq. (32) for the initial condition $c_+(0) = 1$ and $c_-(t)$ considering the approximation $\cos(\delta\varphi\, t/2\tau) \simeq 1$.

terization (27) of $\mathbf{B}(t)$, we obtain

$$\frac{dc_+(t)}{dt} = -\frac{\delta\varphi}{4\tau}\cos\left(\frac{\delta\varphi}{2\tau}t\right)\exp\left(-i\omega_0 t\right)c_-(t), \quad (32a)$$

$$\frac{dc_-(t)}{dt} = \frac{\delta\varphi}{4\tau}\cos\left(\frac{\delta\varphi}{2\tau}t\right)\exp\left(i\omega_0 t\right)c_+(t), \quad (32b)$$

considering $\theta_0 = 0$, $g_\theta(t) = 0$ and $g_\varphi(t) = t/\tau$.

Figure (7) shows the real and imaginary parts of the solutions of (32) as functions of $\omega_0\tau$ considering the approximation $\cos\left(\delta\varphi\, t/2\tau\right) \simeq 1$, since we are in the regime $\delta\varphi \ll 1$ (see appendix B for the analytical form of them). Since the initial conditions are $c_+(0) = 1$ and $c_-(0) = 0$, we should have a finite-time conservation of the adiabatic invariant every time we get a recurrence of this values. In Fig. (7), we see that this hold true for $\omega_0\tau = n\,2\pi$, although due to our approximations the imaginary part of $c_-(t)$ does not vanish at these values of τ.

V. COMPLEX SYSTEMS

The two case studies in Secs. III and IV are analytically solvable and pedagogically elucidating. In particular, we obtained exact expressions for the response functions (9) and (29). However, this is not feasible for general and more realistic systems with more degrees of freedom. However, it has been shown [22, 23, 27, 28] that linear response theory performs well when only phenomenological information is known about the system of interest. In other words, even when the response function is not exact the predictions of linear response theory provide good approximations. Finding shortcuts from linear response theory and by the optimizing $\langle W_{ex}\rangle$ circumvents the difficult problem of having to solve for the full quantum dynamics.

It has been shown that $\langle W_{ex}\rangle$ will have finite-time minima, or non-monotonic behavior as a function of τ, if the relaxation function is sufficiently oscillatory. This can be illustrated for instance using the following phenomenological ansatz [23, 28],

$$\Psi(t) = \Psi(0)\,\exp\left(-\alpha|t|\right)\left(\cos\left(\omega t\right) + \frac{\alpha}{\omega}\sin\left(\omega t\right)\right), \quad (33)$$

for the relaxation function. Plugging the expression above in Eq. (7), we obtain the results shown in Fig. (8) for different values of α/ω. As this ratio decreases, the excess work starts to show minima whose value approach zero. There are several systems for which Eq. (33) describes the relaxation dynamics very well. Among them, we mention a system composed of weakly interacting magnetic moments in the regime where Bloch equations are valid [40].

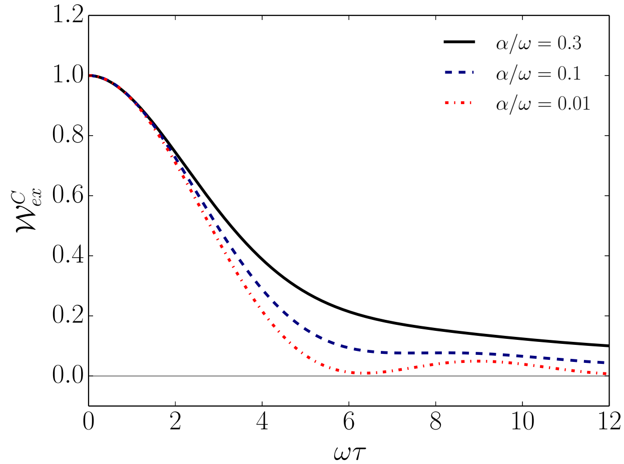

FIG. 8. (color online) Excess work $\mathcal{W}_{ex}^C$ in units of $(\delta\varphi)^2\Psi(0)/2$ for the linear protocol $g_\varphi(t) = t/\tau$ and the relaxation function (33).

VI. CONCLUDING REMARKS

Identifying optimal quantum processes with suppressed or even vanishing nonequilibrium excitations is an important topic, which has recently been attracting intense research efforts. However, all methods currently available necessitate the solution of the full quantum dynamics. In the present work, we have proposed a phenomenological alternative. By generalizing our previous result for the excess work from linear response theory to quantum system we have shown that shortcuts to adiabaticity can be identified from a mathematically simple theory. This observation has been proven for two paradigmatic examples of quantum thermodynamics, namely the parametric harmonic oscillator and the spin-1/2 in a time-dependent magnetic field.

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Appendix A: Approximate solution within linear response

The full expressions for the approximate solutions $\mathcal{X}_t$ and $\mathcal{Y}_t$ in Eqs. (21) and (22) are given in terms of the three constants a, b, c. These are determined by solving the force free equation of motion (14) with the boundary conditions, $\mathcal{F}_0 = a$, $\dot{\mathcal{F}}_0 = b$ and $\mathcal{G}_0 = -b$ and $\dot{\mathcal{G}}_0 = c$. We have,

$$a = \frac{-1 - 2\lambda_0\tau^2 + \cos(2\sqrt{\lambda_0}\tau) - 2\sqrt{\lambda_0}\tau\sin(2\sqrt{\lambda_0}\tau)}{8\lambda_0^2\tau} \quad \text{and} \quad c = \frac{-1 + 2\lambda_0\tau^2 + \cos(2\sqrt{\lambda_0}\tau) - 2\sqrt{\lambda_0}\tau\sin(2\sqrt{\lambda_0}\tau)}{8\lambda_0\tau} \tag{A1}$$

and

$$b = \frac{1}{8\lambda_0\sqrt{\lambda_0}\tau}\left[2 + \sqrt{4 + 2\lambda_0\tau^2 - 4\cos(2\sqrt{\lambda_0}\tau)} + 2\sqrt{\lambda_0}\tau\cos(2\sqrt{\lambda_0}\tau) + \sin(2\sqrt{\lambda_0}\tau)\right]. \tag{A2}$$

Appendix B: Derivation of time-dependent coefficients c_+ and c_-

According to the Ref. [39], the coefficients c_+ and c_- satisfy the differential equations for Eq. (27),

$$\frac{dc_+(t)}{dt} = -\frac{\delta\varphi}{4\tau}\cos\left(\frac{\delta\varphi}{2\tau}t\right)\exp\left(-i\omega_0 t\right)c_-(t), \tag{B1a}$$

$$\frac{dc_-(t)}{dt} = \frac{\delta\varphi}{4\tau}\cos\left(\frac{\delta\varphi}{2\tau}t\right)\exp\left(i\omega_0 t\right)c_+(t). \tag{B1b}$$

In the regime $\delta\varphi \ll 1$, we make the approximation $\cos[\delta\varphi/2\tau\, t] \simeq 1$. Next, we solve exactly the equations with the initial conditions $c_+(0) = 1$ and $c_-(0) = 0$. After making $t = \tau$, we obtain the following equations

$$\begin{aligned} c_+(\omega_0\tau) = \frac{e^{-\frac{i\omega_0\tau}{2}}}{\delta\varphi^2 + 4(\omega_0\tau)^2}\Bigg[&(\delta\varphi^2 + 4(\omega_0\tau)^2)\cosh\left(\frac{1}{4}\sqrt{-(\delta\varphi^2 + 4(\omega_0\tau)^2)}\right) \\ &- 2i\omega_0\tau\sqrt{-(\delta\varphi^2 + 4(\omega_0\tau)^2)}\sinh\left(\frac{1}{4}\sqrt{-(\delta\varphi^2 + 4(\omega_0\tau)^2)}\right)\Bigg] \end{aligned} \tag{B2}$$

$$c_-(\omega_0\tau) = \frac{e^{\frac{i\omega_0\tau}{2}}\delta\varphi}{\delta\phi^2 + 4(\omega_0\tau)^2}\sinh\left(\frac{1}{4}\sqrt{-(\delta\varphi^2 + 4(\omega_0\tau)^2)}\right), \tag{B3}$$

where $\omega_0 = \gamma B$.

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