Shortcuts to Thermodynamic Quasistaticity

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Shortcuts to thermodynamic quasistaticity

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The operation of near-term quantum technologies requires the development of feasible, implementable, and robust strategies of controlling complex many body systems. To this end, a variety of techniques, so-called "shortcuts to adiabaticty", have been developed. Many of these shortcuts have already been demonstrated to be powerful and implementable in distinct scenarios. Yet, it is often also desirable to have additional, approximate strategies available, that are applicable to a large class of systems. In this work, we hence take inspiration from thermodynamics and propose to focus on the macrostate, rather than the microstate. Adiabatic dynamics can then be identified as such processes that preserve the equation of state, and systematic corrections are obtained from adiabatic perturbation theory. We demonstrate this approach by improving upon fast quasi-adiabatic driving, and by applying the method to the quantum Ising chain in the transverse field.

The word "adiabatic" is derived from the Greek *adiabatos*, which means literally "impassable". In thermodynamics, an adiabatic constraint is a "wall" that is impassable to heat, and thus an adiabatic process is a thermodynamic state transformation during which no heat is exchanged [1]. However, the notion of adiabaticity has found a much broader application in Hamiltonian dynamics [2]. In classical mechanics, an "adiabatic invariant" is any quantity that remains constant under the Hamiltonian equations of motion, given infinitely slow variations of the Hamiltonian [2].

This insight led Born to the formulation of the quantum adiabatic theorem [3], which states that during infinitely slow variation of the Hamiltonian no transitions between energy levels occur. Obviously, such adiabatic processes are highly desirable in quantum technological applications. Recent years have seen tremendous research efforts in facilitating such excitation-free processes also in finite time driving. Under the umbrella of *shortcuts to adiabaticity* (STA) [4, 5] a large variety of techniques has been developed, of which counterdiabatic driving [6–11], invariant based inverse engineering protocols [12–16], and the fast-forward technique [17–23] have arguably received the most attention, with applications in vastly different physical scenarios. For instance, counterdiabatic driving is particularly well-suited to optimally control the dynamics of cold ion traps [24, 25]. However, implementing STA in more complex quantum system can become rather involved [26–31]. Thus, it appears very desirable to find alternative and approximate schemes, that may provide more universally applicable control strategies. This has already led to the development of "resource friendly" control strategies [32–37], that provide alternative means to suppress excitations arising from populating energetically high-lying microstates.

One of the main causes for the complexity of finding realistically useful STA rests in the fact that, to a certain degree, all methods originate in circumventing the quantum adiabatic theorem [3]. Hence, the focus is on preserving the occupation probabilities of the energy eigenstates, i.e., microstates [1]. However, in most experimental settings quantum states cannot be easily measured, and rather *thermodynamic observables* are monitored. Therefore, *thermodynamic control* has been suggested as a possible way to construct approximate STA [38], see Ref. [39] for a recent perspective. However, thermodynamic control methods are usually applied with a focus on lowering the energetic cost of a given thermodynamic process [40–44].

In the present letter, we change the paradigm of this approach by proposing genuine *shortcuts to thermodynamic quasistaticity*. To this end, we fully accept the thermodynamic mindset, namely we seek STA that preserve the *adiabatic macrostate*, and not the occupations of microscopic energy eigenstates of a quantum system. Hence, we demand that the macrostate of a driven system (approximately) fulfills an instantaneous equation of state. Such a control strategy is constructed by exploiting *adiabatic perturbation theory* [45], which has recently proven powerful in assessing nonequilibrium excitations in driven quantum Ising chains [46, 47]. To demonstrate the versatility of the approach, we benchmark our results against other STA, in particular against *fast quasi-adiabatic driving* [48–51], which is closest in spirit to our approach.

Preliminaries We start by establishing notions and notations. Consider a quantum system described by a Hamiltonian $H(\lambda) = \sum_n E_n(\lambda) \left|n(\lambda)\right\rangle \left\langle n(\lambda)\right|$, where $E_n(\lambda)$ and $\left|n(\lambda)\right\rangle$ are parametric, non-degenerate eigenvalues and eigenstates, respectively. Moreover, λ is an external control parameter, such as the volume of a gas container or a magnetic field. In the following, we will be interested in thermodynamic state transformations that are driven by varying $\lambda = \lambda(t)$ (also called a protocol), between times t_i and t_f, taking the external parameter from an initial value λ_i to a final value λ_f. Moreover, we assume that the quantum system is thermally insulated and, therefore, its time evolution is unitary. Note that unitary dynamics are necessarily thermodynamically adiabatic in the traditional sense, since no heat is exchanged. Thus, unless otherwise stated, "adiabatic" means "quasistatic" henceforth.

We further assume that the system is initially prepared in a quantum state that is diagonal in the energy eigenbasis, $\rho_i = \sum_n p_n \left|n_i\right\rangle \left\langle n_i\right|$, where the subscript i means that a given quantity is evaluated at t_i, here simply $\left|n_i\right\rangle = \left|n(\lambda_i)\right\rangle$. The time-dependent state is then determined by the von Neumann equation, $i\hbar\,\dot{\rho}(t) = [H(\lambda), \rho(t)]$, and we denote derivatives with respect to time by a dot.

It is worth emphasizing that even if the initial state, ρ_i, is chosen to be an equilibrium state, $\rho(t > t_i)$ may be arbitrarily far from equilibrium. Given an initially canonical state ($\rho_i \propto \exp\left(-\beta H_i\right)$), even an infinitely slow process will generally not keep the system in canonical equilibrium. This is because the quasistatic evolution preserves the statistical weights in the initial Hamiltonian. However, in the present analysis our main focus is also not the microstate, but rather the thermodynamic macrostate.

In (quantum) thermodynamics a macrostate is fully characterized by its state variables [1, 52], which fulfill an equation of state (EOS). At any instant, the EOS can be obtained by calculating the equilibrium average of the generalized force, $F(\lambda)$, which is given by [1]

$$F(\lambda) = -\frac{\partial H(\lambda)}{\partial \lambda}, \tag{1}$$

and $\Lambda \equiv \operatorname{tr}\left\{\rho F\right\}$ is the state variable conjugate to λ. For any driven process, and writing the time-dependent quantum state as $\rho(t) = \sum_n p_n \left|\psi_n(t)\right\rangle \left\langle \psi_n(t)\right|$, the corresponding average generalized force reads

$$\Lambda(t) = \sum_n p_n \left\langle \psi_n(t)\right| F(\lambda) \left|\psi_n(t)\right\rangle . \tag{2}$$

Here, $\left|\psi_n(t)\right\rangle$ is a solution of the corresponding Schrödinger equation.

Thermodynamic state transformations Before we analyze the more general out of equilibrium situation, we inspect Eq. (2) in the adiabatic limit $\tau \to \infty$. The adiabatic theorem dictates that, if the evolution is slow enough, the solution to Schrödinger's equation can be written as [53]

$$\left|\psi_n^{(0)}(t)\right\rangle = e^{i\phi_n(t)} \left|n(\lambda)\right\rangle , \tag{3}$$

where the superscript (0) denotes the adiabatic limit and $\phi_n(t)$ is the usual adiabatic phase (dynamic plus geometric). In this case, Eq. (2) simplifies to

$$\Lambda^{(0)} = \sum_n p_n F_{nn}(\lambda), \tag{4}$$

where $F_{mn}(\lambda) = \left\langle m(\lambda)\right| F(\lambda) \left|n(\lambda)\right\rangle$. Notice the lack of explicit time-dependence in Eq. (4): this is the conventional EOS. For infinitely slow variations of λ, Eq. (4) describes the evolution of the macroscopic state in any mechanically adiabatic (and thermodynamically adiabatic) process, i.e., for a thermodynamic state transformation.

Beyond the adiabatic limit Using adiabatic perturbation theory (APT), whose details we leave for the Supplemental material [54], we can systematically compute finite-time corrections to the EOS (4). Using Eqs. (1)–(3) of the Supplemental Material [54] in Eq. (2) and keeping terms up to $\mathcal{O}(\tau^{-1})$, the first-order correction becomes

$$\begin{aligned}\Lambda^{(1)}(t) &= \sum_{\substack{m,n\\ m\neq n}} p_n \Re\left\{2C_{mn}^{(1)}(t) F_{mn}^{*}(\lambda)\right\}\\ &= 2\hbar\dot{\lambda}_i \sum_{\substack{m,n\\ m\neq n}} p_n \Im\left\{F_{mn,i}\frac{e^{i\phi_{mn}(t)}}{E_{mn,i}^2}F_{mn}^{*}(\lambda)\right\},\end{aligned} \tag{5}$$

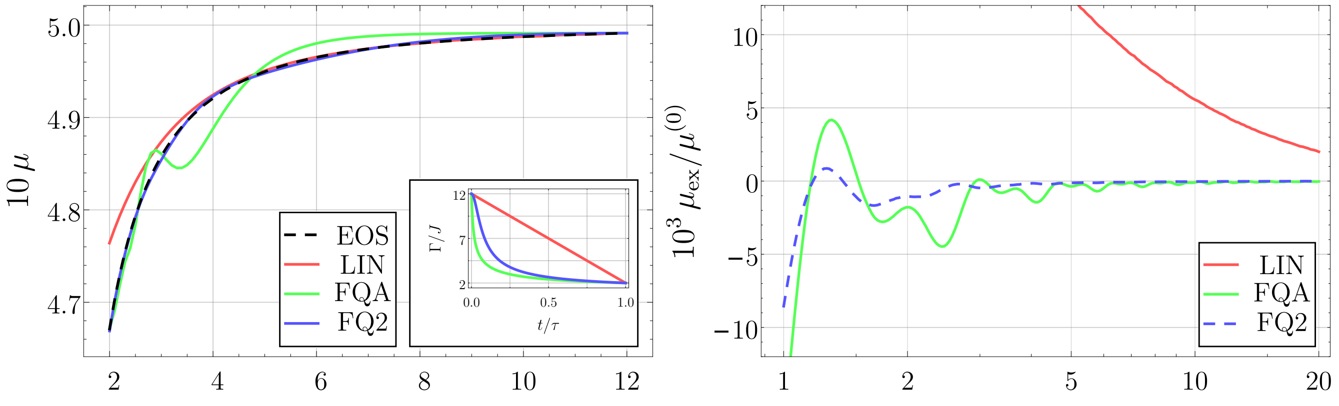
where we used the fact that the product of $F^{*}_{mn}(\lambda)$ and the first term of Eq. (2) of the Supplemental Material [54] is purely imaginary. We immediately observe that the first-order correction to the EOS is directly proportional to the time derivative of the external parameter *at the beginning of the process*. Hence, for all protocols with $\dot{\lambda}_i = 0$, the EOS is preserved up to $\mathcal{O}(\tau^{-2})$ in any sufficiently slow process. We stress that this conclusion is independent of the Hamiltonian considered, only depending on the validity of APT. Thus, we have unveiled a universal design principle for optimal control strategies applicable in any gapped quantum system, simple as well as complex.

Strategies where the time derivatives of the protocols vanish at the end points of the evolution have already been discussed as ways to guarantee adiabaticity in the microstate [55–58]. However we emphasize that the first-order result for the macrostate only depends on the initial derivative, and not the final derivative. This still leaves a lot of freedom in finding "optimal" and experimentally implementable protocols. Thus it should be obvious that even better results can be achieved by complementing our macroscopic strategy with microscopic methods.

Fast quasi-adiabatic driving One strategy to ensure APT convergence is the application of fast quasi-adiabatic (FQA) protocols [48–51] and related approaches [5]. If there is only one relevant energy gap $E_{mn}(\lambda)$ in the quantum system, FQA provides a protocol $\lambda(t)$ for which first-order APT transitions between eigenstates m and n are equally likely at any instant. This protocol is the solution to a first order differential equation [48–51]

$$\hbar\left|\frac{\dot{\lambda}(t) F_{mn}(\lambda)}{E_{mn}^2(\lambda)}\right| = c_1, \tag{6}$$

where c_1 is a constant that, together with the integration constant, is uniquely defined by the boundary conditions $\lambda(t_i) = \lambda_i$ and $\lambda(t_f) = \lambda_f$. For a generic protocol, microscopic adiabaticity is secured if the left-hand side of Eq. (6) is much smaller than unity for any t, the quantitative adiabatic condition [59, 60] [Eq. (4) of the Supplemental Material [54]]. The boundary conditions always lead to $c_1 \propto \tau^{-1}$, which means that the FQA protocol still requires large enough τ for the adiabatic condition



(a)

(b)

FIG. 1. Magnetization of the TI chain in the entirely paramagnetic process with $N = 100$ starting at zero temperature. The results were numerically obtained from the exact time-dependent dynamics. (a) State diagram of the TI chain for an adiabatic (quasistatic) evolution (EOS), the LIN, the FQA and the FQ2 protocols for $J\tau = 3$, starting from the top right corner. The inset shows the time-dependence of each protocol. (b) Excess magnetization $\mu_{\rm ex} = \mu - \mu^{(0)}$ at the end of the process vs. process duration.

to be fulfilled. FQA's advantage is that it *naturally slows down* where $E_{mn}(\lambda)$ is small (see Eq. (6)), and thus it may reach the adiabatic condition and make APT converge for a smaller τ, when compared to a generic protocol.

Curiously, FQA is limited to suppressing first-order transitions. The authors of Ref. [51] remark that considering transitions of higher-than-one order APT is not possible, since the associated differential equation would not have enough constants to satisfy the boundary conditions on λ and its derivatives. For example, demanding the second-order APT transition probabilities to be uniform along the process gives a second-order differential equation,

$$\hbar^2 \left| \frac{1}{E_{mn}(\lambda)} \frac{d}{dt} \left(\frac{\dot{\lambda}(t) F_{mn}(\lambda)}{E^2_{mn}(\lambda)} \right) \right| = c_2, \qquad (7)$$

which was obtained from Eq. (6) with the proper substitution to second order coefficients, discussed in the Supplemental Material [54]. The three available constants (c_2 plus two integration constants) in the solution of Eq. (7) are insufficient to satisfy the four boundary conditions — two on λ (same as FQA) and two on $\dot{\lambda}$, which are necessary to make the second-order APT correction be the relevant correction.

Above we have seen that from the macroscopic dynamics, Eq. (5), optimal driving protocols obey $\dot{\lambda} = 0$ at the beginning (and not at the end). This additional condition permits us to uniquely solve Eq. (7), if we impose the same boundary conditions as the FQA method *plus* $\dot{\lambda}(t_i) = 0$, which leads to $c_2 \propto \tau^{-2}$. We will be referring to this strategy as FQ2, and as we will see shortly, FQ2 clearly outperforms FQA. We once again bring attention to the fact that making $\dot{\lambda}(t_i) = 0$ gives null first order APT correction for the EOS of *any gapped system*. Equations (6) and (7), which do depend on the system through its eigenspectrum, are primarily used to guarantee early APT validity and can be applied even when the Hamiltonian is only numerically diagonalizable. In fact, at low temperature, knowledge of only a few eigenlevels may be necessary, since only transitions between the lowest energy eigenstates are relevant (see Fig. 2 of the Supplemental Material [54]).

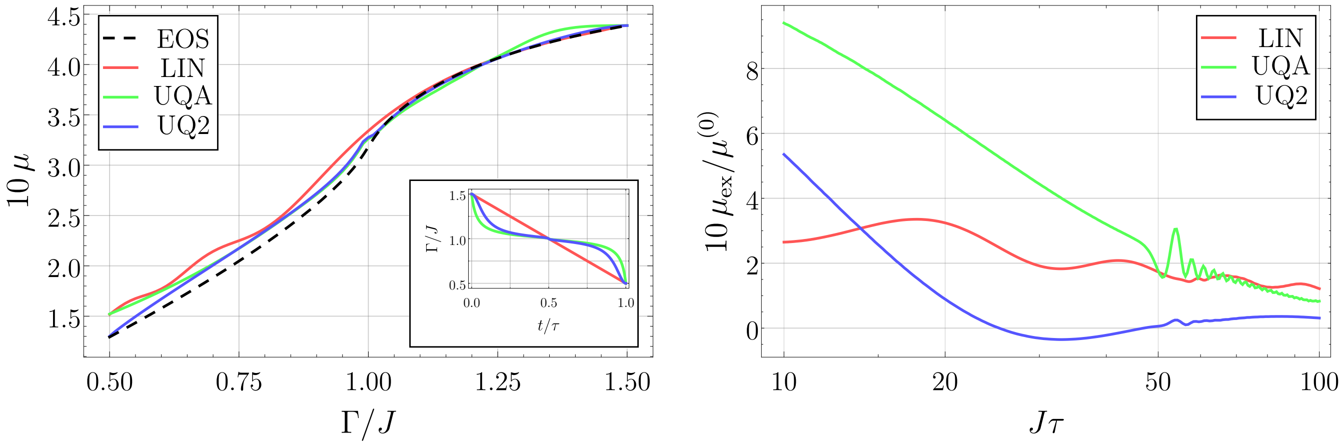
Illustrative example: quantum Ising chain We now apply the above developed strategy to control a thermodynamically relevant, exactly solvable system: the transverse field Ising model (TI) [61, 62]. The Hamiltonian reads

$$H_{\rm TI}(\Gamma) = -\frac{1}{2} \left(J \sum_{j=1}^{N} \sigma^z_j \sigma^z_{j+1} + \Gamma \sum_{j=1}^{N} \sigma^x_j \right), \qquad (8)$$

where J is the coupling constant, Γ is the external magnetic field and $\sigma^{x,z}_j$ are standard Pauli matrices for each spin j (with periodic boundary conditions). In the thermodynamic limit $N \to \infty$, this system displays a quantum critical point (QCP) at $\Gamma = J$, where the energy gap between ground and first excited states vanishes. For simplicity, we assume N to be even and that the system is initially prepared in its ground state. The force is $F_{\rm TI} = \sum_{j=1}^{N} \sigma^x_j/2$, while the nonequilibrium magnetization per spin reads

$$\mu(t) = \frac{1}{2N} \sum_{j=1}^{N} \left\langle \sigma^x_j \right\rangle (t). \qquad (9)$$

In any finite time process, the magnetization can be separated into an adiabatic contribution $\mu^{(0)}$ and an excess contribution $\mu_{\rm ex}$. Details for how to calculate the nonequilibrium average in Eq. (9) can be found in the Supplemental Material [54].



(a)

(b)

FIG. 2. Magnetization of the TI chain in the QCP crossing process starting at zero temperature with $N = 100$. The results of both panels were numerically obtained from the exact time-dependent dynamics. (a) State diagram of the TI chain for an adiabatic (quasistatic) evolution (EOS), the LIN, the UQA and the UQ2 protocols for $J\tau = 50$, starting from the top right corner. The inset shows the time-dependence of each protocol. (b) Excess magnetization $\mu_{\rm ex} = \mu - \mu^{(0)}$ at the end of the process vs. process duration.

First, we consider a process keeping the chain entirely in its paramagnetic phase ($\Gamma > J$) and starting at zero temperature, i.e., with the chain initially prepared in its ground state. We solve FQA and FQ2 for the smallest gap of the system and compare them to a naive linear protocol (LIN) — the results for a chain of finite size are shown in Fig. 1. In Fig. 1a, we show μ of Eq. (9) vs. Γ in a process that approaches, but does not cross, the QCP. The inset contains the time-dependence of each protocol, where it can be seen that both FQA and FQ2 adapt to the system's spectrum, but FQ2 does so while still keeping null first derivative at the start. FQA has a very high first derivative at the initial time, and this ultimately make its evolution have notable oscillations around the EOS. On the other hand, LIN follows the EOS closely, up until a point where the gap gets too small and it ends up breaking adiabaticity. Finally, FQ2 follows the EOS right until the end, which is a consequence of its compromise to attain adiabaticity while zeroing the first order correction to the EOS. In Fig. 1b, we depict the excess magnetization $\mu_{\rm ex}$ at t_f as a function of τ. It is clear that FQ2 outperforms FQA for a generic τ, even if FQ2 first crosses the "adiabatic" $\mu_{\rm ex} = 0$ line for a marginally bigger τ than FQA.

As a second case, we consider the crossing of the QCP, from the paramagnetic phase to the ferromagnetic phase. In a finite size chain, the gap at the QCP is small but non-zero, which makes adiabaticity difficult but possible to achieve. In this scenario, the smallness of the energy gap forces the FQA protocol to slow down dramatically around the QCP and, consequently, to speed up around the end points. This speed-up is detrimental in the ferromagnetic phase of the TI chain, where the gap of many other sub-levels are comparable to the gap of the lowest sub-level (see Fig. 1 of the Supplemental Material [54]). Other energy differences can be taken into account when building FQA protocols (see Ref. [63]), but the associated differential equation is not exactly solvable and hardly numerically solvable when traversing the QCP. Thus, to circumvent this issue, we apply a similar strategy known as uniform quasi-adiabatic (UQA) [64] to the lowest sub-level of the TI chain. It is the solution to Eq. (6) with the substitution $F_{mn}(\lambda) \to \partial_\lambda E_{mn}(\lambda)$ [5], motivated by the Kibble-Zurek mechanism of second-order quantum phase transitions. Thus, we define a UQ2 protocol as the solution of Eq. (7) with the aforementioned substitution and we compare it to LIN and UQA in Fig. 2. Figure 2a is the equivalent of Fig. 1a, but with a considerably larger process duration, which evidences the difficulty of crossing the QCP while maintaining adiabaticity (in the mechanical sense). The inset once again shows the time-dependence of each strategy, and it is clear that both UQA and UQ2 slow down around the QCP. The conclusion is the same as in the paramagnetic process: UQ2 follows the EOS more closely. Furthermore, as can be seen in Fig. 2b, UQ2 gives final $\mu_{\rm ex} = 0$ for a significantly smaller τ than the other two protocols, which is a consequence of its final first derivative also being null at the end point (see inset of Fig. 2a).

Concluding remarks Controlling complex many body quantum systems is an involved task. While some strategies have been successfully employed in platforms with great technological promise, such as counterdiabatic driving in ion traps [24, 25], more universally applicable paradigms appear desirable. To this end, we have proposed to take inspiration from the mother of all control theories — thermodynamics. Rather than aiming to control the microstate, we have suggested to control the macrostate and identify protocols that preserve the equation of state. This approach is somewhat akin to invariant based strategies [5, 13], on which we comment in the Supplemental Material [54], where we study thermodynamic shortcuts for the driven harmonic oscillator [65–67]. However, our approach significantly goes beyond existing methods, since using adiabatic perturbation theory, finite-time corrections can be systematically computed, which gives systematic conditions for the optimal driving protocols. The utility of the approach has been demonstrated by improving upon fast quasi-adiabatic driving, and its applicability has been demonstrated for the driven Ising chain.

The analyses of state diagrams demonstrate the difference between microscopic adiabaticity and macroscopic adiabaticity. More specifically, strategies that are better suited for parametric following of microstates (eigenstates) are not necessarily better for parametric following of macrostates (state variables). It is also worth noting that a notion of relaxation time seems to be absent, which is perhaps expected in isolated systems where relaxation to some sort of equilibrium is not guaranteed. Nonetheless there is still the notion of a time scale to which the driving rate must be compared with, related to the energy gap between eigenstates. Lastly, it is interesting to see that, even though is is possible to stay close to the equation of state in finite time driving, such possibility does not lead to thermodynamic reversibility. In other words, applying the same "optimal" protocol in the reverse process does not give the same curve in the state diagram as in the forward process and, in fact, the FQ2 strategy we devised to better follow the equation of state does not provide protocols with time-reversal symmetry.

Finally, we note that the present paper fills the gap in a hierarchy of strategies developed for securing adiabaticity in finite time. First, there are standard shortcuts to adiabaticity, where one seeks to follow the parametric eigenstates of the system. Second, we have the thermodynamic shortcuts introduced in the present letter, which follow the equation of state. Third, we have the methods from thermodynamic control, where the focus is on making sure that the energetic cost of a certain manipulation of the system is as close as possible to the cost in an quasistatic process. It is expected that the further down you go in the hierarchy, the less information is needed to determine the associated optimal driving protocol.

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