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Shortcut to Equilibration of an Open Quantum System

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We present a procedure to accelerate the relaxation of an open quantum system towards its equilibrium state. The control protocol, termed *Shortcut to Equilibration*, is obtained by reverse-engineering the non-adiabatic master equation. This is a non-unitary control task aimed at rapidly changing the entropy of the system. Such a protocol serves as a shortcut to an abrupt change in the Hamiltonian, i.e., a *quench*. As an example, we study the thermalization of a particle in a harmonic well. We observe that for short protocols the accuracy improves by three orders of magnitude.

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Introduction Equilibration is a natural process, describing the return of a perturbed system back to a thermal state. The relaxation to equilibrium is present in both the classical [1–3] and quantum [4] regimes. Gaining control over the relaxation rate of quantum systems is crucial for enhancing the performance of quantum heat devices [5–9]. In addition, fast relaxation is beneficial for quantum state preparation [10, 11] and open system control [12–17]. To address these issues, we present a scheme to accelerate the equilibration of an open quantum system, serving as a shortcut to the natural relaxation time τ_R . The protocol is termed Shortcut To Equilibration (STE).

This control problem is embedded in the theory of open quantum systems [4]. The framework of the theory assumes a composite system, partitioned into a system and an external bath. The Hamiltonian describing the evolution of the composite system reads $\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{H}_I$, where $\hat{H}_S(t)$ is the system Hamiltonian, \hat{H}_B is the bath Hamiltonian and \hat{H}_I is the systembath interaction term. When the system depends explicitly on time, the driving protocol influences the systembath coupling operators and consequently, the relaxation time.

Quantum control in open systems has been addressed in the past utilizing measurement and feedback [18–23]. Typically, the effect of non-adiabatic driving on the dissipative dynamics was ignored [24–27]. Here, we present a comprehensive theory that incorporates the non-adiabatic effects. The formalism is based on the recent derivation of the Non Adiabatic Master Equation (NAME) [28]. This master equation is of the Gorini-Kossakowski-Lindblad-Sudarshan (GKLS) form, guaranteeing a complete positive trace-preserving dynamical map [29–31]. A further prerequisite is the *inertial theorem* [32]. This theorem allows extending the validity of the NAME for processes with small 'acceleration' of the external driving.

We consider a driven quantum system, the Hamiltonian of which varies from $\hat{H}_{S}\left(0\right)$ to a final Hamiltonian

 $\hat{H}_S(t_f)$, while coupled to a thermal bath (see Fig. 1). Our aim is to exploit the non-adiabatic effects of the driving to accelerate the systems return to equilibrium. By reverse-engineering the NAME, we find a protocol that transforms the thermal state of $\hat{H}_S(0)$ at temperature T to the corresponding thermal state of $\hat{H}_S(t_f)$.

Controlling the equilibration rate differs from the control tasks treated by shortcuts to adiabaticity [33–42]. The latter protocols generate an entropy-preserving unitary transformation, which is effectively the identity map between initial and final diagonal states in the energy representation. Conversely, the STE procedure is a non-unitary transformation, which is designed to rapidly change the entropy of the system.

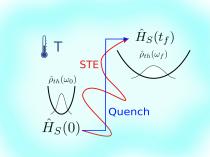


FIG. 1: Scheme of the Shortcut To Equilibration (STE) protocol (curved red line) and the quench protocol (blue step line), transforming an initial thermal state at temperature T and frequency ω_i to a final thermal state with an equivalent temperature and frequency ω_f .

System dynamics We consider a quantum particle in contact with a thermal bath while confined by a time-dependent harmonic trap. The system Hamiltonian reads

$$\hat{H}_{S}(t) = \frac{\hat{P}^{2}}{2m} + \frac{1}{2}m\omega^{2}(t)\,\hat{Q}^{2},$$
 (1)

where \hat{Q} and \hat{P} are the position and momentum operators, respectively, m is the particle mass and $\omega\left(t\right)$ is the time-dependent oscillator frequency. We assume a Bosonic bath with 1D Ohmic spectral density and an interaction Hamiltonian of the form $\hat{H}_{I}=-\hat{D}\otimes\hat{B}$, where $\hat{D}=d\hat{a}+d^{*}\hat{a}^{\dagger}$ (a and a^{\dagger} are the annihilation and creation operators of the oscillator, respectively), d is the interaction strength and \hat{B} is the bath interaction operator. Throughout the paper, we choose units related to the minimum frequency ω_{min} , time $2\pi/\omega_{min}$ and energy $\hbar\omega_{min}$ with $\hbar=1$.

At initial time, the open quantum system is in equilibrium with the bath, and the state is of a Gibbs canonical form $\hat{\rho}_S(0) = Z^{-1}e^{-\hat{H}_S(0)/k_BT}$, where Z is the partition function, k_B is the Boltzmann constant and T is the temperature of the bath. We search for a protocol that varies the Hamiltonian toward $\hat{H}_S(t_f)$ with a target thermal state $\hat{\rho}_S^{Th}(t_f) = Z^{-1}e^{-\hat{H}_S(t_f)/k_BT}$. This procedure serves as a shortcut to an isothermal process. The accuracy of this transformation can be quantified using the fidelity \mathcal{F} , which is a measure of the distance between the final state $\hat{\rho}_S(t_f)$ of the protocol and $\hat{\rho}_S^{Th}(t_f)$ [43–45]. A classical analogous problem has been addressed by Martinez et al. [3].

The most straightforward protocol is a quench protocol. 'Quench' means abruptly changing the Hamiltonian from $H_S(0)$ to $H_S(t_f)$, and then letting the system equilibrate with the bath, Cf. Supplemental Material (SM) III. We assume the open system dynamics are Markovian, safeguarding the relaxation of the Harmonic oscillator towards a thermal state. When $\hat{H}_{S}\left(0\right)$ and $\hat{H}_{S}\left(t_{f}\right)$ do not commute, which is the case for a non-rigid harmonic oscillator, such a sudden change generates coherence in the energy basis, leading to deviations from equilibrium. The quenched system relaxes at an exponential rate toward equilibrium, which leads to an asymptotic exponential convergence of the fidelity toward unity $1 - \mathcal{F}(t) \propto e^{-kt}$, for t/k > 1, with $k = k_{\downarrow} - k_{\uparrow}$, where k_{\downarrow} and k_{\uparrow} are decay rates, Cf. SM IIIA. We use the quench protocol as a benchmark to assess the STE protocol's performance.

To describe the reduced dynamics under the STE, we follow the derivation presented in Refs. [28, 32]. First, we obtain a solution for the unitary propagator $\hat{U}_S(t,0)$ for a protocol determined by a constant adiabatic parameter $\mu = \dot{\omega}/\omega^2$. The closed-form solution of $\hat{U}_S(t,0)$ allows constructing a master equation that includes the bath's influence on the reduced dynamics. Then, by utilizing the inertial theorem, we extend the description to protocols where μ varies slowly $(d\mu/dt \ll 1)$. This condition sets a lower bound for the minimum protocol duration. For protocols faster than the minimum time, the condition $d\mu/dt \ll 1$ is no longer satisfied and the inertial approximation loses its validity [32, 46]. The bound is given by $t_f > f \cdot \max_s \left(\frac{1}{\omega} \sqrt{\frac{\omega''(s)}{2\omega} \frac{1}{8-\mu^2}}\right)$, where $s = t/t_f$

and f < 1 is a small scalar, dependent on the desired precision, Cf. SM II. For example, if f = 0.05, the lower bound is $t_f > 4.38 \ (2\pi/\omega_{min})$, where $\omega_{min} = 5$ a.u.

The range of validity of the NAME sets a number of conditions: (i) weak coupling between system and bath, which also allows for a reduced description of the system's dynamics in terms of $\hat{\rho}_S$ [4]; (ii) Markovianity [47]; (iii) large Bohr frequencies relative to the relaxation rate τ_R ; (iv) slow driving relative to the decay of the bath correlations. In the following, we consider a regime where the NAME and *inertial theorem* are valid.

The dynamics of the externally driven open quantum system, in the interaction representation, is described by

$$\frac{d}{dt}\tilde{\rho}_{S}(t) = k_{\downarrow}(t) \left(\hat{b}\tilde{\rho}_{S}(t) \hat{b}^{\dagger} - \frac{1}{2} \{ \hat{b}^{\dagger}\hat{b}, \tilde{\rho}_{S}(t) \} \right)
+ k_{\uparrow}(t) \left(\hat{b}^{\dagger}\tilde{\rho}_{S}(t) \hat{b} - \frac{1}{2} \{ \hat{b}\hat{b}^{\dagger}, \tilde{\rho}_{S}(t) \} \right) \quad . \quad (2)$$

Here, the density operator in the interaction picture reads $\tilde{\rho}_{S}\left(t\right) = \hat{U}_{S}\left(t,0\right)\hat{\rho}_{S}\left(t\right)\hat{U}_{S}^{\dagger}\left(t,0\right)$.

$$k_{\downarrow}(t) = k_{\uparrow}(t) e^{\alpha(t)/k_B T} = \frac{\alpha(t) |\vec{d}|^2}{4\pi\varepsilon_0 \kappa \hbar c} (1 + N(\alpha(t))) ,$$
(3)

where N is the occupation number of the Bose-Einstein distribution and α is a modified frequency, determined by the non-adiabatic driving protocol and $\kappa = \sqrt{4 - \mu^2}$ [28]. In terms of the oscillator frequency, the modified frequency is given by

$$\alpha(t) = \sqrt{1 - \left(\dot{\omega}(t)/\left(2\omega^2(t)\right)\right)^2}\omega(t) \quad . \tag{4}$$

The Lindblad jump operators become $\hat{b} \equiv \hat{b}(0) = \sqrt{\frac{m\omega(0)}{\kappa\hbar}} \frac{\kappa + i\mu}{2} \left(\hat{Q}(0) + \frac{\mu + i\kappa}{2m\omega(0)} \hat{P}(0) \right)$.

In the interaction representation the Lindblad operators are time-independent. This property provides an explicit solution in terms of the second-order moments $\mathcal{B} = \{\hat{b}^{\dagger}\hat{b}, \hat{b}^{2}, \hat{b}^{\dagger 2}\}$ [28, 32], Cf. SM I, which, together with the identity operator, form a closed Lie algebra. The solution is given by a generalized canonical state, which has a Gaussian form in terms of \mathcal{B} . Such states are canonical invariant under the dynamics described by Eq. (2), implying that the system can be described by the generalized canonical state throughout the entire evolution [48–51]. The system state in the interaction representation is given by

$$\tilde{\rho}_S(t) = Z^{-1} e^{\gamma(t)\hat{b}^2} e^{\beta(t)\hat{b}^{\dagger}\hat{b}} e^{\gamma^*(t)\hat{b}^{\dagger 2}} ,$$
 (5)

which is completely defined by the time-dependent coefficients γ and β and the driving protocol. The partition function reads $Z\left(\beta,\gamma\right)=\frac{e^{-\beta}}{(e^{-\beta}-1)\sqrt{1-4|\gamma|^2/(e^{-\beta}-1)^2}}.$ In the adiabatic limit, the adiabatic parameter μ approaches zero, the state follows the adiabatic solution, and $\hat{b}^{\dagger}\hat{b}\rightarrow\hat{a}^{\dagger}\hat{a}.$

Substituting $\tilde{\rho}_S(t)$ into the master equation, Eq. (2), multiplying by $\tilde{\rho}_S^{-1}$ from the right and comparing the terms proportionate to the operators $\tilde{b}^{\dagger}\tilde{b}$, \tilde{b}^2 and $\tilde{b}^{\dagger 2}$ leads to

$$\dot{\beta} = k_{\downarrow} \left(e^{\beta} - 1 \right) + k_{\uparrow} \left(e^{-\beta} - 1 + 4e^{\beta} |\gamma|^2 \right),
\dot{\gamma} = \left(k_{\downarrow} + k_{\uparrow} \right) \gamma - 2k_{\downarrow} \gamma e^{-\beta} .$$
(6)

These equations describe the evolution of the system for any initial squeezed thermal state. Here, we assume that the system is in a thermal state at the initial time, which infers $\gamma(0) = 0$. This simplifies the expression of the state to

$$\tilde{\rho}_S(\beta(t), \mu(t)) = Z^{-1} e^{\beta \hat{b}^{\dagger} \hat{b}(\mu)} , \qquad (7)$$

and consequently the system dynamics are described by a single non-linear differential equation

$$\dot{\beta} = k_{\downarrow}(t) \left(e^{\beta} - 1 \right) + k_{\uparrow}(t) \left(e^{-\beta} - 1 \right) \quad , \tag{8}$$

with initial conditions $\beta\left(0\right)=-\frac{\hbar\omega\left(0\right)}{k_{B}T}$ and $\mu\left(0\right)=0$. Equation (8) constitutes the basis for the suggested control scheme.

Control The control target is to transform a thermal state, defined by frequency ω_i , to a thermal state of frequency ω_f , while interacting with a bath at temperature T. The control utilizes the fact that at all times, the state is fully defined by $\mu(t)$ and $\beta(t)$. This property implies $\beta(0) = -\frac{\hbar\omega_i}{k_BT}$, $\beta(t_f) = -\frac{\hbar\omega_f}{k_BT}$ and $\mu(0) = \mu(t_f) = 0$. The initial and final β are connected through Eq. (8), where the protocol defines the rates $k_{\uparrow}(t)$ and $k_{\downarrow}(t)$. These rates are determined by the parameter $\alpha(t)$ in Eq. (3), which in turn is completely defined by the control parameter $\omega(t)$ in Eq. (4). Furthermore, $\mu(t)$ is determined by $\omega(t)$, and therefore $\omega(t)$ fully determines the state of the system at all times.

The strategy to solve the control equation is based on a reverse-engineering approach, and the protocol is denoted by *Shortcut To Equilibration* (STE). The method proceeds as follows: we define a new variable $y = e^{\beta}$, and propose an ansatz for y that satisfies the boundary conditions. Then we solve for $\alpha(t)$, and from $\alpha(t)$ determine $\omega(t)$.

The initial and final thermal states determine the boundary conditions of $\mu(t)$, which implies that the state is stationary at initial and final times. This leads to additional boundary conditions $\dot{\beta}(0) = \dot{\beta}(t_f) = \dot{\alpha}(0) = \dot{\alpha}(t_f) = 0$.

When $\mu = 0$ ($\dot{\omega} = 0$) the Lindblad jump operator \hat{b} converges to the annihilation operator \hat{a} . This implies that the final state is a thermal state with a frequency ω_f at a temperature T [52].

A fifth-degree polynomial is sufficient to obey all of the constraints. Introducing $s = t/t_f$, the solution reads

$$y(s) = y(0) + c_3 s^3 + c_4 s^4 + c_5 s^5$$
, (9)

where $c_3 - c_5$ are determined from the boundary conditions $y(0) = e^{\beta(0)}$, $y(t_f) = e^{\beta(t_f)}$, $\dot{y}(0) = \dot{y}(t_f) = \ddot{y}(0) = \ddot{y}(t_f) = 0$. In principle, more complicated solutions for Eq. (8) exist; however, here we restrict the analysis to a polynomial solution [53]. The implicit equation for $\alpha(t)$ becomes

$$t_{f} \frac{d}{ds} y(s) = k_{\downarrow} (\alpha(s)) y(s)^{2} - y(s) (k_{\downarrow} (\alpha(s)) + k_{\uparrow} (\alpha(s))) + k_{\uparrow} (\alpha(s)) . \quad (10)$$

Solving the equation by numerical means generates $\alpha(s)$. This solution is substituted into Eq. (4) and the control $\omega(t)$ is obtained by an iterative numerical procedure. The protocol satisfies the inertial condition on μ , inferring that the derivation is self-consistent.

The solution of the STE incorporates the adiabatic result in the limit of slow driving. For large protocol time duration $(t_f \to \infty)$, the system's instantaneous state is a thermal state at temperature T with frequency $\omega(t)$, see SM V. A similar derivation can be obtained for a SU(2) algebra, see SM VII.

We compare the STE protocol to a quench protocol involving a sudden change from $\omega\left(0\right)=\omega_{i}$ to $\omega\left(t_{f}\right)=\omega_{f}$. Two cases are studied, a compression of the potential, which corresponds to the transition $\omega\left(0\right)=5\rightarrow\omega\left(t_{f}\right)=10$, and a reversed expansion, associated with the transition $\omega\left(0\right)=10\rightarrow\omega\left(t_{f}\right)=5$. Both protocols are presented in Fig. 2 panels (a) and (b). We add, as a reference, an adiabatic process obtained in the limit $t_{f}\rightarrow\infty$. The initial stage of the quench protocol is effectively isolated, as the change in frequency is rapid relative to the relaxation rate toward equilibrium. As a result, the state stays constant while the Hamiltonian abruptly transforms to $\hat{H}_{S}\left(t_{f}\right)$. Coherence is generated with respect to $\hat{H}_{S}\left(t_{f}\right)$, because $\left[\hat{H}_{S}\left(0\right),\hat{H}_{S}\left(t_{f}\right)\right]\neq0$. After the initial stage energy is exchanged with the bath and the coherence dissipates.

In figure 3, we compare the fidelity with respect to the target thermal state of the expansion and compression protocols, for increasing stage times t_f . The STE protocol transfers the system to the target thermal state with fidelities close to unity $\mathcal{F} \approx 1$, while the quench target has lower fidelity due to the slow relaxation. Therefore, the STE protocol equilibrates the system faster and with higher accuracy than the quench protocol. For a given fidelity, the STE achieves the target state up to five times faster than the quench protocol.

Figure 2 panels (c) and (d) presents a comparison of the quantum state's energy for the STE, quench and adiabatic protocols. During the quench protocol, there is a sudden change in the energy, which is followed by a slow exponential decay toward the thermal energy. The adiabatic and STE protocols are characterized by an overshoot beyond the final thermal energy. In the final stage of the STE protocol, the energy rapidly converges to the

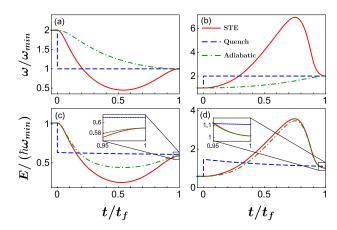


FIG. 2: Control protocols as a function of the scaled time t/t_f : (a,b) the oscillator frequency ω and (c,d) energy for the STE (red line), quench (dashed blue line) and adiabatic (dot-dashed green line) protocols. (a,c) Expansion, (b,d) compression protocols. The dynamics of the STE and quenched systems are shown for $t_f=8$ a.u, and the adiabatic dynamics are obtained in the limit $t_f\to\infty$ (c,d) Inset: details of the final approach to the target state. Model parameters (atomic units): ω (0) $/\omega_f=5/10$ for the compression, and reverse for the expansion and bath temperature T=2.

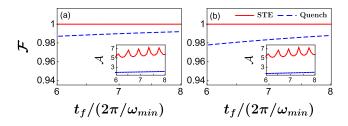


FIG. 3: The fidelity of the final state relative to the target thermal state for the short-cut to equilibration (red) and quench (blue) protocols. (a) Expansion protocol, (b) compression protocol. The error of the STE is dominated by the accuracy of the inertial solution (see SM VI). The fidelity was therefore estimated from the deviation between the inertial solution and the exact free propagation. The inset shows the accuracy $\mathcal{A} = -\log_{10}{(1-\mathcal{F})}$, highlighting the 3-digit accuracy of the STE protocol. Model parameters are the same as in Fig. 2

desired thermal energy, whereas the quenched system remains far from equilibrium (see insets in Fig. 2 panels (c) and (d)).

Energy and entropy cost A control task can be evaluated by the work and entropy cost required to implement the control. Restrictions on the cost can be connected to quantum friction [8, 54], which implies that quicker transformations are accompanied by a higher energy cost [38, 55–58]. Moreover, in any externally controlled process there is an additional cost in energy and entropy to generate faster driving [59, 60]. The work cost for the STE protocol with a duration time t is defined by $W(t) = \int_0^t \operatorname{tr} \left(\hat{\rho}_S(t') \frac{\partial \hat{H}(t')}{\partial t'} \right) dt'$.

For the *quench* protocol, the sudden transition occurs on a much faster timescale than the exchange rate of energy with the bath. This implies that the change in internal energy is equal to the work cost. For the expansion

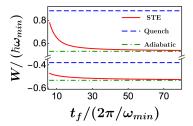


FIG. 4: Work required to perform the driving protocol as a function of the normalized time. Model parameters are identical to Fig. 3. Upper part: compression, lower part: expansion.

stroke (Fig. 4) work is generated by the system. The minimum work is achieve for the quench protocol, the STE is superior and the the optimal work is obtained in the adiabatic limit. When the system is compressed, the STE and quench protocols require additional work compared to the adiabatic process. This result is in accordance with thermodynamic principles, as any rapid driving will induce irreversible dynamics, which in turn leads to sub-optimal performance. For long times, the work of the STE procedure approaches the adiabatic result according to a t^{-1} scaling law. At this limit, the global entropy production approaches zero. For shorter times, the system entropy change, for the STE procedure, is almost independent of protocol duration as a result of the accurate control. The price for shorter protocols is an increase in irreversibility, manifested by larger global entropy production (see SM VI).

Discussion Quantum control is achieved by manipulating the system Hamiltonian via a change of an external control parameter. In turn, the change in the system Hamiltonian influences the system-bath interaction and the equation of motion. Hence, manipulating the Hamiltonian indirectly controls the dissipation rate.

The control procedure is based on *canonical invariance*, where the state of the system can be described by a generalized Gibbs state, Eq. (5), throughout the process. This description requires that the system dynamics are characterized by a closed Lie algebra. The algebraic structure is also incorporated in the equations of motion, it forms the basis for the *inertial theorem* and consequently to the non-adiabatic master equation, Eq. (2) [28].

Substituting the generalized canonical form in the equation of motion, Eq. (2), leads to a set of coupled non-linear differential equations of the state parameters, γ and β , which define the generalized canonical state, Eq. (5). These equations completely describe the system dynamics and implicitly depend on the control parameter. They are the basis for the control procedure.

The open-system protocol controls both the system's entropy and the coherence in the instantaneous energy

representation. In contrast a unitary control leaves the system's entropy invariant. For example, the unitary shortcut to adiabaticity protocol controls only the final coherence in free dynamics (see SM VII).

To solve the control problem, we insert a functional form for the state parameters which obeys the correct boundary conditions. Specifically, the parameters are associated with the initial and final thermal states, $\beta\left(0\right)=-\hbar\omega_{0}/k_{B}T$ and $\beta\left(t_{f}\right)=-\hbar\omega_{f}/k_{B}T$, with vanishing derivatives at the boundaries. The considered functional form is a fifth-order polynomial, the coefficients of which are determined by the boundary conditions. This leads to an implicit equation in terms of the control parameter $\omega\left(t\right)$.

At first glance, it would seem that the quench protocol is optimal, since the approach to equilibrium is exponentially fast. However, a superior solution is obtained by the STE protocol. The advantage of the latter is that it incorporates both the dissipative and unitary parts of the dynamics, changing the rates and engineering the state simultaneously.

The STE protocol can be generalized beyond the isothermal example studied here, for three different kinds of scenarios: (i) the temperature of the initial state differs from the bath temperature; (ii) the case of varying bath temperature (with the help of Eq. (3)); (iii) squeezed initial and final states. These general control tasks should be approached by reverse-engineering of both β and γ in Eq. (6). Furthermore, once a non-adiabatic master equation is obtained [28, 32], the method can be generalized to systems characterized by a closed Lie algebra, for example the SU(2) algebra see SM VII.

To conclude, the STE result demonstrates the feasibility of controlling the entropy of an open quantum system. Such control can be combined with fast unitary transformations to obtain a broad class of states within the system algebra. This will pave the way to faster high-precision quantum control, altering the state's entropy.

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