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Energetic advantages of non-adiabatic drives combined with non-thermal quantum states

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Unitary drivings of quantum systems are ubiquitous in experiments and applications of quantum mechanics and the underlying energetic aspects, particularly relevant in quantum thermodynamics, are receiving growing attention. We investigate energetic advantages in unitary driving obtained from initial non-thermal states. We introduce the non-cyclic ergotropy to quantify the energetic gains, from which coherent (coherence-based) and incoherent (population-based) contributions are identified. In particular, initial quantum coherences appear to be always beneficial whereas non-passive population distributions not systematically. Additionally, these energetic gains are accessible only through non-adiabatic dynamics, contrasting with the usual optimality of adiabatic dynamics for initial thermal states. Finally, following frameworks established in the context of shortcut-to-adiabaticity, the energetic cost related to the implementation of the optimal drives are analysed and, in most situations, are found to be smaller than the energetic cost associated with shortcut-to-adiabaticity. We treat explicitly the example of a two-level system and show that energetic advantages increase with larger initial coherences, illustrating the interplay between initial coherences and the ability of the dynamics to consume and use coherences.

Introduction.—Most quantum experiments and quantum technologies require manipulation of quantum systems’ Hamiltonian. Among the infinite variety of drivings realizing the desired Hamiltonian transformation, the least energy-consuming ones are of high interest for energy controlled applications, like in thermodynamics but soon in quantum information processing and computation [1, 2]. These least energy-consuming unitary evolutions are commonly associated with the well-known family of adiabatic drives. The traditional criterion for adiabaticity relies on the slow variation of the driving with respect to the velocity of the system’s evolution [3] (see also [4–6] for recent reformulation and extension). The energetic aspects and the origin of non-adiabaticity—the breakdown of adiabaticity—were recently shown to stem from the non-commutativity of the time dependent Hamiltonian [7–9], giving rise to generation of quantum coherences and consequently extra energetic costs [10] as well as *irreversible work* [11–13]. Such manifestations of *quantum friction* [7–9] can be circumvented using techniques like shortcut-to-adiabaticity [14–17], widely applied in theoretic and experimental thermodynamics [18–23, 25], adiabatic quantum computing [26], experimental state engineering [27], and quantum information processing [28].

Nevertheless, the above considerations and results are valid for initial thermal states. Here, we focus on initial non-thermal states and the energetic consequences for driving operations. We show that non-adiabatic drives become energetically optimal, highlighting the ongoing interplay between the initial coherences contained in the system and the capacity of the drive to consume coherences. We introduce the concept of *non-cyclic ergotropy* to quantify the corresponding energetic gains. We also investigate the energetic cost required for the

implementation of the optimal drives. Compared to shortcut-to-adiabaticity techniques, we show explicitly in an example with a two-level system that non-adiabatic drives combined with initial non-thermal states can bring higher energetic gains simultaneously with lower energetic costs.

Let us consider the operation consisting in driving a quantum system S from an initial Hamiltonian H_i to a final one H_f , with their respective eigenvalues and eigenvectors denoted by e_n^x and $|e_n^x\rangle$, for $x = i, f$, in increasing order, $e_{n+1}^x \geq e_n^x$. We start the analysis by one of the central quantity of the problem: $E_f := \text{Tr}(\rho_f H_f)$, the energy of the final state ρ_f , reached at the end of the driving. For a given arbitrary initial state ρ_i of initial energy $E_i := \text{Tr}(\rho_i H_i)$, there is an infinite variety of driving Hamiltonians $H(t)$ satisfying $H(t_i) = H_i$ and $H(t_f) = H_f$, leading to an infinity of different final energy. Independently of whether the driving operation injects energy in S ($E_f \geq E_i$) or extracts energy from S ($E_f \leq E_i$), the optimal drive, which is in fact not unique, has to minimise E_f , so that it minimises the energetic costs or maximises the energetic gains of the operation. Therefore, our first aim is to find the minimum $\tilde{E}_f := \min_{U \in \mathcal{U}} \text{Tr}(U \rho_i U^\dagger H_f)$, where \mathcal{U} is the ensemble of unitary operations generated by drives $H(t)$ satisfying $H(t_i) = H_i$ and $H(t_f) = H_f$. As we will see in the following, \mathcal{U} is indeed simply equal to the ensemble of all unitary transformations – in other words, any unitary transformation can be expressed as a unitary transformation generated by a time dependent Hamiltonian satisfying $H(t_i) = H_i$ and $H(t_f) = H_f$.

Since all unitarily accessible final states have necessarily the same entropy as ρ_i , one might first think of \tilde{E}_f as the smallest energy over the ensemble of states of

same entropy as ρ_i . Then, given that the state of smallest energy at fixed entropy is a thermal state, one would conclude that \tilde{E}_f corresponds to the energy of $(\rho_i)_f^{\text{th}}$, the thermal state with respect to H_f of same entropy as ρ_i . However, reminding that unitary evolutions conserve eigenvalues, $(\rho_i)_f^{\text{th}}$ cannot in general be reached unitarily, unless the eigenvalues r_n of the initial state ρ_i are equal to the populations of a thermal state of H_f , as highlighted in [29]. Therefore, the state of lower energy which is always achievable through unitary operations is not $(\rho_i)_f^{\text{th}}$ but $(\widetilde{\rho_i})_f$, a state diagonal in the eigenbasis of H_f with eigenvalues equal to r_n ,

$$(\widetilde{\rho_i})_f := \sum_n r_n |e_n^f\rangle\langle e_n^f|, \quad (1)$$

where $r_{n+1} \leq r_n$. The associated minimal difference of energy is

$$-\mathcal{E}_{\text{nc}} := \text{Tr}[(\widetilde{\rho_i})_f H_f] - \text{Tr}(\rho_i H_i) = \sum_n r_n e_n^f - \text{Tr}(\rho_i H_i). \quad (2)$$

The state in (1) belongs to the family of passive states [30, 31], defined as follows. For a given Hamiltonian $H = \sum_n e_n |e_n\rangle\langle e_n|$, where the energies are ordered in increasing order, $e_{n+1} \geq e_n$, a state ρ is said to be *passive with respect to H* if: (i) it is diagonal in the energy eigenbasis $\{|e_n\rangle\}_n$; (ii) it has decreasing populations, $p_{n+1} = \langle e_{n+1} | \rho | e_{n+1} \rangle \leq p_n = \langle e_n | \rho | e_n \rangle$. The violation of any of these two conditions leads to two different types of *non-passivity*: non-passivity stemming from populations when (ii) is not fulfilled, and non-passivity stemming from coherences when (i) is not fulfilled. These different physical origins of non-passivity will be used in the next paragraph. Of course, it is also possible to have non-passivity stemming from both populations and coherences when neither (i) nor (ii) is fulfilled. Finally, a famous example of passive states is the thermal states.

In the context of cyclic work extraction, where the aim is to extract as much work as possible from a quantum state ρ through time-dependent driving under the *cyclic* constraint $H(t_i) = H(t_f) = H$, it was shown in pioneering studies [29, 32] that no work can be cyclically extracted from passive states with respect to H . For states which are not passive, the maximal amount of cyclically extractable work is called *ergotropy*. Contrarily to what one could have expected, the ergotropy is not directly related to the minimal energy difference $-\mathcal{E}_{\text{nc}}$ – the relevant quantity in our problem. We call the quantity \mathcal{E}_{nc} the *non-cyclic ergotropy* since it is related to non-cyclic operations $H_i \neq H_f$. In particular, contrasting with the ergotropy, the non-cyclic ergotropy can be positive or negative. When positive, it represents the maximal energy extractable from ρ_i while realising the driving from H_i to H_f . When negative, its absolute value represents the minimal energy needed to take the system from H_i to H_f when starting from ρ_i . Additionally, passive states with respect to H_i are not always the states of smallest non-cyclic ergotropy,

as shown in the following (neither are the passive states with respect to H_f). Before continuing, a small note on the notations: $\tilde{\sigma}$ denotes the passive state of same entropy as σ (also called the passive state of σ) with respect to H_i . $(\widetilde{\sigma})_f$ denotes the passive state of σ with respect to H_f .

Necessity of incoherent and coherent non-adiabatic transformations.—It should be emphasised that any dynamics leading to a final passive state is necessarily non-adiabatic if and only if the initial state is a non-passive state with respect to H_i , contrasting with the usual adiabatic dynamics required for initial thermal states [10–13]. This can be easily seen by writing the initial state in its diagonal form.

Furthermore, we notice that there are two kinds of non-adiabatic transformations: the incoherent ones, which generate transitions between different initial and final energy levels but do not generate coherences in the eigenbasis of H_f , and the coherent ones, which do generate coherences in the eigenbasis of H_f . This finds an interesting parallel with the type of non-passive features – with respect to H_i – initially present in ρ_i . If the initial state contains non-passive features stemming only from populations, non-adiabatic evolutions yielding $(\rho_i)_f$ are incoherent (see Appendix A). Alternatively, if the non-passivity of ρ_i is coherence-based, evolutions yielding $(\widetilde{\rho_i})_f$ are necessarily coherent non-adiabatic. This highlights the interplay between coherences contained in ρ_i and the ability of the evolution to consume and use coherences.

This difference in the nature of the required transformation is mirrored in \mathcal{E}_{nc} : the non-cyclic ergotropy can be decomposed in a sum of an incoherent, a passive and a coherent contributions, $\mathcal{E}_{\text{nc}} = \mathcal{E}_{\text{nc}}^{\text{inc}} + \mathcal{E}_{\text{nc}}^{\text{pas}} + \mathcal{E}_{\text{nc}}^{\text{coh}}$. The incoherent contribution can be defined as $\mathcal{E}_{\text{nc}}^{\text{inc}} := \text{Tr}(\rho_i H_i) - \text{Tr}[\widetilde{\rho_{i|D}} H_i]$, where $\rho_{i|D} := \sum_n \langle e_n^i | \rho_i | e_n^i \rangle |e_n^i\rangle\langle e_n^i|$ is the “diagonal cut” of ρ_i and $\widetilde{\rho_{i|D}}$ its associated passive state with respect to H_i . The passive contribution can be identified as $\mathcal{E}_{\text{nc}}^{\text{pas}} := \text{Tr}[\widetilde{\rho_{i|D}} H_i] - \text{Tr}[(\widetilde{\rho_{i|D}})_f H_f]$ where $(\widetilde{\rho_{i|D}})_f$ is the passive state of $\rho_{i|D}$ with respect to H_f . Finally, the coherent contribution can be identified as $\mathcal{E}_{\text{nc}}^{\text{coh}} = \text{Tr}[(\widetilde{\rho_{i|D}})_f H_f] - \text{Tr}[(\widetilde{\rho_i})_f H_f]$. Additional technical details can be found in Appendix A. This extends similar considerations presented in [12, 33] on ergotropy.

Energetic gains.—We are now in position of evaluating the energetic advantages in driving operations provided by non-passivity. These advantages are given by the amount of energy gained (or saved) thanks to the use of the best strategy starting from a non-thermal state compared to the best strategy starting from a thermal state of same energy. As detailed in the following, such energy gain is directly given by the difference of non-cyclic

ergotropies between the initial thermal and non-thermal states.

More precisely, for an initial thermal state, it is well-known, as mentioned in the introduction, that energetically optimal drives are either adiabatic (quasi-static), or use shortcut-to-adiabaticity techniques [14–17]. Then, from the initial thermal state $\rho_i^{\text{th}} = \sum_n p_{i,n}^{\text{th}} |e_n^i\rangle\langle e_n^i|$, where $p_{i,n}^{\text{th}} := Z^{-1} e^{-\beta e_n^i}$, $Z := \text{Tr}(e^{-\beta H_i})$ and β plays the role of the inverse temperature, such drives yield the final passive state $(\rho_i^{\text{th}})_f$, given by (1) substituting r_n by $p_{i,n}^{\text{th}}$. Note that $(\rho_i^{\text{th}})_f$ is generally not a thermal state if the energy spectrum of H_f is not “proportional” to the one of H_i . The non-cyclic ergotropy, applicable also for initial thermal states, is reached by these optimal drives and is given by (2) $\mathcal{E}_{\text{nc}} = \text{Tr}(\rho_i^{\text{th}} H_i) - \text{Tr}[(\rho_i^{\text{th}})_f H_f] = \sum_n p_{i,n}^{\text{th}} (e_n^i - e_n^f)$.

Thus, the non-cyclic ergotropy difference, representing the energy difference between the best strategies starting either from a thermal state ρ_i^{th} or from a non-thermal ρ_i of same energy, is given by

$$\begin{aligned} \Delta\mathcal{E}_{\text{nc}} &:= \text{Tr}[(\rho_i^{\text{th}})_f H_f] - \text{Tr}[(\rho_i)_f H_f] \\ &= \sum_n (p_{i,n}^{\text{th}} - r_n) e_n^f. \end{aligned} \quad (3)$$

Is $\Delta\mathcal{E}_{\text{nc}}$ always positive? Quite surprisingly, the answer is no, contrasting with cyclic ergotropy. It means that, some thermal states have a larger non-cyclic ergotropy than some non-passive states of same energy, or in other words, more work can be extracted non-cyclicly from some thermal states than from some non-passive states of same energy. We provide explicit examples in Appendix B.

A general condition guaranteeing the positivity of $\Delta\mathcal{E}_{\text{nc}}$ is given by the property of majorization. We recall that for any two density operators ρ and σ , ρ majorizes σ when [29, 34]

$$\sum_{n=1}^k r_n \geq \sum_{n=1}^k s_n \quad (4)$$

for all $k \geq 1$, where r_n and s_n are respectively the eigenvalues of ρ and σ , in decreasing order. Then, the positivity of $\Delta\mathcal{E}_{\text{nc}}$ is guaranteed when ρ_i majorizes ρ_i^{th} , which can be seen using summation by part [29], $\Delta\mathcal{E}_{\text{nc}} = \sum_n (p_{i,n}^{\text{th}} - r_n) e_n^f = \sum_{k \geq 1} (e_{k+1}^f - e_k^f) \sum_{n=1}^k (r_n - p_{i,n}^{\text{th}}) \geq 0$.

In particular, this implies that coherence-based non-passivity *always* lead to positive $\Delta\mathcal{E}_{\text{nc}}$, while this is not true for population-based non-passivity. This unexpected difference stems from the passive contribution to $\Delta\mathcal{E}_{\text{nc}}$, which is zero for coherence-based non-passivity whereas it can take any sign – and in particular the negative one – for population-based non-passivity, Appendix A 3.

We mention briefly an alternative figure of merit quantifying the energetic advantages stemming from the optimal driving itself. It simply consists in the energy gained or saved by applying an optimal drive to a given initial state ρ_i instead of applying an adiabatic drive or a shortcut-to-adiabaticity. It is given by $G_{\rho_i} := \text{Tr}\left\{ \left[U_{\text{ad}} \rho_i U_{\text{ad}}^\dagger - (\rho_i)_f \right] H_f \right\} = \sum_n (p_n^i - r_n) e_n^f$, where U_{ad} denotes the unitary transformation generated by the adiabatic drive or shortcut-to-adiabaticity and $p_n^i := \langle e_n^i | \rho_i | e_n^i \rangle$ are the populations in the initial energy eigenbasis. This quantity corresponds to the *cyclic* ergotropy of the state $U_{\text{ad}} \rho_i U_{\text{ad}}^\dagger$ (and therefore also of ρ_i) with respect to H_f , and thus is always positive by contrast with $\Delta\mathcal{E}_{\text{nc}}$. Note that for initial states with non-passivity stemming from coherences, as in the examples considered below, we have $\Delta\mathcal{E}_{\text{nc}} = G_{\rho_i}$.

Upper bound and achievability.—The non-cyclic ergotropy is naturally upper bounded by

$$\begin{aligned} \mathcal{E}_{\text{nc}} &= \text{Tr}(\rho_i H_i) - \text{Tr}[(\rho_i)_f H_f] \\ &\leq \text{Tr}(\rho_i H_i) - \text{Tr}[(\rho_i)_f^{\text{th}} H_f] \end{aligned} \quad (5)$$

where $(\rho_i)_f^{\text{th}}$ is the thermal state of H_f of same entropy as ρ_i , already introduced previously. We denote by β_i its inverse temperature. The ergotropy difference (3) is therefore upper bounded by

$$\begin{aligned} \Delta\mathcal{E}_{\text{nc}} &\leq \text{Tr}[(\rho_i^{\text{th}})_f H_f] - \text{Tr}[(\rho_i)_f^{\text{th}} H_f] \\ &= \beta_i^{-1} \Delta S + \beta_i^{-1} S[(\rho_i)_f^{\text{th}} | (\rho_i)_f^{\text{th}}] \end{aligned} \quad (6)$$

where $\Delta S := S(\rho_i^{\text{th}}) - S(\rho_i)$ is the difference of Von Neumann entropy and is positive since ρ_i^{th} and ρ_i have the same energy. This upper bound is automatically saturated when the final passive state $(\rho_i)_f$ is a thermal state (and therefore equal to $(\rho_i)_f^{\text{th}}$). However, when $(\rho_i)_f \neq (\rho_i)_f^{\text{th}}$, the upper bound can still be saturated asymptotically by using many copies of the non-thermal state ρ_i , see Appendix C. This relies on the theorem shown in [32]. Similarly, G_{ρ_i} is upper bounded by $G_{\rho_i} \leq \text{Tr}\left\{ \left[U_{\text{ad}} \rho_i U_{\text{ad}}^\dagger - (\rho_i)_f^{\text{th}} \right] H_f \right\}$, which can be saturated in the same conditions as Eq. (6) thanks to [32].

As a result, any non-thermal features is energetically beneficial in the asymptotic limit of many copies, whereas for a single copy, non-thermality and even non-passivity are not sufficient to guarantee some energetic benefits with respect to initial thermal states – only majorization is sufficient.

Cost of driving.—The remaining questions concern the existence, the explicit form, and the associated energetic cost of optimal drivings saturating the non-cyclic ergotropy. For a given initial non-thermal state $\rho_i = \sum_n r_n |r_n^i\rangle\langle r_n^i|$, we are looking for Hamiltonians $H(t)$ that generate the final unitary transformation $R =$

$\sum_n e^{i\phi_n} |e_n^f\rangle \langle r_n^i|$ with the constraints $H(t_i) = H_i$ and $H(t_f) = H_f$ at initial and final times t_i and t_f . The phases ϕ_n can be chosen freely if one assumes an experimental setup able to control and adjust them, otherwise they will be left random.

For arbitrary initial and final Hamiltonian H_i and H_f we define $H_0(t) := \lambda_i(t)H_i + \lambda_f(t)H_f$, where $\lambda_i(t)$ and $\lambda_f(t)$ are real positive functions such that $\lambda_i(t_i) = \lambda_f(t_f) = 1$ and $\lambda_i(t_f) = \lambda_f(t_i) = 0$. Besides these initial and final conditions, $\lambda_i(t)$ and $\lambda_f(t)$ can be chosen freely, in particular to suits experimental constraints.

One can show (Appendix D) that a family of drivings reaching $(\rho_i)_f$ is of the form $H(t) = H_0(t) + V(t)$ with $V(t) = -\hbar \dot{f}(t) U_0(t) \chi U_0^\dagger(t)$. We introduced $U_0(t) := e^{-\frac{i}{\hbar} \mathcal{T} \int_{t_i}^t du H_0(u)}$ as the unitary transformation generated by the original drive $H_0(t)$, \mathcal{T} is the time-ordering operator, $\chi := -i \ln [U_0^\dagger(t_f) R]$ represents a kind of “overlap” between the aimed transformation R and the one actually generated by the original drive $H_0(t)$, and $f(t)$ is a real function which can be chosen freely besides the following conditions $f(t_i) = \dot{f}(t_i) = \dot{f}(t_f) = 0$ and $f(t_f) = 1$. This also shows that the ensemble \mathcal{U} introduced in the beginning of the paper contains indeed all unitary evolutions since the above reasoning can be repeated for any unitary instead of R .

The additional driving $V(t)$ seems energetically costless at first sight since it does not contribute explicitly to the total work, $\int_{t_i}^{t_f} du \text{Tr} [\rho_u \frac{d}{du} [H_0(u) + V(u)]] = \text{Tr}(\rho_f H_f) - \text{Tr}(\rho_i H_i)$. Still, there is a intrinsic energetic cost associated with the additional driving $V(t)$. This was pointed out in the context of shortcut-to-adiabaticity [35–38] and captured by the time-averaged norm of the additional Hamiltonian or instantaneous additional driving energy [39]. Note that the Hamiltonian norm is also shown to be the relevant quantity to express energetic cost in extended Landauer principle [40]. Following these energetic analysis, the energetic cost associated with the additional drive $V(t)$ is $w := \frac{1}{\tau} \int_{t_i}^{t_f} dt \|V(t)\|$, where $\tau := t_f - t_i$ and $\|V(t)\|$ is the Frobenius norm of $V(t)$, equal to

$$\|V(t)\| := [\text{Tr} [V(t) V^\dagger(t)]]^{1/2} = \hbar |\dot{f}(t)| [\text{Tr} (\chi \chi^\dagger)]^{1/2}. \quad (7)$$

The relation defining χ can be re-written as $e^{i\chi} = \sum_n e^{i\phi_n} |e_n^i\rangle \langle r_n^i|$ with $|e_n^i\rangle := U_0^\dagger(t_f) |e_n^f\rangle$. Since $\sum_n e^{i\phi_n} |e_n^i\rangle \langle r_n^i|$ is a unitary matrix, it is diagonalisable in the form $\sum_n e^{i\theta_n} |u_n\rangle \langle u_n|$, with $\theta_n \in [-\pi; \pi]$ and $|u_n\rangle$ is the associated eigenvector. Then, a suitable choice is $\chi = \sum_n \theta_n |u_n\rangle \langle u_n|$, implying $\|V(t)\| = \hbar |\dot{f}(t)| (\sum_n \theta_n^2)^{1/2}$, and an energetic cost equal to $w = (\sum_n \theta_n^2)^{1/2} \frac{\hbar}{\tau} \int_{t_i}^{t_f} dt |\dot{f}(t)|$. Since $\int_{t_i}^{t_f} dt |\dot{f}(t)| \geq 1$, with the inequality saturated when $\dot{f}(t) \geq 0$ for all $t \in [t_i; t_f]$,

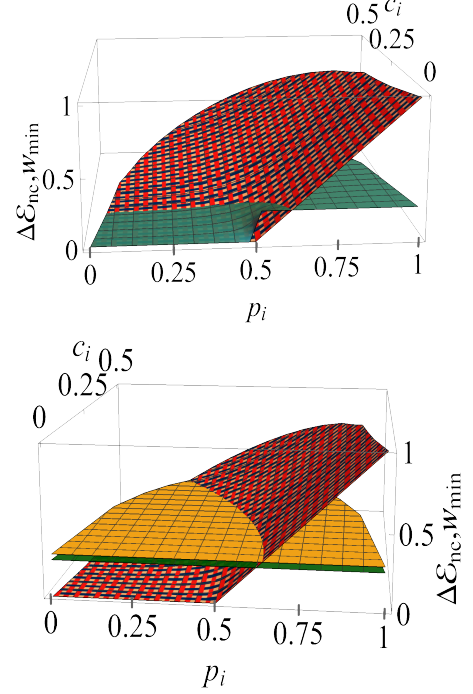


FIG. 1. Top Panel: Plot of the energy gain $\Delta\mathcal{E}_{nc} = G_{\rho_i}$ (texturised surface) and the energetic cost w_{\min} (solid green surface) both in unit of $\hbar\lambda_f\omega$, in function of the initial population $p_i \in [0; 1]$ and coherence $|c_i| \in [0; \sqrt{p_i(1-p_i)}]$. We assume a driving velocity slower than the free evolution, setting $1/\tau = \lambda_f\omega/10$, which allows one to convert \hbar/τ in unit of $\hbar\lambda_f\omega$. Bottom Panel: Same plot with the upper bound $0.89\frac{\hbar\pi}{\tau}$ (yellow horizontal plane) and the lower bound $0.77\frac{\hbar\pi}{\tau}$ (green horizontal plane just below the yellow plane) of the average energetic cost \bar{w}_{\min} (when no experimental control of the phases is available).

we have the following achievable lower bound

$$w \geq w_{\min} := \frac{\hbar}{\tau} \left(\sum_n \theta_n^2 \right)^{1/2}. \quad (8)$$

The term $(\sum_n \theta_n^2)^{1/2}$ can depend on the choice of the phases ϕ_n . If we assume that we have experimentally the full control of such phases, we can choose them in order to minimise $(\sum_n \theta_n^2)^{1/2}$. Otherwise, the phases are random and we will simply average $(\sum_n \theta_n^2)^{1/2}$ over all possible phases to obtain an average cost. Finally, note that $(\sum_n \theta_n^2)^{1/2}$ is upper bounded by $\pi\sqrt{d}$, where d is the dimension of the system.

Illustrative examples.— So far, we showed that non-thermal features can be used to gain or save energy in driving operations. On the other hand, we also saw that there is an intrinsic energetic cost associated with optimal drives. Then, comes the following question: how large the energetic gains and the intrinsic energetic costs can be? We answer this question in two practical exam-

ples involving a two-level system. In the first example, we analyse the situation where H_i is proportional to H_f and compare the energetic gains provided by quantum coherences versus the energetic costs associated with the optimal drives. In the second example, we consider the more general situation where H_i and H_f are not proportional. Then, the bare dynamics $U_0(t)$ is not adiabatic and shortcuts-to-adiabaticity are needed in order to reach $(\rho_i^{\text{th}})_f$ when starting from a thermal state ρ_i^{th} . Thus, in this second example, beyond evaluating the energetic gains provided by quantum coherences, we also compare the intrinsic energetic costs between the optimal drives and shortcut-to-adiabaticity.

Example 1.—We start by analysing the simple but common situation of a two-level system driven by a drive of the form $H_0(t) := \lambda(t)\hbar\frac{\omega}{2}\sigma_z$, which is naturally adiabatic since $[H_0(t), H_0(t')] = 0$ for all t and t' [7, 8]. The time-dependent parameter takes the initial and final positive value $\lambda(t_i) := \lambda_i$ and $\lambda(t_f) := \lambda_f$, and σ_z denotes the z-Pauli matrix, with $|1\rangle$ and $|0\rangle$ the excited and ground states, respectively. A general initial non-thermal state is of the form $\rho_i = \begin{pmatrix} p_i & c_i \\ c_i^* & 1-p_i \end{pmatrix}$ in the basis $\{|1\rangle, |0\rangle\}$. The associated non-cyclic ergotropy is given by (2) with the eigenvalues r_1 and r_0 functions of c_i and p_i (expressions detailed in Appendix E). The minimum energetic cost associated with the family of optimal drivings $V(t)$ is, according to the previous paragraph, given by $w_{\min} = \frac{\sqrt{2}\hbar}{\tau} \arctan \frac{p_i - r_1}{r_0 - p_i}$.

On the other hand, the initial thermal state of same energy as ρ_i is simply $\rho_i^{\text{th}} = \text{diag}(p_i, 1-p_i)$, and the original drive $H_0(t)$ is already adiabatic as commented above. Then, the energetic gain provided by the coherences c_i is given by the non-cyclic ergotropy difference (3), which gives here

$$\Delta\mathcal{E}_{\text{nc}} = \hbar\lambda_f\omega \left[\sqrt{(1/2 - p_i)^2 + |c_i|^2} - 1/2 + p_i \right] \geq 0,$$

and is also equal to the alternative figure of merit G_{ρ_i} .

Fig. 1 (a) presents a plot of $\Delta\mathcal{E}_{\text{nc}} = G_{\rho_i}$ and w_{\min} assuming a driving velocity slower than the free evolution, $1/\tau = \lambda_f\omega/10$. One can see that the energetic gain is always larger than the cost for large initial coherences, as long as $p_i \geq 0.025$ (obtained numerically, not visible on the figure). Note that, rigorously speaking, $\Delta\mathcal{E}_{\text{nc}}$ becomes ill-defined for $p_i \geq 1/2$ because then ρ_i^{th} is not anymore passive (negative temperature). Still, we can use G_{ρ_i} to consider the energetic gain beyond $p_i = 1/2$. Then, the sudden step in the driving cost at $p_i = 1/2$ happens because at this point the populations become inverted. This implies that, for $c_i = 0$, optimal drives must swap the two eigenstates $|0\rangle$ and $|1\rangle$, whose cost is precisely $\frac{\pi\hbar}{\tau\sqrt{2}}$. If the experimental setup does not offer control of the phases ϕ_1 and ϕ_2 , the average energetic cost $\overline{w_{\min}}$ takes value between $0.77\pi\frac{\hbar}{\tau}$ and $0.89\pi\frac{\hbar}{\tau}$, displayed in Fig. 1 (b).

Example 2.—We consider now the same system but

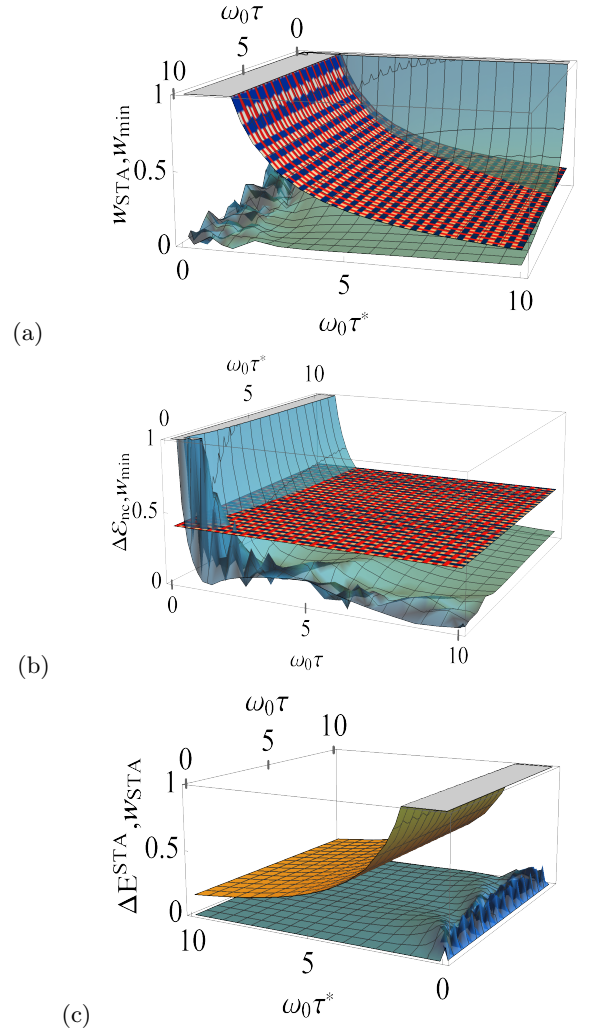


FIG. 2. Plots of (a) w_{STA} (texturised surface) and w_{\min} (blue solid surface); (b) $\Delta\mathcal{E}_{\text{nc}} = G_{\rho_i}$ (horizontal texturised plane) and w_{\min} (blue solid surface); and (c) $\Delta\mathcal{E}^{\text{STA}}$ (lower blue surface) and w_{STA} (upper yellow surface). All plots are in unit of $\hbar\omega_0$ and in function of $\omega_0\tau$ and $\omega_0\tau^*$, for $p_i = 0.4$ and $c_i = \sqrt{0.4 \times 0.6}$.

with $H_i := \frac{1}{2}\hbar\omega_0\sigma_z$ and $H_f := \frac{\hbar\omega_f}{2}\sigma_z + \frac{\hbar\epsilon_f}{2}\sigma_x$ not commuting, implying that $H_0(t)$ is necessarily non-adiabatic. We focus on the following family of driving, $H_0(t) = \frac{1}{2}\hbar\omega(t)\sigma_z + \frac{1}{2}\hbar\epsilon(t)\sigma_x$, with $\omega(t_i) = \omega_0$, $\epsilon(t_i) = 0$, $\omega(t_f) = \omega_f$, and $\epsilon(t_f) = \epsilon_f$. In order to allow for analytic treatment of the dynamics, we assume that the time-dependent frequencies are such that $\mu := \frac{\dot{\omega}(t)\epsilon(t) - \dot{\epsilon}(t)\omega(t)}{\Omega^3(t)}$ is constant [8, 23], where $\Omega(t) := \sqrt{\omega^2(t) + \epsilon^2(t)}$. This includes for instance time dependent frequencies of the form $\omega(t) = \omega_0 \cos[\pi(t - t_i)/2\tau^*]$ and $\epsilon(t) = \omega_0 \sin[\pi(t - t_i)/2\tau^*]$, commonly used experimentally [24]. Such choice implies $\mu = -\pi/(2\omega_0\tau^*)$, $\omega_f = \omega_0 \cos[\pi\tau/2\tau^*]$ and $\epsilon_f = \omega_0 \sin[\pi\tau/2\tau^*]$, whose exact value will depend on one's choice of τ^* . In particular, for $\omega_0\tau^* \rightarrow \infty$, the adiabatic parameter [23] μ

goes to zero, indicating adiabaticity, while $|\mu| \rightarrow \infty$ for $\omega_0\tau^* \rightarrow 0$, indicating strong non-adiabaticity.

Since $H_0(t)$ is non-adiabatic (at least for finite $\omega_0\tau$), optimal drives for initial thermal states ρ_i^{th} use shortcut-to-adiabaticity [18–23, 25]. It consists in adding an extra drive, like for instance the so-called counter-diabatic drive $V_{\text{CD}}(t)$ [14–17], whose aim is to suppress generation of coherences and level transitions. Then, for an initial thermal state $\rho_i^{\text{th}} = p_i|1\rangle\langle 1| + (1-p_i)|0\rangle\langle 0|$, the addition of the counter-diabatic drive $V_{\text{CD}}(t)$ yields the final passive state $(\rho_i^{\text{th}})_f := p_i|e_1^f\rangle\langle e_1^f| + (1-p_i)|e_0^f\rangle\langle e_0^f|$ (which happens to be also a thermal state since there is only two energy levels), and reaches the non-cyclic ergotropy equal to $\mathcal{E}_{\text{nc}}^{\text{STA}} = E_i - \text{Tr}[(\rho_i^{\text{th}})_f H_f]$. The expression of $V_{\text{CD}}(t)$ tailored for our problem is provided in Appendix F 2 (see also [8, 23]) as well as the derivation of the associated energetic cost w_{STA} according to the criteria discussed above. We find $w_{\text{STA}} = |\mu| \frac{\hbar\bar{\Omega}}{\tau}$, with $\bar{\Omega} := \int_{t_i}^{t_f} dt \Omega(t)$.

It is also interesting to estimate how much energy is indeed gained or saved thanks to the shortcut-to-adiabaticity, and compare it to w_{STA} . This requires to compute the energy of the final state ρ_f we would obtain using only the bare drive $H_0(t)$. We obtain $\text{Tr}(\rho_f H_f) = \Omega_f(p_f - 1/2)$, where $\Omega_f := \Omega(t_f)$ and $p_f = \langle e_1^f | \rho_f | e_1^f \rangle$ is the population in the final excited state (analytical expression provided in Appendix F). Thus, the energetic gain associated with the counter-adiabatic drive is $\Delta E^{\text{STA}} := \text{Tr}(\rho_f H_f) - \text{Tr}[(\rho_i^{\text{th}})_f H_f] = \hbar\Omega_f(\frac{1}{2} - p_i) \frac{\mu^2(1-\nu_c)}{1+\mu^2}$, with $\nu_c := \cos \bar{\Omega} \sqrt{1+\mu^2}$. Note that the energetic gain ΔE^{STA} is positive only for initial positive temperature ($p_i \leq 1/2$). This is because thermal states of negative temperature are non-passive, and then shortcut-to-adiabaticity techniques stop being optimal.

We now focus on the non-cyclic ergotropy achieved by an arbitrary non-passive state $\rho_i = \begin{pmatrix} p_i & c_i \\ c_i^* & 1-p_i \end{pmatrix}$ (in the initial eigenbasis). Using the family of optimal drives $V(t)$ we can achieve the optimal final state $(\rho_i)_f = r_1|e_1^f\rangle\langle e_1^f| + r_0|e_0^f\rangle\langle e_0^f|$, with the expressions of r_1 and r_0 as in the example 1. The energetic gain with respect to the performance of shortcut-to-adiabaticity technique applied to initial thermal states is $\Delta \mathcal{E}_{\text{nc}} = \mathcal{E}_{\text{nc}} - \mathcal{E}_{\text{nc}}^{\text{STA}} = \hbar\Omega_f \left[\sqrt{(\frac{1}{2} - p_i)^2 + |c_i|^2} - (\frac{1}{2} - p_i) \right] \geq 0$, same as in example 1, which is also equal to the alternative figure of merit G_{ρ_i} . However, differently from the example 1, one can now compare the energetic costs w_{STA} and w_{min} , which provides a fairer comparison of performances between initial thermal states and non-passive states. The values taken by w_{min} now depends on some phases like the phase of the initial coherence c_i (see technical details in Appendix F 1). We find that w_{min} belongs to the interval $\frac{\sqrt{2}\hbar}{\tau} |\theta_{1,\text{min}} - \theta_{2,\text{min}}| \leq w_{\text{min}} \leq \frac{\sqrt{2}\hbar}{\tau} \pi$, where $\theta_{1,\text{min}} := \arctan \sqrt{\frac{p_i - r_1}{r_0 - p_i}}$ corresponds to the minimal ener-

getic cost in example 1 and $\theta_{2,\text{min}} := \arctan \frac{|\mu| \sqrt{1-\nu_c}}{\sqrt{2+\mu^2(1+\nu_c)}}$ is only due to the non-adiabaticity of $U_0(\tau)$. Importantly, if one has experimental control of the phases, the minimal energetic cost $\frac{\sqrt{2}\hbar}{\tau} |\theta_{1,\text{min}} - \theta_{2,\text{min}}|$ can always be achieved.

In Fig. 2 (a), we compare these energetic costs providing a plot of w_{STA} for $p_i = 0.4$ and w_{min} for $p_i = 0.4$ and $c_i = \sqrt{0.4 \times 0.6}$. We use the specific form of the time dependent frequencies mentioned above, implying $\Omega(t) = \omega_0$, $\bar{\Omega} = \omega_0\tau$, and $w_{\text{STA}} = \frac{\hbar\pi}{2\tau^*}$. Thus, the plots are in unit of $\hbar\omega_0$ and in function of $\omega_0\tau^*$, directly related to the level of non-adiabaticity, and $\omega_0\tau$, related to how fast is the driving with respect to the free evolution of the system. One can see that w_{min} is smaller than w_{STA} for most values of $\omega_0\tau$ and $\omega_0\tau^*$. In particular, while w_{STA} diverges for high non-adiabaticity, w_{min} remains finite. However, w_{min} diverges for very fast drives. Interestingly, one can show that this divergence of w_{min} is only due to the contribution from $\theta_{1,\text{min}}$. In particular, for $c_i = 0$, w_{min} remains finite and strictly smaller than w_{STA} , meaning that the driving $V(t)$ is more performant than shortcut-to-adiabaticity.

In Fig. 2 (b), we compare the energetic gain $\Delta \mathcal{E}_{\text{nc}} = \mathcal{E}_{\text{nc}} - \mathcal{E}_{\text{nc}}^{\text{STA}}$ (also equal to G_{ρ_i}) brought by the optimal drives with its energetic cost w_{min} . In Fig. 2 (c), we compare the energetic gain ΔE^{STA} brought by shortcut-to-adiabaticity with its energetic cost w_{STA} . One can see that the performances of the optimal drives are significantly better than the performances of shortcut-to-adiabaticity. Additional plots in function of the more general parameters $\bar{\Omega}$ and $|\mu|$ are available in Appendix F 3, allowing us to conclude that the above tendency remain valid in more general settings.

Conclusion.— We initiate the exploration of energetic advantages in driving operations of quantum systems obtained from non-thermal states. These energetic advantages with respect to initial thermal states are captured by the non-cyclic ergotropy, composed by the sum of a coherent (coherence-based) contribution, an incoherent (population-based) contribution and a passive contribution. A more specific figure of merit can be introduced, G_{ρ_i} , focusing on the energetic gain brought by the optimal drive itself. It was shown to be equal to the non-cyclic ergotropy difference $\Delta \mathcal{E}_{\text{nc}}$ for coherence-based non-passive states, as considered in the examples.

We saw that any non-thermal feature can bring energetic gains in the limit of many copies of the state. By contrast, for single state, we show, relying on majorization properties, that only quantum coherences can systematically bring energetic gains compared to initial thermal states. In particular, such gains are only achieved by dynamics able to consume coherences, emphasising the interplay between the presence of coherences and the ability to use them. It would be interesting to see if this mechanism could be the underlying phenomena behind the interferences effects enhancing the performance of cyclic engines pointed out in [41], which

would allow to extend its applications.

Additionally, the energetic costs associated with optimal drives can be significantly smaller than the ones associated with shortcut-to-adiabaticity technics while energetic gains can be significantly larger. Future investigations should be conducted to analyse other systems and potentially other criteria to evaluate the energetic costs of drives [21].

All these energetic advantages rely on the availability of non-thermal states. There are indeed many realistic situations producing non-thermal states, including strong interaction with a thermal bath [42, 43], many-body systems interacting with a common bath [44–50], non-Markovian evolution [51, 52], and interaction with several thermal baths at different temperatures [53].

Additional applications could be to explore questions suggested by our approach, like the lower energetic cost offered by the driving $V(t)$ compared to shortcut-to-adiabaticity, the tradeoff speed versus energetic cost of usual (cyclic) work extraction, as well as non-cyclic work extractions in quantum batteries. Finally, we anticipate direct applications in quantum engines operating with strong bath coupling [54–58] or with structured bath [59], where it has been reported mostly negative effects from the non-thermal properties and coherences naturally generated by these rich dynamics. A possible reason could be that such resources have not been fully exploited. Our results provide one possible direction.

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Appendix A: Incoherent and coherent non-adiabatic transformations

1. Non-adiabatic transformations

Any evolution leading to a passive state with respect to H_f is necessarily non-adiabatic if and only if the initial state is a non-passive state with respect to H_i . This can be easily seen by writing the initial state in its diagonal form, $\rho_i = \sum_n r_n |r_n^i\rangle\langle r_n^i|$. The final state is passive if and only if the applied evolution U satisfies the condition $\langle e_n^f | U | r_{n'} \rangle = \delta_{n,n'}$, where $\delta_{n,n'}$ is the Kronecker delta. Then, if ρ_i is a passive state, we have $|r_{n'}\rangle = |e_{n'}^i\rangle$ for all n' , and the previous condition becomes $\langle e_n^f | U | e_{n'}^i \rangle = \delta_{n,n'}$, which corresponds to an adiabatic transformation, or more precisely, to an “integral or global” adiabatic transformation, a looser condition than a dynamics which is adiabatic at all intermediate times. By contrast, if ρ_i is not passive, it means there exists at least one n such that $|r_n^i\rangle \neq |e_n^i\rangle$, implying

that there exists at least another index $m \neq n$ satisfying $\langle e_m^i | r_n^i \rangle \neq 0$. The condition for having a final passive state requires $\langle e_n^f | U | r_n \rangle = 1$, implying in fine that U contains the transition $|e_n^f\rangle\langle e_m^i|$, so that U necessarily realises a non-adiabatic transformation.

2. Coherent and incoherent contributions

Non-thermal and non-passive features have two distinguished contributions: one from populations and one from coherences. It is possible to separate these two contributions in the non-cyclic ergotropy, extending similar considerations presented in [33] on ergotropy. However, for non-cyclic ergotropy, it is convenient to introduce a passive contribution, described in the following. For an initial state ρ_i , we denote by $\rho_{i|D} := \sum_n \langle e_n^i | \rho_i | e_n^i \rangle |e_n^i\rangle\langle e_n^i|$ the corresponding dephased state. The incoherent contribution to the non-cyclic ergotropy is $\mathcal{E}_{nc}^{inc} := \text{Tr}(\rho_i H_i) - \text{Tr}[\widetilde{\rho_{i|D}} H_i]$, where $\widetilde{\rho_{i|D}} = \sum_n p_{\sigma(n)}^i |e_n^i\rangle\langle e_n^i|$ is the passive state of $\rho_{i|D}$ with respect to H_i , with $p_n^i := \langle e_n^i | \rho_i | e_n^i \rangle$ are the populations in the initial energy basis, and $\sigma(n)$ is a permutation of the indices such that $p_{\sigma(n+1)}^i \leq p_{\sigma(n)}^i$. Obviously, in the particular situation where the populations p_n^i of ρ_i are already in decreasing order we have $\widetilde{\rho_{i|D}} = \rho_{i|D}$ and the incoherent contribution is null since $\text{Tr}(\rho_{i|D} H_i) = \text{Tr}(\rho_i H_i)$. By defining the unitary transformation $U_\sigma := \sum_n e^{i\psi_n} |e_n^i\rangle\langle e_{\sigma(n)}^i|$, where ψ_n is a phase factor, we obtain $\widetilde{\rho_{i|D}} = U_\sigma \rho_{i|D} U_\sigma^\dagger = (U_\sigma \rho_i U_\sigma^\dagger)_{|D}$. Alternatively, $\widetilde{\rho_{i|D}}$ can be defined as [33] $\widetilde{\rho_{i|D}} = \text{argmin}_{\sigma \in \mathcal{S}^{inc}} \text{Tr}(\sigma H_i)$, where $\mathcal{S}^{inc} := \{U_\xi \rho_{i|D} U_\xi^\dagger\}_{U_\xi \in \mathcal{U}^{inc}}$ and \mathcal{U}^{inc} denotes the ensemble of incoherent unitary transformations with respect to the initial energy eigenbasis. Incoherent unitaries are of the form $\sum_n e^{i\Theta_n} |e_n^i\rangle\langle e_{\xi(n)}^i|$, where $\xi(n)$ is a permutation of the indices and Θ_n a phase factor. Importantly, \mathcal{E}_{nc}^{inc} is always positive.

The second contribution is the passive one, defined as $\mathcal{E}_{nc}^{pas} := \text{Tr}[\widetilde{\rho_{i|D}} H_i] - \text{Tr}[(\widetilde{\rho_{i|D}})_f H_f]$ with $(\widetilde{\rho_{i|D}})_f := \sum_n p_{\sigma(n)}^i |e_n^f\rangle\langle e_n^f|$ is the passive state of $\rho_{i|D}$ with respect to H_f . Note that $(\widetilde{\rho_{i|D}})_f$ is related to $\widetilde{\rho_{i|D}}$ through adiabatic transformations which are of the form $U_{ad} = \sum_n e^{i\phi_n} |e_n^f\rangle\langle e_n^i|$. Additionally, \mathcal{E}_{nc}^{pas} can be positive or negative.

The coherent contribution to the non-cyclic ergotropy can be defined as $\mathcal{E}_{nc}^{coh} = \text{Tr}[(\widetilde{\rho_{i|D}})_f H_f] - \text{Tr}[(\widetilde{\rho_i})_f H_f]$. \mathcal{E}_{nc}^{coh} is always positive since $\text{Tr}[(\widetilde{\rho_{i|D}})_f H_f] = \text{Tr}[U_{ad} U_\sigma \rho_i U_\sigma^\dagger U_{ad}^\dagger H_f]$ and $(\widetilde{\rho_i})_f$ is the passive state associated with ρ_i but also to $U_{ad} U_\sigma \rho_i U_\sigma^\dagger U_{ad}^\dagger$. A similar expression as in [33] can be obtained for the coherent

non-cyclic ergotropy:

$$\mathcal{E}_{\text{nc}}^{\text{coh}} = \beta^{-1} \left[\mathcal{C}(\rho_i) + S[(\widetilde{\rho_{i|D}})_f | \rho_f^{\text{th}}(\beta)] - S[(\widetilde{\rho_i})_f | \rho_f^{\text{th}}(\beta)] \right] \quad (\text{A1})$$

where $\rho_f^{\text{th}}(\beta)$ denotes a thermal state of the final Hamiltonian at arbitrary inverse temperature β , and $\mathcal{C}(\rho_i) = S[\rho_{i|D}] - S[\rho_i]$ is the amount of initial coherences measured with the relative entropy of coherence [60]. While $(\widetilde{\rho_{i|D}})_f$ can be reached by incoherent non-adiabatic evolutions, for instance $U_{\text{ad}}U_{\sigma}$, $(\widetilde{\rho_i})_f$ can be reached only via coherent non-adiabatic evolutions. It can be easily seen by remembering that applying an incoherent non-adiabatic evolution to an initial state containing coherences necessarily yields a final state with coherences. Alternatively, one can see it by noticing that an evolution able to consume coherences is also able to generate coherences.

Finally, the three contributions add up to give the non-cyclic ergotropy: $\mathcal{E}_{\text{nc}} = \mathcal{E}_{\text{nc}}^{\text{inc}} + \mathcal{E}_{\text{nc}}^{\text{pas}} + \mathcal{E}_{\text{nc}}^{\text{coh}}$. Note that the passive contribution can alternatively be defined before the incoherent one or after the coherent one. This could in general change the respective value of each contribution but without changing their nature.

3. Consequences for energetic gain

The above decomposition of \mathcal{E}_{nc} is insightful to understand the difference between coherence and population-based non-passivity. For coherence-based non-passivity, the energetic gain, given by the difference of non-cyclic ergotropy (Eq.3 of the main text), can be decomposed as

$$\begin{aligned} \Delta \mathcal{E}_{\text{nc}} &= \mathcal{E}_{\text{nc}}(\rho_i) - \mathcal{E}_{\text{nc}}(\rho_i^{\text{th}}) \\ &= \mathcal{E}_{\text{nc}}^{\text{pas}}(\rho_i) + \mathcal{E}_{\text{nc}}^{\text{coh}}(\rho_i) - \mathcal{E}_{\text{nc}}^{\text{pas}}(\rho_i^{\text{th}}). \end{aligned} \quad (\text{A2})$$

Since we assumed that ρ_i contains only coherence-based non-passive features, the populations are the same as the thermal state ρ_i^{th} of same energy, and consequently the passive contributions are also the same, $\mathcal{E}_{\text{nc}}^{\text{pas}}(\rho_i) = \mathcal{E}_{\text{nc}}^{\text{pas}}(\rho_i^{\text{th}})$. Consequently,

$$\Delta \mathcal{E}_{\text{nc}} = \mathcal{E}_{\text{nc}}^{\text{coh}}(\rho_i) \geq 0, \quad (\text{A3})$$

from which we conclude that coherences always bring energetic gains.

By contrast, for a population-based non-passive state, the populations can be very different from the thermal state of same energy, so that the passive contributions can be very different too. Then, we have

$$\begin{aligned} \Delta \mathcal{E}_{\text{nc}} &= \mathcal{E}_{\text{nc}}^{\text{pas}}(\rho_i) + \mathcal{E}_{\text{nc}}^{\text{inc}}(\rho_i) - \mathcal{E}_{\text{nc}}^{\text{pas}}(\rho_i^{\text{th}}) \\ &= \Delta \mathcal{E}_{\text{nc}}^{\text{pas}} + \mathcal{E}_{\text{nc}}^{\text{inc}}(\rho_i), \end{aligned} \quad (\text{A4})$$

which can be of any sign since $\Delta \mathcal{E}_{\text{nc}}^{\text{pas}} := \mathcal{E}_{\text{nc}}^{\text{pas}}(\rho_i) - \mathcal{E}_{\text{nc}}^{\text{pas}}(\rho_i^{\text{th}})$ can be positive or negative. This is illustrated in the next section with three-level systems.

Appendix B: Larger non-cyclic work extraction from passive states than from non-passive states

In this Appendix we provide explicit example that for non-cyclic transformations, initial passive states can yield a larger work extraction (for positive non-cyclic ergotropy) or require less driving energy (for negative non-cyclic ergotropy) than non-passive states. We consider a three-level system and a non-cyclic process with initial Hamiltonian $H_i = \sum_{n=1}^3 e_n^i |e_n^i\rangle\langle e_n^i|$ and the final Hamiltonian $H_f = \sum_{n=1}^3 e_n^f |e_n^f\rangle\langle e_n^f|$. Without loss of generality, we assume that $e_1^i = e_1^f = 0$ and $e_3^i = e_3^f = 1$, which implies that e_2^i and e_2^f belong to the interval $[0; 1]$. As passive state, we consider a thermal state ρ_i^{th} at inverse temperature β . We denote by p_n^{th} its initial populations associated with the eigenvector $|e_n^i\rangle$. We are looking for a non-passive state such that its non-cyclic ergotropy is strictly smaller than the one of the thermal state. Since we saw in the main text that initial coherences always increase the non-cyclic ergotropy, we choose a diagonal non-passive state $\rho_i = \sum_{n=1}^3 q_i |e_n^i\rangle\langle e_n^i|$. In other words, we need to find q_1 , q_2 , and q_3 such that $\tilde{E}_f = q_3^* + q_2^* e_2^f > \text{Tr}[(\widetilde{\rho_i^{\text{th}}})_f H_f] = p_3^{\text{th}} + p_2^{\text{th}} e_2^f$, remembering that $(\widetilde{\rho_i^{\text{th}}})_f$ is the final passive state associated with ρ_i^{th} . We introduced $q_3^* := \min_{n=1,2,3} q_n$ and q_2^* is the second smallest population.

One can show for instance that choosing e_2^i such that $\beta(1 - e_2^i) \ll 1$, with $q_3 = p_3^{\text{th}} + \alpha$, $q_2 = p_2^{\text{th}} - \alpha/e_2^i$, and $q_1 = 1 - q_2 - q_3$, where $\alpha := e^{-\beta} \beta (e_2^i - (e_2^i)^2)/3$ guarantees $q_3^* > p_3^{\text{th}}$. This implies that we can always have $\tilde{E}_f > \text{Tr}[(\widetilde{\rho_i^{\text{th}}})_f H_f]$ by choosing e_2^f small enough.

Explicitly, let us take $\beta = 1$ (in unit of k_B) and $e_2^i = 0.9$. With these values we obtain according to the above choices $p_1^{\text{th}} \simeq 0.564$, $p_2^{\text{th}} \simeq 0.229$, $p_3^{\text{th}} \simeq 0.207$, $q_1 \simeq 0.565$, $q_2 \simeq 0.217$, and $q_3 \simeq 0.218$. Thus, we have for the final populations $q_3^* - p_3^{\text{th}} = q_3 - p_3^{\text{th}} \simeq 0.00954$ and $p_2^{\text{th}} - q_2^* = p_2^{\text{th}} - q_3 = 0.0108$, so that any value of e_2^f smaller than 0.88 leads to $\tilde{E}_f > \text{Tr}[(\widetilde{\rho_i^{\text{th}}})_f H_f]$.

Appendix C: Asymptotic achievability of the upper bound Eq.(7)

The theorem shown in [32] states that for any state ρ and for N going to infinity, there exists a unitary transformation U_N (not unique) such that

$$\frac{1}{N} \text{Tr} \left(U_N \otimes^N \rho U_N^\dagger H_N \right) \xrightarrow{N \rightarrow \infty} \text{Tr}(\rho^{\text{th}} H), \quad (\text{C1})$$

where H can be an arbitrary Hamiltonian, $H_N := \sum_{k=0}^{N-1} \otimes^k \mathbb{I} \otimes H \otimes^{N-k-1} \mathbb{I}$, \mathbb{I} is the identity, and ρ^{th} is the thermal state of same entropy as ρ associated with the Hamiltonian H . Then, it implies the existence of a unitary transformation mapping asymptotically well

(in the sense stated above) $\otimes^N \rho_i$ to $\otimes^N (\rho_i)_f^{\text{th}}$, remembering that $(\rho_i)_f^{\text{th}}$ denotes the thermal state with respect to H_f of same entropy as ρ_i . In particular, it also means that we can find a time dependent Hamiltonian $H_N(t)$ such that the generated unitary transformation realises this mapping with the additional constraints $H_N(t_i) = \sum_{k=0}^{N-1} \otimes^k \mathbb{I} \otimes H_i \otimes^{N-k-1} \mathbb{I}$ and $H_N(t_f) = \sum_{k=0}^{N-1} \otimes^k \mathbb{I} \otimes H_f \otimes^{N-k-1} \mathbb{I}$.

Appendix D: Optimal drivings

One can verify easily that the family of driving $V(t)$ given in the main text brings the initial state ρ_i to the optimal final state $\tilde{\rho}_f$. The complete transformation is given by

$$\begin{aligned} U &= e^{-i\mathcal{T} \int_{t_i}^{t_f} dt H(t)} \\ &= e^{-i\mathcal{T} \int_{t_i}^{t_f} dt H_0(t)} \\ &\quad \times e^{-i\mathcal{T} \int_{t_i}^{t_f} dt e^{iA \int_{t_i}^t du H_0(u)} V(t) e^{-i\mathcal{T} \int_{t_i}^t du H_0(u)}} \\ &= e^{-i\mathcal{T} \int_{t_i}^{t_f} dt H_0(t)} e^{i\chi \int_{t_i}^{t_f} dt \dot{f}(t)} \\ &= e^{-i\mathcal{T} \int_{t_i}^{t_f} dt H_0(t)} e^{i\chi [f(t_f) - f(t_i)]} \\ &= \sum_n e^{i\phi_n} |e_n^f\rangle \langle r_n^i|, \end{aligned} \quad (\text{D1})$$

where we used the definition of χ and the properties $f(t_i) = 0$ and $f(t_f) = 1$. It is then straightforward to see that U brings ρ_i to the optimal final state.

Appendix E: Details on the energetic cost of driving for two-level systems

The eigenvalues and eigenvectors associated with the initial state $\rho_i = \begin{pmatrix} p_i & c_i \\ c_i^* & 1 - p_i \end{pmatrix}$ are respectively

$$r_1 = \frac{1}{2} - \sqrt{(p_i - 1/2)^2 + |c_i|^2}, \quad (\text{E1})$$

$$r_0 = \frac{1}{2} + \sqrt{(p_i - 1/2)^2 + |c_i|^2}, \quad (\text{E2})$$

and

$$|r_1\rangle = \sqrt{\frac{r_0 - p_i}{r_0 - r_1}} |1\rangle - e^{-i\psi_i} \sqrt{\frac{p_i - r_1}{r_0 - r_1}} |0\rangle, \quad (\text{E3})$$

$$|r_0\rangle = e^{i\psi_i} \sqrt{\frac{p_i - r_1}{r_0 - r_1}} |1\rangle + \sqrt{\frac{r_0 - p_i}{r_0 - r_1}} |0\rangle, \quad (\text{E4})$$

where $\psi_i = \arg(c_i)$. The unitary evolution $U_0(t)$ is simply given by $U_0(t) = e^{-i\Lambda \frac{\omega}{2} \sigma_z}$, with $\Lambda := \int_{t_0}^{t_f} dt \lambda(t)$. Since both H_i and H_f are proportional to σ_f , the initial and final energy eigenstates are the same, namely $|1\rangle$ and $|0\rangle$.

As detailed in the main text, optimal drivings can be obtained through the matrix χ which is itself given by

$$\begin{aligned} e^{i\chi} &= \sum_n e^{i\phi_n} U_0^\dagger(t_f) |e_n^f\rangle \langle r_n^i| \\ &= e^{i\phi_1} e^{i\Lambda \frac{\omega}{2}} |1\rangle \langle r_1| + e^{i\phi_0} e^{-i\Lambda \frac{\omega}{2}} |0\rangle \langle r_0|. \end{aligned} \quad (\text{E5})$$

The associated eigenvalues are $e^{i\theta_+}$ and $e^{i\theta_-}$ with

$$\theta_{\pm} = \frac{\phi_0 + \phi_1}{2} + \pi \kappa(\phi_1 - \phi_0) \quad (\text{E6})$$

$$\pm \arctan \sqrt{\frac{r_0 - r_1}{(r_0 - p_i) \cos^2(\phi_1 - \phi_0)/2}} - 1, \quad (\text{E7})$$

where $\kappa(\phi_1 - \phi_0)$ is a function equal to 0 when $\cos(\phi_1 - \phi_0) \geq 0$ and equal to 1 otherwise (explicitly, $\kappa(\phi_1 - \phi_0) = \Theta[-\cos(\phi_1 - \phi_0)]$, where Θ is the Heaviside step function). Assuming one has full control of the phases, one can achieve the following minimal energetic cost

$$\begin{aligned} w_{\min} &= \frac{\sqrt{2}}{\tau} \arctan \sqrt{\frac{p_i - r_1}{r_0 - p_i}} \\ &= \frac{\sqrt{2}}{\tau} \arctan \left(\frac{\sqrt{(1/2 - p_i)^2 + |c|^2} - (1/2 - p_i)}{\sqrt{(1/2 - p_i)^2 + |c|^2} + (1/2 - p_i)} \right)^{1/2}, \end{aligned} \quad (\text{E8})$$

by setting $\phi_1 = \phi_0 = 0$. By contrast, if one has no control of the phases, their value for each realisation is random, and the average cost is given by

$$\bar{w} := \frac{1}{\tau} \frac{1}{4\pi^2} \int_{-\pi}^{\pi} d\phi_1 \int_{-\pi}^{\pi} d\phi_2 \sqrt{\theta_+^2 + \theta_-^2}. \quad (\text{E9})$$

The analytical expression is challenging to obtain, but one can instead show that $\frac{1}{4\pi^2} \int_{-\pi}^{\pi} d\phi_1 \int_{-\pi}^{\pi} d\phi_2 \sqrt{\theta_+^2 + \theta_-^2}$ takes value within the interval $[0.77\pi; 0.89\pi]$ depending on the values of p_i and c_i .

Appendix F: Non-adiabatic dynamics

The time dependent Hamiltonian considered in the last part of the paper is of the form

$$H_0(t) = \frac{1}{2} \omega(t) \sigma_z + \frac{1}{2} \epsilon(t) \sigma_x, \quad (\text{F1})$$

and generates a non-adiabatic dynamics since $[H(t), H(t')] \neq 0$ in general. Such kind of dynamics are challenging to integrate. Still, analytical integrations are possible when the Hamiltonian parameters are such that $\mu := \frac{\dot{\omega}(t)\epsilon(t) - \dot{\epsilon}(t)\omega(t)}{\Omega^3(t)}$ is constant [8, 23]. A simple way to integrate the dynamics is using a closed set of orthogonal observables $\{B_k\}_{0 \leq k \leq 3}$ forming a basis of the Hilbert space. We use the same set as in [8, 23], namely $B_0 = \mathbb{I}$, $B_1 = H_0(t) = \omega(t)S_z + \epsilon(t)S_x$,

$B_1 = \epsilon(t)S_z - \omega(t)S_x$, and $B_3 = \Omega(t)S_y$. In the Heisenberg picture $B_i(t) := e^{i\mathcal{A} \int_{t_i}^t du H_0(u)} B_i e^{-i\mathcal{T} \int_{t_i}^t du H_0(u)}$ the dynamics is given by $\dot{B}_i(t) = i[H_0^*(t), B_i(t)] + \frac{\partial}{\partial t} B_i(t)$, where $H_0^*(t) := e^{i\mathcal{A} \int_{t_i}^t du H_0(u)} H_0 e^{-i\mathcal{T} \int_{t_i}^t du H_0(u)}$ and the partial derivative denotes the derivative with respect to the intrinsic time-dependence of the operator B_i . The

dynamics of the basis can be written in a matrix form

$$\frac{1}{\Omega} \dot{X}(t) = \left(A + \frac{\dot{\Omega}}{\Omega^2} \mathbb{I} \right) X(t) \quad (\text{F2})$$

where $X(t) = \{B_1(t), B_2(t), B_3(t)\}^T$ is a three-component column vector and

$$A = \begin{pmatrix} 0 & \mu & 0 \\ -\mu & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \quad (\text{F3})$$

a 3×3 -matrix. This can be integrated after diagonalising A , yielding (see also [8, 23])

$$X(t) = \frac{\Omega(t)}{(\mu^2 + 1)\Omega(0)} \begin{pmatrix} 1 + \mu^2 \nu_c & \mu \nu_s \sqrt{\mu^2 + 1} & (1 - \nu_c)\mu \\ -\mu \nu_s \sqrt{\mu^2 + 1} & \nu_c(\mu^2 + 1) & \nu_s \sqrt{\mu^2 + 1} \\ \mu(1 - \nu_c) & -\nu_s \sqrt{\mu^2 + 1} & \mu^2 + \nu_c \end{pmatrix} X(0), \quad (\text{F4})$$

with $\nu_c := \cos \bar{\Omega} \sqrt{1 + \mu^2}$, $\nu_s := \sin \bar{\Omega} \sqrt{1 + \mu^2}$, and $\bar{\Omega} := \int_{t_i}^{t_f} dt \Omega(t)$. Note that from $B_i(t)$ we have directly the expressions of $S_z(t)$, $S_y(t)$, and $S_x(t)$, from which we obtain the time dependent Bloch vector to reconstruct the final state, $\rho_f = \begin{pmatrix} p_f & c_f \\ c_f^* & 1 - p_f \end{pmatrix}$ in the basis $\{|e_1^f\rangle, |e_0^f\rangle\}$. We obtain $p_f = \frac{1}{2(1+\mu^2)}[2p_i + \mu^2 - \mu^2 \nu_c(1 - 2p_i)]$ and $c_f = -\frac{\mu(1-2p_i)}{2(1+\mu^2)} \text{sign}(\epsilon_f) [\nu_s \sqrt{1 + \mu^2} - i(1 - \nu_c)]$. The final eigenstates are given by $|e_1^f\rangle = [(\omega_f + \Omega_f)^2 + \epsilon_f^2]^{-1/2} [(\omega_f + \Omega_f)|1\rangle + \epsilon_f|0\rangle]$ and $|e_0^f\rangle = [(\omega_f - \Omega_f)^2 + \epsilon_f^2]^{-1/2} [(\omega_f - \Omega_f)|1\rangle + \epsilon_f|0\rangle]$.

1. Energetic cost of the family of optimal drive

The minimal energetic cost of an optimal drive is given by (see main text) $w_{\min} = \frac{1}{\tau} [\text{Tr} \chi \chi^\dagger]^{1/2}$, where χ is such that $e^{i\chi} = \sum_n e^{i\xi_n} |e_n^i\rangle \langle r_n^i|$. The expression of $|r_1\rangle$ and $|r_0\rangle$ are the same as in (E3) and (E4) respectively. We can derive the expression of $|e_1^i\rangle$ and $|e_0^i\rangle$ (up to a phase factor included in ξ_n) from the above expression of ρ_f ,

taking respectively $|1\rangle\langle 1|$ and $|0\rangle\langle 0|$ as initial state. We obtain

$$|e_1^i\rangle = \alpha e^{-i\phi_\alpha} |1\rangle - \beta |0\rangle \quad (\text{F5})$$

$$|e_0^i\rangle = \beta |1\rangle + \alpha e^{i\phi_\alpha} |0\rangle \quad (\text{F6})$$

with $\alpha e^{i\phi_\alpha} = \frac{1}{\sqrt{2(1+\mu^2)}} [\text{sign}(s) \sqrt{(1 + \mu^2)(1 + \nu_c)} - i\sqrt{1 - \nu_c}]$ and $\beta = \frac{1}{\sqrt{2(1+\mu^2)}} \text{sign}(\epsilon_f) \mu \sqrt{1 - \nu_c}$.

Combining with (F5) and (F6) with (E3) and (E4) we have

$$\sum_n e^{i\phi_n} |e_n^i\rangle \langle r_n^i| = \begin{pmatrix} \cos \eta e^{i\zeta} & \sin \eta e^{-i(\delta - \xi_1 - \xi_0)} \\ -\sin \eta e^{i\delta} & \cos \eta e^{-i(\zeta - \xi_0 - \xi_1)} \end{pmatrix} \quad (\text{F7})$$

in the initial energy eigenbasis $\{|1\rangle, |0\rangle\}$ with η , ζ , and δ are implicitly defined by the relations $\cos \eta e^{i\zeta} = \alpha \sqrt{\frac{r_0 - p_i}{r_0 - r_1}} e^{i(\xi_1 - \phi_\alpha)} + \beta \sqrt{\frac{p_i - r_1}{r_0 - r_1}} e^{i(\xi_0 - \psi_i)}$ and $\sin \eta e^{i\delta} = \beta \sqrt{\frac{r_0 - p_i}{r_0 - r_1}} e^{i\xi_1} - \alpha \sqrt{\frac{p_i - r_1}{r_0 - r_1}} e^{i(\xi_0 + \phi_\alpha - \psi_i)}$, reminding that ψ_i is the argument of the initial coherence c_i . As a result, the eigenvalues of $e^{i\chi}$ are $e^{i\theta_+}$ and $e^{i\theta_-}$ with

$$\theta_{\pm} = \frac{\xi_1 + \xi_0}{2} + \pi \kappa(\xi_1, \xi_0, \alpha, \eta) \pm \arctan \sqrt{\frac{1}{\left[\alpha \sqrt{\frac{r_0 - p_i}{r_0 - r_1}} \cos(\phi_\alpha - \xi_1/2 + \xi_0/2) + \beta \sqrt{\frac{p_i - r_1}{r_0 - r_1}} \cos(\psi_i + \xi_1/2 - \xi_0/2) \right]^2} - 1}, \quad (\text{F8})$$

where $\kappa(\xi_1, \xi_0, \alpha, \eta)$ is a function equal to 0 when $\cos \eta \cos(\zeta - \xi_1/2 - \xi_0/2) \geq 0$, and equal to 1 otherwise. Assuming

one has control of the phase ξ_1 and ξ_0 , the minimum energetic cost is

$$w_{\min} = \frac{\sqrt{2}}{\tau} \arctan \sqrt{\left[\alpha^2 \frac{r_0 - p_i}{r_0 - r_1} + \beta^2 \frac{p_i - r_1}{r_0 - r_1} + 2\beta\alpha \frac{\sqrt{(r_0 - p_i)(p_i - r_1)}}{r_0 - r_1} \cos(\psi_i + \phi_\alpha) \right]^{-1}} - 1. \quad (\text{F9})$$

Contrasting with the first situation where $H_0(t)$ generates an adiabatic transformation, the energetic cost after minimisation over ξ_1 and ξ_0 depends on ψ_i , the initial phase of the coherence c_i , and on ϕ_α (which depends on the original dynamics $U_0(t_f)$). Then, one can consider again the same alternative. If experimentally one has control of these phases, meaning that they have well-defined values which can be adjusted by some controls on the experimental apparatus, then, the minimum energetic cost can be brought down to (for $\psi_i + \phi_\alpha = 0$ if $\epsilon_f \mu \geq 0$, and for $\psi_i + \phi_\alpha = \pi$ if $\epsilon_f \mu \leq 0$)

$$w_{\min} = \frac{\sqrt{2}}{\tau} |\theta_{1,\min} - \theta_{2,\min}|, \quad (\text{F10})$$

with $\theta_{1,\min} = \arctan \sqrt{\frac{p_i - r_1}{r_0 - p_i}}$, contribution from the initial state, and $\theta_{2,\min} = \arctan \frac{|\beta|}{\alpha} = \arctan \frac{|\mu| \sqrt{1 - \nu_c}}{\sqrt{2 + \mu^2(1 + \nu_c)}}$, contribution from the original dynamics $U_0(t_f)$. Conversely, if one has no control over ψ_i and ϕ_α , the energetic cost can take any value between $\frac{\sqrt{2}}{\tau} |\theta_{1,\min} - \theta_{2,\min}|$ and $\frac{\sqrt{2}}{\tau} (\theta_{1,\min} + \theta_{2,\min})$.

Finally, without any control on the phases ξ_1 and ξ_0 and therefore left random, the energetic cost takes values between $\frac{\sqrt{2}}{\tau} |\theta_{1,\min} - \theta_{2,\min}|$ and $\frac{\sqrt{2}}{\tau} \pi$.

2. Counterdiabatic driving and energetic cost

According to [14–17], for a given time dependent Hamiltonian $H(t)$, the counterdiabatic drive is given by

$$H_{\text{CD}} = \sum_n \left(\frac{d}{dt} \pi_n \right) \pi_n \quad (\text{F11})$$

where $\pi_n := |e_n\rangle\langle e_n|$ are projectors onto the instantaneous eigenstates $|e_n\rangle$ of $H(t)$. The corresponding energetic cost is given by the time average of the Hamiltonian norm $\|H(t)\|$. One obtains $\|H(t)\| = (\sum_n \langle \dot{e}_n | e_n \rangle)^{1/2}$, using the property $\langle \dot{e}_n | e_n \rangle = 0$, where $|e_n\rangle$ stands for $\frac{d}{dt}|e_n\rangle$. Recalling that we consider the family of driving $H_0(t) = \frac{\omega(t)}{2} \sigma_z + \frac{\epsilon(t)}{2} \sigma_x$, the instantaneous eigenstates

are given by

$$|e_1\rangle = \sqrt{\frac{\Omega(t) + \omega(t)}{2\Omega(t)}} |1\rangle + \sqrt{\frac{\Omega(t) - \omega(t)}{2\Omega(t)}} |0\rangle \quad (\text{F12})$$

and

$$|e_0\rangle = -\sqrt{\frac{\Omega(t) - \omega(t)}{2\Omega(t)}} |1\rangle + \sqrt{\frac{\Omega(t) + \omega(t)}{2\Omega(t)}} |0\rangle. \quad (\text{F13})$$

This leads to $\|H(t)\| = \frac{|\dot{\omega}(t)\epsilon(t) - \omega(t)\dot{\epsilon}(t)|}{\Omega^2(t)} = |\mu|\Omega(t)$, implying that the energetic cost is $w_{\text{STA}} = |\mu|\bar{\Omega}/\tau$.

3. Some additional plots

We finally provides some plots additional to the one presented in the main text. The following plots are in function of the more general parameters $\bar{\Omega}$ and $|\mu|$. In Fig. 3 (a), we compare the energetic cost w_{\min} and w_{STA} in unit of \hbar/τ and in function of the dimensionless parameters $\mu \in [0; 4]$ and $\bar{\Omega} \in [0; 4]$, and setting $p_i = 0.4$ and $c_i = \sqrt{0.4 \times 0.6}$. One can see that w_{\min} is almost always smaller than w_{STA} . Additionally, for some initial non-passive states, the energetic cost w_{\min} is zero, meaning that the transformation $U_0(t_f)$ is already optimal for these particular initial states. Without the phase controls mentioned above, w_{\min} takes random values between $\frac{\sqrt{2}\hbar}{\tau} |\theta_{1,\min} - \theta_{2,\min}|$ and $\frac{\sqrt{2}\hbar}{\tau} \pi$, so one could say that on average the energetic costs w_{\min} and w_{STA} are comparable for moderate values of $\bar{\Omega}$ and μ . For large values of these parameters, the w_{\min} is always smaller than w_{STA} .

In Fig. 3 (b) we compare the energetic gain ΔE^{STA} in unit of $\hbar\Omega_f$ brought by shortcut-to-adiabaticity with its energetic cost w_{STA} in unit of \hbar/τ . Since these two parameters are in principle independent, in order to be able to plot these two functions on the same graph we have to fixed a “conversion rate” of $\hbar\Omega_f$ into \hbar/τ . We choose $\Omega_f = 20/\tau$. One can see that the energetic balance is negative for most parameter values. In Fig. 3 (c), using the same unit, we compare the energetic gain $\Delta \mathcal{E}_{\text{nc}} = \mathcal{E}_{\text{nc}} - \mathcal{E}_{\text{nc}}^{\text{STA}}$ brought by the initial coherences with the relative energetic cost $w_{\min} - w_{\text{STA}}$, still assuming $\Omega_f = 20/\tau$. Overall, it seems that the performances of the optimal drive are significantly better than the performances of shortcut-to-adiabaticity.

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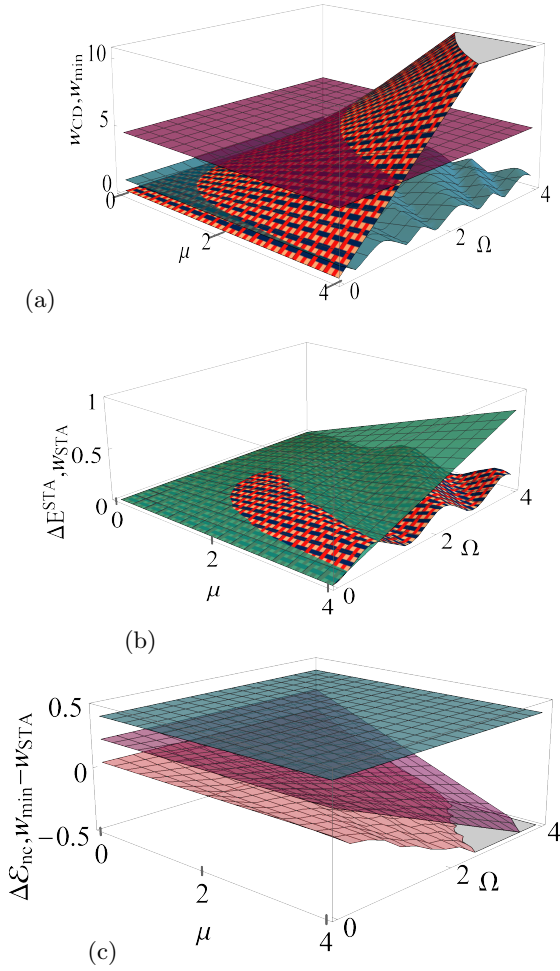


FIG. 3. (a) Plot of w_{STA} (texturised surface) and w_{min} (blue solid lower surface) in unit of \hbar/τ , in function of the dimensionless parameters $\mu \in [0; 4]$ and $\bar{\Omega} \in [0; 4]$, for $p_i = 0.4$ and $c_i = \sqrt{0.4 \times 0.6}$. The purple upper plane is the upper bound of w_{min} equal to $\pi\sqrt{2}$. (b) Plot of w_{STA} (green solid surface) and ΔE_{STA} (texturised surface), both in unit of $\hbar\Omega_f$, in function of $\mu \in [0; 4]$ and $\bar{\Omega} \in [0; 4]$, assuming $\Omega_f = 20/\tau$, which allows to convert \hbar/τ in unit of $\hbar\Omega_f$. (c) Plot of $w_{min} - w_{STA}$ (pink lower surface) and ΔE_{nc} (upper blue horizontal plane), both in unit of $\hbar\Omega_f$, in function of $\mu \in [0; 4]$ and $\bar{\Omega} \in [0; 4]$, still assuming $\Omega_f = 20/\tau$. The purple intermediate surface is the upper bound of $w_{min} - w_{STA}$, equal to $\pi\sqrt{2} - w_{STA}$.

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