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Work extremum principle: Structure and function of quantum heat engines

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We consider a class of quantum heat engines consisting of two subsystems interacting with a work-source and coupled to two separate baths at different temperatures $T_h > T_c$. The purpose of the engine is to extract work due to the temperature difference. Its dynamics is not restricted to the near equilibrium regime. The engine structure is determined by maximizing the extracted work under various constraints. When this maximization is carried out at finite power, the engine dynamics is described by well-defined temperatures and satisfies the local version of the second law. In addition, its efficiency is bounded from below by the Curzon-Ahlborn value $1-\sqrt{T_c/T_h}$ and from above by the Carnot value $1-(T_c/T_h)$. The latter is reached—at finite power—for a macroscopic engine, while the former is achieved in the equilibrium limit $T_h \to T_c$. The efficiency that maximizes the power is strictly larger than the Curzon-Ahloborn value. When the work is maximized at a zero power, even a small (few-level) engine extracts work right at the Carnot efficiency.

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I. INTRODUCTION

Heat engines are natural or artificial devices, the goal of which is to extract work (high-graded energy) from nonequilibrium sources of heat (low-graded energy) [1–4]. There are *three* basic characteristics of the engine operation: (i) the work extracted per cycle; (ii) the efficiency with which the input heat is converted into work; and (iii) the power of work-extraction, i.e., the work-extracted per cycle divided over the cycle duration.

Heat engines may evolve in time toward states that provide (constrained) optimization of their functional characteristics. Here are three examples from largely different fields.

(1) Engineering: the modern man-made engines which are much more powerful and efficient than those which started the Industrial Revolution. The cause of this improvement is efforts driven by our desire to get more high-graded energy at a lower cost.

(2) Biology and ecology: driven by evolution, higher organisms and more developed ecosystems have more refined and more optimal means of extracting energy from their respective environment [5]. This observation led to several quantitative formulations [5].

(3) Physical systems: the Earth's atmosphere can be approximately regarded as a huge heat-engine operating between two thermal baths (cold bath of the Earth's surface and eventually the hot bath of the sun) and producing as output large-scale turbulent motion of air and vapor [6]. As verified by observation [6], this engine is also tuned to extract the maximal work [6], although the precise mechanism of this tuning is unclear yet.

It is needless to stress that the optimization of heat engines would have to proceed in the presence of constraints that determine the very path of the engine evolution. This fact is obvious in the above bioecological perspective.

Our present aim is to understand the structure of quantum heat engines emerging from the maximization of work (produced per cycle) under specific constraints. The study of quantum engines started in the 1960s [7], when it was realized that many models of lasers and masers are in fact quantum heat engines. A good review of this early activity is given in [8]. Nowadays the physics of quantum heat engines is a rich field [9–22] related to other branches of modern quantum theory; see [23] for a recent review of engines in the context of quantum information theory. We see two basic reasons for studying quantum heat engines: (i) understanding of how thermodynamics emerges from the quantum mechanics; and (ii) clarifying the principal possibilities of nanoscale devices.

Our analysis starts from quantum mechanics [1] and does not rely on the validity of thermodynamical concepts normally invoked in studying heat engines [2–4]. We allow the intermediate states of the engine to be arbitrary far from equilibrium. We shall, however, see that local thermodynamical concepts—such as the existence of local temperatures in the intermediate stages of the engine functioning, or the validity of local formulations of the second law—emerge as a result of maximizing the produced work.

Our model will consist of two quantum systems R and S interacting with thermal baths at temperatures T_h and T_c, respectively ($T_h > T_c$); see Fig. 1. The number of energy levels for R and S is finite, but it can be made very large going to the macroscopic limit. R and S interact with an external work-source producing work and then relax back to equilibrium under the influence of the baths. For given temperatures (and given number of subsystem energy levels) work maximization can be introduced on three different levels.

(1) The extracted work is maximized over the interaction of R and S with the external source of work.

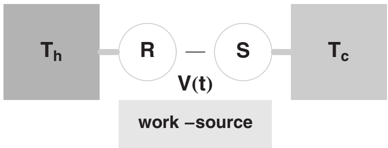

FIG. 1. Schematic representation of the considered quantum engine. Quantum systems R and S interact with thermal baths at temperatures T_h and T_c, respectively. The mutual interaction between them is governed by the potential $V(t)$ that also serves to deliver work to an external source. The mutual interaction is switched on for a short time only. Once it is switched off, the systems S and R do relax to equilibrium under influence of the respective thermal baths. Similar constructions of quantum heat engines appeared in [9,12,24].

(2) One optimizes the work, in addition, over the spectral structure of R and S.

(3) Finally, the extracted work is maximized also over the interaction of R and S with their respective thermal baths. In the following we will investigate these strategies in full detail.

This paper is organized as follows. Section II describes the studied model for a quantum heat engine. Here we also recall the derivation of the Carnot bound for the efficiency and address the problem of the power of work. In Sec. III we discuss the optimization of work over the interaction with the sources. In Sec. IV we report the results emerged from maximizing the work over the spectral structure of the involved quantum systems. In Sec. V we describe the finite-power condition, and show that a finite-level quantum engine can extract work right at the Carnot efficiency. The last section presents our conclusions, discusses some open questions, and compares our findings with the results obtained previously. Several technical issues are discussed in the appendixes.

II. MODEL

The engine consists of two quantum systems R and S which individually and in parallel couple to two different thermal baths and interact with a source of work; see Fig. 1. In the first step R and S undergo a work extraction process driven by the source. In the second step R and S relax back to their initial states under influence of the baths. Thus a cycle is performed.

Let H_R and H_S be the Hamiltonian of R and S, respectively. R (S) has n (m) energy levels. In the scenarios studied here almost all operators involved will be diagonal in the energy representation. Thus we write

$$H_R = \mathrm{diag}[\varepsilon_n, \ldots, \varepsilon_1], \quad \varepsilon_n \geq \cdots \geq \varepsilon_1, \tag{1}$$

$$H_S = \mathrm{diag}[\mu_m, \ldots, \mu_1], \quad \mu_m \geq \cdots \geq \mu_1, \tag{2}$$

where $\mathrm{diag}[a, \ldots, b]$ is a diagonal matrix with entries $(a, \ldots, b)$. We will take

$$\varepsilon_1 = \mu_1 = 0, \tag{3}$$

that is the energies of both systems are measured from zero. It will be seen below that this choice does not imply any loss of generality. The total Hamiltonian reads

$$H = H_R \otimes 1 + 1 \otimes H_S = \sum_{\alpha=1}^{nm} E_\alpha |E_\alpha\rangle\langle E_\alpha| \tag{4}$$

$$= \mathrm{diag}[\varepsilon_n + \mu_n, \varepsilon_n + \mu_{n-1}, \ldots, \varepsilon_1 + \mu_2, \varepsilon_1 + \mu_1], \tag{5}$$

where $\{E_\alpha\}_{\alpha=1}^{nm}$ and $\{|E_\alpha\rangle\}_{\alpha=1}^{nm}$ are, respectively, eigenvalues and eigenvectors of $H_R \otimes 1 + 1 \otimes H_S$.

A. Initialization

Subsystem R (S) is now assumed to couple to a thermal bath at temperature T_h (T_c); see Fig. 1. We shall assume:

$$T_h > T_c. \tag{6}$$

At this stage there is no mutual coupling between R and S, and each bath drives its corresponding subsystem to an equilibrium state specified by the Gibbs density matrices

$$\rho = \frac{e^{-\beta_h H_R}}{\mathrm{tr}\, e^{-\beta_h H_R}},$$

$$\sigma = \frac{e^{-\beta_c H_S}}{\mathrm{tr}\, e^{-\beta_c H_S}}, \tag{7}$$

where $T_h = 1/\beta_h$ and $T_c = 1/\beta_c$. Alternatively,

$$\rho = \mathrm{diag}[r_n, \ldots, r_1], \quad r_n \leq \cdots \leq r_1, \tag{8}$$

$$\sigma = \mathrm{diag}[s_m, \ldots, s_1], \quad s_m \leq \cdots \leq s_1, \tag{9}$$

$$\varepsilon_k = T_h \ln \frac{r_1}{r_k}, \quad k = 1, \ldots, n, \tag{10}$$

$$\mu_l = T_c \ln \frac{s_1}{s_l}, \quad l = 1, \ldots, m. \tag{11}$$

The overall initial density matrix is thus

$$\Omega_{\mathrm{in}} = \rho \otimes \sigma = \sum_{\alpha=1}^{nm} P_\alpha |P_\alpha\rangle\langle P_\alpha| \tag{12}$$

$$= \mathrm{diag}[r_n s_n, r_n s_{n-1}, r_n s_{n-2}, \ldots, r_1 s_1], \tag{13}$$

and the average initial energy

$$\mathrm{tr}[H\Omega_{\mathrm{in}}] = \sum_{\alpha=1}^{nm} P_\alpha E_\alpha. \tag{14}$$

Note that in Eq. (7) we did not take into account the coupling of R and S to thier baths. This aspect is discussed in Sec. II C below.

B. Two step process

1. First step: Unitary transformation

Now $R+S$ are taken to interact via a time-dependent potential $V(t)$ so that their Hamiltonian reads

$$\mathcal{H}(t) = H_R \otimes 1 + 1 \otimes H_S + V(t), \tag{15}$$

$$V(t) = 0 \quad \text{for} \quad t < 0 \quad \text{and} \quad \text{for} \quad t > \tau. \tag{16}$$

This means that the initial and final Hamiltonian (i.e., before and after this first step) are both given by Eq. (4). The potential $V(t)$ in Eq. (15) is assumed to be sufficiently strong (and to act in a sufficiently short time) so that the influence of the thermal baths between the times 0 and τ can be neglected.[1] These are the standard conditions of a thermally isolated process [2]. We require this step to be thermally isolated, since, otherwise, for the couplings to the baths being on, one would get a direct heat exchange between the baths, a factor that should decrease the overall efficiency of the work-extraction. Thus the dynamics of $R+S$ is unitary for $0 \leq t \leq \tau$:

$$\Omega_{\text{fin}} = \mathcal{U}\Omega_{\text{in}}\mathcal{U}^\dagger, \quad \mathcal{U} = \mathcal{T}\exp\left[-i\int_0^\tau d\bar{t}\mathcal{H}(\bar{t})\right], \tag{17}$$

where Ω_{in} is the initial density matrix defined in Eq. (12), Ω_{fin} is the final density matrix, $\mathcal{U}$ is the unitary evolution operator, and $\mathcal{T}\exp$ is the chronologically ordered exponent. The work extracted in this step reads [1–4]

$$W_{nm}(T_h, T_c, \varepsilon, \mu, V) = \text{tr}[\mathcal{H}(\Omega_{\text{in}} - \Omega_{\text{fin}})]. \tag{18}$$

This work W depends on a set of parameters: the number of energy levels n and m for R and S, respectively, the spectra ε and μ according to Eq. (2), and the potential $V(t)$. In the following we do not make explicit the dependence of W on the temperatures T_h and T_c, which are taken to be fixed conditions in all cases.

Equation (18) is the standard definition of work for a thermally isolated process [1–4]. This is the energy which goes from the thermally isolated system to the source of work [3]. In fact Eq. (18) is the general definition for work, since any process can be regarded as a thermally isolated one, provided that one enlarges suitably the definition of the thermally isolated system [3]. The relation of Eq. (18) with the idea of high-graded (mechanical) energy is analyzed in Ref. [3].

2. Second step: Relaxation

After $V(t)$ has been switched off, which means that the final Hamiltonian is again given by Eq. (4), R and S return to the initial states (7) and (12) after some relaxation time. This completes the two-step cycle; now the same heat-to-work transformation can be repeated.

During the relaxation the thermal baths at temperatures T_h and T_c get, respectively, the amounts of heat

$$Q_h = \text{tr}(H_R\rho) - \text{tr}(H_R \otimes 1\Omega_{\text{fin}}), \tag{19}$$

$$Q_c = \text{tr}(H_S\sigma) - \text{tr}(1 \otimes H_S\Omega_{\text{fin}}). \tag{20}$$

The work (18) is expressed as

$$W_{nm}(\varepsilon, \mu, V) = Q_h + Q_c. \tag{21}$$

Following [1,24,25] (see also Ref. [26] in this context) we determine how Q_h and Q_c relate to the temperatures. Recall that the relative entropy between two density matrices ρ_1 and ρ_2 is defined as [27]

$$S[\rho_1 \| \rho_2] = \text{tr}[\rho_1 \ln \rho_1 - \rho_1 \ln \rho_2]. \tag{22}$$

This non-negative quantity reflects the difference between ρ_1 and ρ_2: $S[\rho_1\|\rho_2]=0$ if and only if $\rho_1=\rho_2$ [27]. Due to the unitarity of the work-extracting process (17), $\text{tr}[\Omega_{\text{in}} \ln \Omega_{\text{in}}] = \text{tr}[\Omega_{\text{fin}} \ln \Omega_{\text{fin}}]$, where Ω_{in} and Ω_{fin} are defined by Eqs. (12) and (17). We get

$$-S[\Omega_{\text{fin}} \| \Omega_{\text{in}}] = \frac{Q_h}{T_h} + \frac{Q_c}{T_c} \leq 0. \tag{23}$$

If a non-negative amount of work is extracted, $W_{nm}(\varepsilon,\mu,V) \geq 0$, Eqs. (21) and (23) imply $W_{nm}(\varepsilon,\mu,V) \leq (1-\frac{T_c}{T_h})Q_h$. Together with $T_h > T_c$ this means that the heat flows from the higher temperature to the lower one:

$$Q_h \geq 0 \quad \text{and} \quad Q_c \leq 0. \tag{24}$$

For the efficiency of the work-extraction we get that it is always bound from above by the Carnot value

$$\eta_{nm}(\varepsilon,\mu,V) \equiv \frac{W_{nm}(\varepsilon,\mu,V)}{Q_h} \tag{25}$$

$$\leq \eta_{\text{Carnot}} \equiv 1 - \frac{T_c}{T_h}. \tag{26}$$

Equations (24)–(26) are, of course, well-known in the ordinary thermodynamics. Here their validity is confirmed out of the local equilibrium [24].

C. System-bath interaction

In constructing the heat engine we did not take into account the interaction of S and R to their baths. This is validated by assuming that the couplings to the baths are weak, i.e., the system-bath interaction energy is much smaller than the relevant energies of S and R. The weak-coupling suffices to drive S and R to the equilibrum states (7), but the contribution of the system-bath interaction to the work can be neglected, provided that the latter is not very small. In Appendix C we estimate this contribution for the standard setup of the system-bath interaction.

Alternatively, we can assume that S and R are subjected to the collisional interaction with their baths; see Appendix A for a discussion on this system-bath interaction mechanism. During the collisional relaxation the coupling to the bath is not weak—thus the relaxation time to equilibrium can be short—but it is switched on only for the relatively short collision time. In between two collisions one can implement the fast work-extracting transformation without taking into an explicit account the system-bath interaction.

A constantly switched-on nonweak interaction will change the situation, since now in calculating the work via Eq. (18) one should account for the contribution of the system-bath interaction energy; see Appendix C.

D. Power

As discussed above, the engine operation consists of two steps: work extraction during a reversible unitary transforma-

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[1] In more detail this procedure is described in [20].

tion, which can be implemented in an arbitrary short time, and the heat gathering step, when the baths drive R and S back to their initial states. This relaxation is in general irreversible, since, as will be seen below, at the moment when the second stage starts, the state of R (S) as given by Eq. (34) is not at local equilibrium with the hot (cold) bath.

Recall that the power is defined as the ratio of the work extracted per cycle to the cycle time: $\frac{W}{\tau_{\mathrm{cycle}}}$. To quantify whether this dimensional quantity is large or small, we compare it with the ratio $\frac{E_{\mathrm{char}}}{\tau_{\mathrm{char}}}$ of the characteristic energy of the engine (e.g., the input thermal energy) to its characteristic time (e.g., the relaxation time). A small power means that

$$\frac{W}{E_{\mathrm{char}}}\frac{\tau_{\mathrm{char}}}{\tau_{\mathrm{cycle}}} \ll 1. \tag{27}$$

Recalling the discussions in Sec. II C, we see that for the setup described in Sec. II B the power of work-extraction will be finite, since in general we shall have $W \sim E_{\mathrm{char}}$, while the cycle duration τ_{cycle} will be of order of the characteristic relaxation time, because the work-extracting step of the cycle takes a short time.

III. FIRST LEVEL MAXIMIZATION STRATEGY

We first optimize the work $W_{nm}(\varepsilon,\mu,V)$ in Eq. (18) over all unitary evolutions (17). This is equivalent to maximizing $W_{nm}(\varepsilon,\mu,V)$ over all potentials $V(t)$, defined in Eqs. (15) and (16):

$$W_{nm}(\varepsilon,\mu) \equiv \max_V[W_{nm}(\varepsilon,\mu,V)]. \tag{28}$$

This is a known problem in thermodynamics [1–4]. However, the standard textbook answer to this problem applies only to macroscopic, weakly nonequilibrium systems S and R. The solution to the maximal work-extraction problem for a given initial state Ω_{in} was given in [28–30]. For the considered situation (7)–(12) this solution amounts to the following [28–30]. Once the initial state (and thus the initial energy) is fixed, for maximizing the work (18) one has to minimize the final energy [cf. Eqs. (12)–(14)]:

$$\mathrm{tr}[H\Omega_{\mathrm{fin}}] = \sum_{\alpha=1}^{nm}\sum_{\beta=1}^{nm} C_{\alpha\beta}P_\beta E_\alpha, \tag{29}$$

where

$$C_{\alpha\beta} = \langle E_\alpha|\mathcal{U}|E_\beta\rangle\langle E_\beta|\mathcal{U}^\dagger|E_\alpha\rangle. \tag{30}$$

Note that $C_{\alpha\beta}$ is a double-stochastic matrix, i.e., (i) $C_{\alpha\beta}\geq 0$ and (ii) $\Sigma_{\alpha=1}^{n}C_{\alpha\beta}=1$ and $\Sigma_{\beta=1}^{n}C_{\alpha\beta}=1$. Conversely, any matrix that satisfies the features (i) and (ii) can be presented as in Eq. (30) for some unitary operator $\mathcal{U}$ [31]. A particular case of double-stochastic matrices are permutation matrices, which on each row and on each column contain one element equal to 1, while other elements are equal to zero. For this simplest case, which will be most relevant for our purpose, the relation with unitaries is especially clear, since the transpose Π^T of a permutation matrix Π coincides with its inverse Π^{-1}. Thus Π is already orthogonal (unitary).

It was shown in [28–30] that the double-stochastic matrix $C_{\alpha\beta}$ which minimizes the sum in the right-hand side (rhs) of Eq. (29) is a permutation matrix that enforces the largest element in E to appear in Eq. (29) paired with the smallest element in P. The one but the largest in E gets the one but the smallest element in P, and so on. Finally, the smallest element in P is paired with the largest element in E. These features explain heuristically why the above permutation matrix minimizes the rhs of Eq. (29). The complete proof of this fact is given in [28–30]. In a purely mathematical context this result appears in [31].

To write down the optimal permutation matrix, let Π_H be the permutation that orders the sequence E in Eq. (5) in the nonincreasing order

$$(\Pi_H E)_{nm} \geq (\Pi_H E)_{nm-1} \geq \cdots \geq (\Pi_H E)_1, \tag{31}$$

where $(\Pi_H E)_{nm}$ is the largest element of $\Pi_H E$ which is obviously equal to $\varepsilon_n+\mu_n$ due to Eq. (8), $(\Pi_H E)_{nm-1}$ is the one but the largest element of E which in general is not anymore equal to $\varepsilon_n+\mu_{n-1}$, etc.

In the same fashion, let Π_Ω be the permutation that orders in the nondecreasing order the sequence P in Eq. (13):

$$(\Pi_\Omega P)_{nm} \leq (\Pi_\Omega P)_{nm-1} \leq \cdots \leq (\Pi_\Omega P)_1. \tag{32}$$

Note that $(\Pi_\Omega P)_{nm}=r_n s_m$ and $(\Pi_\Omega P)_{11}=r_1 s_1$ due to Eq. (9). Then the minimal final energy can be written as $\Sigma_{\alpha=1}^{nm}(\Pi_\Omega P)_\alpha(\Pi_H E)_\alpha=\Sigma_{\alpha=1}^{nm}(\Pi_H^{-1}\Pi_\Omega P)_\alpha E_\alpha$, where Π_H^{-1} is the inverse permutation to Π_H: $\Pi_H^{-1}\Pi_H=1$. The relation between $\Pi_H^{-1}\Pi_\Omega P$ and E is that if for any two indices $E_\alpha\geq E_\beta$, then $(\Pi_H^{-1}\Pi_\Omega P)_\alpha\leq(\Pi_H^{-1}\Pi_\Omega P)_\beta$.

Thus the maximum of the work W over all interactions $V(t)$ in Eq. (15) is equal to [recall Eq. (14)]

$$W_{nm}(\varepsilon,\mu) = \sum_{\alpha=1}^{nm} P_\alpha E_\alpha - \sum_{\alpha=1}^{nm}(\Pi_H^{-1}\Pi_\Omega P)_\alpha E_\alpha. \tag{33}$$

The maximum (33) is achieved for the final state

$$\Omega_{\mathrm{fin}} = \mathrm{diag}[\Pi_H^{-1}\Pi_\Omega P], \tag{34}$$

which obviously has the same (but differently ordered) eigenvalues as Ω_{in}, since eigenvalues (but not their order) are invariants of any unitary transformation. Thus $\mathrm{tr}(\mathrm{diag}[\Pi_H E]\mathrm{diag}[\Pi_\Omega P])=\Sigma_{\alpha=1}^{nm}(\Pi_H^{-1}\Pi_\Omega P)_\alpha E_\alpha$ is the lowest possible energy that can be achieved by permuting the eigenvalues of Ω_{in} [28–30].

Introducing the separate final states of R and S,

$$\rho_{\mathrm{fin}} = \mathrm{tr}_S\Omega_{\mathrm{fin}},$$

$$\sigma_{\mathrm{fin}} = \mathrm{tr}_R\Omega_{\mathrm{fin}}, \tag{35}$$

and using Eq. (16) one can write

$$W_{nm}(\varepsilon,\mu) = \mathrm{tr}[(\rho-\rho_{\mathrm{fin}})H_R] + \mathrm{tr}[(\sigma-\sigma_{\mathrm{fin}})H_S]. \tag{36}$$

Note that ρ_{fin} and σ_{fin} commute with the respective Hamiltonians

$$[\rho_{\mathrm{fin}},H_R] = 0,$$

$$[\sigma_{\mathrm{fin}},H_S] = 0, \tag{37}$$

and that they provide a larger probability for a smaller energy, i.e., the analog of Eqs. (8) and (9) is valid for ρ_{fin} and

$\sigma_{\rm fin}$. Would not both these properties have to hold, one could extract more work from R and S. Note as well that in general $\rho_{\rm fin}$ and $\sigma_{\rm fin}$ do not have the Gibbsian form, i.e., they are not described by definite temperatures. The general form of the maximal work extracting interaction $V(t)$ [see Eq. (15) for the definition] is given in [29].

IV. SECOND LEVEL MAXIMIZATION STRATEGY

A. Optimal spectral form

We saw how to maximize the work over all interactions $V(t)$. We now maximize the work $W_{nm}(\varepsilon,\mu)$ also over all energy levels $\{\varepsilon_k\}_{k=1}^n$ and $\{\mu_l\}_{l=1}^m$, i.e., over the initial state (12). The obtained value of work W will still be a function of T_h, T_c, n, and m.

So far we have not been able to carry out analytically the maximization of W over the energy levels. Thus we have to settle for a numerical optimization of W employing the standard optimization packages of MATHEMATICA 5.[2] The result that emerged for

$$n=m \tag{38}$$

has the following form. (i) The maximal work

$$W_{nm}\equiv \max_{\varepsilon,\mu}[W_{nm}(\varepsilon,\mu)] \tag{39}$$

is attained for

$$\varepsilon_n=\varepsilon_{n-1}=\cdots=\varepsilon_2>\varepsilon_1=0, \tag{40}$$

$$\mu_n=\mu_{n-1}=\cdots=\mu_2>\mu_1=0, \tag{41}$$

that is when both upper levels ε_2 and μ_2 are $(n-1)$ fold degenerate.[3] (ii) The parameters ε_2 and μ_2 are obtained from maximizing the work. In other words the maximization over $2(n-1)$ parameters $\varepsilon_n, \varepsilon_{n-1}, \ldots, \varepsilon_2, \mu_n, \mu_{n-1}, \ldots, \mu_2$ reduces to the maximization over two parameters ε_2 and μ_2. This result has been checked numerically for $n=3, 4,$ and 5 and we expect it to hold for an arbitrary $n=m$.[4]

The intuition behind Eqs. (40) and (41) is that the energy is concentrated—as much as the thermal equilibrium allows—at higher energy levels creating a sort of instability that facilitates the subsequent work-extraction.

For the occupation numbers one gets from Eqs. (40) and (41):

$$r_n=r_{n-1}=\cdots=r_2<r_1, \tag{42}$$

$$s_n=s_{n-1}=\cdots=s_2<s_1. \tag{43}$$

In the context of Eqs. (40)–(43) we note that any state with occupation (42) and energies (40) admits a well-defined temperature. While we shall elaborate on this point in Secs. IV B 1 and IV B 2 below, it is important to stress already now that the existence of final temperatures came out as the result of maximization: in general the final state (35) does not admit any well-defined temperature. Note that few-level systems with an almost degenerate upper energy level (so-called V-configuration) are well in quantum and atomic optics; see [32] for examples.

Once the fact of Eqs. (40) and (41) is recognized, it is not difficult to get the explicit expressions for the maximal work and the corresponding efficiency at maximal work. Assuming Eqs. (40)–(43) we get from Eqs. (33) and (34) for the work and the optimal work-extraction transformation, respectively (see Appendix D for details of the derivation),

$$W_{nn}(\varepsilon_2,\mu_2)=(n-1)(\varepsilon_2-\mu_2)(r_2s_1-r_1s_2), \tag{44}$$

$$\Omega_{\rm in}=\rho\otimes\sigma,$$

$$\Omega_{\rm fin}=\sigma\otimes\rho. \tag{45}$$

Thus the optimal work extracting operation exchanges the states of S and R (SWAP). The meaning of the factorization in Eq. (45) is discussed after Eq. (95).

Equation (44) can be rewritten in a more convenient form by introducing new variables (Boltzmann weights):

$$u\equiv e^{-\beta_h\varepsilon_2},$$

$$v\equiv e^{-\beta_c\mu_2}, \tag{46}$$

so that

$$r_2=\frac{u}{1+(n-1)u},$$

$$r_1=\frac{1}{1+(n-1)u}, \tag{47}$$

$$s_2=\frac{v}{1+(n-1)v},$$

$$s_1=\frac{1}{1+(n-1)v}, \tag{48}$$

$$\varepsilon_2=T_h\ln\frac{1}{u},$$

$$\mu_2=T_c\ln\frac{1}{v}. \tag{49}$$

Equation (44) thus reads

$$W_{nn}(u,v)=\frac{(n-1)[u-v]\left[T_h\ln\frac{1}{u}-T_c\ln\frac{1}{v}\right]}{[1+(n-1)u][1+(n-1)v]}. \tag{50}$$

According to the discussion after Eq. (41), u and v in Eq. (50) are obtained by maximizing $W_{nn}(u,v)$. This makes the work positive for $T_h>T_c$. However, for several purposes (ex-

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[2] More specifically, we used three packages based, respectively, on genetic algorithms, random-gradient search, and stimulated annealing, to ensure that we get the correct results.

[3] Appendix B discusses in which sense the system with spectrum (40) is equivalent to a two-level system

[4] The reader who does not want to accept this expectation can still regard this as an anzatz providing a lower bound for the actual maximal work.

plored in detail below) it is useful to understand the behavior of $W_{nn}(u,v)$ as a function of free parameters u and v requiring only that $W_{nn}(u,v)>0$. (It should be clear that if for some u and v the latter condition is not satisfied, no work can be extracted for those values of u and u, and one should implement no work-extraction operation at all.)

Recalling Eq. (6), for the positivity of $W_{nn}(u,v)$ in Eq. (50) it is necessary to have[5]

$$u>v \quad \text{and} \quad T_h \ln\frac{1}{u} > T_c \ln\frac{1}{v}, \tag{51}$$

which together with Eqs. (6), (46), (40), and (41) leads to

$$1<\frac{\varepsilon_2}{\mu_2}<\frac{T_h}{T_c}. \tag{52}$$

Conditions (51) and (52) hold automatically after maximizing over u and v; see Eqs. (61) and (62).

For the efficiency of work-extraction we get from Eqs. (19), (25), and (51):[6]

$$\eta_{nn}(u,v)=1-\frac{\min\left[T_h \ln\frac{1}{u}, T_c \ln\frac{1}{v}\right]}{\max\left[T_h \ln\frac{1}{u}, T_c \ln\frac{1}{v}\right]}=1-\frac{T_c \ln\frac{1}{v}}{T_h \ln\frac{1}{u}}. \tag{53}$$

Comparing Eq. (50) with Eq. (53) we see that for a finite n the efficiency tending to the Carnot value $1-T_c/T_h$ means that the work extracted per cycle goes to zero (recall that the cycle duration is finite).

B. Structure of the target state

1. Temperatures after work-extraction

Recall with Eq. (6) that Ω_{in} is a nonequilibrium state. The final density matrix Ω_{fin} is also nonequilibrium, but it is expected to be closer to equilibrium than Ω_{in}.

Let us see in which sense this expectation is going to be correct. Recalling Eqs. (10), (11), (40), and (41), the final temperatures T_h' and T_c' of R and S, respectively, are deduced from Eq. (45),

$$\begin{aligned} e^{-\beta_h'\varepsilon_2}&=\frac{s_2}{s_1}=v,\\ e^{-\beta_c'\mu_2}&=\frac{r_2}{r_1}=u, \\ T_h'&=T_h\frac{\ln\frac{1}{u}}{\ln\frac{1}{v}},\end{aligned} \tag{54}$$

$$T_c'=T_c\frac{\ln\frac{1}{v}}{\ln\frac{1}{u}}. \tag{55}$$

With help of Eq. (53) and of the Carnot bound (26) we get

$$\begin{aligned} T_h&>T_h',\\ T_c&<T_c'. \end{aligned} \tag{56}$$

Thus the initially hotter system R cools down, while initially cooler S heats up. Recall that the physical meaning of the Carnot bound is closely tied to the second law, i.e., to the impossibility of transferring heat completely into work. Equations (56) provide a somewhat different perspective on the Carnot bound related to the zeroth law.

Another inequality is derived via Eqs. (55) and (52):

$$\frac{T_h'}{T_c'}<\frac{\varepsilon_2}{\mu_2}<\frac{T_h T_h'}{T_c T_c'}. \tag{57}$$

This means that the analog of the condition (52) is not satisfied for the final temperatures T_c' and T_h', so that one cannot, again, employ the final state in Eq. (45) for work extraction via a thermally isolated process.

2. Relation with the Curzon-Ahlborn efficiency

If R initially having a higher temperature than S still has this property after the work extraction, i.e., if

$$T_h'>T_c', \tag{58}$$

we get, employing Eq. (55) that Eq. (58) is equivalent to

$$\eta_{nn}>1-\sqrt{\frac{T_c}{T_h}}=\eta_{\mathrm{CA}}. \tag{59}$$

Here η_{CA} is known as the Curzon-Ahlborn efficiency [33,34]; see Sec. VI A 1 for a discussion of its various aspects. For u and v satisfying to the work-extraction condition (51), inequality (59) may or may not be satisfied. We show now that if the maximal work (over u,v) is extracted, Eq. (59) always holds.

C. Maximization of work over u and v

1. Efficiency

It remains to maximize the work $W_{nn}(u,v)$ over the parameters u and v:

$$W_{nn}=\max_{u,v}[W_{nn}(u,v)]. \tag{60}$$

Differentiating $W_{nn}(u,v)$ we get the following equations for u_{m} and v_{m}:

$$\frac{1+(n-1)u_{\mathrm{m}}}{1+(n-1)v_{\mathrm{m}}}=\sqrt{\theta}\sqrt{\frac{u_{\mathrm{m}}}{v_{\mathrm{m}}}}, \tag{61}$$

$$\left(1-\frac{v_{\mathrm{m}}}{u_{\mathrm{m}}}\right)\frac{1+(n-1)u_{\mathrm{m}}}{1+(n-1)v_{\mathrm{m}}}=\ln\frac{1}{u_{\mathrm{m}}}-\theta\ln\frac{1}{v_{\mathrm{m}}}, \tag{62}$$

where

---

[5] The inverse conditions $u<v$ and $T_h \ln\frac{1}{u}<T_c \ln\frac{1}{v}$ are not compatible with each other due to condition (6).

[6] Note that from Eqs. (46) and (53) that for a fixed ε_2 and μ_2 we get the well-known Otto-cycle result $\eta=1-\frac{\mu_2}{\epsilon_2}$, which is constrained by Eq. (52), but otherwise does not depend on temperatures. The Otto cycle is realized via two isothermal and two adiabatically (slow) processes; see, e.g., [12,18]. Thus in this scenario the power of work is very small. In contrast, as we stressed already, in our situation the efficiency (53) is obtained with a finite power.

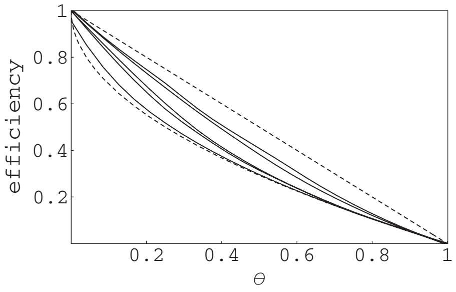

FIG. 2. Normal curves: efficiency η_{nn} at the maximal work versus the temperature ratio $\theta = \frac{T_c}{T_h}$ for various values of the energy level number n. From bottom to top: $n = 2,\ 501,\ 1001,\ 10\,001$, and $100\,001$. Upper dashed line: Carnot efficiency $\eta_{\rm Carnot} = 1 - \theta$. Lower dashed line: Curzon-Ahlbron efficiency $\eta_{\rm CA} = 1 - \sqrt{\theta}$. It is seen that $\eta_{\rm Carnot} > \eta_{nn} > \eta_{\rm CA}$.

$$\theta \equiv \frac{T_c}{T_h} \leq 1. \tag{63}$$

We see that $u_{\rm m}$ and $v_{\rm m}$—and thus $\frac{W_{nn}(u_{\rm m},v_{\rm m})}{T_h}$ and the efficiency $\eta_{nn}(u_{\rm m},v_{\rm m})$ at the maximal work—depend only on the ratio θ and the number n of the energy levels.

For $\theta = 1$, Eqs. (61) and (62) lead to $u_{\rm m} = v_{\rm m}$, and thus to $W_{nn} = \eta_{nn} = 0$, as expected. For a fixed spectrum the efficiency η would not depend on θ at all. This changes upon maximization of W: The behavior of η_{nn} as a function of $\theta = T_c/T_h$ is shown in Fig. 2. While the Carnot efficiency $\eta_{\rm Carnot} = 1 - \theta$ is always an upper bound for η_{nn}, it appears that η also has a definite lower bound given by the Curzon-Ahlborn efficiency:

$$\eta_{nn} \equiv \eta_{nn}(u_{\rm m}, v_{\rm m}) > \eta_{\rm CA} \equiv 1 - \sqrt{\theta}, \tag{64}$$

i.e., Eqs. (58) and (59) hold indeed. In particular, η_{nn} converges toward $\eta_{\rm CA}$ for $T_h \to T_c$; see next section and Fig. 2. For small values of n, η_{nn} is closer to $\eta_{\rm CA}$ than to $\eta_{\rm Carnot}$. For larger values of n and for θ not very close to 1, η_{nn} is closer to $\eta_{\rm Carnot}$.

In addition, Fig. 2 shows that η_{nn} (for a fixed θ) monotonically increases with the number n of energy levels. A similar monotonous increase holds for the dimensionless maximal work W_{nn}/T_h; see Fig. 3.

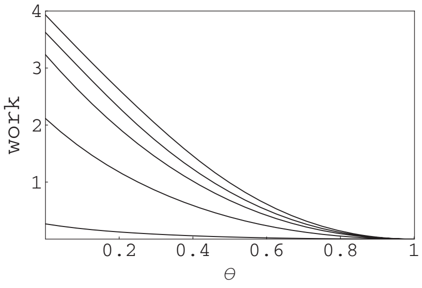

FIG. 3. Dimensionless maximal work $\frac{W_{nn}}{T_h}$ versus the temperature ratio $\theta = \frac{T_c}{T_h}$ for various values of the energy level number n. From bottom to top: $n = 2,\ 51,\ 251,\ 501$, and 1001.

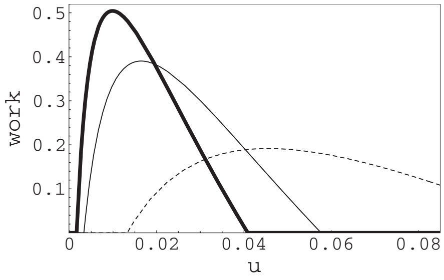

FIG. 4. The dimensionless work $\frac{W_{nn}(u,v_{\rm m})}{T_h}$ versus the parameter u. The parameter v is set at its optimal value $v_{\rm m}$ that provides the unconditional maximum of $\frac{W_{nn}}{T_h}$. Here $T_c/T_h = 0.5$. Heavy line: $n = 100$, normal line: $n = 50$, and dashed line: $n = 10$. It is seen that the maximum of $\frac{W_{nn}}{T_h}$ gets larger and sharper for larger values of n. As explained after Eq. (50), for some $u \neq u_{\rm m}$ no work can be extracted at all.

Note that according to the Clausius formulation of the second law, if there is a heat exchange between two thermal systems, the heat goes from the hotter system to the colder one. Thus the temperature of the initially hotter system is always larger than or equal to the one of the initially colder system. Now recall that the Clausius formulation in the present setup always holds globally in the sense that after the engine cycle is completed, the hotter thermal bath (attached to R) always has lost heat, while the colder bath (attached to S) always has gained heat; see Eqs. (23) and (24). Condition (58) tells that the heat goes from hot to cold not only globally (i.e., for the overall cyclic process of the engine functioning), but also locally, in the work-extraction stage. Indeed, the inverse condition $T_h' < T_c'$ will mean that the initially colder system got hotter at the end of the work-extracting stage. Thus according to Eq. (59) the maximal work extraction is related to the local version of the Clausius formulation.

Recall from Eq. (52) that for the work extraction at fixed spectra we need a finite difference between the temperatures. Condition (58), which is related to the maximization of work, shows that the final temperatures T_h' and T_c' have also to be different, in contrast to the classic thermodynamic case, where after the maximal work extraction the overall system has one single temperature [2,4].

2. Tuning to the maximum

Figure 4 presents a projection of the landscape of the dimensionless work $\frac{W_{nn}(u,v)}{T_h}$. We see that upon increasing n, the maximum of $\frac{W_{nn}}{T_h}$ not only gets larger, but it also becomes sharper. (For increasing the visibility of this effect, $\frac{W_{nn}}{T_h}$ is presented as a function of one parameter u, with another being fixed at its optimal value; other reasonable ways of taking projections around the maximum lead to similar qualitative conclusions.) Imagine that various engines with different characteristics u, v, and n operate between the two thermal baths. Now the engine with the best characteristics, i.e, larger n and with u and v closer to their optimal values for the given temperatures, will produce the largest amount of work, and will thus overdominate the others. This could explain how the optimization might occur even without explicit selection.

D. Special parameter windows

Equilibrium limit

For the close to equilibrium situation $T_h \approx T_c$ one introduces the small parameter ε in the following way:

$$\theta \equiv \frac{T_c}{T_h} = 1 - \epsilon,$$

$$\frac{u_{\mathrm{m}}}{v_{\mathrm{m}}} = 1 + \epsilon\omega, \tag{65}$$

Using Eq. (65) in Eqs. (61) and (62) and keeping terms $\sim O(\epsilon)$, we get

$$v_{\mathrm{m}} = e^{-2\omega}, \tag{66}$$

$$\frac{1}{\omega} = \frac{1-(n-1)e^{-2\omega}}{1+(n-1)e^{-2\omega}}. \tag{67}$$

Equation (66) expresses v_{m} via ω, while Eq. (67) is a transcendental equation for ω. As graphical construction shows, Eq. (67) has a unique positive solution for $n \geq 2$. Combining Eqs. (66) and (67) with Eqs. (50) and (53) we get for the maximal work W_{nn} and for the efficiency η_{nn} at the maximal work:

$$W_{nn} = \frac{\epsilon^2\omega^2 e^{-2\omega}}{(1+ne^{-2\omega})^2} + O(\epsilon^2), \tag{68}$$

$$\eta_{nn} = \frac{\epsilon}{2} + O(\epsilon^2), \tag{69}$$

where $\omega > 0$ is the solution of Eq. (67). As Eq. (69) shows, in the considered order η_{nn} coincides with the Curzon-Ahlborn efficiency: $\eta_{\mathrm{CA}} = 1 - \sqrt{1-\epsilon} = \epsilon/2$.

E. Macroscopic limit: Work and efficiency

Here we restrict ourselves with the specific spectra as given by Eqs. (40) and (41). If S and R are macroscopic, then $\ln n$ is large:

$$\ln n \gg 1. \tag{70}$$

Indeed for a system containing $N \gg 1$ particles, the number of energy levels scales as $e^{\mathrm{const}\ N}$.

The solution of Eqs. (61) and (62) is found via expanding over the large parameter $\ln[n-1]$:

$$u_{\mathrm{m}} = \frac{\theta(1-\theta)\ln[n-1]}{n-1} - \frac{\phi+1-\theta^2}{n-1}, \tag{71}$$

$$v_{\mathrm{m}} = \frac{\theta}{(1-\theta)[n-1]\ln[n-1]} + \frac{\phi-1+\theta^2}{(1-\theta)^2(\ln[n-1])^2}, \tag{72}$$

$$\phi \equiv \theta \ln\{\theta(1-\theta)\ln[n-1]\} + \theta^2 \ln\left[\frac{1-\theta}{\theta}\ln[n-1]\right]. \tag{73}$$

The first terms in the rhs of Eqs. (71) and (72), respectively, are the dominant ones, while the second terms are the corrections of order $O(\frac{1}{\ln[n-1]})$.

Substituting Eqs. (71) and (72) into Eqs. (50) and (53) we get for the maximal work W_{nn} and for the corresponding efficiency η_{nn}

$$\frac{W_{nn}}{T_h} = (1-\theta)\ln[n-1] - \frac{\phi+1+\theta^2}{\theta} \tag{74}$$

$$+ O\left(\frac{1}{\ln[n-1]}\right), \tag{75}$$

$$\eta_{nn} = 1 - \theta - \frac{2\theta}{\ln[n-1]}\ln\{(1-\theta)\ln[n-1]\} \tag{76}$$

$$+ O\left(\frac{1}{(\ln[n-1])^2}\right), \tag{77}$$

where ϕ is given by Eq. (73), while the factors $O(\frac{1}{\ln[n-1]})$ and $O(\frac{1}{(\ln[n-1])^2})$ in Eqs. (75) and (77) can be recovered with help of the correction in Eqs. (71) and (72), respectively.

It is seen from Eqs. (74) and (76) that the efficiency converges to the Carnot value, while the maximal work converges to the simple expression

$$W_{nn} = T_h(1-\theta)\ln n, \tag{78}$$

which is a characteristic input thermal energy $T_h \ln n$ times the Carnot efficiency $1-\theta$. The corrections to these results,i.e., the last terms in the rhs of Eqs. (74) and (76), are important as well. They show that besides Eq. (70) one should satisfy

$$(1-\theta)\ln n \gg 1, \tag{79}$$

and that due to negativity of the corrections the actual values of W_{nn} and η_{nn} increase in the macroscopic limit.

1. Macroscopic limit: Structure of the engine

An additional implication of the macroscopic limit is that the temperatures T_h' and T_c' defined in Eq. (55) converge to T_h and T_c, respectively. This is clear from Eq. (76) and from $\frac{T_c'}{T_c} = \frac{T_h}{T_h'} = \frac{1-\eta_{nn}}{\theta}$, which follows from Eq. (55).

As follows from Eq. (79), the macroscopic limit is not compatible with the equilibrium limit $T_h \to T_c$. An additional obstacle for the macroscopic limit of the maximal work (but not of the efficiency) is $\theta \to 0$, since then the correction $\frac{1}{\theta}$ in the left-hand side (lhs) of Eq. (74) diverges.

For $\theta \to 1$ (or $T_c \to T_h$) both the work and efficiency go to zero. However, according to Eq. (79) they tend to zero after having left the macroscopic regime [Eqs. (74)–(77)]. For this regime Eq. (79) implies that the relative difference $1-\theta$ should be smaller than $\frac{1}{\ln n}$.

TABLE I. The maximal work W_{23} and the relative difference $\frac{\eta_{23}-\eta_{\rm CA}}{\eta_{\rm CA}}$ between the efficiency at the maximal work and the Curzon-Ahlborn efficiency for various temperatures. Here as in Eq. (80), the hot system R has two energy levels, while the cold system S has three energy levels.

	W_{23}	$\frac{\eta_{23}-\eta_{\rm CA}}{\eta_{\rm CA}}$
$T_h=2\ T_c=1$	0.0891062	0.0292807
$T_h=3\ T_c=1$	0.265928	0.0560355
$T_h=10\ T_c=1$	1.97317	0.112379

We should stress that the considered example with the strongly degenerate upper energy level is not what one usually relates with the macroscopic limit [2,3]. The latter is connected with many nearly equidistant energy levels. We should, however, note that the studied situation does resemble the ordinary macroscopic limit in several ways. Indeed we note from Eqs. (71) and (72) and from Eq. (49) that the energy gaps ε_2 and μ_2 scale as $\ln n$, as should be for macroscopic systems. Another aspect is uncovered when comparing Eqs. (71) and (72) with Eqs. (48) and (49): in the limit (70) for the high-temperature system R the population is concentrated on the higher ($n-1$ times degenerate) energy level ε_2, while for the low-temperature system S the population is concentrated on the lowest ($\mu_1=0$) energy level. In particular, this means that for both S and R in the limit (70), the canonical ensemble is equivalent (in the leading order of $\frac{1}{\ln n}$) to the microcanonic ensemble, where all the population is put on one [possibly (quasi)degenerate] energy level. This is what one expects for a macroscopic system.

2. System with $n \neq m$

So far we studied the case when both subsystems S and R have the same size, i.e., the same number $n=m$ of energy levels. One may want to know what happens for $n\neq m$. One of the simplest models of this type is

$$n=2 \quad \text{and} \quad m=3. \tag{80}$$

While for $m=n$ we had the conditions (40) and (41), which considerably simplified the subsequent analysis, no analog of these conditions holds for Eq. (80). Thus we have to rely on numerical investigations. It appears that we can keep all qualitative conclusions; see Table I. (i) The dimensionless maximal work $\frac{W_{nm}}{T_h}$ is still a function of the temperature ratio $\theta=T_c/T_h<1$. (ii) The optimal values of the energy spacings—though not satisfying any simple condition similar to Eqs (40) and (41)—still depend only on θ. (iii) The efficiency at the maximal work η_{nm} is still bounded from below by the Curzon-Ahlborn value $1-\sqrt{\theta}$ and from above by the Carnot value $1-\theta$.

F. Conditional maximum

When seeking the maximum of W over the spectra one may impose additional constraints. We study two such scenarios below.

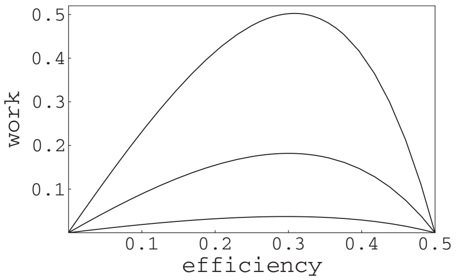

FIG. 5. The dimensionless work $\frac{W_{nn}(\eta)}{T_h}$ defined in Eq. (81) versus the efficiency η. Recall from Eq. (81) that $W_{nn}(\eta)$ is obtained by maximizing the work over all parameters for a fixed efficiency η. For this figure $\theta=\frac{T_c}{T_h}=0.5$, and from bottom to top: $n=2$, 51, and 101. Note that $\frac{W_{nn}(\eta)}{T_h}$ turns to zero two times: for $\eta=0$ and for $\eta=\eta_{\rm Carnot}=1-\theta$. The maximum of $\frac{W_{nn}(\eta)}{T_h}$ corresponds to the overall maximization of work; see Fig. 3.

1. Maximization of work for fixed efficiency

Consider the maximum of $W_{nn}(u,v)$ in Eq. (50), when the maximization over the parameters u and v is carried out under the condition of a given efficiency (53). This defines the dimensionless maximal work $\frac{W_{nn}(\eta)}{T_h}$ for a fixed efficiency η:

$$\frac{W_{nn}(\eta)}{T_h} = \max_u \left[\frac{(n-1)\,\eta[u-u^{1-\eta/\theta}]\ln\frac{1}{u}}{[1+(n-1)u][1+(n-1)u^{1-\eta/\theta}]} \right]. \tag{81}$$

Note that $W_{nn}(\eta)$ is still a function of the temperature ratio $\theta=\frac{T_c}{T_h}$.

As seen in Fig. 5, $\frac{W_{nn}(\eta)}{T_h}$ as a function of η is a bell-shaped curve, which turns to zero once for $\eta=0$ and then for $\eta=\eta_{\rm Carnot}$; recall the discussion after Eq. (53). Figure 5 shows that $\frac{1}{T_h}W_{nn}(\eta)$ increases upon increasing the number of energy levels, while the maximum η_{nn} of $\frac{1}{T_h}W_{nn}(\eta)$ shifts toward larger values, since in the macroscopic limit $\frac{1}{T_h}W_{nn}(\eta)$ will have its maximum very close to the Carnot value $\eta=1-\theta$; recall Eq. (76).

2. Emergence of the Curzon-Ahlborn limit during partial optimization of work: An example

It may be instructive to follow in more detail, but via a particular example, how the Curzon-Ahlborn lower bound for the efficiency emerges during a constrained maximization. Assume that the systems R and S have, respectively, the spectra $\{a_R\varepsilon_k\}_{k=1}^n$ and $\{a_S\varepsilon_k\}_{k=1}^n$, which differ only by positive scaling factors a_R and a_S. The initial states of R and S are given by Eq. (7). We shall not optimize over the interaction with the work sources, but rather impose the SWAP transformation (45) for the work extraction. The work extracted during this transformation is deduced from Eq. (18):

$$W_{nn}(a_R,a_S) = (a_R-a_S)\sum_{k=2}^{n}\varepsilon_k(r_k-s_k), \tag{82}$$

where $r_k \propto e^{-\beta_h a_{\rm R}\varepsilon_k}$ and $s_k \propto e^{-\beta_h a_{\rm S}\varepsilon_k}$. In the second step the systems R and S are subjected to free relaxation, as described in Sec. II B 2. Without loss of generality we assume $\frac{T_c}{T_h} < \frac{a_S}{a_R}$, which means that R (S) has higher (lower) temperature.[7] The efficiency of work extraction is obtained from Eqs. (82), (19), and (25):

$$\eta_{nn}(a_R, a_S) = 1 - \frac{a_S}{a_R}. \tag{83}$$

We now employ a necessary condition $\frac{\partial W_{nn}}{\partial a_R} = \frac{\partial W_{nn}}{\partial a_S} = 0$, for the work (82) to be optimal over a_S and a_R. Working out $\frac{\partial W_{nn}}{\partial a_R} + \frac{\partial W_{nn}}{\partial a_S} = 0$ we get

$$1 - \frac{a_S}{a_R} = 1 - \sqrt{\frac{T_c C_c}{T_h C_h}}, \tag{84}$$

where $C_h = \beta_h^2 a_R^2 [\langle \varepsilon^2 \rangle_h - \langle \varepsilon \rangle_h^2]$ and $C_c = \beta_c^2 a_S^2 [\langle \varepsilon^2 \rangle_c - \langle \varepsilon \rangle_c^2]$ are the equilibrium specific heats of R and S, respectively, calculated for the initial states at the temperatures T_h and T_c (recall that $T_h > T_c$).

For a finite number of energy levels n, the equilibrium specific heat C is a nonmonotonous function of temperature: for low temperatures C naturally goes to zero, while for very large temperatures it is zero again, since there is a maximal energy a finite-level system can have. For $n = \infty$ the equilibrium specific heat can be (but need not be) a monotonically increasing function of the temperature, since now the system can accept infinitely large energies.[8] Thus now $\frac{C_c}{C_h} < 1$, since $T_h > T_c$, and Eq (84) implies that the Curzon-Ahlborn value is a lower bound for the efficiency (83).

We draw two conclusions: (i) upon partial maximization the Curzon-Ahlborn value may or may not be a lower bound for the efficiency depending on the system details; and (ii) the emergence of the Curzon-Ahlborn lower bound is facilitated for systems with a classical (i.e., unlimited from above) spectrum, since now the equilibrium specific heat can be an increasing function of the temperature.

V. THIRD LEVEL MAXIMIZATION STRATEGY

Eventually we optimize also the second step, i.e., we try to extract work also during the relaxation of R and S. We start at the initial state (12) of $S+R$. The maximal work-extracting transformation is applied, the work (33) is extracted, and R (S) is left in the final state $\rho_{\rm fin}$ ($\sigma_{\rm fin}$), as given by Eq. (35). Recall from Eq. (37) that $\rho_{\rm fin}$ and $\sigma_{\rm fin}$ commute with their Hamiltonians. In Sec. II C we described two scenarios of coupling of R and S to their thermal baths. This is either the weak-coupling regime or the collisional relaxation. In both these cases the joint initial state of R (S) and the hot (cold) bath is factorized before the work-extracting transformation: $\rho \otimes \rho_{\rm B}$ ($\sigma \otimes \sigma_{\rm B}$), where $\rho_{\rm B}$ ($\sigma_{\rm B}$) is the equilibrium state of the hot (cold) bath. Since the interaction with the bath is not essential during the work-extracting step, the same factorization holds after this step: $\rho_{\rm fin} \otimes \rho_{\rm B}$ and $\sigma_{\rm fin} \otimes \sigma_{\rm B}$.

If we just let R (S) to interact with the thermal bath at temperature T_h (T_c), it will relax back to the initial state ρ (σ). We can, however, control this relaxation process and extract an additional amount of work.

According to the standard thermodynamic argument [2,4], the *maximal* work extractable—via a cyclic-Hamiltonian process—from a system in the initial state $\rho_{\rm fin}$ in contact with the thermal bath at temperature T_h is bounded from above by the free energy difference

$$\Delta F_R = \Delta U_R - T_h \Delta S_R, \tag{85}$$

$$\Delta U_R \equiv {\rm tr}[\rho_{\rm fin} H_R] - {\rm tr}[\rho H_R], \tag{86}$$

$$\Delta S_R \equiv -{\rm tr}[\rho_{\rm fin} \ln \rho_{\rm fin}] + {\rm tr}[\rho \ln \rho], \tag{87}$$

where ρ is the equilibrium state (7), and where ΔU_R and ΔS_R are the changes of the energy and the von Neumann entropy, respectively.

A detailed discussion of Eq. (87) and its derivation is given in Appendix E 1. Moreover, in Appendix E 2 we show that if the initial state commutes with the Hamiltonian, $[\rho_{\rm fin}, H_R] = 0$, as is the case according to Eq. (37), the bound (87) is achieved via the following.

(1) *Suddenly* changing the energy spacings of H_R according to Eqs. (E17)–(E19). This brings R to the local equilibrium with the hot bath, since at the end of the sudden change the temperature of R is equal to the bath temperature T_h. The change is sudden as compared to the relaxation time induced by the hot bath, so that the interaction with the hot bath during the change is neglected.

(2) *Slowly* changing the spacings back to their initial values. Now the change is much slower than the relaxation time of R and thus the power of work extraction is small; see Eq. (27). R is always in the local equilibrium with the hot bath; see the discussion around Eq. (E21). The equilibrium state ρ is attained at the end of this isothermal process.

The heat received from the hot thermal bath is [compare with Eq. (19)]:

$$Q_h = {\rm tr}(H_R \rho) - {\rm tr}(H_R \rho_{\rm fin}) + \Delta F_R = -T_h \Delta S_R, \tag{88}$$

where ΔF_R is given by Eq. (87).

The same procedure is applied to S thereby extracting the work ΔF_S:

$$\Delta F_S = \Delta U_S - T_c \Delta S_S, \tag{89}$$

$$\Delta U_S \equiv {\rm tr}[\sigma_{\rm fin} H_S] - {\rm tr}[\sigma H_S], \tag{90}$$

$$\Delta S_S \equiv -{\rm tr}[\sigma_{\rm fin} \ln \sigma_{\rm fin}] + {\rm tr}[\sigma \ln \sigma]. \tag{91}$$

The total work extracted during the cycle reads

$$\mathfrak{W}_{nm}(\varepsilon, \mu) = W_{nm}(\varepsilon, \mu) + \Delta F_R + \Delta F_S \tag{92}$$

---

[7] Since we did not optimize over the interaction with the sources of work, $W_{nn}(a_R, a_S)$ in Eq. (82) can be negative, e.g., for $T_h = T_c$, which means that the work is put into the system.

[8] An example of such a behavior is given by a harmonic oscillator with frequency ω, where $\varepsilon_n = \hbar \omega n$, and the specific heat is $C = b^2 e^b (e^b - 1)^{-2}$, with $b = \hbar \omega / T$.

$$=-T_h\Delta S_R - T_c\Delta S_S, \tag{93}$$

where $W_{nm}(\varepsilon,\mu)$ is the maximal work (36) (optimized over the interaction with the sources of work) extracted during the first stage. Note that the only feature of $W_{nm}(\varepsilon,\mu)$ employed in passing from Eq. (92) to Eq. (93) is that the evolution of $R+S$ in the first stage is themally isolated, i.e., $W_{nm}(\varepsilon,\mu)$ is equal to the energy difference of $R+S$; see Eq. (18).

The efficiency that follows from Eqs. (88) and (93) is

$$\mathfrak{e}_{nm}(\varepsilon,\mu) = 1 + \frac{T_c}{T_h}\frac{\Delta S_S}{\Delta S_R}. \tag{94}$$

The work (93) is now optimized over the spectra $\varepsilon_n,\ldots,\varepsilon_2$ and $\mu_n,\ldots,\mu_2$ of R and S, respectively, for fixed temperatures.

For R and S having the same number of energy levels: $n=m$, the numerical optimization of Eq. (93) produced the same result [Eqs. (40) and (43)] as for the work extraction at a finite power: the optimal work is achieved for the upper levels being $n-1$ fold degenerate.

As we already know, Eqs. (40) and (41) imply the factorized final state (34): $\rho_{\rm fin}=\sigma$ and $\sigma_{\rm fin}=\rho$; see Eq. (45). Recalling the definitions (87) and (91) of ΔS_S and ΔS_R, we get

$$\Delta S_S + \Delta S_R = 0. \tag{95}$$

The physical meaning of this condition becomes clear when noting that if the factorization (45) was invalid, i.e., if there were correlations in the final state (34), the sum $\Delta S_S+\Delta S_R$ would be larger than zero, as implied by the subadditivity of the von Neumann entropy.[9] Since after the second step of the engine operation, the systems R and S return to their initial states (7), the surplus entropy $\Delta S_S+\Delta S_R$ has to be consumed by the thermal baths, thereby increasing their entropy. Thus the factorization condition (45) eliminates this potential channel for entropy generation.

Equations (94) and (95) imply that the efficiency is equal to the *maximally possible* Carnot value:

$$\mathfrak{e}_{nn} = \eta_{\rm Carnot} = 1 - \frac{T_c}{T_h}. \tag{96}$$

Using Eqs. (46)–(49) we get for the work (93)

$$\mathfrak{W}_{nn}(u,v) = (T_h - T_c)(\mathrm{tr}[\sigma \ln \sigma] - \mathrm{tr}[\rho \ln \rho]) \tag{97}$$

$$=(T_h - T_c)\left[\ln\frac{1+(n-1)u}{1+(n-1)v} + (n-1)\right.$$
$$\left.\times\frac{v\ln v - u\ln u + (n-1)uv\ln\frac{v}{u}}{[1+(n-1)u][1+(n-1)v]}\right]. \tag{98}$$

The latter expression is to be optimized over u and v. It should be clear from our constructions that

TABLE II. The maximal value of $\mathfrak{W}_{33}$, given by Eq. (98) with maximization over the parameters u and v, compared to the maximal value of W_{33}; see Eq. (60). The maximization is done for $n=m=3$ (two three-level systems). We also present the relative difference $\frac{\eta_{33}-\eta_{\rm CA}}{\eta_{\rm CA}}$ between the efficiency η_{33} at the maximal work W_{33} and the Curzon-Ahlborn efficiency $\eta_{\rm CA}=1-\sqrt{T_c/T_h}$. Recall that the work $\mathfrak{W}_{33}$ is extracted with the Carnot efficiency; see Eqs. (94) and (96).

	W_{33}	$\frac{\eta_{33}-\eta_{\rm CA}}{\eta_{\rm CA}}$	$\mathfrak{W}_{33}$
$T_h=2$ $T_c=1.7$	0.009271	0.000931	0.0198908
$T_h=2$ $T_c=1$	0.128486	0.0142578	0.478908
$T_h=10$ $T_c=1$	3.07425	0.0711658	9.20744

$$\mathfrak{W}_{nn} \equiv \max_{u,v}[\mathfrak{W}_{nn}(u,v)] \geq W_{nn}. \tag{99}$$

It is seen that $\frac{\mathfrak{W}_{nn}}{T_h}$—analogously to W_{nn} in Eq. (60)—is a function of the temperature ratio $\theta\equiv\frac{T_c}{T_h}$.

The difference $\mathfrak{W}_{nn}-W_{nn}$ quantifies how much work has been traded in by sacrificing the power. As Table II shows, especially for $T_h\approx T_c$, the ratio $\frac{\mathfrak{W}_{nn}}{W_{nn}}$ can approach $\sim$20.

VI. DISCUSSION AND CONCLUSIONS

A. Relation to previous work

1. Curzon-Ahlborn efficiency

The Curzon-Ahlborn (or more precisely Chambadal-Novikov-Curzon-Ahlborn) value [33,34] was first obtained as the efficiency of an irreversible (endoreversible) Carnot engine operating at the maximal power; see [33] for reviews. This result was generalized in [35,36], where it was found that the Curzon-Ahlborn value is an *upper* bound for the efficiency of a heat engine operating at the maximum power and according to the rules of the linear transport theory. Reference [9] studies a quantum heat engine model and derives the Curzon-Ahlborn value, but in the limit of vanishing interaction with sources of work. The Curzon-Ahlborn efficiency appears as well in several reversible heat engine models [37].

In contrast, we show that the Curzon-Ahlborn value is the *lower* bound for the efficiency at the maximal work and a finite power of work. Within the presented approach the cycle time is fixed, thus the maximization of the power amounts to the work maximization. In our model the efficiency which maximizes the work is thus strictly larger than the Curzon-Ahlborn efficiency.

2. Carnot efficiency

According to standard thermodynamics the efficiency of any heat engine is bounded by the Carnot value [2,4]. Although this result was derived within (nearly) equilibrium thermodynamics, it can be extended to a rather general class of nonequilibrium heat engines; see Eqs. (23) and (26) and [24]. While useful as an upper bound, the Carnot efficiency by itself is often considered to lack practical significance,

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[9] If $S_{12}=-\mathrm{tr}\,\rho_{1+2}\ln\rho_{1+2}$ is the von Neumann entropy of a composite system with density matrix ρ_{1+2}, then the subadditivity implies [27]: $S_{1+2}\leq S_1+S_2$, where $S_i=-\mathrm{tr}\,\rho_i\ln\rho_i$, $i=1,2$, and where $\rho_1=\mathrm{tr}_2\,\rho_{1+2}$, $\rho_2=\mathrm{tr}_1\,\rho_{1+2}$.

since the the power of work goes to zero in this limit. This has been a motivation to develop the so-called finite-time (finite-power) thermodynamics [33].

For a finite-level quantum heat engine operating close to the Carnot efficiency we have two related results. First we show that for such an engine operating with a finite cycle duration, the work extracted per cycle goes to zero when the efficiency approaches the Carnot value; see our discussion at the end of Sec. IV A. The second result is that the same quantum engine can extract a nonzero amount of work—but with a long cycle duration—sharply at the Carnot efficiency, provided one properly optimizes the bath-engine interaction.

Results on small quantum [7,13,14,16,17] or classical [38,39] engines working at zero power, but with the Carnot efficiency, were already reported in literature. Most of these results [7,16,17,38,39] concern continuously [not cyclically] working engines, where the external source of work is absent and the work is performed by moving particles against an external force; see [40] for a review on the energetics of such engines. In contrast, Refs. [13,14] report on a cyclically operating quantum heat engine that (at a small power) deliver with the Carnot efficiency a finite amount of work per cycle to an external source of work. Both these works attempt to model a quantum Carnot cycle. Various limits in achieving the Carnot limit for small systems are studied in [41].

In this context we show that the macroscopic engine can extract a finite amount of work at a finite power and with (almost) the Carnot efficiency.

B. Summary

Our purpose has been to deduce the physics of quantum heat engines from maximizing the work (extracted per cycle) under various constraints. The work maximization can be introduced on three different levels.

(1) One optimizes the extracted work over the interaction of the quantum systems S and R with the external source of work. In general, this procedure is not sufficient for extracting a finite amount of work at $T_h \neq T_c$. In addition, the intermediate stages of the engine functioning are not described by well-defined temperatures: if S and R had well-defined temperatures before the work-extraction, they are not guaranteed to have definite temperatures after (or during) this process.

(2) One maximizes the work, in addition, over the spectral structure of S and R. The optimal spectral structure has been found to be effectively two-level. This level of maximization turns out to be a crucial step, since after this optimization one finds that (i) S and R are described by well-defined temperatures in the intermediate stages of the engine operation. (ii) The Clausius formulation of the second law—heat goes from higher to lower temperature—is satisfied not only for the total work-extracting cycle (as it should), but also locally for the intermediate stages of the process. Thus the local thermodynamic structure emerges as a result of work optimization. (iii) The efficiency at the maximal work is bounded from *below* by the Curzon-Ahlborn efficiency $1-\sqrt{T_c/T_h}$. This is in addition to the upper Carnot bound $1-T_c/T_h$, which holds for this model generally (with or without any optimization). The important feature of these limits is that they are system-independent.

The Curzon-Ahlborn bound is approached close to equilibrium $T_h \to T_c$, while the Carnot upper bound is reached—at a finite power—for a large system S and R. In the latter macroscopic limit S and R (tuned to extract the maximal work) have the expected features of macroscopic systems, e.g., canonic and microcanonic ensembles are equivalent for them. The equilibrium and macroscopic limits do not commute. We demonstrated that for a system with an unbound energy spectrum even a partial maximization over the spectrum may lead to efficiency larger than the Curzon-Ahlborn value. Within the present approach the cycle time is fixed and the power is in general finite.

The optimal work-extraction unitary operation appears to be the so-called SWAP, well-known—especially for the particular case $n=2$—as one of the basic gates of quantum computation [27]. Although SWAP is normally realized via composition of several more elementary unitary operations [27], its direct implementation for atomic few-level systems was argued to be feasible [42].

(3) Finally, one optimizes the extracted work also over the interaction of S and R with their respective thermal baths. This optimization was carried out via increasing the cycle duration and thus reducing the power of work extraction. The main result is that the Carnot value for the efficiency—with a finite amount of work extracted at a small power—is reached for finite systems S and R. Thus there are two options for operating close to the Carnot efficiency: either one extracts a finite amount of work per a very long cycle, or a small amount of work per a finite cycle.

Several important questions have to be left open, among those are How generic are the optimization conditions? How could a given operating engine tune itself to the maximum, and under which constraints? What are quantum effects proper? Can one extract work at finite power by employing a finite-level engine operating at the Carnot-efficiency?

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APPENDIX A: COLLISIONAL RELAXATION

The purpose of this discussion is to outline a realistic example of a finite-duration (collisional) relaxation process which is consistent with the thermally isolated work extracting setup described in Sec. II B 1. Our presentation follows [25,43,44].

The thermal bath is modeled as a collection of $N \gg 1$ independent equilibrium systems (particles) with density matrices $\omega_i = \frac{1}{Z_i}\exp[-\beta H_i]$ and Hamiltonians H_i, where $i=1,\ldots,N$, and where $1/\beta = T$ is the bath temperature. This formalizes the intuitive notion of the bath as a collection of many weakly interacting equilibrium systems.

The target system R starts in (an arbitrary) initial state ρ and has Hamiltonian H_R. The collisional relaxation is realized when the particles of the bath sequentially interact [collide] with R. Consider the first collision. The initial state of R and the first bath particle is $\Omega_{1+R}=\rho\otimes\omega_1$, the interaction between them is realized via a unitary operator $\mathcal{V}$, so that the final state after the first collision is $\Omega'_{1+R}=\mathcal{V}\Omega_{1+R}\mathcal{V}^\dagger$. Define separate final states:

$$\rho' = \mathrm{tr}_1\Omega'_{1+R},$$

$$\omega'_1 = \mathrm{tr}_R\Omega'_{1+R}, \tag{A1}$$

where tr_1 and tr_R are the partial over the first particle and R, respectively. Recall the definition (22) of the relative entropy. The unitarity of $\mathcal{V}$ implies

$$S[\Omega'_{1+R}\,\|\,\rho'\otimes\omega_1] = \mathrm{tr}[\Omega_{1+R}\ln\Omega_{1+R}] - \mathrm{tr}[\Omega'_{1+R}\ln(\rho'\otimes\omega_1)]. \tag{A2}$$

Employing $\omega_1=\frac{1}{Z_1}\exp[-\beta H_1]$ and $S[\Omega'_{1+R}\|\rho'\otimes\omega_1]\geq 0$ in Eq. (A2) we get

$$T\Delta S_R + \Delta U_1 \geq 0, \tag{A3}$$

where $\Delta S_R=\mathrm{tr}[-\rho'\ln\rho'+\rho\ln\rho]$ and $\Delta U_1=\mathrm{tr}(H_1[\omega'_1-\omega_1])$ are, respectively, the change of the entropy of R and the average energy of the first particle.

We now require that the that interaction $\mathcal{V}$ conserves the energy: $\Delta U_1=-\Delta U_R$. Using this in Eq. (A3) one has

$$\Delta U_R - T\Delta S_R \leq 0. \tag{A4}$$

Since we did not use any special feature of the initial state of R, Eq. (A4) holds for subsequent collisions of R with the bath particles. Thus $\Delta U_R-T\Delta S_R$ decays in time, and it should attain its minimum. It is well-known [2] that this minimum is reached for the Gibbs matrix $\rho\propto e^{-\beta H_R}$: the collisions drive R to equilibrium starting from an arbitrary state. The coupling with the bath is switched on during the collision only, but since this coupling can be sizable, the relaxation time can be very short [25].

Further results and concrete scenarios of collisional relaxation are given in [25,43–45]. This includes the rate of (exponential) convergence to equilibrium which was favorably compared to experiments in [43].

As for the implementation of the work extracting pulse described in Sec. II B 1, one notes that within the present relaxation model, the duration of the pulse has to be shorter than the time between the collisions. If the latter time is much larger than both the collision time and the pulse time, almost any implementation of the pulse will amount to a thermally isolated process.

APPENDIX B: SYSTEM WITH $n-1$ FOLD DEGENERATE SPECTRUM

Consider an n-level quantum system R whose upper $n-1$ energy levels are degenerate; see Eq. (40). Let us show that the behavior of R is equivalent to that of a two-level system ($n=2$) with respect to all transformations that do not resolve the $n-1$ fold degeneracy of the spectrum (40). To this end we introduce for $n=3$ generalized Pauli matrices (extending to $n>3$ is straightforward)

$$\hat{\tau}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$\hat{\tau}_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix},$$

$$\hat{\tau}_2 = i\hat{\tau}_1\hat{\tau}_3. \tag{B1}$$

It is clear that (i) the algebra of these matrices is identical to that of the Pauli matrices; (ii) any perturbation of the Hamiltonian H_R of R by an arbitrary linear combination of $\{\hat{\tau}_i\}_{i=1}^3$ does not change the double-degeneracy of H_R; and (iii) if the initial state of R can be expressed only via $\{\hat{\tau}_i\}_{i=1}^3$, then during any interaction with another quantum system, which is written only via $\hat{\tau}_i$ and arbitrary operators of this system, R is dynamically equivalent (via the Heisenberg representation) to a two-level system. An example of such an initial state is when R is described by a definite temperature.

APPENDIX C

Here we shall analyze a scenario of the interaction between R (S) and the thermal bath at temperature T_h (T_c). We assume that the system-bath coupling is always on, and analyze the contribution to the work coming from the system-bath interaction energy.

Recall from Eq. (40) that the optimal work-extraction engine consists of effectively two-level systems R and S; see Eq. (40). The full Hamiltonian of R and S together with their interactions with the corresponding thermal (macroscopic) baths reads [46]:

$$\mathcal{H} = \mathcal{H}_R + \mathcal{H}_S \tag{C1}$$

$$= \frac{\varepsilon}{2}(1+\hat{\tau}_3^{[R]}) + \frac{\mu}{2}(1+\hat{\tau}_3^{[S]}) \tag{C2}$$

$$+ g\,\hat{\tau}_1^{[R]}\otimes B^{[R]} + g\,\hat{\tau}_1^{[S]}\otimes B^{[S]} \tag{C3}$$

$$+ H_{\mathrm{bath}}^{[R]} + H_{\mathrm{bath}}^{[S]}, \tag{C4}$$

The rhs of Eq. (C2) contains the Hamiltonians of R and S, where $\hat{\tau}_{1,3}^{[R,S]}$ are the (generalized) Pauli matrices as defined in Appendix B, and where ε and μ are the energy gaps of R and S. Equation (C3) accounts for the interaction Hamiltonians of R and S to their baths. Here $B^{[R]}$ ($B^{[S]}$) is the collective operators of the bath attached to R (S). All particles of the (macroscopically large) bath contribute into $B^{[\mathrm{R}]}$ ($B^{[S]}$), which lives in the Hilbert space of the bath. The fact of $[\hat{\tau}_1,\hat{\tau}_3]\neq 0$ is necessary for ensuring the proper relaxation of the two-level system.

In Eq. (C3) $g>0$ is the system-bath coupling constant; for simplicity we take the same coupling for R and S.

Finally, $H_{\rm bath}^{[R]}$ ($H_{\rm bath}^{[S]}$) is the separate Hamiltonian of the bath R (S). The thermal baths are frequently modeled via noninteracting spins or noninteracting oscillators (spin-boson model) [46]. For our purposes the concrete form of $B^{[R,S]}$ and $H_{\rm bath}^{[R,S]}$ will not be needed.

In Eqs. (C1)–(C4) we did not include the time-dependent interaction between R and S, so that the full Hamiltonian $\mathcal{H}$ is the sum of partial Hamiltonians $\mathcal{H}_R$ and $\mathcal{H}_S$. Before this interaction is switched on as in Eqs. (15) and (16), R (S) together with its bath is described by the Gibbsian density matrix at temperature T_h (T_c):

$$\widetilde{\rho} = \frac{1}{Z_R} e^{-\beta_h \mathcal{H}_R},$$

$$\widetilde{\sigma} = \frac{1}{Z_S} e^{-\beta_c \mathcal{H}_S}. \tag{C5}$$

It is known [46] that for an important class of open systems (including the spin-boson model [47]) the separate state of the two-level system interacting with the bath is Gibbsian by itself:

$$\rho = {\rm tr}_{\rm bath}\, \widetilde{\rho} \propto \exp\left[-\frac{\varepsilon}{2} \bar{\beta}_h (1 + \hat{\tau}_3^{[R]}) \right], \tag{C6}$$

$$\sigma = {\rm tr}_{\rm bath}\, \widetilde{\sigma} \propto \exp\left[-\frac{\mu}{2} \bar{\beta}_c (1 + \hat{\tau}_3^{[S]}) \right]. \tag{C7}$$

If the system-bath coupling constant g is not small, the effective temperatures $\bar{T}_h$ and $\bar{T}_c$ do not coincide with T_h and T_c, respectively. It follows from Eqs. (C6) and (C7) that the equilibrium averages of $\hat{\tau}_1^{[R]}$ and $\hat{\tau}_1^{[S]}$ are equal to zero:

$${\rm tr}[\rho \hat{\tau}_1^{[R]}] = {\rm tr}[\sigma \hat{\tau}_1^{[S]}] = 0. \tag{C8}$$

As we know from Sec. IV A, the optimal work extraction transformation—obtained without taking into account the system-bath interaction—amounts to the SWAP operation; see Eq. (45). We shall now obtain the work extracted via the SWAP operation under the system-bath interaction (C3), and thereby estimate the contribution of this interaction in the work.

When calculating the work we recall that the SWAP operation is implemented in the pulsed regime: the corresponding potential $V(t)$—defined analogously to Eqs. (15) and (16)—is assumed to be so strong that the terms (C2) and (C3) in the total Hamiltonian can be neglected; see the discussion in Sec. II B 1. (The bath Hamiltonians need not be neglected; they drop out themselves.) We also note that it is easier to calculate the work directly in the Heisenberg representation:

$$W = {\rm tr}[\widetilde{\rho} \otimes \widetilde{\sigma} \mathcal{H}] - {\rm tr}[\widetilde{\rho} \otimes \widetilde{\sigma} \mathcal{U}_{\rm SWAP}^{\dagger} \mathcal{H} \mathcal{U}_{\rm SWAP}] \tag{C9}$$

$$= {\rm tr}\left[\frac{\varepsilon}{2}(1 + \hat{\tau}_3^{[R]})(\rho - \sigma) + \frac{\mu}{2}(1 + \hat{\tau}_3^{[S]})(\sigma - \rho) \right] \tag{C10}$$

$$+ g\, {\rm tr}[\widetilde{\rho} \hat{\tau}_1^{[R]} \otimes B^{[R]}] + g\, {\rm tr}[\widetilde{\sigma} \hat{\tau}_1^{[S]} \otimes B^{[S]}], \tag{C11}$$

where we took into account Eq. (C8), and noted that the bath Hamiltonians $H_{\rm bath}^{[R]}$ and $H_{\rm bath}^{[S]}$ do not contribute directly into the work due to the assumed pulsed character of the SWAP operation.

The two terms in Eq. (C10) are the contribution to the work that we already studied in Eq. (44). The two terms in Eq. (C11) arise due to the system-bath interaction energy. Expectedly they are just equal to the (average) interaction energies calculated over the initial states (C5).

The interaction energies in Eq. (C10) are negative. Indeed, employing Eq. (C5) one calculates

$$-T_h \frac{\partial}{\partial g} {\rm tr}[\widetilde{\rho} \hat{\tau}_1^{[R]} \otimes B^{[R]}] = {\rm tr}[\widetilde{\rho} (\hat{\tau}_1^{[R]} \otimes B^{[R]})^2] - ({\rm tr}[\widetilde{\rho} \hat{\tau}_1^{[R]} \otimes B^{[R]}])^2 \geq 0. \tag{C12}$$

Once $\frac{\partial}{\partial g} {\rm tr}[\widetilde{\rho} \hat{\tau}_1^{[R]} \otimes B^{[R]}] \leq 0$ and ${\rm tr}[\widetilde{\rho} \hat{\tau}_1^{[R]} \otimes B^{[R]}]$ is equal to zero for $g=0$ [see Eq. (C8)], both $g\, {\rm tr}[\widetilde{\rho} \hat{\tau}_1^{[R]} \otimes B^{[R]}]$ and $g\, {\rm tr}[\widetilde{\sigma} \hat{\tau}_1^{[S]} \otimes B^{[S]}]$ are negative for $g > 0$.

For $g \to 0$ the magnitude of the interaction energy is at least $O(g^2)$,

$$g\, {\rm tr}[\widetilde{\sigma} \hat{\tau}_1^{[R]} \otimes B^{[R]}] = O(g^2), \tag{C13}$$

since $\frac{\partial}{\partial g} {\rm tr}[\widetilde{\sigma} \hat{\tau}_1^{[R]} \otimes B^{[R]}]$ is constant for $g \to 0$. Indeed, Eq. (C12) implies

$$\frac{\partial}{\partial g} {\rm tr}\, [\widetilde{\rho} \hat{\tau}_1^{[R]} \otimes B^{[R]}]\big|_{g=0} = -\beta_h\, {\rm tr}[\widetilde{\rho} (B^{[R]})^2], \tag{C14}$$

which means that the for $g \to 0$ the interaction energy mainly reduces to the average of $(B^{[R]})^2$ over the thermal state of the bath.

We conclude that the constantly switched on system-bath interaction normally decreases the work obtained under SWAP operation. (One can, of course, optimize the work in the presence of the system-bath interaction; the resulting optimal transformation will be different from SWAP, but it is at the moment not clear to us whether the resulting work will be larger or smaller than the one extracted via SWAP operation.)

APPENDIX D: DERIVATION OF EQS. (44) AND (45)

Assuming Eqs. (40) and (41) we get from Eq. (4):

$$E = [\underbrace{\underbrace{\varepsilon_2 + \mu_2}_{n-1 \text{ times}}, \varepsilon_2}_{n-1 \text{ times}}, \underbrace{\underline{\mu_2}}_{n-1 \text{ times}}, 0]. \tag{D1}$$

Analogously we get from Eqs. (12), (42), and (43):

$$P = [\underbrace{\underbrace{r_2 s_2}_{n-1 \text{ times}}, \underline{r_2 s_1}}_{n-1 \text{ times}}, \underbrace{\underline{r_1 s_2}}_{n-1 \text{ times}}, r_1 s_1]. \tag{D2}$$

When comparing E with P, we see that the action of $\Pi_E^{-1} \Pi_\Omega$, as defined in Eqs. (31) and (32), amounts to interchanging the underlined elements of P in Eq. (D2):

$$\Pi_H^{-1}\Pi_\Omega P = [\,\underbrace{\underbrace{r_2 s_2}_{n-1 \text{ times}},\ r_1 s_2}_{n-1 \text{ times}},\ \underbrace{r_2 s_1}_{n-1 \text{ times}},\ r_1 s_1]. \tag{D3}$$

This then leads to Eqs. (44) and (45).

APPENDIX E

1. Free energy bound for the maximal work extractable from a system in contact with a bath

We are given a quantum system in a nonequilibrium initial state Φ and with Hamiltonian H. Some work is to be extracted from this system via a cyclic Hamiltonian,

$$H(0) = H(\tau) = H, \tag{E1}$$

thermally isolated process. We want to give an upper bound for this work. The work-extraction process is unitary, and thus it conserves the eigenvalues of Φ. In particular, it conserves the von Neumann entropy

$$S[\Phi] = -\,\mathrm{tr}[\Phi \ln \Phi]. \tag{E2}$$

Recall that the (positive) extracted work is defined as the difference between the initial and final energies. We can give an upper bound for the maximal extractable work by looking for a final state with the *minimal* energy compatible with the above conservation of the von Neumann entropy [2,4]. The corresponding minimization procedure is standard in statistical physics [2]—since it is dual to the maximization of the entropy for a fixed average energy—and it produces for the final state a Gibbsian density matrix

$$\Phi(\beta_{\mathrm{f}}) = \frac{1}{Z} e^{-\beta_{\mathrm{f}} H}, \quad Z = \mathrm{tr}\, e^{-\beta_{\mathrm{f}} H}, \tag{E3}$$

with an inverse final temperature β_{f} defined via the entropy conservation:

$$S[\Phi] = S[\Phi(\beta_{\mathrm{f}})]. \tag{E4}$$

The upper bound for the maximal work is now

$$W_{\mathrm{th}} = \mathrm{tr}[H\Phi] - \mathrm{tr}[H\Phi(\beta_{\mathrm{f}})]. \tag{E5}$$

This is the standard solution of the maximal work extraction problem given in thermodynamics [2,4].

Let us now adopt the above reasoning assuming that the overall system consists of a large thermal bath B and a small system R. Initially B is in equilibrium at inverse temperature β, while R is in an arbitrary state ρ. Thus the initial state is

$$\Phi = \rho \otimes \rho_B(\beta),$$

$$\rho_B(\beta) = \frac{1}{Z_B} e^{-\beta H_B}, \tag{E6}$$

where H_B is the bath Hamiltonian. The overall initial Hamiltonian is

$$H = H_R \otimes 1 + 1 \otimes H_B, \tag{E7}$$

where H_R is the Hamiltonian of R.

We now employ the following facts.

(1) The number of bath degrees of freedom is much larger than that for the small system R.

(2) Since the bath started from a passive equilibrium state, the extracted work is expected to be of the same order as the energy of R. Thus the extracted work is much smaller than the bath energy.

(3) Since $\beta = O(H_R)$, the difference between the initial bath temperature β and the final temperature β_{f} is expected to be much smaller than H_R.

(4) The interaction between B and R occurs only during the work-extraction process. It is negligible both before and after the process. The interaction may be sizable during the work extraction, but the corresponding energy costs for switching it on and off are already included in the work.

Let us now write Eq. (E4) as

$$S[\rho] + S[\rho_B(\beta)] = S[\rho(\beta)] + S[\rho_B(\beta_{\mathrm{f}})], \tag{E8}$$

where $\rho(\beta) \propto \exp[-\beta H_R]$, and where the lhs follows from the fact that initially the bath and the small system were in a factorized state (E6). The rhs follows from the Gibbs density matrix (E3) of the final state, taking into account in the final state that R and B do not interact.

In Eq. (E8) we neglected the difference between β and β_{f} in $S[\rho(\beta)]$. For the bath this small difference should not be neglected, since it is multiplied by the large number of the bath degrees of freedom. We write

$$S[\rho_B(\beta_{\mathrm{f}})] = S_B(U_B + \delta U_B), \tag{E9}$$

where U_B is the initial bath energy, and where δU_B is the change of the bath energy due to its interaction with the small system. Using $dS_B/dU_B = \beta$ and expanding

$$S_B(U_B + \delta U_B) = S_B(U_B) + \beta \delta U_B, \tag{E10}$$

we get from Eq. (E8): $\delta U_B = T(S[\rho] - S[\rho(\beta)])$. Putting this into Eq. (E5) we get

$$W_{\mathrm{th}} = \mathrm{tr}[H\rho] - \mathrm{tr}[H\rho(\beta)] - T\{S[\rho] - S[\rho(\beta)]\} \tag{E11}$$

$$= F_{\mathrm{i}} - F_{\mathrm{f}}. \tag{E12}$$

This is the difference $F_{\mathrm{i}} - F_{\mathrm{f}}$ between the free energies, provided the latter is defined as

$$F = \mathrm{tr}[H\rho] - TS[\rho]. \tag{E13}$$

Note that W_{th} in Eq. (E12) can be written as $W_{\mathrm{th}} = TS[\rho \| \rho(\beta)]$, where $S[\rho \| \rho(\beta)]$ defined in Eq. (22) is the relative entropy between the initial state ρ and the final equilibrium state $\rho(\beta)$ of R.

2. Reachability of the thermodynamical upper bound via a slow process

One may hope that the thermodynamical bound (E12) could indeed be reached by some realistic work extraction dynamics [2,4,22,29]. This is because for a macroscopic system (for the present case $R+B$) the conservation of entropy alone is expected to characterize a thermally isolated process. More specifically, we should demand from a physical realization of the bound (E12) that the work sources act on the system and, at worst, at the system bath coupling, but not on the bath itself, since the latter is supposed to be out of a direct control.

A realization of the bound (E12) for restricted initial states ρ was outlined in [22]. This realization takes a long time and thus amounts to zero power of work extraction. A finite power protocol of extracting Eq. (E12) from an arbitrary initial state ρ is given in [48]. However, this protocol has another serious drawback, namely one has to allow direct interactions between the source of work and the thermal bath (uncontrollable degrees of freedom).

The result presented in [22] focused on the zero Hamiltonian case $H_R=0$. It is, however, possible to generalize this result assuming that the initial state ρ is diagonal in the representation of H_R. This restriction is essential, as we discuss below. Thus we write H_R and ρ as

$$H_R = \mathrm{diag}[\varepsilon_n, \ldots, \varepsilon_1], \quad \varepsilon_n \geq \cdots \geq \varepsilon_1 = 0, \tag{E14}$$

$$\rho = \mathrm{diag}[r_n, \ldots, r_1], \tag{E15}$$

where $\mathrm{diag}[a, \ldots, b]$ is a diagonal matrix with entries $(a, \ldots, b)$. For simplicity we assume that the eigenvalues r_k are ordered as

$$r_n \leq \cdots \leq r_1. \tag{E16}$$

This assumption is not essential. If it does not hold, one should supplement step (1) below by the unitary transformation that orders properly the spectrum of ρ.

The work extraction consists of the following two steps.

(1) One changes with time the level spacings from their initial values $\{\varepsilon_n, \ldots, \varepsilon_2\}$ to final values $\{\varepsilon_n', \ldots, \varepsilon_2'\}$:

$$\{\varepsilon_n, \ldots, \varepsilon_2\} \to \{\varepsilon_n', \ldots, \varepsilon_2'\}. \tag{E17}$$

The change occurs much *faster* than the relaxation time induced by the bath, so that the interaction with the bath can be neglected during the change. Since the corresponding time-dependent Hamiltonian commutes with the initial density matrix for all times, the populations $\{r_n, \ldots, r_1\}$ remain constant during this process. The purpose of Eq. (E17) is to achieve the *local equilibrium* of the system at the bath temperature β:

$$r_n = \frac{e^{-\beta\varepsilon_n'}}{Z}, \ldots, r_2 = \frac{e^{-\beta\varepsilon_2'}}{Z}, \quad r_1 = \frac{1}{Z}, \tag{E18}$$

where $Z \equiv \sum_{k=1}^{n} e^{-\beta\varepsilon_k'}$. Together with Eqs. (E14) and (E16), Eqs. (E18) define the new spacings $\{\varepsilon_n', \ldots, \varepsilon_2'\}$:

$$\varepsilon_n' = T_\mathrm{i} \ln\frac{r_1}{r_n}, \ldots, \varepsilon_n' = T_\mathrm{i} \ln\frac{r_1}{r_2}. \tag{E19}$$

The full work W_1 done during Eq. (E17) is (initial average energy minus final average energy)

$$W_1 = \sum_{k=2}^{n} r_k[\varepsilon_k - \varepsilon_k']. \tag{E20}$$

(2) The spacings $\varepsilon_n', \ldots, \varepsilon_2'$ are now slowly moved back to their original values $\varepsilon_n, \ldots, \varepsilon_2$. Here slow means that the characteristic time of the variation is much larger than the relaxation time of the system (determined by the coupling to the bath). It is at this point that the work-extraction process is going to take a long time.

During this process the density matrix is

$$\rho_2(t) = \frac{1}{Z(t)} \mathrm{diag}[e^{-\beta\varepsilon_n(t)}, \ldots, e^{-\beta\varepsilon_2(t)}, 1], \tag{E21}$$

$$Z(t) \equiv \sum_{k=1}^{n} e^{-\beta\varepsilon_k(t)}, \tag{E22}$$

where at the initial stage of this second step $\varepsilon_k(t_\mathrm{i}) = \varepsilon_k'$, while at the final stage $\varepsilon_k(t_\mathrm{f}) = \varepsilon_k$.

The work done during this process reads

$$W_2 = -\int_{t_\mathrm{i}}^{t_\mathrm{f}} ds \rho_2(s) \partial_s H(s) = \int_{t_\mathrm{i}}^{t_\mathrm{f}} ds \frac{d[T \ln Z(s)]}{ds}, \tag{E23}$$

where $Z(t)$ is defined in Eq. (E22). Working out Eq. (E23) one gets that W_2 is equal to the free energy difference:

$$W_2 = -\{\mathrm{tr}[\rho(\beta)H] - TS[\rho(\beta)]\} \tag{E24}$$

$$+ \sum_{k=2}^{n} r_k \varepsilon_k' + T\sum_{k=1}^{n} r_k \ln r_k, \tag{E25}$$

where the rhs of Eq. (E24) is the minus final free energy with $\rho(\beta) = \rho_2(t_\mathrm{f})$ being the final equilibrium state of R, and where Eq. (E25) is the free energy at the end of the sudden change defined in Eq. (E17). It is clear that the sum $W_1 + W_2$ defined via Eqs. (E20), (E24), and (E25) is equal to the thermodynamic bound (E12).

Since the local equilibrium is related to the simultaneously diagonal form for H and ρ_0, should there be initial coherences (nondiagonal elements of ρ_0), there is no unitary operation that could bring the system to the local equilibrium with the bath at the end of the first step. Thus the restriction (E15) on the initial state is essential.

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