The multilevel four-stroke swap engine and its environment

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Abstract
A multilevel four-stroke engine where the thermalization strokes are generated by unitary collisions with thermal bath particles is analyzed. Our model is solvable even when the engine operates far from thermal equilibrium and in the strong system–bath coupling. Necessary operation conditions for the heat machine to perform as an engine or a refrigerator are derived. We relate the work and efficiency of the device to local and non-local statistical properties of the baths (purity, index of coincidence, etc) and put upper bounds on these quantities. Finally, in the ultra-hot regime, we analytically optimize the work and find a striking similarity to results obtained for efficiency at maximal power of classical engines. The complete swap limit of our results holds for any four-stroke quantum Otto engine that is coupled to the baths for periods that are significantly longer than the thermal relaxation time.

Keywords: quantum thermodynamics, heat engine, multilevel, Otto engine

1. Introduction

Present day technology is on the verge of enabling different realizations of quantum heat machines where the engine core (‘working substance’) comprises of a single particle in a discrete level system (e.g. a qubit). In analogy to their classical counterparts, quantum heat machines can be used to cool or to produce work. Furthermore, similarly to classical
thermodynamics, performance analysis of heat machines without going into the details of a specific realization is a key theme in quantum thermodynamics (QT). There are several approaches to QT. The more recent one comes from quantum information resource theory. In this approach thermal states are considered free while non-equilibrium states are considered as a resource ([1–3] and references therein). An energy conserving unitary is used to couple the system and the bath. A different viewpoint to QT is dynamical, and uses the framework of quantum generators of open systems [4]. In this approach, models of a quantum heat machine are constructed and analyzed. The methodology in this study overlaps with both approaches. On the one hand, an explicit dynamical analysis of an engine is carried out, and on the other hand the thermalization process is based on energy-conserving unitary operation between the system and bath. This is different from studies in the dynamical approach where the interaction with the bath is modeled by some effective reduced-dynamics non-unitary evolution (Lindblad equation). A third approach called typicality aims to find the conditions when complex interactions lead to thermal behavior for a typical set of states (see [5] and references therein).

A useful theory of QT should provide simple and efficient tools to evaluate the performance of quantum heat machines. However, as we show here, in a multilevel system, it is far from trivial to even map the parameter regimes where the machine operates as an engine or as a refrigerator (let alone their performance). The goal of this work is to gain a more comprehensive understanding of the operation of multilevel quantum heat machines and to study the regimes in which the machines operate as an engine or as a refrigerator. In particular, in our model the dynamics can be solved analytically even when the coupling between the bath and the system is strong (this is a very difficult and subtle limit in the standard open systems approach [4]). Our analysis emphasizes the difference between ‘non-local’ quantities that cannot be evaluated using a single bath, and ‘local’ quantities that can be evaluated using a single bath. In principle, we wish to express non-local quantities of interest such as work, heat and efficiency in terms of simpler local quantities (temperature, purity of the baths, entropy of the baths, etc).

Various quantum engine models have been suggested—some are continuous (where the baths are always connected to the engine) and some are reciprocating (where in different strokes different processes take place). The equivalence between a laser and the Carnot engine [6] has inspired the study of quantum heat engines. For example, studying maximum power operation [7–10], the role of coherence and entanglement [11–17], quantum refrigerators and the third law of thermodynamics [18–25], and the connection to quantum information [26, 27]. Recently, machines powered by non-thermal baths have been studied as well [28–30].

Different quantum working mediums have been considered: two-level systems, N-level systems or harmonic oscillators [31–37]. In most previous studies the system bath dynamics was modeled by a reduced description where the dynamics of the system is described explicitly by a master equation with a generator cast into the Lindblad form [38, 39]. In the reduced formalism the bath is only considered implicitly, therefore the effect of the engine on the baths is almost always ignored. In this paper we take the opposite point of view and study the heat machine operation using the properties of the baths. One of the main difficulties in the Lindblad approach is that the reduced dynamics generators are not uniquely defined. Various choices of the Lindblad generator lead to the same reduced dynamics of the working medium but to different entropy fluxes to and from the baths. As it turns out, the Lindblad operators have to be carefully chosen in order to be consistent with the second law of thermodynamics [4].
The problem becomes more severe when time dependent external fields drive the system [40, 41]. The analysis carried out in this paper overcomes this problem by considering a very simple yet physically plausible bath model that is based on collisions [42, 43]. In this model the bath consists of non-interacting particles which are initially in the same thermal state. The engine interacts with the bath particles via a two-particle collision described by a unitary operation. We choose to model the collision by the unitary swap operation but other unitary operations such as CNOT and random unitaries have been considered as well [44, 45] even though they were not applied to the study of heat machines. As will be discussed later on, the swap operation has two interesting physical limits. The first is the full swap that describes full thermalization and the other is the weak partial swap that mimics quasi-static evolution where the heat is equal to the bath temperature multiplied by the entropy difference.

Typically, in these collisions based baths the system that interacts with the bath is taken to be a single qubit but qudits and a chain of coupled qubits have been considered as well [46, 47]. The collision model can also represent a general non-Markovian dynamics [48, 49]. If, however, the bath is very large, a particle that interacted with the system is unlikely to affect the system again. In such cases the dynamics is Markovian. See [50, 51] and reference therein for more studies on collision-generated Markovian dynamics. In this article we consider Markovian collisions in order to study the salient features of an engine driven by collision baths.

The importance of studying multilevel heat machines is twofold. First, experimentally speaking, in some systems it is not possible or not practical to interact with only two levels. Secondly, two-level systems may contain some non-generic features and it is highly important to isolate the more general features of quantum heat machines by considering multilevel engines. For example, in a two-level system temperature is always well defined if the density matrix is diagonal in the energy basis. Clearly this is not true if there are more than two levels.

While in a two-level engine it is fairly simple to map the parameter space where the system operates as an engine and as a refrigerator, when the number of levels is three or more it is a considerably more complicated task [37]. In a two-level system the different operation regimes are determined by the temperature and the gap energy associated with the cold and hot strokes. It is not straightforward what energy scale replaces the two-level energy gap in the multilevel case (the variance? the maximal gap?). Furthermore, it is not clear at this point if necessary and sufficient conditions for engine (or refrigerator) operation can be formulated without explicitly solving the full dynamics of the system. In this work we provide the necessary conditions for the operation of a multilevel Otto engine as engine or a refrigerator. In particular, in the ultra-hot regime we obtain a necessary and sufficient condition. Another important issue addressed in our analysis is work output optimization. In the ultra-hot regime we find the optimal way to compress (or expand) a generic multilevel working substance in order to produce maximal work output per cycle.

This study can be related to ‘finite time thermodynamics’ [52–54] although there is no explicit reference to time. Implicitly the cycle can be related to the collision timescale and in addition there is no assumption of thermal equilibration of the device with the baths upon contact.

The article is organized as follows: section 2 contains the description of our engine and bath model. In section 3 we analyze the steady state operation of the engine and discuss the difference between quantum swap and classical random swap. Next, section 4 explores various aspects of the engine evolution: Clausius and, generalized Clausius inequality and the baths’
purity reduction. Necessary conditions for operation of a multilevel swap engine as an engine or refrigerator are derived in section 5. In section 6 we set upper bounds on the work and efficiency in terms of statistical quantities like purity, index of coincidence and Wootters distance. Finally, section 7 presents two possible regimes of operation: the ultra-hot bath regime and the quasi-static regime.

2. The baths, engine, and their interaction

2.1. The bath

Our bath model is based on the ‘quantum homogenizer’ introduced in [42, 43, 55]. This bath contains a very large amount of single species non-interacting multilevel particles. At the beginning all the particles are in the same thermal state. However, each time a bath particle interacts with the engine the population of the particle and of the engine changes according to the simple partial swap rule that will be described shortly. The special case of a complete population swap was used in [33, 56, 57] to generate a thermal distribution in a finite time. For other studies of reduced dynamics using unitary interaction with ancillary systems see [58–60].

Every time the system (engine) interacts with the bath it collides with a new thermal particle in the bath. If the system is coupled only to one bath then repeated collision would lead to thermalization of the engine particle at an exponential rate. In this work, however, we will assume that there is only one collision or none at all at each thermal stroke of the engine. Therefore, the engine will typically not be in a Gibbs state. The extension to multiple collisions in each thermal stroke is straightforward.

The bath is assumed to be large enough so that the probability to re-collide with a bath particle that already interacted with the system is negligible. Consequently, the resulting dynamics is Markovian. We assume that the particles do not interact with each other in the bath but only with the system particle at the bath–system interface. That is, in our model there is no thermalization inside the bath. In principle, for large baths, this has no impact on the engine’s operation. If the bath is sufficiently large it does not matter if the scattered particle gets thermalized again or not as the engine will (almost) always interact with a new thermal particle. Nevertheless, it is interesting to explore the operation of small baths with and without intra-bath thermalization.

There is a different class of quantum engines where the baths are always connected to the engine but different levels are connected to different baths [18]. This implies that if only one bath is connected the relative probabilities of the specific coupled levels will be thermal but the engine as a whole will not be in a Gibbs state. Alternatively stated, these bath models have a continuum of steady states. In our model the Gibbs state is the only single bath steady state.

2.2. The engine’s cycle

Our engine comprises a multilevel system that is driven to a four-stroke Otto cycle [61]. Figure 1(a) illustrates the engine’s operation for a two-level system. In stroke A the gap spacing is increased by applying an external field. The engine is decoupled from the baths at this stage. The state evolution is such that the system’s density is diagonal in the energy basis at the beginning and at the end of the stroke. Adiabatic change of the Hamiltonian will achieve such a
transformation but other faster options exist (see section 2.5). Despite the existence of faster alternatives, for simplicity, we refer to this part of the cycle as an ‘adiabatic stroke’.

In stroke $B$ the gap is kept fixed in time, but the engine is allowed to interact with the hot bath. During this time interval there may be one collision, multiple collisions or none at all. The average collision rate is a parameter that characterizes the bath and its coupling to the engine. It encapsulates within the particle density in the bath, the engine cross-section for collision, etc. The collision entangles the engine and the particles in the bath. However since the interacting bath particles will not interact with the engine again (the top spheres in figure 1(a) with temperature denoted by prime), we consider the reduced dynamics of the engine by tracing out the scattered particle of the bath. This stage changes the entropy of the engine and involves heat exchange with the hot bath. In stroke $C$ the external field is changed again so that the gap returns to its initial value. Finally, in stroke $D$, the system is coupled to the cold bath.

In the multilevel case the energy levels’ evolution can be considerably more intricate. First, we do not assume that all the levels are increased or decreased by the same ratio (figure 1(c)). Second, we allow the levels to cross (figure 1(d)). The engine scheme described here requires external time-dependent control of the energy level. An autonomous implementation of this engine that requires no control at all will be described elsewhere.

2.3. The collision model

We assume that at the initial state, the system and the bath particles are in a product of a thermal Gibbs state:
\[ \rho = \rho_b \otimes \rho_b \otimes \rho_b \ldots \quad (1) \]
\[ \rho_{b,ij} = e^{E_{b,j} \tau_b / \hbar} \sum_{j=1}^N e^{E_{b,i} \tau_b / \hbar} = e^{E_{b,j} - E_{b,i} \tau_b / \hbar}, \quad (2) \]
\[ \rho_{b,i \neq j} = 0, \quad (3) \]

where ‘b’ stands for ‘c’ (cold bath) or ‘h’ (hot bath). The free energy \( F_b \) takes care of normalization. Let \( U \) be some two-particle unitary operation that conserves the total energy of the two particles. The reduced density matrices after the interaction are:
\[ \rho_s' = \text{tr}_b \left( U \rho_b \otimes \rho_s U^\dagger \right), \quad (4) \]
\[ \rho_b' = \text{tr}_s \left( U \rho_b \otimes \rho_b U^\dagger \right). \quad (5) \]

When the collision Hamiltonian that generates \( U \) is invariant under the transformation \( b \leftrightarrow s \) one can show that:
\[ \rho_s' - \rho_s = - \left( \rho_b' - \rho_b \right). \quad (6) \]

This condition, together with the total energy conservation, implies that the energy levels of the bath and the system have to be equal.

**2.4. Density matrix swap and energy population swap**

In this work we focus on collisions that induce a single parameter convex transformation for the system’s reduced density matrix or for the system’s energy population. The density swap rule is:
\[ \rho_s' = (1-x)\rho_s + x\rho_b, \quad (7) \]
\[ \rho_b' = (1-x)\rho_b + x\rho_s, \quad (8) \]
\[ 0 \leq x \leq 1, \quad (9) \]

where \( x \) is the swap parameter. For \( x = 0 \) the density matrices remain as they were, and for \( x = 1 \) the density matrix of the bath and the particle completely interchange. It is easy to verify that this transformation satisfies (6), and that the only steady state of this transformation is \( \rho_b = \rho_s \).

Re-colliding the system particles with new bath particles in a thermal state will lead to exponential decay of \( \rho_s \) towards \( \rho_b \). Yet, in this work, we do not assume that equilibrium is reached. In fact we will mostly consider a single collision at most in a given stroke (B or D).

Although the density swap rule has a very simple structure, our framework is valid for a more general type of swap operation. Let \( p_b \) and \( p_s \) denote the energy level populations of the bath and system particles. We shall use bold face characters to denote quantities that have a level index such as the probability or energies of a bath \( E_b \). The energy population swap rule is:
\[ p_s' = (1-x)p_s + xp_b, \quad (10) \]
\[ p_b' = (1-x)p_b + xp_s, \quad (11) \]
where as before the prime relates to the traced-out outcome after the collision. We do not claim that the swap operation in its current form is general enough to describe many typical thermal baths used in experiments. Yet, such bath could in principle be built. One advantage of this bath model is that it leads to a solvable dynamics that can be used as a reference for other more complex models. Another advantage, as will be shown later on, is that it helps to formulate new questions and new points of view concerning the operation of heat machines. Nevertheless, in a two-level system an energy population swap follows immediately from (6) since only one parameter is needed to describe the population transfer in a two-level system. For example, the Einstein rate equation for an interaction of two levels with thermal radiation describes such an energy population swap interaction.

In appendix A, we show examples of two (partial) swap Hamiltonians. One generates a density matrix swap and the other an energy population swap.

2.5. The adiabatic evolution step

Stroke A and C are termed ‘adiabatic’ as we require that the evolution will be diagonal in the energy basis at the beginning and the end of the stroke. The coherences will remain zero and the energy populations will remain as they are. Such a process does not have to be slow. For example, consider the following Hamiltonian that commutes with itself at all times:

\[
\sum_{i=1}^{N} E_i(t) |i\rangle \langle i|.
\]

A density matrix that is diagonal in the energy basis \( |i\rangle \) will be invariant under this type of Hamiltonian regardless of how fast the energy levels are changing. In a two-level spin system this Hamiltonian will be \( H_{\text{adiab}} = B(t) \sigma_z \), where \( \sigma_z \) is the \( z \) Pauli matrix.

The population and coherence evolution can be obtained by more general time dependent Hamiltonians that do not commute at different times \( [H(t_1), H(t_2 \neq t_1)] \neq 0 \). Nevertheless the possibility of an adiabatic transformation is guaranteed by the coherent control theorem [62, 63]. Alternatively it is possible to use a method known as ‘quantum driving’ or ‘shortcut to adiabaticity’ [64–69] to generate an evolution that preserves the energy-basis diagonal form of the density matrix at the end of the process.

In principle, we allow the energy levels to cross1. However in such a case it important to remember that the energy index is a level index and not some order index that indicates how the levels are ordered. For example, in figure 1(b) \( E_{c,1} < E_{c,2} < E_{c,3} < E_{c,4} \) but at the hot bath \( E_{h,4} < E_{h,1} < E_{h,2} < E_{h,3} \).

3. The average populations in steady state operation

Next we explore the dynamics and the properties of the system’s (engine) reduced density \( \rho_s \). We assume that during stroke B a single particle interacts with the engine with probability \( R \). The description can easily be generalized to include the possibility of more than one collision during each thermal stroke. The probability \( R \) appears naturally in a collisions model as there is

\[ 0 \leq x \leq 1, \]

1 This will not automatically generate strong non-adiabatic effects (e.g. if (13) drives the system).
no certainty that a particle from the a bath particle will be available to interact with the engine. For simplicity we assume that the bath parameters are identical for both baths: they have same $R$ and the same swap parameter $x$. A generalization to different $x$ and $R$ for different baths is straightforward using the same methods.

Even though for some applications transient behavior may be of interest, here we focus on the steady state operation. The average engine population at stage $C$, $\rho^C_s$, is related to that of stage $A$, $\rho^A_s$, via:

$$\rho^C_s = (1 - R) \rho^A_s + R \left[ (1 - x) \rho^A_s + x \rho_h \right]. \quad (14)$$

The first term describes a no-collision event and the other describes a collision with a swap parameter $x$. Equation (14) simplifies to:

$$\rho^C_s = (1 - xR) \rho^A_s + xR \rho_h. \quad (15)$$

Here $x$ and $R$ are inseparable since both of them have the same effect on the average population. In the same manner we can write the equation for $\rho^A_s$:

$$\rho^A_s = (1 - xR) \rho^C_s + xR \rho_h. \quad (16)$$

By combining (15) and (16) we get:

$$\rho^C_s = \frac{\rho_h + \rho_s - xR \rho_h}{2 - xR}, \quad (17)$$

$$\rho^A_s = \frac{\rho_h + \rho_s - xR \rho_h}{2 - xR}. \quad (18)$$

Note that a combination of Gibbs states is not a thermal state if there are more than two levels. Hence, as expected in a finite time thermodynamic framework, the multilevel swap engine is never in a Gibbs state for $xR < 1$. The expectation value of the population change is:

$$d\rho^A_{s \rightarrow C} = \rho^C_s - \rho^A_s = \frac{xR}{2 - xR} (\rho_h - \rho_s). \quad (19)$$

Inspection of (17) and (18) shows that even if the initial density matrix of the engine has some coherences they have no impact on the energy diagonal steady state. Thus for all energy observables computed locally (i.e., with the reduced density matrices of the baths or the engine) it is sufficient to consider the population vector $\rho_i = \text{diag}(\rho_i)$ where $i = \text{s}', \text{c}', \text{h}'$. Hence, in this notation:

$$d\rho^A_{s \rightarrow C} = \frac{xR}{2 - xR} (\rho_h - \rho_s). \quad (20)$$

In general, the population change under a swap operation in steady state is proportional to $\rho_h - \rho_s$, even when $x$ and $R$ are not the same for both baths. This result will have a large impact later on. We point out that if the baths are only coupled to some of the system levels as in [6], then the result is different.

When $xR = 1$ in a single collision, or $xR < 1$ with a vast number of collisions a complete thermalization of the engine’s population takes place. Therefore, many of the results in the limit $xR = 1$ apply to a much more general setup than the swap collision used above. They apply
wherever the engine is connected long enough to effectively reach a Gibbs state (and not some other state).

For work and efficiency investigations, only the populations in the energy basis are important. Hence, it is not necessary that the whole density matrix is swapped as in (7)–(9), rather it is sufficient that an energy population swap takes place (see (10)–(12)).

3.1. Quantum versus classical swap and entropy generation

In equation (20) \( x \) and \( R \) are lumped together in a product form \( xR \). Yet, they are not physically equivalent. \( R \) controls how deterministic the system is, and \( x \) determines the interaction strength and the ‘quantumness’ (coherences and entanglement before the partial trace). Note that the quantum behavior is not monotonically increasing with \( x \), since the system is classical when \( x = 1 \) (bath and engine particles switch places).

In the quantum case, where \( R = 1 \) and \( x < 1 \), \( x \) can generate coherences and entanglement in the joint density matrix of two interacting particles. The increase in the sum of entropies of the reduced density matrices is the result of ignoring entanglement and classical correlations.

In contrast, in the classical case where \( x = 1 \), and \( R < 1 \), the particles are either fully swapped or left as they are. Therefore entanglement cannot be produced from the initial product state. Here, the sum of the entropies of the individual particles also increases since the information if a collision took place or not is discarded.

In both cases the increase of the bath particle entropy is encapsulated in the mutual information of the colliding particles. In the quantum case, the mutual information contains a contribution from entanglement. The separation to quantum and classical correlations can be studied using the quantum discord tool [70]. This, however, is outside the scope of this work. Furthermore in our model the observables we studied depend only on \( xR \) so they can equally be obtained from a classical or a quantum realization. However, we do not expect this to hold for observables that are not functions of the steady state population.

4. Thermodynamic properties

4.1. First law

In this model the expectation value of the engine’s energy is:

\[
\frac{dU}{dt} = \frac{d}{dt}(p_s \cdot E) = E \cdot \frac{dp_s}{dt} + p_s \cdot \frac{dE}{dt}
\]

(21)

\[
= \frac{d}{dt} \text{Heat} + \frac{d}{dt} \text{Work}
\]

(22)

For the identification of work and heat see, for example [71, 72]. In short, work is associated with internal energy change when the population is fixed in time, and heat is a change in energy when the Hamiltonian is fixed in time. On average in a complete cycle \( \langle U \rangle_{\text{initial}} = \langle U \rangle_{\text{final}} \) we have:
\[\Delta U = 0 = \left\langle p_s^A \right\rangle (E_h - E_c) + E_h \cdot \left( \left\langle p_s^C \right\rangle - \left\langle p_s^A \right\rangle \right) + \left\langle p_s^C \right\rangle \cdot (E_c - E_h) + E_c \cdot \left( \left\langle p_s^A \right\rangle - \left\langle p_s^C \right\rangle \right), \tag{23}\]

where the first term on the right-hand side corresponds to stroke \(A\), the second term to stroke \(B\), and so forth. Regrouping we identify:

\[\langle Q_h \rangle = E_h \cdot \left\langle dp_s^A - C \right\rangle, \tag{24}\]
\[\langle Q_c \rangle = -E_c \cdot \left\langle dp_s^A + C \right\rangle, \tag{25}\]
\[\langle W \rangle = \left\langle dp_s^A + C \right\rangle \cdot (E_h - E_c), \tag{26}\]

where we used the ‘positive heat in, positive work out’ sign convention. Note that these quantities are invariant to any constant shift of the levels in one or two of the baths: \(E_{h,i} \rightarrow E_{h,i} + G_h, E_{c,i} \rightarrow E_{c,i} + G_c\) where \(G_c\) and \(G_h\) are some constants. The probabilities themselves are invariant to such transformation by virtue of the form of the Gibbs state. In the heat expressions, the energy is clearly not invariant to such a shift but the extra term cancels out when summed over the probability difference. Equations (24)–(26) lead to the averaged form of the first law:

\[\langle Q_h \rangle + \langle Q_c \rangle = \langle W \rangle. \tag{27}\]

Note that the energy at the end of the cycle is equal to the energy at the beginning of the cycle only on average. In a specific cycle it is, in general, not zero. Using (20) and (26) we obtain:

\[\langle W \rangle = \frac{xR}{2 - xR} (p_h - p_c) \cdot (E_h - E_c). \tag{28}\]

As mentioned before, the limit \(xR = 1\), (28) holds for any interaction that leads to a complete thermalization (or very close to it) and not just for a swap interaction. The modes of operation of a two-level swap machine are shown in figure 2. In a general multilevel system it is not straightforward to write analytically the condition for engine or refrigerator operation using the energy levels and the temperature due to the exponential dependence of the probabilities on the energy levels. Yet, in some temperature regimes this is considerably simpler as discussed in section 7.

4.2. The second law and the Clausius number

In cyclic processes in classical thermodynamics the second law can be expressed in terms of the Clausius inequality \(\oint \frac{dQ}{T} \geq 0\). In our case we calculate:

\[\mathcal{R} = \frac{\langle \dot{Q}_h \rangle}{T_h} + \frac{\langle \dot{Q}_c \rangle}{T_c}, \tag{29}\]

where, as before, the \(\langle \cdot \rangle\) brackets denotes the average value in steady state and the tilde signifies a heat flow to the bath and not to the system (the sign is opposite). Hereafter we shall refer to \(\mathcal{R}\) as the Clausius number. Strictly speaking, this is not the classical Clausius inequality. The swap collision process is not an isotherm at all. For a multilevel system a temperature cannot even be assigned to the bath or engine particles since they are not in a Gibbs state after...
(or during) the collision. In this section we find that $R \geq 0$ holds in steady state for any multilevel swap engine and that it has an information theoretic interpretation. Furthermore, it is shown that $R \geq 0$ belongs to a family of more general inequalities. It is easy to verify that $R \geq 0$ entails within the second law. For $T = T_h$ we get $\langle W \rangle \leq 0$. That is, in steady state, no work can be extracted from a single bath. Alternatively, when calculating the efficiency, $\eta = 1 - \langle Q_c \rangle / \langle Q_h \rangle$, $R \geq 0$ ensures that the efficiency is smaller than the Carnot efficiency (see section 6.2).

Using the expressions for heat we want to show that for swap heat machines:

$$R = \sum_{i=1}^{N} \left( d p_i^A - C \right) \left( \frac{E_{h,i}}{T_h} - \frac{E_{c,i}}{T_c} \right) \geq 0.$$  \hfill (30)

In a specific cycle this does not have to be true. Our aim is to show that it holds on average when the system is in steady state. To obtain the average we use (20) and get:

$$R = \frac{xR}{2 - xR} \sum_{i} \left( p_{c,i} - p_{h,i} \right) \left( \frac{E_{h,i}}{T_h} - \frac{E_{c,i}}{T_c} \right)$$

$$= \frac{xR}{2 - xR} \sum_{i} p_{c,i} \ln \frac{p_{c,i}}{p_{h,i}} + p_{h,i} \ln \frac{p_{h,i}}{p_{c,i}},$$ \hfill (31)

which leads to the following result for swap engines:

$$R = \frac{xR}{2 - xR} J(p_c, p_h),$$ \hfill (32)
\[ J = D_{KL}(p_i|p_h) + D_{KL}(p_h|p_i), \]  

(34)

where \( J \) is the Jeffreys divergence and \( D_{KL}(p||q) = \sum p_i \ln \frac{p_i}{q_i} \) is the Kullback–Leibler divergence or the relative entropy. A similar result is known for processes that start or end in a thermal state [71, 73]. Since \( D_{KL}(p||q) \geq 0 \) for any two probability vectors (also known as Klein’s inequality), \( R \geq 0 \) follows naturally as an information theory inequality.

4.3. Generalized Clausius inequality

The Clausius number inequality is a special case of a more general inequality that holds for swap heat machines. We find that the more general inequality is:

\[
R_{2m-1} = \sum_{i=1}^{N} \left( \theta - C \right) \left( \frac{E_{h,i}}{T_h} - \frac{E_{c,i}}{T_c} \right)^{2m-1} \geq 0. 
\]

(35)

Clearly, if this equality holds, it holds for any odd analytic and monotonically increasing function of \( \frac{E_{h,i}}{T_h} - \frac{E_{c,i}}{T_c} \) as well. While \( R \equiv R_1 \) can be understood in thermodynamics terms of heat, temperature and entropy, for \( m > 1 \) higher energy powers are involved and there is no straightforward thermodynamic interpretation.

The proof of (35) is straightforward. Denoting \( \epsilon_{h,i} = E_{h,i}/T_h \) and \( D_i = \epsilon_{h,i} - \epsilon_{c,i} \) we get that inequality (35) is equivalent to:

\[
R_{2m-1} = \sum_k e^{-\varepsilon_{c,k}} \sum_{ij} e^{-\varepsilon_{j,i}} \left( e^{-D_{ij}} - e^{-D_i} \right) D_{ij}^{2m-1}. 
\]

(36)

Next we write \( R_{2m-1} = \frac{1}{2} R_{2m-1} + \frac{1}{2} R_{2m-1} \), exchange the indices names in the second term and obtain:

\[
R_{2m-1} = N_h \frac{1}{2} \sum_k e^{-\varepsilon_{c,k}} \sum_{k'} e^{-\varepsilon_{h,k'}} \times \sum_{ij} e^{-\varepsilon_{j,i}} \left( e^{-D_{ij}} - e^{-D_i} \right) \left( D_{ij}^{2m-1} - D_{j}^{2m-1} \right). 
\]

(37)

The term \( D_{ij}^{2m-1} - D_{j}^{2m-1} \) has the same sign as \( D_{ij} - D_j \) and the same sign as \( (e^{-D_{ij}} - e^{-D_i}) \), hence the product of the two differences that appears in (37) is always positive. The rest of the multipliers are positive and symmetric under \( i \leftrightarrow j \) and therefore \( R_{2m-1} \geq 0 \).

4.4. Clausius dominated level

An immediate consequence of this generalized Clausius number inequality follows from considering \( m \to \infty \). In this case, the term with the largest \( |(E_{h,i}/T_h) - (E_{c,i}/T_c)| \) becomes enormously larger than all the other terms. Therefore, this single term in \( R_{\infty} \) must be positive. If this term is positive, it is positive also in \( R_1 \) and therefore the Clausius dominated level \( i_{\text{max}} \) defined by:
\[ \frac{E_{h,i \max}}{T_h} - \frac{E_{c,i \max}}{T_c} \geq \frac{E_{h,i}}{T_h} - \frac{E_{c,i}}{T_c}, \]  

satisfy:

\[ \text{sign} \left( \frac{dp_{A \to C}}{t_{\max}} \right) = \text{sign} \left( \frac{E_{h,i \max}}{T_h} - \frac{E_{c,i \max}}{T_c} \right), \]  

where we assume that \( (E_{h,i}/T_h) - (E_{c,i}/T_c) \) has a single maximum and that \( \langle dp_{A \to C} \rangle \neq 0 \). Equation (39) allows us to immediately determine the direction of heat flow into the baths for this level. Of course, this can be done explicitly by evaluating the probabilities numerically. This equality is not trivial since the Clausius dominated level is not necessarily the largest element in the Clausius number sum (30).

4.5. Local and non-local quantities

We call a quantity ‘local scalar’ if the scalar quantity can be written in terms of the single-bath parameters \( E_b \) and \( T_b \) (i.e. \( f(E_b, T_b) \)). The mean energy \( p_b \cdot E_b \) of the bath particle, its purity \( p_b \cdot p_b \), its entropy, its energy variance, its free energy and so on, are all examples of local scalars. A local function is a function of local scalars.

Many other quantities of prime importance cannot be written in this form: the index coincidence \[ [74] \] \( p_c \cdot p_h \), the fidelity of the two baths \( \sum_i \sqrt{p_{c,i}} \sqrt{p_{h,i}} \), the Jeffreys and Kullback–Leibler divergence \[ [75] \], the Wootters distance \[ [76] \] etc. Hence these scalars are ‘non-local scalars’. More importantly heat, work and efficiency are non-local scalars.

In our analysis, thermodynamics amounts to finding relations between non-local scalars of interest (e.g. work and efficiency) and local scalars (temperature entropy, etc).

4.6. Purity reduction

Let us define the purity of the bath after the collision by the purity of the reduced density formed by tracing out the engine and the other bath. Although the purity does not have all the appealing properties of the von Neumann entropy, it provides a simple and convenient measure of impurity. Furthermore, in contrast to entropy, it is not sensitive to whether we keep track of the particles’ position or not (i.e. there is no mixing entropy issue). In addition the purity will naturally emerge in the derivation of bound on maximal work and efficiency.

The purity change in one cycle in one bath is:

\[ \Delta P_b = \left| p_b + dp_b \right|^2 - \left| p_b \right|^2 = dp_b^2 + 2p_b \cdot dp_b, \]  

where the absolute value of a vectors refers to the standard \( L_2 \) norm \( |y| = \sqrt{\sum_{i=1}^{N} |y_i|^2} \equiv \sqrt{\mathbf{y}^2} \). Using \( dp_c = -dp_h \) for steady state operation we obtain:

\[ \Delta P_h + \Delta P_c = 2 \left( \frac{1 - xR}{xR} \right) dp_h^2 \]  

\[ = -\frac{xR(1-xR)}{(2-xR)^2} \left| p_h - p_c \right|^2. \]  

In a refrigerator the cold bath purity increases while the hot bath becomes more mixed. Yet, the change in the hot bath is larger so the purity of the whole system decreases. For \( xR < 1 \) the sum
of individual purities of the whole system (engine+baths) becomes increasingly more mixed in all modes of operations.

In the spirit of section 4.5 we want to express the purity reduction using local functions. This can be achieved by applying the inverse triangular inequality:

\[
|\Delta P_h + \Delta P_i| \geq \frac{xR(1-xR)}{(2-xR)^2} \left( |p_h| - |p_i| \right)^2
\]

Interestingly, in contrast to the Clausius inequality, we did not assume a thermal distribution. In fact, in steady state this device will decrease the total purity for any bath population that is diagonal in the energy basis. While the Clausius number is not well defined (there is no notion of temperature for non thermal baths) the purity decrease still holds.

Finally, we note that using the Jensen inequality for the \( \ln \) function it is straightforward to show that the purity is related to the entropy through:

\[
P \geq e^{-S},
\]

where \( S = - \sum p_i \ln p_i \) is the standard entropy function. This inequality can be interpreted in the following way: the Chebyshev sum inequality yields \( P \geq 1/N \) where the equality holds for uniform distributions. \( e^S \) is the Shannon’s effective number of degrees of freedom. The right-hand side of (45) is also equal 1/N for uniform distribution. Hence (45) expresses the relation between two measures that count the degrees of freedom in the system.

5. Index of coincidence necessary conditions for engines and refrigerators

The engine regime is defined by the condition

\[
\langle W \rangle = xR/(2-xR) \left( p_h \cdot E_h + p_e \cdot E_e - p_h \cdot E_h - p_h \cdot E_e \right) \geq 0.
\]

Using the mean bath energy \( \langle E_b \rangle = p_h \cdot E_h \) and the free energy defined through \( p_b = e^{-\frac{E_b}{T_b}} \)
we get:

\[
\langle W \rangle \geq \langle E_h \rangle + \langle E_e \rangle + \sum_i p_{c,i} \left( T_h \ln p_{h,i} - F_h \right) + p_{h,i} \left( T_e \ln p_{c,i} - F_e \right).
\]

After rearranging and using the Jensen inequality to get

\[
\ln p_c \cdot p_h \geq \sum_i p_{c,i} \ln p_{h,i}, \quad \ln p_e \cdot p_h \geq \sum_i p_{h,i} \ln p_{c,i}
\]

we get that the work satisfies the inequality:

\[
\langle W \rangle \leq T_c S + T_h S_h + \left( T_h + T_e \right) \ln p_h \cdot p_c,
\]

where we used: \( T_b S_b = \langle E_b \rangle - F_b \). If the right-hand side is smaller than zero so will be \( \langle W \rangle \). Thus, demanding that the right-hand side of (47) is positive we get a necessary (but not sufficient) condition for the heat machine to perform as an engine:

\[
P_{ch} \geq e^{-\frac{T_c S_e + T_h S_h}{T_c + T_h}},
\]

(48)
where $\mathcal{P}_{ch}$ is the index of coincidence $\mathcal{P}_c \cdot \mathcal{P}_h$ \[74\]. While the purity describes the probability that the same result will appear when measuring the energy of two particles in the same bath, $\mathcal{P}_{ch}$ describes the probability that particles from different baths will be in the same level. $\mathcal{P}_{ch}$ is often used in cryptography and code ciphering. Note, that it does not imply a correlation but simply the likelihood of identical events in both baths.

Equation (48) also imposes a restriction on the individual purities since:

$$e^{-\frac{T_c S_c + T_h S_h}{T_c + T_h}} \leq \mathcal{P}_c \cdot \mathcal{P}_h \leq \sqrt{\mathcal{P}_c \mathcal{P}_h} \leq \frac{\mathcal{P}_c + \mathcal{P}_h}{2},$$ \hspace{1cm} (49)

where we used the Cauchy–Schwarz inequality to go from the second step to the third. The last stage before the end of (49) can be expressed using the second order Rényi entropy \[77\]

$$S_{R_{2:ch}} = -\ln \mathcal{P}_h:$$

\[\frac{T_c S_c + T_h S_h}{T_c + T_h} \geq \frac{S_{R_{2:c}} + S_{R_{2:h}}}{2}.\] \hspace{1cm} (50)

Now we wish to find the analogue condition for the refrigerator regime. Cooling occurs when the cold bath gives away heat to the system\[2\]:

$$(\mathcal{P}_c - \mathcal{P}_h) \cdot E_c > 0.$$ \hspace{1cm} (51)

Repeating the same procedure as before we get a necessary refrigerator condition:

$$\mathcal{P}_{ch} \geq e^{-S_c}.$$ \hspace{1cm} (52)

In contrast to other measures like fidelity, $\mathcal{P}_{ch}$ has a very simple statistical interpretation which also makes it easier to measure it in practice. $\sum \mathcal{P}_{c,i} \mathcal{P}_{h,i}$ is the probability that two particles chosen from different baths will be in the same state (like getting the same result with two different unbalanced dices). To evaluate it, there is no need to keep track of the exact result and then to estimate the probabilities $\mathcal{P}_{c,i}$ and $\mathcal{P}_{h,i}$ through their frequencies. One only needs to keep track of if the results are the same or not. Thus, $\mathcal{P}_{ch}$ corresponds to a binary random variable (a coin flip). Like the purity, $\mathcal{P}_{ch}$ also satisfies $\mathcal{P}_{ch} \geq 1/N$ (if the levels do not cross) but this is true for any two monotonic distributions and in contrast to (48) and (52) it does not give any indication of the heat machine’s functionality.

6. Upper bounds on work and efficiency

6.1. Bounds on the maximal work production

The first work upper bound can be obtained from (47) where the inequality $\ln \mathcal{P}_c \cdot \mathcal{P}_h \leq \frac{1}{2} \ln \mathcal{P}_c \mathcal{P}_h$ is used to bring it to the local form:

$$\langle W \rangle \leq \frac{x R}{2 - x R} \left[ T_h S_h + T_c S_c + \frac{T_h + T_c}{2} \ln \mathcal{P}_c \mathcal{P}_h \right].$$ \hspace{1cm} (53)

\[2\] For the refrigerator regime the work is not a good indicator since it is possible to apply work to the system without cooling the cold bath (e.g. the rightmost regime in figure 2).
A different bound can be obtained by writing the work in a different form:

$$\langle W \rangle = \frac{xR}{2 - xR} \left[ (T_h - T_c)(S_h - S_c) - T_c D_{KL}(p_h|p_c) - T_h D_{KL}(p_c|p_h) \right].$$  \hspace{1cm} (54)

The last two terms are always negative (including the minus sign). Therefore the first term must be positive for the machine to perform as an engine. $S_h \geq S_c$ is expected for engines as engine transfer entropy from the hot bath to the cold bath but (54) quantifies how large the entropy difference must be:

$$S_h - S_c \geq \frac{T_c D_{KL}(p_h|p_c) + T_h D_{KL}(p_c|p_h)}{T_h - T_c}.$$ \hspace{1cm} (55)

The work expression (54) contains within the non-local quantity $D_{KL}$. To obtain a local upper bound we use the inequality:

$$D_{KL}(p_c|p_h) \geq \frac{1}{2} \left( \sum \left| p_{c,i} - p_{h,i} \right| \right)^2 \geq \frac{1}{2} \left( \sum \left| p_c \right|^2 + \sum \left| p_h \right|^2 - 2 \left| p_c \right| \left| p_h \right| \right) = \frac{1}{2} \left( \sqrt{p_c} - \sqrt{p_h} \right)^2,$$ \hspace{1cm} (56)

and get:

$$\langle W \rangle \leq \frac{xR}{2 - xR} \left[ (T_h - T_c)(S_h - S_c) - \frac{T_c}{2} + \frac{T_h}{2} \left( \sqrt{p_c} - \sqrt{p_h} \right)^2 \right].$$ \hspace{1cm} (57)

Different approaches and different inequalities may lead to work upper bounds that can perform better in certain regimes. In addition, further reasonable restrictions on the system can also lead to better results. In appendix C we derive another work bound under some assumptions about the energy levels’ structure.

### 6.2. Upper bounds on the efficiency

In the two-level case the efficiency is simply given by $1 - \frac{E_f - E_i}{E_f - E_i}$ and the population change cancels out. In the multilevel engine the efficiency is:

$$\eta_c = 1 - \frac{\langle dp \cdot E_c \rangle}{\langle dp \cdot E_h \rangle}.$$ \hspace{1cm} (58)

Using the Clausius number defined in section 4.2:

$$\eta_c = 1 - \frac{T_c}{T_h} - \frac{T_c}{\langle dp \cdot E_h \rangle R}.$$ \hspace{1cm} (59)

Notice that this result is still exact. Since $R \geq 0$ we get that the swap engine efficiency is always smaller than the Carnot efficiency. To get a tighter upper bound we use
again the inequality $D_{KL} (p_c | p_h) \geq \frac{1}{2} | p_c - p_h |^2$ and Cauchy–Schwarz in the denominator and obtain:

$$\eta \leq 1 - \frac{T_c}{T_h} - \frac{T_c}{| \mathcal{E}_h |} | p_c - p_h |,$$

where we used $\mathcal{E}_h$ to denote the centered energy vector:

$$\mathcal{E}_{h,i} = E_{h,i} - \frac{1}{N} \sum_{k=1}^{N} E_{h,k}.$$  \hspace{1cm} (60)

The replacement $\mathbf{E}_h \rightarrow \mathcal{E}_h$ is highly important. It keeps the bound invariant to energy shifts and at the same time makes the bound tighter. Equation (60) can be written as

$$\eta \leq 1 - \frac{T_c}{T_h} - \frac{T_c}{| \mathcal{E}_h |} \sqrt{P_c + P_h - 2 P_{ch}}.$$  \hspace{1cm} (62)

In order to obtain a local-quantities bound we use the inequality $P_{ch} \leq \sqrt{P_c} \sqrt{P_h}$ and obtain a weaker yet local upper bound:

$$\eta \leq 1 - \frac{T_c}{T_h} - \frac{T_c}{| \mathcal{E}_h |} \left| \sqrt{P_c} - \sqrt{P_h} \right|.$$  \hspace{1cm} (63)

This inequality is often very close to the Carnot efficiency. Yet, it still shows that the baths’ purity imposes some limitations on the efficiency.

A different upper bound can be written down in term of the Wootters statistical distance [76] between the hot and cold probability distribution:

$$L_w = \arccos \left( \sum_{i=1}^{N} \sqrt{P_{c,i} P_{h,i}} \right) \hspace{1cm} (64)$$

From [73] it follows that the Jeffreys divergence satisfies:

$$J \geq \frac{16}{\pi^2} L_w^2.$$  \hspace{1cm} (65)

The efficiency bound obtained from using (65) in (59) is not always smaller or larger than (60) and it uses the non-local quantity $\sum_{i=1}^{N} \sqrt{P_{c,i} P_{h,i}}$ (fidelity). Yet, it introduces another relation between the difference in the statistics of the baths and the efficiency.

7. The ultra-hot baths and the quasi-static regime

7.1. The ultra-hot baths regime

For systems with small energy gaps (e.g. magnetically induced splitting or translational motion in a trap), the levels are highly excited even for low bath temperatures. The condition $E_h / T_h, E_c / T_c \ll 1$ defines a high temperature limit for the specific system (a more rigorous condition will be given later). In this section we study the multilevel heat engine operation when the baths are so hot that we consider only the first order correction in
$1/T_b$ to the $T_b \to \infty$ limit where $p_{b,i} \to 1/N$. The ultra-hot regime is defined by the small parameters:

\[
\frac{\Delta E_c}{T_c}, \frac{\Delta E_h}{T_h} \ll 1,
\]

where $\Delta E_b = E_{b,\text{max}} - E_{b,\text{min}}$ is the gap of the bath. First order expansion in $\{\beta_c = 1/T_c, \beta_h = 1/T_h\}$ yields:

\[
W_{\text{ultra-hot}} = \frac{xR}{2 - xR N} \left[ (\beta_c + \beta_h) E_c \cdot E_h - \beta_c |E_c|^2 - \beta_h |E_h|^2 \right].
\]  

This time the centered energy form $E_b$ emerges naturally from the free energy normalization factor in the ultra-hot limit. $W > 0$ yields the ultra-hot necessary and sufficient engine condition:

\[
E_c \cdot E_h > \frac{\beta_c |E_c|^2 + \beta_h |E_h|^2}{\beta_c + \beta_h}.
\]

Applying Cauchy–Schwarz we get a necessary condition for ultra-hot swap engines:

\[
1 < \frac{|E_h|}{|E_c|} < \frac{T_h}{T_c},
\]

**Work per cycle optimization**

Next we want to take advantage of the simple energy dependence in the work expression (67) and optimize the work output under some restrictions. First, let us assume that the norms of the energies $|E_c|$ and $|E_h|$ are fixed. Under these two constraints the last two terms in (67) are fixed. To maximize the first term, and consequently the work, $E_c$ must be parallel to $E_h$:

\[
E_{h,i} = CE_{c,i},
\]

\[
1 \leq C \leq \frac{T_h}{T_c},
\]

where $C$ is the compression ratio and (71) follows from (69). For ‘uniform compression’ (70) the device works as a refrigerator when $C < 1$, and as a heater when $C \geq T_h/T_c$. In the regime (71) it performs as an engine. The uniform compression can be studied for any temperature but in the ultra-hot regime it is found that the uniform compression maximizes the work when the energy norms are fixed. Now we remove the restriction that $|E_c|$ is fixed and use (70) in (67). Imposing $\partial_c W = 0$ we get:

\[
C_{\text{max}} |E_{c,i}| = \frac{T_h}{2(T_h + T_c)} \leq 2,
\]

where $|E_{h,i}|$ subscript signifies the $|E_h| = \text{const}$ optimization constraint. This result is a bit surprising. If the hot levels are fixed we find that there is no point in compressing them by more than a factor of two (or $C_{\text{max}} |E_{c,i}$ to be exact) to reach the maximal output work. The efficiency is:
\[ \eta_{\text{ultra-hot}}^{\text{max}, \{E_a\}} = 1 - \frac{1}{C_{\text{Wmax}, \{E_a\}}} = \frac{T_h - T_c}{2 T_h} = \frac{1}{2} \eta_c \leq \frac{1}{2}, \]  
(73)

where \( \eta_c \) is the Carnot efficiency. The optimal compression and the efficiency at maximum work critically depends on the constraint we impose. If we impose that the cold bath energy norm is fixed and optimize over the hot bath levels we obtain:

\[ C_{\text{Wmax}, \{E_a\}} = \frac{1}{2} \frac{(T_h + T_c)}{T_c}, \]  
(74)

\[ \eta_{\text{ultra-hot}}^{\text{max}, \{E_a\}} = \frac{T_h - T_c}{T_h + T_c} = \frac{\eta_c}{2 - \eta_c}. \]  
(75)

Interestingly, the same expression for the efficiency was obtained in [78] for a classical engine operating at maximum power.

In [79] both (73) and (74) were obtained for slow classical engines when the engine is close to reaching equilibrium with the bath during the thermal strokes. Depending on whether the hot bath relaxation time of the cold bath overwhelms the cold bath relaxation time or vice versa (73) and (74) are obtained. If the time scales are the same (the symmetric case) then the Chambadal, Novikov, Curzon and Ahlborn (CNCA) efficiency bound [53, 80, 81]

\[ \eta_{\text{CA}} = 1 - \sqrt{T_c/T_h} \]  
is obtained. In our system we can get CNCA result as well by imposing the constraint \( |E_c| \parallel |E_h| = \text{const} \) (or equivalently fixing the geometric mean of the norms) that lead to:

\[ C_{\text{Wmax}, \{E_a\}} = \frac{T_h}{T_c}, \]  
(76)

\[ \eta_{\text{ultra-hot}}^{\text{max}, \{E_a\}} = 1 - \frac{T_c}{T_h} = 1 - \sqrt{1 - \eta_c}. \]  
(77)

Despite the similarity of our final results (73), (74) and (76) to [79] the physical scenario is completely different. First, we optimize work per cycle and not power. Second, our result does not reach the Carnot efficiency if the cycle (the collisions) is slower. In our case, the deviation from Carnot is due to the levels’ structure and the deviation persists regardless of the degree of thermalization. To see this one can take the swap parameter to be one where complete thermalization takes place or take it to be tiny where the state is hardly affected by the bath. However the efficiency at maximal work is independent of the swap parameter and the level of thermalization.

Once \( C_{\text{Wmax}} \) is found then together with the constraint it can be used to get an expression for the maximal work. Let us write it explicitly just for the \( |E_h| = \text{const} \) case in order to clarify a point:

\[ W_{\text{max}, \{E_a\}}^{\text{ultra-hot}} = \frac{x R}{2 - x R N} \frac{1}{4 T_c T_h^2} \left( \frac{T_h - T_c}{T_h} \right)^2 \]  
(78)

At first sight, it may seem that the \( \frac{1}{N} \) term suggests that the work becomes smaller when the number of levels increases. Yet, \( E_h^2 \) may also depend on \( N \). For example if the levels are degenerate so that there are \( N/2 \) replicas of two levels, we get that the work does not depend on the number of replicas, as expected.
To conclude this section we evaluate the Clausius number in the ultra-hot limit and get:

\[
\mathcal{R}_{\text{ultra-hot}} = \frac{xR}{2 - xR} \sum_i \left( \frac{\mathcal{E}_{h,i}}{T_h} - \frac{\mathcal{E}_{c,i}}{T_c} \right) \left( \frac{\mathcal{E}_{h,i}}{T_h} - \frac{\mathcal{E}_{c,i}}{T_c} \right)
\]

\[
\mathcal{R}_{\text{ultra-hot}} = \frac{xR}{2 - xR} \sum_i \left( \frac{\mathcal{E}_{h,i}}{T_h} - \frac{\mathcal{E}_{c,i}}{T_c} \right) \left( \frac{\mathcal{E}_{h,i}}{T_h} - \frac{\mathcal{E}_{c,i}}{T_c} + \text{const} \right). \tag{79}
\]

The constant term can be dropped since it contributes zero to the total sum. After the constant term is removed, all the terms in the Clausius sum are positive. This is not true for temperatures below the ultra-hot bath regime. In this regime, the Clausius inequality holds since the probability difference and the Clausius factor \( (\mathcal{E}_{h,i}/T_h) - (\mathcal{E}_{c,i}/T_c) \) have the exact same form.

7.2. Almost ‘quasi-static evolution’ at finite time

Consider the case where the swap parameter is sufficiently small so that after a collision the change in a bath particle population, \( \Delta p_{b,i} \), is small with respect to the original bath population \( \delta p_{b,i} \ll p_{b,i} \). At the end of appendix A it is shown that the energy basis diagonal form of the density matrices is conserved in an energy population swap (this trivially holds in a density swap interaction). Consequently, it is possible to use just \( p_b \) and \( \delta p_b \) to calculate the von Neumann entropy change. To first order in \( \delta p_{b,i} \) the change in the bath particle’s entropy is given by:

\[
\langle \delta S_b \rangle = S\left( \bar{p}_b + \delta \bar{p}_b \right) - S\left( \bar{p}_b \right) = \langle \delta p_b \rangle \frac{\Delta E_b}{T_b} = \frac{\langle \delta Q_b \rangle}{T_b}. \tag{80}
\]

Note that this equation holds only for the bath particles and for tiny deviations from the Gibbs state. The engine is not in a thermal state at all, and cannot be assigned a temperature. However, in a complete cycle, on average, the engine returns to its initial state so the engine does not contribute to the average entropy production of the total system. Therefore the total increase in both baths and the system satisfies:

\[
\langle \delta S_b \rangle + \langle \delta S_c \rangle \geq 0, \tag{81}
\]

by virtue of the Clausius inequality for swap heat machines proven earlier.

Assuming that on average there are \( n \) cold collisions and \( n \) hot collision, the work can be expressed in terms of the entropy changes:

\[
\langle W \rangle = nT_h \langle \delta S_h \rangle + nT_c \langle \delta S_c \rangle. \tag{82}
\]

Although (80) seems like a plausible property for a bath, it is not mandatory and in our model it emerges only in the weak coupling limit (small population change per collision).

Even though we assumed the change in a single collision is small it does not mean that the heat exchange in strokes \( B \) or \( C \) must be small in our model. If we allow multiple collisions, it is possible to have large changes while still satisfying \( \Delta Q_b = T_b \Delta S_b = T_b n \delta S_b \).

In our entropy considerations we have not included the mixing entropy so it is not claimed that (80) is the change in the entropy of the system but just the part of the entropy change that is responsible for the heat exchange.

20
8. Conclusion

We have presented an analysis of a multilevel heat machine that is driven by a sequential partial swap interaction with a hot and cold bath. In the limit of the complete swap our results describe any ‘slow’ four-stroke Otto cycle where the interaction with the bath (not necessarily a swap interaction) has sufficient time to bring the engine very close to thermal equilibrium. We derived necessary conditions for the engine and refrigerator regimes and produced refined upper bounds on the work and efficiency using the relative entropy and Jefferies divergence of the baths. Our analysis emphasizes the difference between ‘local’ quantities that are evaluated using the properties of a single bath, and ‘non-local’ quantities that require both baths to be evaluated. Bounds on non-local quantities of interest such as work, heat and efficiency were expressed in terms of simpler local quantities such as the purity and entropy of the baths.

The equivalent of Clausius inequality in this system was generalized to higher order energy moments. We identified a quasi-static regime in finite time evolution and an ultra-hot regime where stronger statements can be made and work optimization can be carried out analytically.

While our findings are valid for any multilevel engine and collisions that can bring the system to a Gibbs state, it is interesting to consider other bath models like the ones used in continuous engines where different levels interact with different baths or where the thermalization rate is different for different levels.

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Appendix A. The two-level swap Hamiltonian

The partial swap unitary is given by:

\[ U = e^{-i\frac{\phi}{2} \sum \sigma_i \otimes \sigma_i}, \]

where \( \sigma_i \) are the Pauli matrices and \( \phi \) is the swap angle. \( \phi = \pi/2 \) corresponds to a complete swap. The reduced density matrix of particle 1 after applying \( U \) is:

\[ \rho_1' = \text{tr}_2 \left( U \rho_1 \otimes \rho_2 U^* \right). \]

One can verify that the density swap rule is satisfied:

\[ \rho_1' = \cos^2 \phi \rho_1 + \sin^2 \phi \rho_2. \]

Since the Hamiltonian in the exponent of \( U \) is written in terms of the Pauli matrices it is not straightforward to generalize it to a multilevel swap operation. For energy population swap, the generalization is simpler when two-particle states are considered. A complete swap operation yields: \( U_{\phi} |li, i\rangle = U_{\phi} |lj, i\rangle \). The states \( |li, i\rangle \) are invariant under this operation. The complete swap unitary in the two-particle state can be written as:
The column to the left shows how the states are ordered in the two-particle density matrix. In this form the unitary has a clear block diagonal structure. In the space of each non-identical state $\langle ij \rangle$ a simple spin flip takes place:

$$a \langle ij \rangle + b \langle ji \rangle \rightarrow a \langle ji \rangle + b \langle ij \rangle.$$  

Replacing the spin flip by a more general rotation in this Hilbert subspace, it is easy to deduce the partial swap time-independent Hamiltonian:

$$H = \sum_{ij} \phi_{ij} \langle ij \rangle \langle ji \rangle.$$  

The $\phi_{ii}$ terms just contribute a phase to the invariant states. A complete swap takes place when $\phi_{i \neq j} = \pm \pi/2$.

In general, there is no particular reason why the rotation rate, $\phi_{ij}$ should be the same for all pairs of states. However, when it is the same, $\phi_{i \neq j} = \phi$ can show that the energy population swap rule follows:

$$\rho_{12} = \rho_1 \otimes \rho_2 = \sum_{ij} \phi_{ij} \langle ij \rangle \langle ji \rangle.$$  

This swap model is specially designed for the energy basis. Consequently, for partial swap, in general, it does not satisfy the ‘density swap’ rule but the energy basis probability rule. Yet, a proper choice of $\phi_{ij}$ leads to the density swap Hamiltonian that appears in the exponent of (A.1).

We conclude by noting the important fact that the energy population Hamiltonian preserves the energy diagonal form after the partial trace. That is, if the input state is $\rho_1 \otimes \rho_2$ where $\rho_1$, $\rho_2$ are diagonal in the energy basis then $\rho^\prime_{1(2)} = \text{tr}_{2(1)}(U\rho_1 \otimes \rho_2 U^\dagger)$ will be diagonal in the energy basis as well. For simplicity we illustrate this for the $\phi_{i \neq j} = \phi$ case. The density matrix after the collision and before the trace is:

$$U\rho_1 \otimes \rho_2 U^\dagger = \cos^2 \phi \rho_1 \otimes \rho_2 + \sin^2 \phi \rho_2 \otimes \rho_1 + \sum_{i \neq j} f_{ij} \langle ij \rangle \langle ji \rangle,$$

where $f_{ij}$ are some complex coefficients. The third term vanishes when taking partial trace on either particle. Due to the block structure (A.4) this holds even when $\phi_{i \neq j}$ depends on $i$ and $j$.

**Appendix B. Markovian swap formulation**

As shown in section 3, in the steady state all coherences of the density matrix vanish. Thus only the diagonal elements are important and the Markov chain formalism can be used to describe the evolution of the diagonal elements (probabilities). In this appendix it will be more
convenient to use Dirac’s ‘Bra–Ket’ notation for the probability vectors in order to distinguish between right vectors and left vectors. However the normalization is still the regular probability normalization.

The probabilities before and after the collision with the hot bath satisfy:

\[ p_s' = K_h p_s, \]  
\[ K_h = \bar{x} |p_{Th}\rangle \langle 1, 1, 1.. \rangle + (1 - \bar{x}) I_{N \times N}, \]

where \( \bar{x} \) is an effective swap parameter that may contain a ‘classical’ contribution from the collision probability \( R \) and a quantum contribution from a quantum partial swap (\( x < 1 \) or \( \phi < \pi/2 \)). \( I_{N \times N} \) is the identity operator. One can verify that the above equations lead to the population swap rule \( p_s' = (1 - \bar{x}) p_s + \bar{x} p_h \). A Markov chain with a single steady state vector is always associated with a left eigenvector of the form \( \langle 1, 1, 1.. \rangle \). Thus, \( |p_{Th}\rangle \) is a right eigenvector of \( K_h \) and it has a unity eigenvalue: \( K_h |p_{Th}\rangle = |p_{Th}\rangle \).

The engine operation over one cycle starting from stroke \( A \) is given by:

\[ K_{A\rightarrow A} = K_e K_h \]
\[ = \left[ \bar{x}^2 |p_{Th}\rangle \langle 1, 1, 1.. \rangle + \bar{x}(1 - \bar{x}) |p_{Th}\rangle \langle 1, 1, 1.. \rangle + (1 - \bar{x})^2 I_{N \times N} \right]. \]

This operator has a clear interpretation. The \( \bar{x}^2 |p_{Th}\rangle \langle 1, 1, 1.. \rangle \) term describes two complete swaps that occur with probability \( \bar{x}^2 \). Since both swap events are complete, the population is determined by the last swap with the cold bath. The \( \bar{x}(1 - \bar{x}) \) terms describe the probability for a single complete swap event, and the \( (1 - \bar{x})^2 \) term describes zero swap events.

Clearly the invariant steady state is \( (x(1 - x) + \bar{x}^2)|p_{Th}\rangle + x(1 - x)|p_{Th}\rangle \). After normalization we obtain the steady state eigenvector:

\[ |p_e^A\rangle = \frac{|p_{Th}\rangle + |p_{Th}\rangle - \bar{x} |p_{Th}\rangle}{2 - \bar{x}}. \]

Repeating this for a cycle starting from stroke \( C \) and using \( K_{C\rightarrow C} = K_e K_h \) one gets:

\[ |p_e^C\rangle = \frac{|p_{Th}\rangle + |p_{Th}\rangle - \bar{x} |p_{Th}\rangle}{2 - \bar{x}}. \]

Both \( B.4 \) and \( B.5 \) agree with the steady state population obtained in \( (3) \), when replacing \( \bar{x} \rightarrow xR \)

**Appendix C. Alternative work upper bound**

The expression for the work is a standard inner product over the real vectors. By using the Cauchy–Schwarz inequality we get:

\[ |\langle W \rangle| \leq \frac{xR}{2 - xR} |p_l - p_h| |E_e - E_h|. \]

At first, it seems, that this separation between statistics and energy is not very useful. If all \( p_l \) and \( p_h \) have to be known, then there is not much difference from calculating the exact value of
the work. However, $|\mathbf{p}_c - \mathbf{p}_h|$ can be expressed in terms of simple scalar quantities that characterize the baths.

$$\begin{align*}
|\mathbf{p}_c - \mathbf{p}_h|^2 &= |\mathbf{p}_c|^2 + |\mathbf{p}_h|^2 - 2\mathbf{p}_c \cdot \mathbf{p}_h = \mathcal{P}_c + \mathcal{P}_h - 2\mathcal{P}_{ch}. 
\end{align*}$$

(C.2)

The upper bound (C.1) holds for any diagonal distribution and even if the distribution is not known exactly it is enough to measure $\mathcal{P}_c$, $\mathcal{P}_h$ and $\mathcal{P}_{ch}$. Since $\mathbf{p}_c$ and $\mathbf{p}_h$ are ordered if there are no level crossings, we can use Chebyshev’s sum inequality and get $\mathbf{p}_c \cdot \mathbf{p}_h \geq 1/N$ so that:

$$\begin{align*}
|\langle W \rangle| &\leq \frac{xR}{2 - xR} \sqrt{\mathcal{P}_c + \mathcal{P}_h - 2\mathcal{P}_{ch}} \left| E_c - E_h \right| 
\end{align*}$$

(C.3)

$$\begin{align*}
\leq \frac{xR}{2 - xR} \sqrt{\mathcal{P}_c + \mathcal{P}_h - \frac{2}{N}} \left| E_c - E_h \right|.
\end{align*}$$

(C.4)

Note that: $\sqrt{\mathcal{P}_c + \mathcal{P}_h - (2/N)} \leq \sqrt{2} \sqrt{(N - 1)/N}$. If all the levels are compressed (not necessarily by the same factor) so that:

$$E_{c,i} = \frac{1}{C_i} E_{h,i}$$

(C.5)

$C_i \geq 1$, 

(C.6)

in this case, we can use $(a - b)^2 \leq |a - b| |a + b| = |a^2 - b^2|$ $\forall a b > 0$ and get the following local form:

$$\begin{align*}
|\langle W \rangle|_{C_i \geq 1} &\leq \frac{xR}{2 - xR} \sqrt{\mathcal{P}_c + \mathcal{P}_h - \frac{2}{N}} \left| E_h - E_c \right| 
\end{align*}$$

(C.7)

$$\begin{align*}
\leq \frac{xR}{2 - xR} \sqrt{\mathcal{P}_c + \mathcal{P}_h - \frac{2}{N}} \sqrt{E_h^2 - E_c^2}.
\end{align*}$$

(C.8)

We cannot use the centered level $E$ here, as it may violate (C.5). The advantage of this bound is that it separates the statistical properties of the baths from the energy structure of the baths and that all the quantities used are local.

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