Universal features in the efficiency at maximal work of hot quantum Otto engines

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Abstract – Classically, external power optimization over the coupling times of a heat engine to its baths leads to universal features in the efficiency. Here we study internal work optimization over the energy levels of a multilevel quantum Otto engine, and find similar universal features. It is shown that in the ultra-hot regime the efficiency is determined solely by the energy level optimization constraint, and is independent of the engine’s details. Constraints on the energy levels naturally appear due to physical limitations or design goals. For some constraints the results significantly differ from the classical universality.

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Carnot’s discovery of a universal efficiency upper bound for heat engines had a profound impact on physics and engineering. Yet, in practice to approach this efficiency bound the system needs to be reversible, which implies an infinitely slow cycle time and vanishing power output. This has motivated extensive studies under the title of “finite-time thermodynamics” (see [1,2] for review articles). More importantly, efficiency is only a secondary design goal. First the engine must be capable of doing the task it is designed to do: lifting a weight in a given time, accelerating a car, etc. In general, the efficiency depends on the heat transfer mechanism between the system and the bath. Nevertheless, some universal features were discovered when the power output is maximal. In this work we study the universality of efficiency at a maximal output of quantum Otto engines. In the engines studied here, the working substance is a single particle that constitutes an N-level system. In the adiabatic stroke of the quantum Otto engine the levels of the particle must be varied in time. In real systems this level variability is limited by practical considerations. For example, in Zeeman splitting the maximal gap is determined by the maximal available external magnetic field. In other systems it can be the power of the laser. In this work we study the optimal output of engines subjected to this type of constraints. We find that the details of the engine are irrelevant when the baths are very hot. The efficiency at maximal output is determined only by the nature of the constraint and the temperatures.

Typically, in classical engines the equation of state of the working substance is known and the output optimization is done by changing the coupling time to the baths. The output power may change from system to system but it was observed that for some classes of classical engines the efficiency at maximum power has universal features. In particular, in [3,4] it was shown that in the low-dissipation limit the efficiency at maximum power satisfies

\[
\eta \leq \eta_{LD} \leq \frac{\eta_c}{2} - \frac{\eta_c^2}{8} + O(\eta_c^3),
\]

(1)

where \(\eta_c\) is the Carnot efficiency \(\eta_c = 1 - T_c/T_h\). The same results were obtained in [5,6] for different thermalization mechanisms. In the low-dissipation scenario, the special case where the coupling coefficients to the cold and hot baths is the same (symmetric case), yields the Curzon-Ahlborn (CA) [7–9] efficiency,

\[
\eta_{CA} = 1 - \sqrt{T_c/T_h}.
\]

(2)

\(\eta_{CA}\) was originally obtained by applying the Newton heat transfer law. The CA efficiency was observed in a reciprocating hot quantum engine in [10] and in a continuous engine in [11]. Classically, features of universality appear in the Taylor expansion of the efficiency in terms of the Carnot efficiency. In [12] it was shown that

\[
\eta_{\text{Pmax,sym}} = \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + O(\eta_c^3).
\]

(3)
The one-half factor of the linear term is universal and the second term is universal for systems that have a "left-right" symmetry. For studies of efficiency in different models see [13–16] and references therein.

In this work we study work optimization in multilevel quantum Otto engines [17]. The working substance is a single N-level particle coupled periodically to hot and cold baths. The properties of this quantum working substance are determined by the level structure of the particle when it is coupled to the hot and cold baths. We optimize the level structure to get maximal work output per cycle. When the cycle time is fixed this is equivalent to power optimization. The classical optimization described earlier can be called "external" as it involves the optimization of the coupling process to the external baths. The maximum power in this case originates from the fact that reaching a thermal equilibrium with the baths is time consuming. Yet our optimization is "internal" as we optimize over the working medium properties (the level structure). We will assume that the baths are coupled for a sufficiently long period to effectively reach equilibrium for all practical purposes. This assumption is very reasonable when only one particle needs to be thermalized (and not a whole medium filled with particles). Here, the analysis includes the case of partial "swap" thermalization [17]. It is remarkable that for the most basic constraints the results of this internal structure quantum optimization are identical to the classical external coupling optimization.

We consider a generic single particle four-stroke Otto cycle. In the adiabatic strokes the energy levels of the particle (engine) change in time without changing the populations (see discussion in [17] on ways of achieving this in a short time). In the thermal strokes the system is coupled to hot and cold baths. If the system is coupled for periods that exceed a few relaxation times, it is plausible to assume that a full thermalization has taken place. As shown in the present work, some universal engine-independent features appear in the ultra-hot limit where only first order in β (inverse of the temperature) is non-negligible. In some cases, our results hold to order β² as well. For a study of refrigerators in hot regime see [18].

The work output of an N-level ultra-hot swap engine is [17]

\[ W_{\text{ultra-hot}} = \frac{\xi}{2 - \xi} \left( |E_c| - |E_h| \right)^2 \right) \left[ E_c - \beta c E_c^2 - \beta h E_h^2 \right], \]

where \( E_{c(h)\beta} \) is the i-th cold (hot) energy level of the engine, and \( |E|^2 = E \cdot E \) is the standard Euclidean L2 norm squared (not to be confused with the energy variance of the energy distribution). The energy levels are shifted so that \( \text{Mean}(E) = 0 \). The work is energy shift invariant, but a zero mean lead to a more compact form. The swap parameter \( 0 \leq \xi \leq 1 \) determines the degree of thermalization in the thermal strokes of the engine. When \( \xi = 1 \) a full thermalization takes place. This case should hold for any interaction that leads to a practically full thermalization regardless of the mechanism that generates it. Before proceeding, we note that the norm of the levels in the ultra-hot regime is directly related to several key quantities. For example, the internal energy when coupled to one bath is \( \text{tr}(\rho_0 \mathcal{H}_0) = \frac{1}{N} \beta / |E|^2 \), the purity and entropy is \( \text{tr}(\rho_0^2) = \frac{1}{N} + \frac{1}{N} |E|^2 |E|^2 \), and the heat capacity is \( C = \frac{1}{N} \beta^2 |E|^4 \). Another example for the norm significance will be given later on. In [17] it was shown that once the norm of the hot and cold levels are fixed, the maximum work is obtained when the energy vectors are parallel:

\[ E_c = (1 - \chi) E_h, \]

\[ 0 \leq \chi \leq \eta_c, \]

where \( \chi \), the compression deviation, is related to the compression ratio via \( \eta = \frac{1}{1+\chi} \). Condition (6) follows from the necessary condition for engine operation in the ultra-hot regime \( T_c/T_h \leq |E_c|^2 / |E_h|^2 \leq 1 \) (see [17]). The exact expression for the efficiency of an Otto engine with uniform compression (5) is [17]

\[ \eta = 1 - |E_c|^2 / |E_h|^2 = \chi. \]

Despite the equality of \( \eta \) and \( \chi \), it is useful to keep the different notation in order to prevent confusion. The maximal work in terms of \( \chi \) and the Carnot efficiency is

\[ W_\chi = \frac{\xi}{2 - \xi} \beta c \chi (\eta_c - \chi) |E|^2 / N, \]

where the subscript \( \chi \) indicates that we have already imposed the necessary but not sufficient optimality condition (5). Notice that \( W_\chi (\chi = 0) = 0 \) (no compression) and \( W_\chi (\chi = \eta_c) = 0 \) (reversible limit in Otto engines). Since \( |E_c| \neq 0 \), it follows from (8) that a maximum exists in the domain \( \eta = \eta_c \). The maximal work in the ultra-hot regime has an inherent universality. It depends only on the norms \( |E_c|^2 \) and \( |E_h|^2 \) (or \( |E_c|^2 \) and the compression ratio). The specific energy level structure is insignificant. All quantum Otto engines 1 with the same energy variance 2, and the same temperatures will have the same efficiency and same maximal work per cycle (up to the \( \xi/(2 - \xi) \) factor in (8)). The finer details of the engine manifest themselves only at colder temperatures.

**Work per cycle optimization.** — We start with a few important cases that exemplify the kinship to the classical case with very little algebra. First we choose the constraint \( |E|^2 \right) = \text{const} \). Applying \( \frac{d}{d \xi} W_\chi = 0 \) to (8) with fixed \( |E|^2 \) we obtain

\[ \eta \eta_c = \eta_c / 2. \]
which is the lower limit on the efficiency in the low-dissipation model (1). On the other hand, the opposite constraint $|\mathcal{E}_c| = \text{const}$ ($|\mathcal{E}_h| = \text{const}/(1 - \chi)$) yields

$$\eta_{|\mathcal{E}_c|} = \frac{\eta_c}{2 - \eta_c},$$  \hspace{1cm} (10)

which is the upper limit on the efficiency in the low-dissipation model (1). When applying the symmetric constraint $|\mathcal{E}_c|/|\mathcal{E}_h| = \text{const}$ then:

$$\eta_{|\mathcal{E}_c|/|\mathcal{E}_h|} = \eta_{\text{CA}} = 1 - \sqrt{1 - \eta_c}.$$  \hspace{1cm} (11)

Although this specific symmetric constraint yields CA efficiency (2), we shall see that symmetry does not necessarily lead to the CA efficiency in quantum Otto engines. Furthermore, we will present a non-symmetric constraint that yields the CA efficiency as well. Another important example follows from the constraint $\alpha \{\mathcal{E}_c\} + (1 - \alpha) |\mathcal{E}_h| = \text{const}$ that yields the maximum power efficiency:

$$\eta_\alpha = \frac{\eta_c}{2 - \alpha \eta_c}.$$  \hspace{1cm} (12)

This efficiency form frequently appears in various classical systems such as Brownian engines [14], systems operating in the low-dissipation limit [4], and systems with other thermalization processes [5,6].

The simple linear constraints studied above can be solved in a closed form. In what follows we explore the low-efficiency limit for a general constraint and find universal features.

**A general optimization constraint.** – As an example for a non-trivial physical constraint that is characterized by the energy norms, consider the quantum Otto engine studied in [19,20]. This engine has four energy levels and is comprised of two interacting spins and an external time-dependent magnetic field. In order to have the same population in the beginning and at the end of the adiabatic evolution strokes a certain protocol must be applied. Using the optimal protocol in [20], the minimal time for the adiabatic step is proportional to $\frac{1}{|\mathcal{E}_c|} + \frac{1}{|\mathcal{E}_h|}$ (to simplify (24) in [20] we considered the limit $\omega_f, \omega_i \ll j$). Thus, for the engine to operate at the minimal possible time (e.g., to maximize the power) the constraint is $\frac{1}{|\mathcal{E}_c|} + \frac{1}{|\mathcal{E}_h|} = \text{const}$. This example shows that a completely different optimization process (in this example elimination of non-adiabatic effects), may also lead to energy norm constraint. In addition, it clarifies that for observing universality there is a justified need for a framework valid for more complicated non-linear constraints. Applying $\frac{d}{d\chi} W_\chi = 0$ to (8) we get

$$\frac{d}{d\chi} \frac{|\mathcal{E}_h|}{|\mathcal{E}_c|} = \frac{(\eta_c - 2\chi)}{2(\eta_c - \chi^2)}.$$  \hspace{1cm} (13)

At this point we introduce the constraint function

$$G(|\mathcal{E}_c|, |\mathcal{E}_h|) = \text{const},$$  \hspace{1cm} (14)

that can describe either an implementation constraint or a design goal. Writing

$$G((1 - \chi)|\mathcal{E}_h(\chi)|, |\mathcal{E}_h(\chi)|) = \text{const},$$  \hspace{1cm} (15)

we get the additional equation needed to find $\chi$. The only limitation on $G$ is that (15) must provide a positive continuous solution for $|\mathcal{E}_h|$ in the domain $0 < \chi < \eta_c$. When $|\mathcal{E}_h(\chi)|$ can be solved explicitly from (15), then it can be used to evaluate the left-hand side of (13) and obtain an explicit equation for the optimal $\chi$. Yet, it is simpler to take the derivative of (15), evaluate $\frac{d}{d\chi} |\mathcal{E}_h|/|\mathcal{E}_h|$ and then use it in (13). However, even this simpler method is limited to very simple constraints and it is hard to see the underlying universal structure, and to compare it to the classical results. In what follows, we explore the low-efficiency limit, but before doing so we wish to point out that the solution of (13) and (15) yields an efficiency of the form $\eta = \eta(G, \eta_c)$. That is, an efficiency that depends only on the constraint and on the temperature ratio. It does not depend on the number of levels or on the engine specific details of the energy level structure $\mathcal{E}_h$. Hence, even without an explicit solution it is clear that there is universality to all orders in $\chi$ for hot quantum Otto engines that are subjected to the same constraint (or a design goal). To the lowest order in $\chi$ we can expand:

$$\frac{d}{d\chi} |\mathcal{E}_h|/|\mathcal{E}_h| = A + B\chi.$$  \hspace{1cm} (16)

Using (16) in (13) leads to a cubic equation in $\chi$. Since $\chi$ is small we use the lowest-order solution $\chi = \frac{\eta_c}{2}$ and replace the cubic term by $\chi^3 = \frac{\eta_c^3}{2}$. This yields a quadratic equation that is correct up to order $\eta_c^3$. The solution is

$$\eta = \frac{1}{2} \eta_c + \frac{1}{4} \eta_c^2 + \frac{1}{2} \eta_c^3 + O(\eta_c^4),$$  \hspace{1cm} (17)

$$a = A/4,$$  \hspace{1cm} (18)

$$b = B/8.$$  \hspace{1cm} (19)

In order to obtain $a$ and $b$ we need to specify a constraint function: To evaluate $A$ and $B$ we expand (15) in powers of $\chi$. Since $G = \sum F_k \chi^k$ is constant in $\chi$, all non-zero-order multipliers $F_{i\neq 0}$ should be zero. In particular $F_1 = 0$ yields

$$a = \frac{1}{4} \left( \frac{d}{d\chi} |\mathcal{E}_h|/|\mathcal{E}_h| \right) \bigg|_{\chi=0} = \frac{1}{4} \frac{G_{10}}{G_{10} + G_{01}} \bigg|_{\chi=0},$$  \hspace{1cm} (20)

where the subscript of $G$ specify the order of derivatives with respect to the first and second variable (the values of the variables are omitted for brevity but they are determined by $\chi = 0$: $|\mathcal{E}_c| = |\mathcal{E}_h| = |\mathcal{E}_h|_{\chi=0}$). From (20) two important results immediately follow. First, if the
constraint is symmetric \( G(|E_c|, |E_h|) = G(|E_h|, |E_c|) \), and therefore \( G_{10} = G_{01} \) for \( \chi = 0 \) and therefore
\[
a_{\text{sym}} = \frac{1}{8}.
\]
Using this in (17) we see that the same universality in the second-order coefficient that was observed in the classical case, appears here as well even though the optimization task is completely different.

The second result that follows from (20) concerns the asymmetric case where \( G_{10} \neq G_{01} \). If \( G_{10} \) and \( G_{01} \) have the same sign, then
\[
0 \leq a_{\text{sign}} \leq \frac{1}{4},
\]
The two extreme values 0 and \( \frac{1}{4} \) appear in the \( |E_h| = \text{const} \) and \( |E_c| = \text{const} \) studied earlier. However, in contrast to the classical power optimization studied in [3], in the quantum constraints (QC) framework studied here, the function \( \eta_{E_c} \) is not necessarily an upper bound on the efficiency. For example, this is true if the sign of \( G_{10} \) is different from that of \( G_{01} \). This can be seen by comparing the leading order of the QC case and classical low-dissipation case:
\[
\eta_{\text{QC}} = \frac{\eta_c}{2} + \frac{\eta^2_c}{4(1 + \frac{S_c}{G_{10}})} + O(\eta^3_c),
\]
\[
\eta_{\text{LD}} = \frac{\eta_c}{2} + \frac{\eta^2_c}{4(1 + \frac{S_c}{G_{10}})} + O(\eta^3_c),
\]
where \( S_{c,h} \) are the relaxation time scales of the baths [3]. Since \( S_c \geq 0, S_h \geq 0 \) it follows that \( a \leq 1/4 \) (for \( |E_c| = \text{const} \) \( a = 1/4 \)). In contrast, in the quantum case \( a \) can be larger if \( G_{01}/G_{10} \) is smaller than zero. Consider the constraint \( |E_c| - (1 - d) |E_h| = \text{const} \) for which \( G_{01} = d - 1 \), \( G_{10} = 1 \) thus the quadratic term is \( \frac{\eta^2_c}{G_{10}} \). For \( d = 1 \) we get the expected \( \frac{1}{4} \) for \( |E_c| = \text{const} \), but for smaller \( d \), \( a > 1/4 \). Note that \( d \) should satisfy \( d > \eta_c \). When \( d = \eta_c \) the Taylor series no longer converges. Physically, beyond this point the solution is no longer an engine.

Until now the constraints were due to some physical limitation. Yet, energy constraints can be indirectly imposed by setting a design goal. For example, if we wish to get maximal power but we want the energy expectation value of the particle after interaction with the hot bath to be fixed \( i.e. \text{tr} (\rho_i H) = \beta_h |E_h|^2 = \text{const} \), the efficiency at max power will be \( \eta_{E_h} \) (see (9)). Fixing the cold energy, yields (10). If the average energy is fixed, \( \frac{1}{2} \beta_c |E_c|^2 + \frac{1}{2} \beta_h |E_h|^2 = \text{const} \), the efficiency at max power is exactly \( \eta_{CA} (2) \). This shows that the CA efficiency can appear as a result of very different constrains (in (11) it followed from \( |E_c| |E_h| = \text{const} \)). Notice that the average energy constraint is not symmetric under \( |E_c| \leftrightarrow |E_h| \) if \( \beta_c \neq \beta_h \). From this we conclude that in contrast to the classical low-dissipation model, the CA result is not necessarily associated with hot-cold symmetry.

If we set the average von Neumann entropy (with ultra-hot approximation) \( S_{avg} = S_c + S_h = \frac{1}{2} \beta_c^2 |E_c|^2 + \frac{1}{2} \beta_h^2 |E_h|^2 = \text{const} \), the efficiency compared to the average energy case is
\[
\eta_{S_{avg}} = \frac{\eta_c}{2} + \frac{\eta^2_c}{8} + O(\eta^3_c),
\]
\[
\eta_{E_{avg}} = \frac{\eta_c}{2} + \frac{\eta^2_c}{8} + O(\eta^3_c).
\]

Different thermodynamic constrains lead to different maximal efficiency. In this example, the difference appears only in the third order. In the next section we derive an analytical expression for the third order as a function of the constraint equation. However for simplicity we write down the result only for the symmetric case.

**Next order for symmetric constraints.** – We start by using the \( F_2 = 0 \) condition from const = \( G = F_0 + F_1 \chi + \frac{1}{2} F_2 \chi^2 + O(\chi^3) \), and get for the symmetric case \( (G_{ij} = G_{ji}) \):
\[
\frac{d}{d \chi} |E_h| \left| \frac{\chi}{E_h} \right| = \frac{1}{2} + \frac{1}{4} \left[ 1 + |E_h| \left| \frac{(G_{11} - G_{20})}{G_{10}} \right| \right] \chi.
\]
The multiplier of the linear term is \( B \) and therefore:
\[
\eta_{\text{sym}} = \frac{1}{2} \eta_c + \frac{1}{8} \eta^2_c + \frac{1}{32} \left[ 1 + |E_h| \left| \frac{(G_{11} - G_{20})}{G_{10}} \right| \right] \eta^3_c + O(\eta^4_c).
\]

For example for the CA constraint \( |E_c| |E_h| = \text{const} \), \( G_{11} = 1, G_{20} = 0 \), \( G_{10} = |E_h| \) and indeed we get the correct factor \( \frac{1}{16} \eta^3_c \). As a second example, consider the efficiency \( \eta_{a=1/2} (12) \) obtained from the constraint \( |E_c| + |E_h| = \text{const} \). In this case \( G_{11} = G_{20} = 0 \) so the multiplier of the cubic term is 1/32 as can be verified from the exact expression for the efficiency. Using the same method a similar (yet considerably more cumbersome) formula can be written for the non-symmetric case.

**Colder engines with reflection symmetry.** – Surprisingly, the next order in \( \beta \) only adds the following leading-order terms to the work:
\[
\frac{\xi}{2 - \xi} \sum_{i=1}^{N} \frac{1}{2} \beta^2_c c_{c,i}^3 + \frac{1}{2} \beta^2_h c_{h,i}^3 - \frac{1}{2} \beta^2_c c_{c,i}^2 \eta_{E_h,i} - \frac{1}{2} \beta^2_h c_{h,i}^2 \eta_{E_c,i}.
\]
In principle, it complicates the optimization, however if the \( E_c, E_h \) are symmetric with respect to zero (reflection symmetry) then each term individually sums up to zero and all the results previously obtained still hold. In particular (29) is always zero for two-level systems and systems with evenly spaced spectrum. Notice that this reflection symmetry of the levels is completely unrelated to the hot-cold symmetry of the constraints discussed earlier.

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Conclusion. – We have studied internal optimization of hot quantum Otto engines. Universal features of the efficiency were identified. For some optimization constraints the efficiencies at maximal work are the same as the efficiency at maximum power in the low-dissipation limit. However, we find constraints for which the efficiencies deviate from the classical results. In the present case the optimization is with respect to the internal properties of the working fluid, while in the low-dissipation limit, power is optimized with respect to heat transport. It is interesting to see if similar universality appears in different engines (e.g. continuous engines) and in different operating regimes. In particular, it is intriguing to investigate if similar universality appears in faster engines where coherence is very important.

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