Optimization criteria, bounds, and efficiencies of heat engines

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The efficiency of four different and representative models of heat engines under maximum conditions for a figure of merit representing a compromise between useful energy and lost energy (the Ω criterion) is investigated and compared with previous results for the same models where the efficiency is considered at maximum power conditions. It is shown that the maximum Ω regime is more efficient and, additionally, that the resulting efficiencies present a similar behavior. For each performance regime we obtain explicit equations accounting for lower and upper bounds. The optimization of refrigeration devices is far from being as clear as heat engines, and some remarks on it are finally considered.

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It is well known that the universal validity of the maximum Carnot efficiency $\eta_c = 1 - T_c/T_h \equiv 1-\tau$ for any reversible heat engine operating between reservoirs at temperatures T_h and T_c ($T_h > T_c$) has little practical relevance since it applies to zero-power output heat devices. On the contrary, real heat engines work at nonzero power and evolve along irreversible paths coming from finite-time and finite-size unavoidable constraints. Thus, thermodynamic optimization plays a central role in order to find efficient heat engines operating at nonzero rates [1–3].

In a number of recent papers the subject of efficiency at maximum power, η_{mp}, in heat engines has been addressed for both cyclic and steady state models of stochastic (mesoscopic) or quantum (microscopic) systems [4–14]. From the paradigmatic Curzon-Ahlborn expression for the efficiency at maximum power [15], the universality of η_{mp} has been analyzed through its asymptotic behavior with the Carnot value η_c

$$\eta_{mp}^{CA} = 1 - \sqrt{\tau} \equiv 1 - \sqrt{1-\eta_c} \approx \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \frac{6\eta_c^3}{96} + \cdots. \quad (1)$$

The original Curzon-Ahlborn efficiency applies to a particular class of cyclic irreversible Carnot-like models where all irreversibilities are limited to (linear) finite-rate heat transfers between the working fluid and the external heat sources, so that internal dissipation of the working fluid and heat leaks between reservoirs are avoided (endoreversible model) [2,3].

In particular, we briefly mention three results. First is the one obtained by Schmiedl and Seifert [4] for a stochastic one-dimensional Brownian heat engine performing a Carnot-like cycle driven by a time-dependent harmonic potential. The power output is maximized with respect to the time interval spent by the system along the high- and low-temperature isothermal processes. At maximum power output the system efficiency is given by

$$\eta_{mp}^{SS} = \frac{2\eta_c}{4-\eta_c} \approx \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \frac{3\eta_c^3}{96} + \cdots. \quad (2)$$

Second is the work by Tu [5] for the Feynman ratchet and pawl model working under steady conditions optimized with respect to both the external load and the internal energy required to lift the pawl in absence of heat exchange between the thermal baths,

$$\eta_{mp}^{T} = \frac{\eta_c^2}{\eta_c - (1-\eta_c)\ln(1-\eta_c)} \approx \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \frac{7\eta_c^3}{96} + \cdots. \quad (3)$$

Third is the result by Esposito *et al.* [6] for a nanothermoelectric engine modeled as a single quantum level embedded between two leads at different temperatures and chemical potentials, working under steady conditions and optimized with respect to the scaled electron energy barriers. Using the perturbative method described in [6] we obtain the closed equation given by

$$\eta_{mp}^{ELB} = 1 - \frac{24(\eta_c - 1)[\cosh(a_0) - 1]\log(A+B)}{3a_0(\eta_c - 4)[\cosh(a_0) - 1] + 2\eta_c^2 \sinh(a_0)}, \quad (4)$$

where

$$A = \sqrt{\frac{\cosh\left[a_0 - \frac{a_0\eta_c}{4} - \frac{\eta_c^2}{6}\coth(a_0/2)\right] + 2\eta_c - 1}{2(\eta_c - 1)}},$$

$$B = \frac{\cosh\{\frac{1}{24}[3a_0(\eta_c - 4) + 2\eta_c^2 \coth(a_0/2)]\}}{\sqrt{1-\eta_c}},$$

and $a_0 = 2.399\,36$. This equation, not explicitly reported in Ref. [6], gives the series expansion [6]

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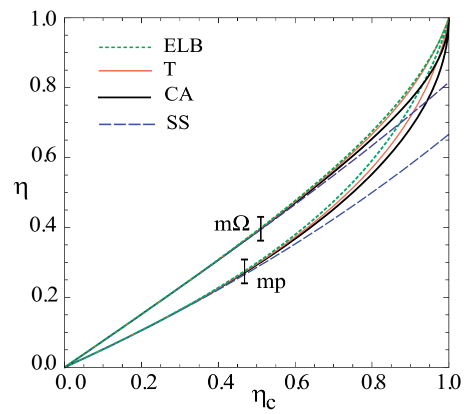

FIG. 1. (Color) Comparison between efficiency at maximum power (mp) and maximum Ω (mΩ) for the indicated models (see text) of heat engines as a function of the Carnot efficiency η_c.

$$\eta_{mp}^{ELB} \approx \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \frac{[7+\mathrm{csch}^2(a_0/2)]}{96}\eta_c^3 + \cdots. \tag{5}$$

The exact η_{mp} results in Eqs. (1)–(3) and (5) are plotted together in Fig. 1 where it is clearly seen that they coincide at small temperature differences, and deviations [below or above the Curzon-Ahlborn (CA) value] are appreciable for relatively large temperature differences.

The approximated results for η_{mp} in Eqs. (1)–(3) and (5) show that the coefficients of the linear and quadratic terms are identical for such systems, while the coefficient of the cubic term seems to be model dependent. Very recent results by Esposito *et al.* [7], using stochastic thermodynamics for a master equation description of a driven open system, have shown that universality of the coefficient 1/8 of the quadratic term is restricted to strong-coupling systems with a left-right symmetry condition (which is satisfied by the systems considered in [4–6]). The coefficient 1/2 of the linear term agrees with results for nonisothermal systems in linear irreversible thermodynamics with perfect coupling between fluxes and forces [9–11]. Its validity has been checked by molecular-dynamics simulations [12] and explicit theoretical calculations of the Onsager coefficients [8,13]. Interestingly, the coefficient 1/2 also appears for steady strong-coupling models used in linear irreversible thermodynamics to describe some biological isothermal energy converters when the coupling parameter tends to unity [16]. As noted, the coefficient 1/8 of the quadratic term depends on particular symmetry conditions.

The main goal in this paper is to show that the mentioned kind of universality is not exclusive of the maximum power regime. It is possible to find other performance regimes (or figures of merit) generating optimized efficiency with the same kind of universality which, additionally, behave as upper bounds. To illustrate our argument we focus on the analysis of the so-called Ω criterion, which represents a compromise between energy benefits and losses for a specific job; it is easy to implement in any energy converter (isothermal or nonisothermal) because it does not require the explicit evaluation of the entropy generation, and it is independent on environmental parameters. Particular details on this unified optimization criterion can be found in [17] and explicit applications for different heat devices models have been also reported: nonlinear systems rectifying thermal fluctuations [18], isothermal adiabatic rocking ratchets [19], harmonic quantum heat devices [20], and coupled Carnot-like heat devices in the context of linear irreversible thermodynamics [10,11]. Moreover, this criterion is also easy to implement in endoreversible refrigeration cycles [17].

Pertinent to our analysis here is that for heat engines the Ω criterion reads as

$$\Omega = (2\eta - \eta_{max})|\dot{W}|/\eta, \tag{6}$$

where $|\dot{W}|$ is the delivered power output and η_{max} is the maximum possible efficiency [17]. From this definition we have obtained the Ω function for the considered models of heat engines, calculated the conditions of maximum in terms of the natural independent variables of each problem, and then obtained the efficiency under maximum Ω conditions, which is denoted as $\eta_{m\Omega}$. For the endoreversible Curzon-Ahlborn model the efficiency at maximum Ω is given by [17] $\eta_{m\Omega}^{CA}=1-\sqrt{\frac{\tau(\tau+1)}{2}}$ (a result first obtained by Angulo-Brown [21] using the so-called ecological criterion), which can be expanded as

$$\eta_{m\Omega}^{CA} = 1 - \sqrt{\frac{(1-\eta_c)(2-\eta_c)}{2}} \approx \frac{3\eta_c}{4} + \frac{\eta_c^2}{32} + \frac{3\eta_c^3}{128} + \cdots. \tag{7}$$

For the stochastic heat engine cycle model of Schmiedl and Seifert [4] the algebra is straightforward although cumbersome, and the result is given by

$$\eta_{m\Omega}^{SS} = \frac{C+D}{E}, \tag{8}$$

where

$$C = 2(1-\eta_c)[\eta_c(3+\sqrt{4-2\eta_c}) - 2(2+\sqrt{4-2\eta_c})],$$

$$D = 8 + 4\sqrt{4-\eta_c} - \eta_c(2+\eta_c),$$

$$E = (2+\sqrt{4-\eta_c})[2(1-\eta_c) + (2+2\sqrt{4-2\eta_c}-\eta_c)],$$

which can be expanded as

$$\eta_{m\Omega}^{SS} \approx \frac{3\eta_c}{4} + \frac{\eta_c^2}{32} + \frac{\eta_c^3}{64} + \cdots. \tag{9}$$

For the Feynman ratchet and pawl model considered by Tu [5] the algebra is also straightforward, and we get

$$\eta_{m\Omega}^{T} = \frac{\eta_c(5\eta_c - 6)}{7\eta_c - 8} \approx \frac{3\eta_c}{4} + \frac{\eta_c^2}{32} + \frac{7\eta_c^3}{256} + \cdots. \tag{10}$$

For the nanothermoelectric engine model reported by Esposito *et al.*, we start with Eqs. (10) and (11) in [6] in order to derive the expression of Ω. Then we apply the condition $\partial_{x_l}\Omega = \partial_{x_r}\Omega = 0$ and following the same perturbative method as in [6], we obtain an identity at order zero, the transcendental equation $a_0 = 2\coth(a_0/2)$ at first order, the condition

$a_1 = -a_0/8$ at second order, and $a_2 = -\coth(a_0/2)/6$ at third order. The closed form for the efficiency at maximum Ω conditions is thus given by

$$\eta_{m\Omega}^{ELB} = 1 - \frac{48(\eta_c - 1)\ln\left(\frac{F+G}{2}\right)}{3a_0(\eta_c - 8) + 4\eta_c^2 \coth(a_0/2)}, \tag{11}$$

where

$$F = \sqrt{\frac{(\eta_c - 2)\cosh\left[a_0 - \frac{a_0\eta_c}{8} - \frac{\eta_c^2}{6}\coth(a_0/2)\right] - 3\eta_c + 2}{\eta_c - 1}},$$

$$G = \sqrt{2 - \frac{2}{\eta_c - 1}}\cosh\left[\frac{1}{48}[3a_0(\eta_c - 8) + 4\eta_c^2 \coth(a_0/2)]\right],$$

which can be expanded as

$$\eta_{m\Omega}^{ELB} = \frac{3\eta_c}{4} + \frac{\eta_c^2}{32} + \frac{19 + \mathrm{csch}^2(a_0/2)}{768}\eta_c^3 + \cdots. \tag{12}$$

It is clear from the approximated results for $\eta_{m\Omega}$ that they are coincident in the coefficients 3/4 and 1/32 of the linear and quadratic terms and model-dependent differences appears at third and higher terms. The 3/4 coefficient has been also reported in the context of the linear irreversible formalism for nonisothermal [10] and isothermal [16] heat engines in the limit of strong coupling when the efficiency is calculated under maximum ecological conditions.

The exact results of the optimized efficiencies $\eta_{m\Omega}$ are also plotted in Fig. 1, where their coincidence at small temperature differences can be observed while deviations (below or above the $\eta_{m\Omega}^{CA}$ value) become appreciable for relatively large temperature differences. By inspection of Fig. 1 it is obvious that the efficiencies under maximum of the Ω function behave as the efficiencies under maximum power for the same models, thus sharing the same kind of universality. Another clear consequence is that in each case the maximum Ω regime yields higher efficiencies, closer to the Carnot values. In fact, it is easy to check numerically that in all cases the exact results of the efficiency at maximum Ω can be approximated by the semisum of the Carnot value and the exact results of the efficiency at maximum power, $\eta_{m\Omega} \approx (\eta_{mp} + \eta_c)/2$ (semisum rule [16,21]), while for the approximated results the equality is strictly verified at first order in η_c.

One first question is in order here. Why so different models of heat engines working at small temperature differences show such a unified behavior when optimized under the same conditions? In this regard we first recall that the original endoreversible Curzon-Ahlborn model assumes a cyclic internally reversible working system where the irreversibilities are only due to the external coupling between (the noninstantaneous upper and lower isothermal paths of) the working system with the external hot and cold reservoirs through a *linear* Fourier heat transfer law, where the proportionality constants are the corresponding thermal conductances (σ_h, σ_c) [15]. Also, relevant in this model is that the maximum power efficiency is only dependent on the reservoir temperatures and thus independent on σ_h and σ_c. With this

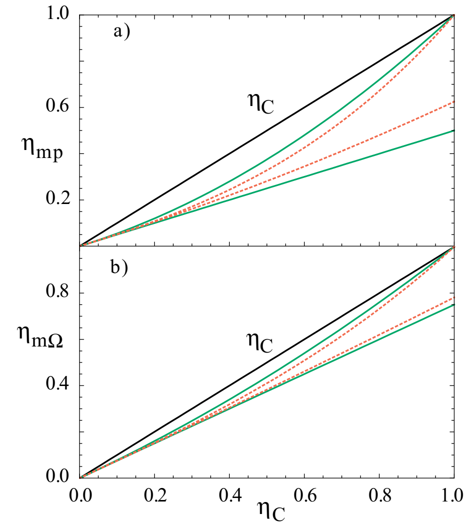

FIG. 2. (Color) (a) Upper and lower bounds for the efficiency at maximum power for systems with left-right symmetry conditions [Eq. (14), dotted red lines] and without symmetry conditions [Eq. (15), solid green lines]; (b) same as in (a) but for the maximum Ω efficiency [Eqs. (16) and (17)]. In both cases we show the universal Carnot value (black lines).

model in mind it is not easy to understand at all the calculated universality of efficiency at maximum power since strongly coupled models are nonlinear and, besides, results of the behavior of heat fluxes on temperature difference are not explicitly reported. In particular, in the work by Schmiedl and Seifert [4] the possibility of a linear thermal conduction gives rise to the existence of a time-dependent thermal conductivity which does not match the assumptions of the endoreversible Curzon-Ahlborn model. Sound and recent results by Esposito *et al.* [22] clarify the meaning of the observed universality for efficiency at maximum power. These authors considered a minimal and generic model of a Carnot-type heat engine where the heat (input and output) is assumed to be inversely proportional to the times during which the system is in contact with the (hot and cold) reservoirs, τ_h and τ_c, respectively. All irreversibilities (dissipations) are incorporated in the corresponding proportionality constants, which play the same role as the thermal conductances of the CA model. The key result is that efficiency at maximum power is exactly the CA value when these constant are equals. Then, the CA value of efficiency is recovered without invoking any specific law for heat transfer and considering the equality of the irreversibility constants as a symmetry condition playing the same role as the left-right symmetry of the fluxes in the strong-coupling systems. Thus, universality of efficiency at maximum power (up to second order) emerges as a general property linked to symmetric conditions. The same reason could explain the observed universality under maximum Ω conditions (up to second order), since behind the mathematics of Eq. (6), the Ω criterion just represents a compromise between useful energy and energy losses (dissipations) for a specific heat converter [17].

Another relevant question arises in relation to the possible existence of universal realistic upper and lower bounds for optimized efficiencies. In this regard some conclusions can be extracted from the above results for efficiencies at maximum power and maximum Ω. Let us consider the maximum power regime and its universal validity up to second order for systems with well-defined left-right symmetry conditions. Then we can write for this kind of systems

$$\eta_{mp}(\eta_c) = \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \sum_3^\infty a_n \eta_c^n. \tag{13}$$

Because of $\eta_{mp}(\eta_c) \le \eta_c$, this series should be convergent to a value of ≤ 1 for any value $\eta_c \le 1$. Then it verifies that $\frac{1}{2} + \frac{1}{8} + \Sigma_3^\infty a_n \le 1$ and $\Sigma_3^\infty a_n \le 1 - \frac{1}{2} - \frac{1}{8} = \frac{3}{8}$. Assuming positivity of all a_n coefficients, then it is easy to show that $\Sigma_3^\infty a_n \eta_c^n \le \frac{3}{8}\eta_c^3$. From this the following relation holds:

$$\frac{\eta_c}{2}\left(1 + \frac{\eta_c}{4}\right) \le \eta_{mp} \le \frac{\eta_c}{2}\left(1 + \frac{\eta_c}{4} + \frac{3\eta_c^2}{4}\right), \tag{14}$$

which accounts for the bounds of maximum power efficiency of systems with left-right symmetry. If such condition is not met, then only the coefficient 1/2 should be considered, and a similar proof shows that the inequality in Eq. (14) becomes

$$\frac{\eta_c}{2} \le \eta_{mp} \le \frac{\eta_c}{2}(1 + \eta_c). \tag{15}$$

The bounds defined in Eqs. (14) and (15) are plotted in Fig. 2(a), and it can be checked that all η_{mp} results considered in Eqs. (1)–(5) lie (as it should be) between the lower and upper bounds of Eq. (14). Also note the more restrictive character of the bounds for the systems with left-right symmetry conditions.

Indeed, for the maximum Ω regime we can proceed in a similar way starting with the expression $\eta_{m\Omega}(\eta_c) = (3\eta_c/4) + (\eta_c^2/32) + \Sigma_3^\infty b_n \eta_c^n$ and assuming positivity of the coefficients b_n $(n \ge 3)$ for the function $\eta_{m\Omega}(\eta_c) \le \eta_c$. In this case the obtained bounds are

$$\frac{3\eta_c}{4}\left(1 + \frac{\eta_c}{24}\right) \le \eta_{m\Omega} \le \frac{3\eta_c}{4}\left(1 + \frac{\eta_c}{24} + \frac{7\eta_c^2}{24}\right), \tag{16}$$

for the systems with left-right symmetry conditions, and

$$\frac{3\eta_c}{4} \le \eta_{m\Omega} \le \frac{3\eta_c}{4}\left(1 + \frac{\eta_c}{3}\right), \tag{17}$$

for the systems without left-right symmetry conditions. These bounds are plotted in Fig. 2(b), and we have checked that all above $\eta_{m\Omega}$ results lie between bounds imposed by Eq. (16).

The derivation of above bounds has been based on the positivity of all Taylor's series coefficients for the approximated $\eta_{mp}(\eta_c)$ and $\eta_{m\Omega}(\eta_c)$ expressions of the CA, SS, T, and ELB models of heat engines. We are not aware of any general mathematical proof from which the positivity of the coefficients $a_n = d^n \eta_{mp}(0)/d\eta_c$ and $b_n = d^n \eta_{m\Omega}(0)/d\eta_c$ $(n \ge 3)$ could be demonstrated for arbitrary functions $\eta_{mp}(\eta_c) \le \eta_c$ and $\eta_{m\Omega}(\eta_c) \le \eta_c$ with the sole conditions $\eta_c \le 1$ and $a_0 \equiv \eta_{mp}(0) = 0$, $a_1 = 1/2$, $a_2 = 1/8$, $b_0 \equiv \eta_{m\Omega}(0) = 0$, $b_1 = 3/4$, and $b_2 = 1/32$. Nevertheless, we think that the reported bounds contain explicit and valuable physical insights in the optimization of heat engines.

Up to now all results apply to heat devices working as heat engines. For inverse cycles the situation is less clear than for heat engines. First, it should be stressed that in the Carnot-like models of refrigerators with two noninstantaneous isotherms and two instantaneous adiabatics (i.e., the endoreversible refrigerator model), the power input is not an objective function to be optimized following the original Curzon-Ahlborn method. In other words, an optimization criterion based on the coefficient of performance (COP), ϵ, at minimum power input of endoreversible refrigerator models is not feasible [23–25]. So, a number of different optimization criteria have been proposed for this kind of models. Yan and Chen [23] reported an optimization study taking as the target function ϵQ_c, where Q_c is the cooling power of the refrigerator. The optimized COP they obtained depends only on τ and was independently reported by Velasco *et al.* [24] using a maximum per-unit-time COP and, very recently, by Allahverdyan *et al.* [25] from a quantum model with two n-level systems interacting via a pulsed external field in the classical limit and taking as the objective function ϵQ_c. Nevertheless, within linear irreversible thermodynamics formalism the analysis of a specific working regime gave [26] a different optimized coefficient of performance. It has been claimed that any of those optimized COPs could be considered as equivalent to the Curzon-Ahlborn efficiency for endoreversible refrigeration cycles [23–26]. This is hard to verify because, as noted before, in such refrigeration cycles the optimization of COP at minimum input power is not feasible. However, the Ω criterion is also easy to implement in an unified way in classical refrigeration systems [17] where the endoreversible limit is well defined [$\epsilon_{m\Omega} = \tau/(\sqrt{2-\tau}-\tau)$] and corroborated by results obtained in the classical limit of some quantum refrigeration cycles [20]. Quite surprising is also the situation with some other quantum cooling models where the protocol involving the minimum amount of work done on the system has been analyzed: a single-level quantum system interacting with a metallic thermal reservoir through a tunneling junction [27] and a Brownian particle in a heat bath [28]. In both cases it has been found that this protocol displays discontinuous jumps at the initial and final states of the cooling process.

In summary, additional work on optimization criteria for inverse cycles or steady systems working as refrigerators (or heat pumps) of stochastic and quantum systems could help one to find unified features of optimized coefficients of performance under appropriate figures of merit. Even more, perhaps a wide variety of energy converters, isothermal or not, could share some universal characteristics, independent of its nature or specific job. Along this line the Ω criterion or other figures of merit based on an appropriate compromise could guide future works on unified optimization criteria for any energy converter.

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