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EFFICIENCY, POWER AND PERIOD AT TWO OPTIMUM OPERATIONS OF A THERMOELECTRIC SINGLE LEVEL QUANTUM DOT

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Abstract

We take a single level quantum dot embedded between two metallic leads at different temperatures and chemical potentials which works as a heat engine. Two optimization criteria were used and their corresponding optimized efficiencies, powers and periods evaluated. Comparison between similar quantities of the two optimization criteria reveals mixed advantage and disadvantage. We quantify the engine's overall performance by suggesting a *figure of merit* that takes into account the contribution of each of the three quantities. Based on the proposed figure of merit, one of the optimization criterion presents a clear advantage. This same criterion is found to be invariably advantageous when applied to three other representative models.

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A heat engine attains a maximum possible value of Carnot efficiency when it operates under an extremely slow process. This corresponds to a quasistatic process taking infinite time to perform one cycle. Hence, power delivered by this quasistatic process is zero.

This theoretical limit is not of practical interest. In real life tasks need to be accomplished in a finite time. One practical interest is whether there is a maximum possible power attainable out of a heat engine. Such task need to be performed in a short enough time. However, performing a task in a short time wastes more energy making it less efficient.

The earliest study in finding efficiency at maximum power was done by Odum and Pinkerton in 1955 by taking an Atwood machine as a mechanical converter [1]. This was followed by the work of Curzon and Ahlborn twenty years later when they derived the efficiency of an endoreversible engine operating at maximum power (η_{CA}) to be [2]

$$\eta_{CA} = 1 - \sqrt{\frac{T_c}{T_h}}, \tag{1}$$

where T_c and T_h are the cold and hot temperatures of the reservoirs. Since then many model systems have been studied and their corresponding efficiencies at maximum power reported [[3]-[14]]. It is now becoming clear that there is some sort of universal value for the efficiency at maximum power similar to that of Carnot efficiency.

Is there a strategy by which these two opposing trends of attaining high (maximum) power on the one hand and high (maximum) efficiency on the other can be compromised to give an optimized value for efficiency? Several optimization methods have been proposed, but most of them lack generality and are only applicable to specific heat devices [15]. Among these methods, the two most often used for optimizing heat devices either require the evaluation of the entropy generation which may be difficult for systems far from equilibrium, or depend on the parameters of the environment which are usually difficult to determine.

About ten years back, Herǹandez et *al.* have come up with a unified optimization criterion (Ω criterion) to identify the point of operation of an engine where trade-off between energy cost and fast transport is compromised [16]. This optimization criterion presents the advantage of being independent of any environment parameter, and does not require the explicit evaluation of entropy generation. Moreover, results obtained from the application of this method on endoreversible Carnot-type engines agree with those obtained by applying ecological-like criteria which involve the explicit derivation of entropy generation [17]. For irrveresible heat engines it gives a performance regime lying between the maximum efficiency and the efficiency at maximum power, a regime that is considered as optimum for traditional heat engines [18]. In addition, an important feature of this method is its potential applicabilty to a large range of engine size starting from nano (molecular motors) up to macroscopic (traditional Carnot-type engines) devices as suggested in [16]. In a previous work, we have applied this optimization criterion to a simple model Brownian heat engine and found its optimized efficiency to lie between efficiency at maximum power, η_{mp}, and Carnot efficiency, η_c [19]. Recently, Sànchez-Salas et *al.* took four repersentative models of heat engines and investigated their optimized efficiencies and compared them with their corresponding efficiencies at maximum power [20]. They showed that the optimized efficiencies are not only larger than the efficiencies at maximum power but found them to have sort of universal behavior.

In addition to comparing the optimized efficiency with the efficiency at maximum power, one should be interested to know how much of the maximum available power is being utilized at this optimum condition. The other physical quantity of interest is the period at the optimum condition in comparison with the period at maximum power. In this work, we will take a particular system and apply the Ω criterion for two cases to determine not only their optimized efficiencies but also the powers and periods at the corresponding optimum conditions. This study will be followed by analysis and comparison of the determined quantities.

The particular system we consider is a nanothermoelectric engine consisting of a single quantum dot whose efficiency at maximum power has been explored by M. Esposito et *al.* [6]. The system is of interest as it addresses timely issues in several areas such as nanotechnology, thermodynamic properties of small systems away from equilibrium, quantum features and thermoelectric generating devices. Note that one of the four representative models investigated by Sánchez-Salas et *al.* is this same system [20]. The model consists of a quantum dot with a single resonant energy in contact with two thermal reservoirs at different temperatures and chemical potentials. The quantum dot can contain one single electron with a sharply defined energy ε. The exchange of electrons between the leads through the dot is described by a stochastic master equation and the corresponding thermodynamic properties such as heat flux and power are obtained from stochastic thermodynamics.

We next find expressions for optimized efficiencies (η_{opt}), optimized powers ($\dot{W}_{opt}$) and optimized periods (τ_{opt}) -defined as the inverse of the current from/to the dot- by applying optimization criteria for two cases and define a *figure of merit* to quantify how well the engine operates under any condition.

In order to implement the optimization criteria, we need to first define the function Ω. The function Ω makes use of two quantities that are the effective useful power $\dot{E}_{u,eff} = (\eta - \eta_{min})\dot{E}_{in}$ and lost useful power, $\dot{E}_{u,lost} = (\eta_{max} - \eta)\dot{E}_{in}$, where $\dot{E}_{in}$ is the input power. An engine operating in a finite time has its efficiency η lying between the maximum efficiency, η_{max} , and minimum efficiency, η_{min} i.e. $\eta_{min} \leq \eta \leq \eta_{max}$. An objective function, Ω, which is the difference between these quantities $(\dot{E}_{u,eff} - \dot{E}_{u,lost})$

$$\Omega = [2\eta - \eta_{min} - \eta_{max}]\dot{E}_{in}, \tag{2}$$

is defined and one searches for a point of operation at which Ω takes a maximum value with respect to natural independent variables of the system. One usually takes the minimum efficiency to be zero while the maximum efficiency to be the Carnot efficiency, η_c (hereafter referred to as case 1). In this case, one considers the physically allowed explorable range of control parameters of the system to search for the optimum. The objective function for case 1, $\Omega^{(1)}$, is then given by:

$$\Omega^{(1)} = [2\eta - \eta_c]\dot{E}_{in}, \tag{3}$$

The second optimization (hereafter referred to as case 2) takes the minimum efficiency to be the efficiency at maximum power, η_{mp}, while the maximum efficiency is again η_c. In this scenario, one considers a limited range of control parameters to be explored for optimization. The corresponding objective function, $\Omega^{(2)}$, is then

$$\Omega^{(2)} = [2\eta - \eta_{mp} - \eta_c]\dot{E}_{in}. \tag{4}$$

Using the corresponding expression for the input power $(\dot{E}_{in})$, efficiency (η), period (τ) and efficiency at maximum power (η_{mp}) from [6], we obtain the values of the three physical quantities η_{opt}, $\dot{W}_{opt}$ and τ_{opt} for the two optimization scenarios under consideration. As a starting point we find the power series expansion of optimized efficiency in the limit of small η_c for the first case of optimization, $\eta^{(1)}_{opt}$, which is given by

$$\eta^{(1)}_{opt} = \frac{3}{4}\eta_c + \frac{1}{32}\eta_c^2 + 0.0253116\eta_c^3 + \vartheta(\eta_c^4), \tag{5}$$

while for the second case of optimization, $\eta_{opt}^{(2)}$, is expressed as

$$\eta_{opt}^{(2)} = \frac{7}{8}\eta_c + \frac{31}{800}\eta_c^2 + 0.0225369\eta_c^3 + \vartheta(\eta_c^4). \quad (6)$$

The expression of the optimized efficiency for the first case (Eq.(5)) is identical to the one obtained by Sánchez-Salas et *al.* [20] for the particular model they studied, a model similar to ours. This is to be expected as we are using similar expression (Eq.(3)) for Ω criterion to evaluate $\eta_{opt}^{(1)}$.

In order to compare the three quantities of interest with their corresponding values at maximum power, we define three scaled quantities ϵ, ω and π such that $\epsilon = \frac{\eta_{opt}}{\eta_{mp}}$, $\omega = \frac{\dot{W}_{opt}}{\dot{W}_{mp}}$ and $\pi = \frac{\tau_{opt}}{\tau_{mp}}$. We are able to express these scaled quantities as series expansion in the limit of small η_c. Accordingly, for the first case of optimization they are given by

$$\epsilon^{(1)} = \frac{3}{2} - \frac{5}{16}\eta_c - 0.136304\eta_c^2 + \vartheta(\eta_c^3), \quad (7)$$

$$\omega^{(1)} = \frac{3}{4} + \frac{1}{8}\eta_c + 0.0638995\eta_c^2 + \vartheta(\eta_c^3), \quad (8)$$

and

$$\pi^{(1)} = 2 - \frac{1}{2}\eta_c - 0.214953\eta_c^2 + \vartheta(\eta_c^3), \quad (9)$$

while for the second case of optimization they are

$$\epsilon^{(2)} = \frac{7}{4} - \frac{9}{25}\eta_c - 0.136304\eta_c^2 + \vartheta(\eta_c^3), \quad (10)$$

$$\omega^{(2)} = \frac{7}{16} + \frac{3}{16}\eta_c + 0.145124\eta_c^2 + \vartheta(\eta_c^3), \quad (11)$$

and

$$\pi^{(2)} = 4 - \frac{1}{2}\eta_c - 0.197\eta_c^2 + \vartheta(\eta_c^3). \quad (12)$$

On the other hand, we can evaluate these scaled quantities numerically for all ranges of possible values of η_c from the optimization relations. Note that the numerical values of the scaled quantities determined from the optimization relations for the case when $\eta_c \to 0$ coincides with the corresponding values found from Eqs. (6) to (11).

Figure 1 shows plots of both $\epsilon^{(1)}$, $\epsilon^{(2)}$ versus the full range of η_c. Both quantities monotonically decrease approaching the same final value of one as η_c goes to a maximum value of unity. The graph clearly indicates that efficiency-wise the second optimization has larger value than the first optimization over the whole range of η_c. However, while this advantage is significant for smaller η_c it shrinks to the same value as η_c goes to unity.

Figure 2 compares how much of the maximum available power is being utilized by the two optimization criteria. The plot of $\omega^{(1)}$ versus η_c clearly shows that the first optimization criterion utilizes a minimum of 75% of the available maximum power at small values of η_c and performs even better (up to 100%) as η_c goes to one. On the other hand, the plot of $\omega^{(2)}$ versus η_c shows that the second optimization criterion utilizes less than half of the maximum available power over the major (75%) range of η_c only doing better (up to $\sim$ 65%) for η_c close to one.

Figure 3 shows plots of $\pi^{(1)}$ and $\pi^{(2)}$ versus η_c. Under the first optimization criterion, the engine performs its task in a cycle twice that of the period at maximum power in the limit of small η_c and its cycle monotonically decreases to that of one period at maximum power as η_c goes to one. On the other hand, the second optimization takes between two and a quarter to four times that of the period at maximum power over the whole range of η_c. Note that completing a task in shorter period must be advantageous.

Efficiency-wise the engine *performs better* under the second optimization criterion than when subject to the first criterion (Fig. 1). On the other hand, under the first criterion the engine *performs better* both power-wise and period-wise than when under the second optimization criterion (Figs. 2 and 3). In order to decide which optimization criterion presents the best trade-off, we introduce a *figure of merit* that makes use of the three quantities. The *figure of merit* (f_m) that we suggest is, thus, defined by

$$f_m = \frac{\epsilon\omega}{\pi}. \tag{13}$$

Note that the particular optimization criterion which presents a larger value of f_m has an overall advantage over the other optimization criterion.

Figure 4 depicts the figures of merit, $f_m^{(1)}$ and $f_m^{(2)}$, versus η_c for the two optimization criteria. Comparing the plots one clearly sees that the first optimization has a better advantage over the second for the whole range of η_c. In fact the figure of merit of the first optimization is larger by about three fold than the f_m of the second optimization over all range of η_c.

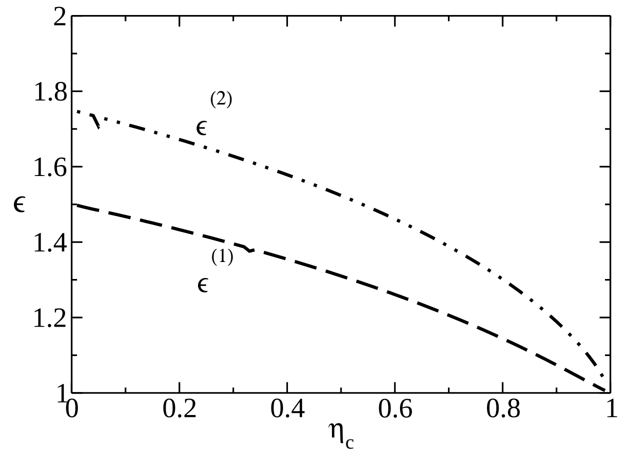

FIG. 1. Plots of the ratio of optimized efficicency to the efficiency at maximum power for the two optimization criteria versus η_c.

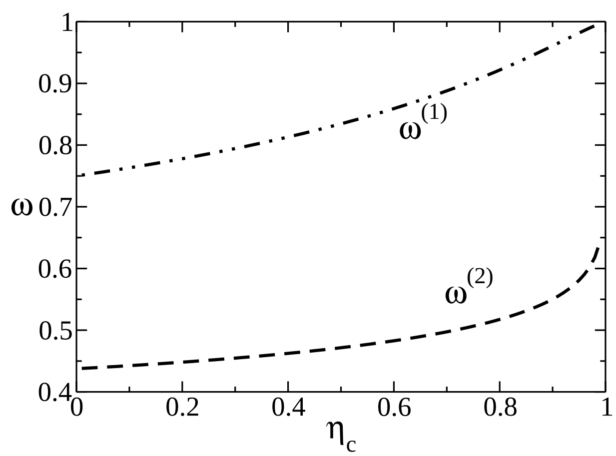

FIG. 2. Plots of the ratio of optimized power to the maximum power for the two cases of optimization criteria versus η_c.

One wonders whether comparison between the two figures of merit for other models of heat engines exhibits similar features to the one depicted in Fig. 4. In order to find out if there is any general feature, we took three other representative models: (i) stochastic heat engine cycle of Schmiedl and Seifert (SS) [3], (ii) Feynman ratchet and pawl model considered by Tu (T) [4] and (iii) Brownian heat engine model of Asfaw and Bekele (AB) [19] and evaluated their corresponding figures of merit over that whole range of η_c. Fig. 5 shows plots of these quantities versus η_c. While the figures of merit for the models of T and

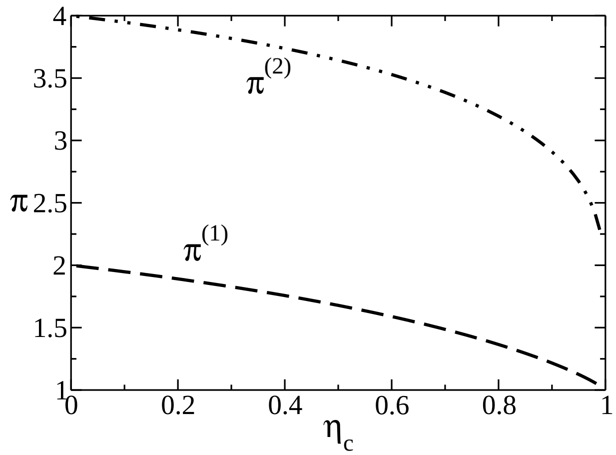

FIG. 3. Plots of the ratio of optimized period to the period at maximum power for the two cases of optimization criteria versus η_c.

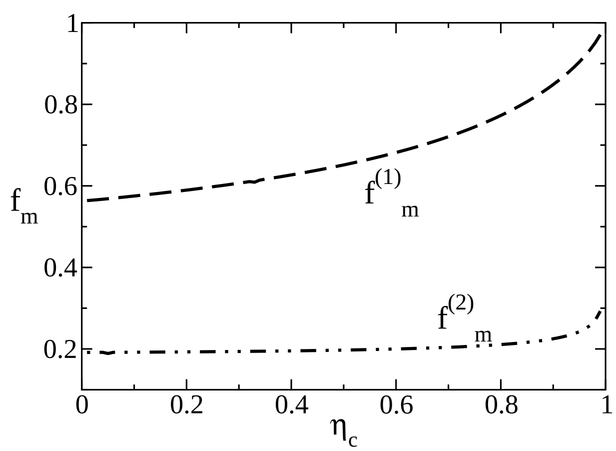

FIG. 4. Figures of merit f_m for the two cases of optimization ctiteria versus η_c.

SS show monotonically increasing functions with increase in η_c similar to that of Fig. 4, AB's model has weak nonmonotonic nature with change in η_c. However, the figure of merit corresponding to the first optimization is about *three times* as large as that of the f_m of the second optimization for *all* the models we considered.

The consistent advantage of the first optimization over the second expressed in terms of f_m can be understood as follows: an optimization carried out by tuning the parameters of the system over a wide range of allowed values is better than a one made using a smaller range. Obviously, the range of possible values of η is directly related to the ranges of accessible values of systems parameters. These simple observations explain why the first optimization is systematically better regardless of the model under consideration. We further suggest that the above might be true for all energy converters. Seen this way, the figure of merit seems to be an appropriate and universal quantifier of the performance of heat engines.

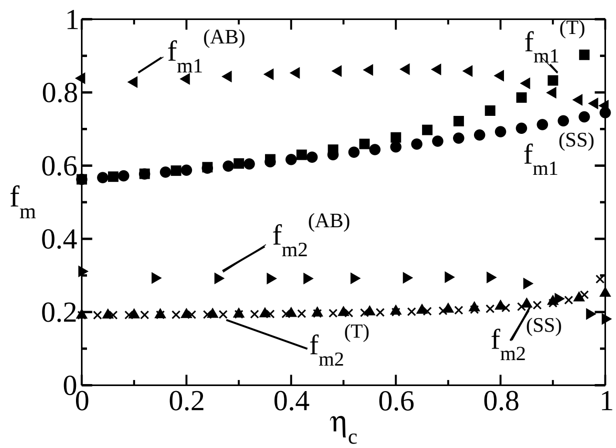

FIG. 5. Plots of figures of merit $f_m^{(1)}$ and $f_m^{(2)}$ for the three model heat engines (SS[3], T[4], AB[19]).

In summary, we have explored the performance (efficiency-wise, power-wise and period-wise) of a thermoelectric engine by applying two optimization criteria. By defining a figure of merit that takes account the contributions of these quantities we have found that the first optimization criterion has a clear advantage over the second not only for the thermoelectric engine but also for three other representative models we considered. Our study, then, suggests that the first optimization criterion might have a universal advantage over the second by about three fold for all heat engines. Lastly, it would be interesting to test the universality of our result for other engines such as molecular motors and chemical engines.

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