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Universality of efficiency at unified trade-off optimization

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We calculate the efficiency at the unified trade-off optimization criterion (the so-called maximum Ω criterion) representing a compromise between the useful energy and the lost energy of heat engines operating between two reservoirs at different temperatures and chemical potentials, and demonstrate that the linear coefficient 3/4 and quadratic coefficient 1/32 of the efficiency at maximum Ω are universal for heat engines under strong coupling and symmetry conditions. It is further proved that the conclusions obtained here also apply to the ecological optimization criterion.

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I. INTRODUCTION

It is well known that the Carnot efficiency $\eta_C = 1 - T_c/T_h$ determines the upper bound of the efficiency for any heat engine operating between two reservoirs at temperatures T_h and T_c ($T_c < T_h$). However, the Carnot efficiency is too high to be practical for real heat engines [1,2]. Additional practical, meaningful work is to find useful optimization criteria to describe the performance of real heat engines. One method widely used in determining such criteria is to determine the efficiency at maximum power (EMP) originating from the work of Curzon and Ahlborn [3]. Curzon and Ahlborn proposed an endoreversible model of the Carnot cycle and found that the EMP is given by the Curzon-Ahlborn (CA) efficiency [4,5] $\eta_{\mathrm{CA}} = 1 - \sqrt{T_c/T_h}$. Since then, various theoretical models have been established for both cyclic [6–11] and steady state [12–16] heat engines, ranging from mesoscopic (stochastic) heat engines [12–14,17,18] to microscopic (quantum) heat engines [15,19–21]. Tu [12] investigated Feynman's ratchet as a heat engine and obtained an analytic expression for its EMP. Later, the same result was derived by Van den Broeck *et al.* [13] for the EMP in a simple model of classical particle transport. Schmiedl and Seifert [15] calculated the EMP for a large class of one-dimensional stochastic Brownian heat engines performing a Carnot-like cycle driven by a time-dependent harmonic potential. Recently, Esposito *et al.* [16] evaluated the EMP of a nanothermoelectric engine consisting of a single quantum level embedded between two reservoirs at different temperatures and chemical potentials and gave the expansion of the EMP in the regime of small η_C. Interestingly, it is found that the EMPs of many models agree with η_{CA} up to quadratic order in η_C, i.e., $\eta_{mP} = \eta_C/2 + \eta_C^2/8 + o(\eta_C^3)$. In the region of linear response, it was proven that the EMP is exactly equal to half of the Carnot efficiency for the strong coupling condition [22]. In the nonlinear region, Esposito *et al.* [23] constructed a general model of heat engines and verified that the EMP is indeed universal up to quadratic order in η_C for the strong coupling system in the presence of a symmetry condition. Subsequently, Uzdin and Kosloff [24] studied hot quantum Otto engines and identified the universal features in the efficiency at the maximum work output. Sheng and Tu [18] applied the generic nonlinear constitutive relation and finite-time thermodynamics to obtain the universality of the EMP for tight-coupling heat engines. Cleuren *et al.* [25] investigated the EMP in a general setting for energy conversion machines and demonstrated how symmetries and constraints at the microscopic level, combined with the fluctuation theorem, emerge at the macroscopic level via the expression for the EMP.

Besides maximum efficiency and power criteria, a unified trade-off optimization criterion (the so-called Ω criterion) for energy converters has been proposed by Hernández *et al.* [26]. The Ω criterion is defined as a compromise between the useful energy and the lost energy of heat engines, i.e. [27],

$$\Omega = \frac{(2\eta - \eta_{\max})P}{\eta}, \tag{1}$$

where η and P are the efficiency and power output of a heat engine, respectively, and $\eta_{\max}$ is the maximum efficiency. For the endoreversible Curzon-Ahlborn model of heat engines, the efficiency at the maximum Ω criterion was given by [27]

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

This result was first derived by Angulo-Brown by applying the so-called ecological optimization criterion [28]. An important feature of the maximum Ω criterion is that it gives an optimized efficiency lying between the maximum efficiency and the EMP, i.e., $\eta_{\mathrm{CA}} \leqslant \eta_{m\Omega}^{\mathrm{CA}} \leqslant \eta_C$. Angulo-Brown *et al.* [29,30] first discussed the possibility of thermodynamic optimization in some biochemical reactions by means of finite-time thermodynamics, and gave some optimization criteria for biological systems in linear irreversible thermodynamics. Recently, some explicit applications for different heat engines, such as classical heat engines [31], stochastic Brownian heat engines [27], Feynman ratchet heat engines [27], quantum dot heat engines [27], low-dissipation heat engines [32], and minimally nonlinear irreversible heat engines [33], and others [34–37], have been reported. These works display a common feature for the efficiency at the maximum Ω criterion up to quadratic order in η_C, i.e., $\eta_{m\Omega} = 3\eta_C/4 + \eta_C^2/32 + o(\eta_C^3)$. Thus, the relevant questions in relation to the universality of efficiency at unified trade-off optimization arise again. Is the efficiency at the maximum Ω criterion of a general nature? What conditions can achieve universal efficiency at the maximum Ω criterion? In this paper, we will solve these problems and further discuss the

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unified trade-off optimization [26] and ecological optimization criteria [28].

II. MODEL AND THEORY

We consider a system exchanging energy and particles with two reservoirs ν $(= h,c)$ with chemical potentials μ_ν and temperatures T_ν, respectively. The states of the system with energy ε_i and number of particles n_i are denoted i. The occupation probability of finding the system in state i is denoted $p_i(t)$. The time evolution of the occupation probability $p_i(t)$ is described by the master equation [38,39]

$$\dot{p}_i(t) = \sum_j [\Gamma_{ij} p_j(t) - \Gamma_{ji} p_i(t)], \tag{3}$$

where the first term on the right-hand side is the rate of gain in state i due to transitions from other states j, the second term is the rate of loss from state i due to transitions to other states j, and Γ_{ij} is the transition rate from state j to state i. Since transitions between the system states are triggered by the reservoirs, the transition rates are expressed as the sums of independent contributions from the two reservoirs, i.e., $\Gamma_{ij} = \sum_\nu \Gamma_{ij}^\nu$. The average matter currents J_M^ν and energy currents J_E^ν entering the system from the reservoir ν are given by

$$J_M^\nu(t) = \sum_{i,j} \Gamma_{ij}^\nu p_j(t)(n_i - n_j) \tag{4}$$

and

$$J_E^\nu(t) = \sum_{i,j} \Gamma_{ij}^\nu p_j(t)(\varepsilon_i - \varepsilon_j). \tag{5}$$

Thus, the average heat flows from the reservoir ν into the system are given by

$$\dot{Q}_\nu(t) = J_E^\nu(t) - \mu_\nu J_M^\nu(t). \tag{6}$$

From now on we will focus on nonequilibrium steady state situations, with particular focus on the situation of the device operating as a heat engine in which a heat flow from a hot to a cold reservoir is used to drive particles uphill from low to high chemical potential. For this purpose, a simple analysis can be done assuming that $T_h > T_c$ and $\mu_h < \mu_c$. Regarding the matter of current conservation at steady state, the absence of an accumulation of particles inside the system implies that $J_M^h = -J_M^c \equiv J_M$ is obvious, while for energy current conservation, $J_E^h = -J_E^c \equiv J_E$ is a consequence of the time-independent steady state solution p_i of the master equation, (3). The average power output of the heat engine, being the amount of the net chemical energy produced, is given by

$$P = (\mu_c - \mu_h) J_M. \tag{7}$$

The efficiency, defined as the ratio of the power output P to the heat flow $\dot{Q}_h$ extracted from the hot reservoir, is given by

$$\eta = \frac{P}{\dot{Q}_h} = \frac{\mu_c - \mu_h}{J_E/J_M - \mu_h}. \tag{8}$$

According to nonequilibrium thermodynamics, the entropy production rate can be written in the traditional bilinear force-flux form as [40,41]

$$\dot{S} = -\frac{\dot{Q}_c}{T_c} - \frac{\dot{Q}_h}{T_h} = J_M X_M + J_E X_E, \tag{9}$$

where $X_M = \mu_h/T_h - \mu_c/T_c$ and $X_E = 1/T_c - 1/T_h$ are the standard expressions for the thermodynamic forces.

In the case of strong coupling between the energy current and the matter current, this condition implies that energy is exclusively transported by particles of a given energy ε and defined as [23]

$$J_E = \varepsilon J_M \equiv \varepsilon J. \tag{10}$$

Equation (9) can be further simplified as

$$\dot{S} = JX. \tag{11}$$

Hence, the two fluxes and forces in Eq. (9) collapse into a single flux J and a single corresponding thermodynamic force X, respectively [23]. The thermodynamic force $X = x_c - x_h$ can be expressed in terms of two parameters, $x_c = (\varepsilon - \mu_c)/T_c$ and $x_h = (\varepsilon - \mu_h)/T_h$. Thus, Eqs. (7) and (8) can be rewritten as

$$P = (T_h x_h - T_c x_c)J = T_h(\eta_C x_c - X)J \tag{12}$$

and

$$\eta = 1 - (1 - \eta_C)\frac{x_c}{x_h} = 1 - (1 - \eta_C)\frac{x_c}{x_c - X}. \tag{13}$$

According to the theory of irreversible thermodynamics, Eq. (9) shows that for the case of the equilibrium state, $\dot{S} = 0$ and $J_M X_M + J_E X_E = 0$. In such a case, there only exist two situations. (i) The thermodynamic fluxes and forces J_M, X_M, J_E, and X_E are not equal to zero simultaneously, the thermodynamic forces X_M and X_E may balance each other, and, consequently, $X = 0$ [42]. (ii) The thermodynamic fluxes and forces J_M, X_M, J_E, and X_E are equal to zero simultaneously so that $X = 0$. Equation (11) shows that when $X = 0$, $J = 0$. When the system is near the equilibrium state, the thermodynamic flow J may be expanded into a Taylor series with respect to the thermodynamic force X as

$$J = LX + MX^2 + o(X^3), \tag{14}$$

where $L = -J_1'(x_c,x_c)$ and $M = J''_{11}(x_c,x_c)/2$ are the expansion coefficients [23] and subscripts 1 and 11 represent the first- and second-order partial derivatives with respect to the first independent variable.

III. MAXIMUM Ω OPTIMIZATION

In the present paper, $\eta_{\max} = \eta_C$. By using Eqs. (12) and (13), Eq. (1) can be expressed as

$$\Omega = \frac{(2\eta - \eta_C)P}{\eta} = T_h[\eta_C x_c - (2 - \eta_C)X]J. \tag{15}$$

Using Eq. (15) and its extremal conditions, we have

$$\frac{\partial \Omega}{\partial X} = T_h\left\{-(2 - \eta_C)J + [\eta_C x_c - (2 - \eta_C)X]\frac{\partial J}{\partial X}\right\} = 0 \tag{16}$$

and

$$\frac{\partial \Omega}{\partial x_c} = T_h\left\{\eta_C J + [\eta_C x_c - (2 - \eta_C)X]\frac{\partial J}{\partial x_c}\right\} = 0. \tag{17}$$

When η_C goes to zero, X has to be equal to zero, and, consequently, the thermodynamic force can be expanded as

$$X = a\eta_C + b\eta_C^2 + o(\eta_C^3), \tag{18}$$

where a and b are two expansion coefficients to be determined. Substituting Eqs. (14) and (18) into Eq. (16), we obtain

$$(x_c - 4a)L\eta_C + (2aL - 4bL - 6a^2M + 2aMx_c)\eta_C^2 + o(\eta_C^3) = 0. \tag{19}$$

It can be found from Eq. (19) that

$$a = \frac{x_c}{4} \tag{20}$$

and

$$b = \frac{4Lx_c + M{x_c}^2}{32L}. \tag{21}$$

Next, substituting Eqs. (14) and (18) into Eq. (17), we obtain

$$a\left(L + x_c\frac{\partial L}{\partial x_c} - 2a\frac{\partial L}{\partial x_c}\right)\eta_C^2 + o(\eta_C^3) = 0. \tag{22}$$

From Eqs. (20) and (22), it is found that

$$x_c = -\frac{2L}{\partial L/\partial x_c}. \tag{23}$$

Substituting Eqs. (18), (20), (21), and (23) into Eq. (13) yields the efficiency at the maximum Ω criterion valid up to quadratic order in η_C, i.e.,

$$\eta_{m\Omega} = \frac{3}{4}\eta_C + \left(\frac{1}{16} + \frac{M}{16\,\partial L/\partial x_c}\right)\eta_C^2 + o(\eta_C^3). \tag{24}$$

In the symmetry condition, the switching of temperatures and chemical potentials leads to inversion of the flux [23], i.e., $J(x_c,x_h) = -J(x_h,x_c)$, from which we have $J_{12}''(x_c,x_c) = 0$. Using the relation $\partial L/\partial x_c = -J_{11}''(x_c,x_c) - J_{12}''(x_c,x_c)$, we obtain $2M = -\partial L/\partial x_c$, and, consequently, Eq. (24) is simplified as [27,31–33]

$$\eta_{m\Omega} = \frac{3}{4}\eta_C + \frac{1}{32}\eta_C^2 + o(\eta_C^3). \tag{25}$$

Equation (25) shows clearly that the linear coefficient 3/4 holds universally for heat engines with the strong coupling condition (Appendix) and the quadratic coefficient 1/32 is also universal for strong coupling heat engines with the symmetry condition.

IV. DISCUSSION

For the so-called ecological criterion [28,43–45], which represents the best compromise between the power output and the product of entropy production and the cold reservoir temperature of heat engines, i.e., $E = P - T_c\dot{S}$, where $T_c\dot{S}$ is called "loss power" (the environment temperature is equal to the cold temperature). In two reservoir systems, the total entropy production is given by $\dot{S} = \dot{Q}_c/T_c - \dot{Q}_h/T_h$ and $\dot{Q}_h = P + \dot{Q}_c$. The ecological function E can be further rewritten as

$$\begin{aligned} E &= P - T_c\dot{S} = P - \dot{Q}_c + \frac{T_c}{T_h}\dot{Q}_h \\ &= 2P - \eta_C\dot{Q}_h = \frac{(2\eta - \eta_C)P}{\eta} = \Omega. \end{aligned} \tag{26}$$

Equation (26) clearly shows that the objective function E is identical to Ω, i.e., the two criteria of unified trade-off optimization and ecological optimization are equivalent to each other, and, consequently, the efficiency at maximum ecological optimization [28,43] is also given by Eq. (25).

V. CONCLUSIONS

We have investigated the efficiency of nonequilibrium heat engines based on the master equation model of heat engines, and verified that the efficiency at the maximum Ω criterion exhibits universality up to quadratic order in the deviation from equilibrium for the strong coupling system in the presence of a symmetry condition. This condition is in agreement with that of the universal efficiency at maximum power. It has been proved the Ω criterion is equivalent to the ecological optimization criterion. Thus, the conclusions obtained from the maximum Ω criterion also apply to the ecological optimization. The results obtained here are meaningful for the optimal design and manufacture of bio- and nano-heat engines in experiments and actual applications in the future.

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APPENDIX: UNIVERSALITY OF EFFICIENCY AT MAXIMUM Ω CRITERION IN LINEAR-RESPONSE REGION

Within the linear-response region of $T_h \approx T_c$, Eq. (9) can be rewritten as

$$\begin{aligned} \dot{S} &\approx J_M X_M + J_E X_E - \mu_h J_M\left(\frac{1}{T_c} - \frac{1}{T_h}\right) \\ &= J_M X_M + \dot{Q}_h X_E \equiv J_M X_M + J_Q X_E, \end{aligned} \tag{A1}$$

Where $J_Q = \dot{Q}_h$. The power output and the efficiency can be given by $P = -J_M X_M T_c$ and $\eta = P/\dot{Q}_h = P/J_Q$, respectively. According to the linear irreversible thermodynamics, the relationship between the thermodynamic fluxes J_M and J_Q and the thermodynamic forces X_M and X_E can be expressed as [40,41]

$$\begin{aligned} J_M &= L_{11}X_M + L_{12}X_E, \\ J_Q &= L_{21}X_M + L_{22}X_E, \end{aligned} \tag{A2}$$

where L_{ij} are the Onsager coefficients with the symmetry relation $L_{12} = L_{21}$. The entropy production rate $\dot{S} \geqslant 0$ leads to the restriction on the Onsager coefficients $L_{11} \geqslant 0, L_{22} \geqslant 0$, and $L_{11}L_{22} - L_{12}^2 \geqslant 0$. Equation (1) can be expressed as

$$\Omega = \frac{(2\eta - \eta_C)P}{\eta} = -2L_{11}T_cX_M^2 - 3L_{12}\eta_C X_M - L_{22}\eta_C X_E. \tag{A3}$$

Using the extremal condition $(\partial\Omega/\partial X_M)_{X_E} = 0$ and Eq. (A3), one can find that when

$$X_{M\Omega} = -\frac{3L_{12}\eta_C}{4L_{11}T_c}, \tag{A4}$$

the efficiency at maximum Ω is given by

$$\eta_{m\Omega} = \frac{3}{4}\eta_C \frac{q^2}{4 - 3q^2}, \tag{A5}$$

where $q = L_{12}/\sqrt{L_{11}L_{22}}$ is the dimensionless coupling strength and obeys $-1 \leqslant q \leqslant 1$ [22]. Equation (A5) was first derived by applying the so-called ecological optimization criterion [46]. For strongly coupled systems, $|q| = 1$ and the efficiency is exactly 3/4 of the Carnot efficiency.

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