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Quantum heat engines: A thermodynamic analysis of power and efficiency

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Abstract – We show that the operation and the output power of a quantum heat engine that converts incoherent thermal energy into coherent cavity photons can be optimized by manipulating quantum coherences. The gain or loss in the efficiency at maximum power depends on the details of the output power optimization. Quantum effects tend to enhance the output power and the efficiency as the photon occupation in the cavity is decreased.

Nano devices, such as solar cells, lasers, and photosynthesis cells, where quantum coherence is involved in their operation, are known as quantum heat engines (QHE). Quantum effects in such systems can reveal themselves in many curious ways, defying our common sense. Lasing without population inversion [1], extracting work from a single thermal bath [2], electromagnetically induced transparency [3,4], enhancing the power [5] and the thermodynamic efficiency [6] of QHE have been demonstrated by the proper manipulation of quantum coherences. Linden *et al.* [7] have recently analyzed fundamental limits on the size of quantum refrigerators that can achieve absolute zero temperature.

One of the most interesting properties of a heat engine is its efficiency, defined as the ratio of the work performed to the absorbed heat. The thermodynamic efficiency of QHEs have been extensively studied [8–11]. The maximum efficiency of a classical heat engine is given by Carnot's efficiency ($\eta_c = 1 - T_c/T_h$). This is reached when the work is done in an adiabatic manner (quasi-equilibrium) where the corresponding power is zero. This renders a Carnot engine impractical. There is a great interest in studying the efficiency of heat engines under real working conditions. In the first study of a QHE, Scovil and Schulz-DuBois have shown that the bound holds for a three-level atom in contact with two thermal reservoirs [12]. In a recent experiment [13], it has been demonstrated that the incoherent energy of crystal phonons can enhance the output power (photons) of light-emitting diodes beyond the consumed electrical power, enhancing the performance of the diode.

Heat engines can be characterized by maximizing their power output with respect to controllable set of parameters and then studying their efficiency. Based on some simple assumptions, Curzon and Ahlborn have obtained an efficiency at maximum power (EMP) of $\eta = 1 - \sqrt{T_c/T_h}$ for an analogue of Carnot's engine [14].

Recently there has been a renewed interest in the behavior of small systems driven away from equilibrium. An extensive research effort is aimed at studying the efficiency at maximum output of small thermodynamic machines. This is motivated in part by the possible universality for systems driven by a small temperature differnece [8,15,16]. It is therefore of interest to investigate how quantum effects may influence the efficiency at maximum output of QHEs [17–21].

In this letter we show how coherences can be tuned to manipulate the power and the efficiency of a QHE. We show that power and EMP can be enhanced simultaneously by careful adjustment of quantum coherences. Conditions under which quantum effects can lead to an enhancement of the output power are derived. We find that lowering the photon occupation in the cavity mode increases the quantum effects which leads to a higher percentage gain in the output power and EMP.

Our QHE model is a set of four levels coupled through two thermal baths and a cavity mode (see fig. 1). The

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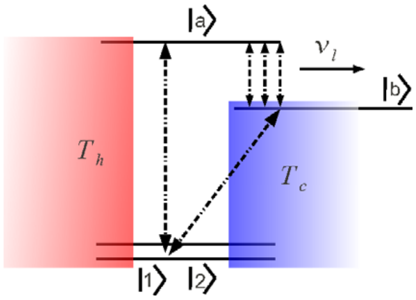

Fig. 1: (Color online) Level scheme of the model quantum heat engine. A pair of degenerate levels $|1\rangle, |2\rangle$ is resonantly coupled to two excited levels $|a\rangle$ and $|b\rangle$ by two thermally populated field modes with hot (T_h) and cold (T_c) temperatures. Levels $|a\rangle$ and $|b\rangle$ are coupled through a non-thermal (cavity) mode of frequency ν_l. Emission of photons into this mode is the work done by the QHE.

generated power can be manipulated by controlling the coherences between states $|1\rangle$ and $|2\rangle$ [5]. The QHE is described by the Hamiltonian

$$\hat{H}_0 = \sum_{\nu=1,2,a,b} E_\nu \hat{B}_{\nu\nu} + \sum_k \epsilon_k \hat{a}_k^\dagger \hat{a}_k + \epsilon_l \hat{a}_l^\dagger \hat{a}_l, \quad (1)$$

where the three terms correspond to the multilevel system, heat baths and the cavity mode, respectively. $\hat{B}_{\nu\nu'} = |\nu\rangle\langle\nu'|$ represents the excitation operator between states $|\nu\rangle$ and $|\nu'\rangle$, $\hat{a}^\dagger(\hat{a})$ denotes creation (annihilation) operators for harmonic modes in thermal baths and in the electromagnetic field. The coupling between the various components is described by

$$\hat{H} = \sum_{k,i=1,2} \sum_{X=a,b} g_{ik} \hat{a}_k \hat{B}_{iX}^\dagger + \text{h.c.}, \quad (2)$$

where index k sums over the modes in hot (if $X = a$) and cold (if $X = b$) baths.

Finally, the coupling of states $|a\rangle$ and $|b\rangle$ via the cavity mode is

$$\hat{V} = g(\hat{a}_l^\dagger \hat{B}_{ba} + \hat{B}_{ba}^\dagger \hat{a}_l), \quad (3)$$

where g is a real number that represents coupling strength between the system and the radiation field in the cavity.

Stimulated emission into a single laser cavity mode is the useful work done by the QHE: converting thermal energy to coherent photons. The QHE can operate as a heat engine, converting incoherent photon energy of the hot thermal bath into coherent photons in the cavity mode by stimulated emission. The rest of the heat is rejected to the cold bath. The engine can also operate in reverse as a refrigerator: transfer heat from the cold to the hot bath by absorbing energy from the coherent cavity mode.

Relaxation caused by coupling to the two thermal reservoirs will be described by the Lindblad equations. These rate-like equations for the reduced system density matrix $\rho(t)$ are obtained by a second-order expansion in the couplings, H and V, combined with the standard approximations and assuming that the two states $|1\rangle$ and $|2\rangle$ are degenerate. For further details see [22] and [5].

The time evolution of the system energy is $\dot{E} = \text{Tr}\{H_s \dot{\rho}(t)\}$, where H_s is the system Hamiltonian (the first term on the LHS of (1)), and $\dot{A} = \frac{\mathrm{d}A}{\mathrm{d}t}$. Using the first law of thermodynamics, we can separate the energy change into work (W) and heat, $\dot{E}(t) = \dot{W}(t) + \dot{Q}_h + \dot{Q}_c$, where $\dot{W}$ is the power (P) and $\dot{Q}_c$ and $\dot{Q}_h$ are the heat currents between the system and the hot and the cold baths, respectively. The efficiency is defined as

$$\eta = -\frac{P}{\dot{Q}_h}. \quad (4)$$

Note that at steady state, $\dot{E} = 0$ and the efficiency can be expressed as $\eta = 1 + (1 - \eta_c)\dot{S}_c/\dot{S}_h$, where $\dot{S}_c(\dot{S}_h)$ is the (reversible) entropy current between the cold (hot) bath and the system [23].

To simplify the analysis, we focus on the case when all the couplings to the hot and cold baths are the same and the coupling to the cavity mode is large [5]. We believe that the results reported here should apply for arbitrary couplings to the baths and the cavity. At steady state the power of the QHE is

$$P = P_0 \frac{f_1}{1 - f_2}, \quad (5)$$

where

$$f_1 = \frac{(\mathrm{e}^{x_c} - 1)[1 - r^2 + \frac{\Gamma}{\gamma}(\mathrm{e}^{x_c + x_l}\mathrm{e}^{-\mathcal{F}} - 1)]}{\mathrm{e}^{x_c} + \mathrm{e}^{x_c + x_l}\mathrm{e}^{-\mathcal{F}} + \frac{\Gamma}{\gamma}(\mathrm{e}^{x_c} - 1)(\mathrm{e}^{x_c + x_l}\mathrm{e}^{-\mathcal{F}} - 1) - 2},$$

$$f_2 = \frac{\mathcal{D}(r)[\mathrm{e}^{x_l + x_c}\mathrm{e}^{-\mathcal{F}} + r(\mathrm{e}^{x_c} - 1) - 1]}{\mathcal{D}[\mathrm{e}^{x_l + x_c}\mathrm{e}^{-\mathcal{F}} + \mathrm{e}^{x_c} + \frac{\Gamma}{\gamma}(\mathrm{e}^{x_c} - 1)(\mathrm{e}^{x_l + x_c}\mathrm{e}^{-\mathcal{F}} - 1) - 2]}, \quad (6)$$

where $\mathcal{D}(r) = r(\mathrm{e}^{x_c} - 1)[1 + \mathrm{e}^{x_l} + 2\mathrm{e}^{x_l + x_c}\mathrm{e}^{-\mathcal{F}}] + (\mathrm{e}^{x_l + x_c}\mathrm{e}^{-\mathcal{F}} - 1)(1 + \mathrm{e}^{x_l} + 2\mathrm{e}^{x_l + x_c})$ and $\mathcal{D} = \mathcal{D}(r = 1)$. Here γ represents the coupling strength between the bath and the system states, Γ is the phenomenological parameter that accounts for induced dephasing due to the environment [5], and $r(= \gamma_{12}/\gamma)$ is the ratio of cross-couplings that induce coherences between states $|1\rangle$ and $|2\rangle$ due to the interaction between the system and the hot bath (γ_{12}) and the cold bath (γ). Thus, coherences induced by the coupling to the cold bath are maximal while $\gamma_{12} \leqslant \gamma$ is arbitrary (see [22] for further details). Note that the parameter $0 \leqslant r \leqslant 1$. $x_h = \beta_h(E_a - E_1)$, $x_c = \beta_c(E_b - E_1)$, and $x_l = \beta_l(E_a - E_b)$, where $\beta_a = 1/(k_B T_a)$ (here we have defined an "effective" temperature β_l for the cavity). $\mathcal{F} = x_l + x_c - x_h$ represents the thermodynamic force that drives the system out of equilibrium. P_0 is the power without coherences,

$$P_0 = \frac{2\gamma(E_a - E_b)(1 - \mathrm{e}^{-\mathcal{F}})}{(\mathrm{e}^{x_l} + 1)[\mathrm{e}^{-\mathcal{F}}(1 + 2\mathrm{e}^{x_c}) - 2\mathrm{e}^{-x_l - x_c}] - 1 - 2\mathrm{e}^{-\mathcal{F}} + \mathrm{e}^{-x_l}}. \quad (7)$$

Note that as $r \to 1$, all the couplings (including the cross-couplings) have the same value, and the power is $P = P_0$, *i.e.*, coherence effects vanish. This is due to the fact that in this case the system becomes symmetric with respect to the degenerate levels $|1\rangle$ and $|2\rangle$ and there is no way to tell them apart. As far as dynamics is concerned, the two lower states effectively become a single state, and hence coherence is irrelevant. Another point to note is that in (5), the limit $\Gamma \to 0$ first and then $r \to 1$, is not physical, which gives $P_0 = 0$. The proper limit is first to set $r \to 1$ and then $\Gamma \to 0$, which gives $P = P_0$. From eq. (5), setting $P = P_0$ gives two values of r. $r = 1$ is trivial as discussed above, while the nontrivial value $r = r_s$ is

$$r_s = \frac{1 + e^{x_l} + 2e^{x_l + x_c - \mathcal{F}}}{1 + e^{x_l} + 2e^{x_l + x_c}}. \tag{8}$$

It is obvious that $r_s \to 1$ as $\mathcal{F} \to 0$. Thus, there are two values of r ($r = 1$ and $r = r_s$) for which the QHE power is unaffected by coherences. For intermediate values of r, the power must show a maximum or a minimum. We find that there is an optimal value (r^*) of r which maximizes the power:

$$r^* = 1 + \frac{\Gamma f_3}{2\gamma}\left[1 - \sqrt{1 + \frac{4\gamma}{\Gamma f_3}\frac{e^{x_c}(1 - e^{-\mathcal{F}})}{1 + e^{-x_l} + 2e^{x_c}}}\right], \tag{9}$$

where

$$f_3 = \frac{(e^{x_l + x_c}e^{-\mathcal{F}} - 1)(1 + e^{-x_l} + 2e^{x_c})}{1 + e^{-x_l} + e^{x_c}(1 + e^{-\mathcal{F}})}. \tag{10}$$

The power is enhanced by the coherences for $r_s \leqslant r \leqslant 1$, reaching a maximum at r^*. For $r < r_s$, it is reduced by the quantum effects. It can be shown (see [22]) that r^* increases as the photon occupation in the cavity mode is increased (x_l decreases), reaching a saturation value

$$r^* = 1 + X\left(1 - \sqrt{1 + \frac{1 - e^{-\mathcal{F}}}{X(1 + e^{-x_c})}}\right), \tag{11}$$

where $X = \Gamma f_3/(2\gamma) \geqslant 0$. The maximum percentage enhancement in the power output is given by $\lim_{r \to r^*}[f_1/(1 - f_2)]$. This gain decreases as x_l is decreases (see [22]). Thus, we conclude that quantum effects become more significant as the occupation in the cavity mode is decreased.

In fig. 2, we show the variation in power with r for several values of the cavity mode occupation [$n_l = (e^{x_l} - 1)^{-1}$]. The vertical solid lines are the optimal values of r, while values of r_s are indicated by the dashed vertical lines. The horizontal dotted lines depict the power in the absence of coherences.

We now turn to the efficiency. At steady state, the power and the heat currents $\dot{Q}_c$ and $\dot{Q}_h$ are proportional, and we can write $P/(E_a - E_b) = \dot{Q}_c/(E_b - E_1) = \dot{Q}_h/(E_a - E_1) = I$. The efficiency (4) then becomes independent of r and is given by

$$\eta = \frac{E_a - E_b}{E_a - E_1}. \tag{12}$$

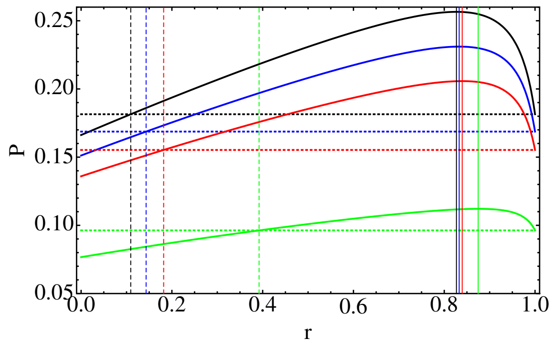

Fig. 2: (Color online) The QHE power (solid curves) *vs.* r for $n_l = 0.01, 0.05, 0.1$, and 0.5 from top to bottom. The horizontal dotted lines represent corresponding power without coherences. The vertical solid lines indicate the optimal values of r, eq. (9), while the dashed vertical lines indicate values for r_s, eq. (8). Here $\gamma = 0.5$, $\Gamma = 0.01$, $T_h = 1.0$, $T_c = 0.2$, $g = 100$, $E_a = 1.5$, $E_b = 0.4$, and $E_1 = 0.1$.

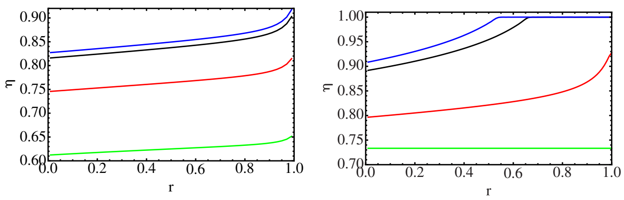

Fig. 3: (Color online) The QHE efficiency at maximum power over a range of r. The four curves are for $n_l = 0.001, 0.01, 0.1, 1$ (top to bottom). Other parameters, except E_b, are the same as in fig. 2. Left (right) panel: when power is maximized with respect to E_b (E_1).

We are interested in efficiency at maximum power. From eq. (12) it is clear that the variation of r considered earlier does not affect the efficiency. We therefore optimized the power with respect to E_a, E_b or E_1 to see how the EMP depends on system parameters. (The value of the energy level, say E_b, that maximize the power output will typically depend on r.) The various cases are discussed separately below. Note that changing E_b or E_a will affect x_l, but we can always modify β_l to keep x_l constant, that is, the photon occupation in the cavity mode is held fixed. Other system parameters are also kept fixed. When $r \to 1$ and the cavity occupation is large $x_l \approx 0$, our model reduces to a simple three level QHE system studied in ref. [8].

To calculate the efficiency in the presence of coherences $r \neq 1$, we numerically computed the optimal values of E_a, E_b and E_1 that correspond to the maximum output power. Substituting this in (12) gives the efficiency at maximum power. We first maximize the power with respect to E_b at fixed $E_a = 1.5$ and $E_1 = 0.1$. This is displayed in left panel of fig. 3 over a range of r values. The EMP is monotonically decreased as r is decreased. Since $r = 1$ corresponds to the classical result (coherences are zero), we find that the effect of coherence is to actually reduce the EMP. We next

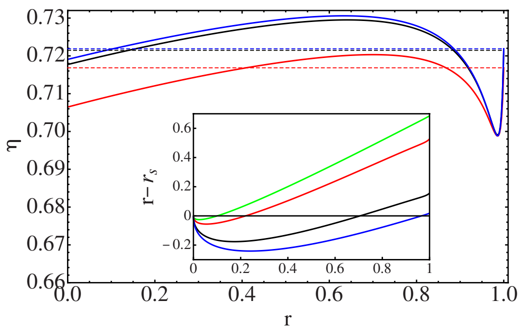

Fig. 4: (Color online) The QHE efficiency at maximum power (EMP) over a range of r for $n_l = 0.001$, 0.01, 0.1, 1 (top to bottom). The power maximization is done with respect to E_a. Other parameters, except E_a, are the same as in fig. 2. Inset: the difference $r - r_s$ as function of r computed for the optimal values of E_a corresponding to efficiencies shown in the main figure. Over the range of r for which $r - r_s > 0$, and η is above the classical result (above dotted lines in the main figure), both the power and the efficiency are enhanced beyond the classical result.

performed the power optimization with respect to E_1 at fixed $E_a = 1.5$ and $E_b = 0.4$. We look for optimal values of E_1 in the range $0 < E_1 < E_b$. We find that for large values of n_l, there is no optimal value of E_1. For small values of n_l, the optimal value of E_1 increases with r and approaches to E_b. Thus, EMP increases with increasing r and approaches to unity (since optimal value of $E_1 \to E_b$). This is shown in the right panel in fig. 3. In the flat region seen for $n_l = 0.001$ and $n_l = 0.01$, the maximum output is found at the boundary of the domain, $E_1 = E_b$. In this region our model loses its physical interpretation because i) the small energy separation between E_1 and E_b conflicts with several assumptions and ii) the field modes belonging to different reservoirs inducing QHE transitions can no longer interact predominantly with a specific reservoir. There is no value of r which enhances the EMP beyond the classical value $r = 1$.

We next optimized the power with respect to E_a, holding $E_b = 0.4$ and $E_1 = 0.1$ fixed. The change in the efficiency with r is plotted in fig. 4. The dashed horizontal lines represent EMP without coherences. In this case, for small values of the occupation in the cavity mode ($n_l < 1$), there is an optimal value of r at which the efficiency is more than the classical value ($r = 1$). Thus, in optimizing the power with respect to E_a, quantum effects can enhance the efficiency beyond the classical value for small values of n_l. The range of r for which the efficiency can be enhanced beyond the classical value, increases with decreasing n_l. In order to find the relative values of the power with respect to the classical result, we compute the values of $r - r_s$ for the same values of E_a which maximizes the power. This is shown in the inset. Recall that for $r - r_s > 0$, the power is enhanced by coherences. Thus, as for the maximum output power, the range of r decreases as the photon occupation in the single cavity mode is decreased. Note that it is different than the result in fig. 2 where we maximize the power with respect to r without having any effect on the efficiency (12). We can therefore enhance both the power and the efficiency simultaneously over a range of r where $r > r_s$ and the EMP is above the classical result.

Thus, for small photon occupation number in the cavity mode, it is possible to enhance the EMP beyond the classical value ($r = 1$) by adjusting the coherences. This however depends on the optimization parameters. Since the optimal value of E_1 and E_b increases as the coherence is increased, the power optimization with respect to these parameters lead to suppression in the efficiency as compared to the classical value for all values of the coherence. On the other hand, when power is optimized with respect to E_a, quantum effects can work in our favor and enhance the EMP. However for large occupation of the cavity mode $n_l \gg 1$, the EMP is always less than the classical value, irrespective of the optimization parameter. This effect is similar to the results reported for the output power in fig. 2, where power output and the coherence effects increase with lowering the cavity population.

In conclusion, we have demonstrated that quantum effects in heat engine operating at maximum power strongly affect the output power and the corresponding efficiency. The relative strength (r) of the induced coherences due to thermal baths determines the strength of the quantum effects, which become increasingly important as the photon occupation in the cavity mode is decreased. By tuning the relative coherences, the output power can be enhanced significantly if $r_s \leqslant r \leqslant 1$. For $r \leqslant r_s$, the quantum effects reduce the output power. We derived a simple expression for r_s and the optimal value, r^*, of the relative coherences that maximizes the output power. The steady-state efficiency given by (12) is in general independent of the quantum effects (r). However, the efficiency at maximum power is strongly influenced by coherences which may lead to an enhancement or to reduction in the EMP, depending on how the power is optimized.

It is the optimization of the output power that brings in the dependence on the coherences. We showed that in order to enhance EMP beyond the classical value, we must optimize the power with respect to E_a, the energy of the highest energy state. The power and the efficiency both can be enhanced beyond classical result. Finally, we emphasize that in order to improve the power output and the EMP, the photon occupation in the cavity mode must be kept at low values ($n_l < 1$). The simultaneous optimization of both the power and the efficiency beyond the classical value is possible, however the range of values of photon occupation in the cavity mode must be adjusted carefully.

* * *

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