Adaptive Quantum Heat Engines

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For heat engines working between two heat baths, functionality is often conditioned on a set of fixed constraints such as given internal structure of the engine and given temperatures for the baths. It is, however, important to devise heat engines which can function adaptively, in particular when the engine is a quantum system and the baths are subject to fluctuations. Here we study a model for an adaptive quantum heat engine whose heat baths can have variable temperatures. We obtain conditions under which such an engine can still operate. Moreover, we propose an enhancement of the heat engine by coupling it with an appropriate controller which changes the internal structure of the engine. Interestingly, we prove that this enhanced engine can always operate and we also obtain conditions for maximum power extraction from this engine for all temperatures of the heat baths.

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\textbf{Introduction}.—Since the inception of thermodynamics, heat engines (machines operating between two reservoirs with different temperatures and converting heat to work) have been a cornerstone concept [1]. Recently with the renewed interest in thermodynamics in quantum regimes [2–5], investigation of quantum heat engines has also been reinvigorated [6–23], e.g., operation of autonomous heat engines has been extensively analyzed [20–27].

A heat engine optimal or close-to-optimal for some given conditions may not necessarily function optimally when its ambient conditions change. For example, in realistic heat engines temperatures of heat baths may have inevitable fluctuations. Thus, it may be important so see whether heat engines can adapt themselves with such variations and continue to function under new conditions [28, 29]. This issue will be more important for small-scale heat engines working in quantum regimes. Here we propose an adaptive quantum heat engine which can extract energy with maximum power on the work source, at different temperatures of its baths.

\textbf{Model}.—We consider a minimal model for a quantum heat engine, a three-level quantum system which interacts with two heat baths [6, 10, 11, 13–18, 20]. The Hamiltonian of the system is $H_0 = \sum_{i=1}^{3} e_i |i\rangle \langle i|$, where $e_i$s are the energies and $\{|i\rangle\}$ are energy eigenstates. Transitions between the energy levels $i$ and $j$ are induced by exchanging energy with a thermal bath of temperature $T_{ij}$, mediated by an appropriate frequency filter passing only $\omega_{ij} = e_j - e_i$ [6] (assuming $\hbar \equiv 1$ hereafter)—Fig. 1. The thermal baths with finite temperatures $T_{23}$ and $T_{13}$ are considered as the cold and hot reservoirs (depending which temperature is higher or lower). However, the temperature of the thermal bath $T_{12}$ is assumed to be infinity, which renders it effectively as a work source [13].

We assume that the dynamics is Markovian and described by the local Lindblad master equation (disregarding the Lamb shift) [30, 31]

$$\dot{\rho}_S = -i[H_0, \rho_S] + \sum_{j>i=1}^{3} L_{ij} [\rho_S],$$

where dot denotes time derivative, $\rho_S$ is the state of the system, and $L_{ij}$ is the local Lindbladian term caused by interaction with the thermal bath $ij$ (typically assumed a bath of quantized radiation fields) given by [30]

$$L_{ij} [\rho] = \gamma_{ij} [S_{ij} \rho S_{ij}^\dagger - \frac{1}{2} \{ S_{ij}^\dagger S_{ij}, \rho \}] + \gamma_{ji} [S_{ij}^\dagger \rho S_{ij} - \frac{1}{2} \{ S_{ij} S_{ij}^\dagger, \rho \}],$$

where $S_{ij} = |i\rangle \langle j|$ are jump operators with rates

$$\gamma_{ij} = \begin{cases} \gamma_0 |\omega_{ij}|^3 \beta_{ij} |\omega_{ij}|^3 (e^{\beta_{ij} |\omega_{ij}|} - 1)^{-1}, & j > i \\ \gamma_0 |\omega_{ij}|^3 (e^{\beta_{ij} |\omega_{ij}|} - 1)^{-1}, & i > j \end{cases}$$

and $\beta_{ij} = 1/(k_B T_{ij})$ and $\gamma_0 > 0$. The average energy $U(t) = \text{Tr}[H_0 \rho_S(t)]$ changes in time as

$$U(t) = J_{12}(t) + J_{13}(t) + J_{23}(t),$$

where the average rate of energy exchange $J_{ij}(t)$ $(i, j \in \{12, 23, 13\})$ between the system and each thermal bath is

$$J_{ij}(t) = \langle \dot{e}_i \rangle \gamma_{ij} \gamma_{i-j} = \gamma_{ij} \gamma_{i-j}.$$
The heat engine operates if $J_{12} < 0$, hence as long as $\theta \equiv T_{32}/T_{13}$ satisfies
\[
-\hat{e}_2 [(1 - \theta) \hat{e}_3 - \hat{e}_2] < 0, \quad (8)
\]
the engine can adapt itself with the change in the temperatures of the heat baths.

If the temperatures vary such that the adaptability condition does not hold, one remedy can be to change the energy levels $e_i$ appropriately. This can be achieved by coupling a controller to the system, whose effect is to modify the system energy levels depending on its degree of freedom. We assume that the controller $C$ is a quantum Brownian particle of mass $m$ with $(x, p)$ position-momentum degrees of freedom and potential $(1/2)kx^2$, coupled to another thermal bath of temperature $T$, which is described by the Caldeira-Leggett model [30, 32]. The dynamics of the state of the controller $\rho_C(t)$ is given by $\dot{\rho}_C = -i[H_C, \rho_C] + \mathcal{L}_{CL}[\rho_C]$, where $H_C = (1/2m)p^2 + (1/2)kx^2$ is the Hamiltonian of the controller and $\mathcal{L}_{CL}[\rho] = -i\hat{\xi}[\rho, \{p, o\}] - 2m\hat{\xi}T[x, \{x, o\}]$, with $\hat{\xi}$ being the friction coefficient and $\{A, B\} = AB + BA$. The stationary state probability density of the controller is given by $p_C(x) = \sqrt{\kappa/(2\pi T)}e^{-\kappa x^2/(2T)}$. Let us introduce
\[
x^* \equiv \text{argmax } p_C(x), \quad (9)
\]
as the most probable position of the controller in the stationary state. We consider the system-controller interaction as [33]
\[
H_{SC} = \sum_{i=1}^3 g_i |i\rangle\langle i| \otimes x, \quad (10)
\]
where the controller is coupled to the levels $|i\rangle$ with different couplings $g_i$. Hence the state of the system-controller in the weak-coupling, Markovian regime is given by
\[
\dot{\rho}_{SC} = -i[H_0 + H_C + H_{SC}, \rho_{SC}] + (\mathcal{L}_{CL} + \sum_{j>i} \mathcal{L}_{ij})[\rho_{SC}], \quad (11)
\]
The controller affects the energy levels of the system and hence its functioning as the heat engine. In order to find the stationary state of the controller and $x^*$, one should use Eq. (11). To obtain the engine’s power associated with the position of the controller, we need to find the conditional state $\hat{\rho}_{S|C} = \text{Tr}_C[\rho_{S|C}]$, which obeys the master equation
\[
\dot{\hat{\rho}}_{S|C} = -i[H(x), \hat{\rho}_{S|C}] + \sum_{j>i} \mathcal{L}_{ij}[\hat{\rho}_{S|C}], \quad (12)
\]
where [16]
\[
H(x) = \sum_i e_i |i\rangle\langle i| = \sum_i (e_i + g_i x)|i\rangle\langle i| \quad (13)
\]
and $\mathcal{L}_{ij}$ has the form as in Eq. (2) with $S_{ij|k} = S_{ij}$ and $\gamma_{i\rightarrow j} \rightarrow \gamma_{i\rightarrow j}(x)$ as in Eq. (3) with the difference that now $\omega_{ij} \rightarrow \omega_{ij}(x) \equiv e_j(x) - e_i(x)$. The stationary solution of Eq. (12) yields populations as in Eq. (5) where all $\gamma_{ab} \rightarrow \gamma_{ab}(x)$. Thus, from Eq. (6) the conditional power is obtained as
\[
J_{12|\bar{x}} = \hat{e}_2(x) j(x), \quad (14)
\]
and similarly $J_{13|\bar{x}} = -\hat{e}_3(x) j(x)$ and $J_{23|\bar{x}} = [\hat{e}_3(x) - \hat{e}_2(x)] j(x)$, where $\hat{e}_i(x) \equiv e_i(x) - e_1(x)$. In this scenario, the adaptation condition $J_{12|\bar{x}} < 0$ yields
\[
-\hat{e}_2(x) [(1 - \theta) \hat{e}_3 - \hat{e}_2] < 0, \quad \bar{x} \approx x^* \quad (15)
\]
which means that the most probable position of the controller should be where the heat engine can perform work on the work source. For later use, here we introduce a position $\bar{x}$ where
\[
\bar{x} \equiv \text{argmax } |J_{12|\bar{x}}|, \quad (16)
\]
at which the extracted power from the engine in optimal. It is ideal to have $\bar{x} = x^*$. Satisfying Eq. (15) reduces to making the quadratic form $y(x) \equiv ax^2 + bx + c$ negative, where $a = (\theta - 1)\hat{e}_2\hat{g}_3 + \hat{g}_2\hat{e}_3$, $b = (\theta - 1)(\hat{e}_2\hat{g}_3 + \hat{g}_2\hat{e}_3) + 2\hat{g}_2\hat{e}_2$, $c =$
\[(\theta - 1)\hat{e}_3\hat{e}_2 + \hat{e}_2^2, \text{ and } \hat{g}_t = g_t - g_1. \text{ Note that the discriminant of } y(x) \text{ is always nonnegative,}\]

\[\left((1 - \theta)(\hat{e}_2\hat{g}_3 - \hat{g}_2\hat{e}_3)\right)^2 \geq 0. \quad (17)\]

Depending on \(x^*\), the sign of \(y(x^*)\) can be positive (unacceptable) or negative (acceptable). However, it is interesting that according to Eq. (17), and provided that \(\hat{e}_2\hat{g}_3 \neq \hat{e}_3\hat{g}_2\), at all temperature of the hot and cold baths, one can always find acceptable ranges for \(x\). In other words, in contrast to the case of classical heat engines [28], by attaching a controller to a quantum heat engine we can always make it adaptive.

We can also calculate the efficiency of the heat engine as

\[\eta(x) = \frac{-J_{12}^{(x)}}{\max\{J_{23}^{(x)}, J_{13}^{(x)}\}} \leq \eta_{\text{Carnot}} = 1 - \min\{\theta, 1/\theta\}, \quad (18)\]

depending on whether \(T_{13} > T_{23}\) or \(T_{23} > T_{13}\). The efficiency is upper bounded by the Carnot efficiency \(\eta_{\text{Carnot}}\), and when the heat engine reaches its maximum efficiency, according to Eq. (15) its power goes to zero—so that it respects the trade-off between power and efficiency [1]. From Fig. 2 (a) it is seen that the power vanishes at two points \(x_0 = -55.5 \text{ [nm]}\) and \(x_1 = -42.1 \text{ [nm]}\), and that in the region \((x_0, x_1)\) the heat engine can perform work on its environment. Note that \(\eta(x_0) = 0\) and \(\eta(x_1) = 1 - \theta = \eta_{\text{Carnot}}\). This can be explained by noting that when the controller is at \(x_0\), we have degeneracy and the energy levels \([1] \text{ and } [2]\) coincide \(\hat{e}_2(x_0) = 0\), hence no work can be extracted from the heat engine, whereby the power and the efficiency both vanish. However, at \(x_1\) the three levels are degenerate \(\hat{e}_2(x_1) = \hat{e}_3(x_1) = 0\), which implies that in the vicinity of that position the power and the heat absorbed from the hot bath approach 0 such that \(\eta(x_1) \rightarrow \eta_{\text{Carnot}}\).

If \(y(x^*) > 0\), the system cannot operate as a heat engine. Thus, we need to move the controller to the acceptable region of \(x\) as given by Eq. (15). This can be achieved by assuming that the controller is a charged particle with charge \(q\) and applying an appropriate electric field \(E'\) on it. In this case, the position of the controller is obtained from \(\hat{\phi} = -i[H_C + H_{CF} + \mathcal{L}_C][\hat{q}_C]\), where \(H_{CF} = \mathcal{E}X\) with \(E \equiv qE'\). This yields that the stationary probability density of the position of the controller is modified to

\[p_C(x) = \langle e^{-iE'/2(xT)} \mathcal{E}X/kT \rangle e^{-E(x + \kappa x^2)/2T}. \quad (19)\]

Under the potential \(H_{CF}\) the dynamical equation (11) changes to

\[\dot{\phi}_{SC} = -i[H_0 + H_C + H_{SC} + H_{CF}, \hat{q}_SC] + \mathcal{L}_C[\hat{q}_SC] + \sum_{j > i} \mathcal{L}_{ij}[\hat{q}_SC], \quad (19)\]

from which one can see that the same conditional master equation (12) and power (14) are obtained; hence the profile of the conditional power does not change by the electric field.

By attaching a programmed learner to the engine, we can simply make its adaptation autonomous and autorn (at the price of energy needed to keep the learner operating). Before applying the electric filed, the learner calculates the position \(\tilde{x}\) and compares it with \(x^*\); then it turns on a proper electric field on the charged controller to enforce \(x^* = \tilde{x}\)—Fig. 2. This way the engine can operate adaptively and with maximum power at different temperatures of its baths—Fig. 1.

Summary and conclusions.—Here we have investigated an adaptive model for a quantum heat engine whose baths may
have nonconstant temperatures. The pivotal ingredient of the model is coupling it with a charged quantum Brownian controller whose position can always be chosen such that the engine can perform work on its environment. We have shown that this adaptation can be performed in an autorun fashion with the assistance of a programmed learner which forces the controller to move to a position at which the engine can operate with maximum power.

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