Universal efficiency at optimal work with Bayesian statistics

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If the work per cycle of a quantum heat engine is averaged over an appropriate prior distribution for an external parameter \(a\), the work becomes optimal at Curzon-Ahlborn efficiency. More general priors of the form \(\Pi(a) \propto 1/a^\gamma\) yield optimal work at an efficiency which stays close to CA value, in particular near equilibrium the efficiency scales as one-half of the Carnot value. This feature is analogous to the one recently observed in literature for certain models of finite-time thermodynamics. Further, the use of Bayes’ theorem implies that the work estimated with posterior probabilities also bears close analogy with the classical formula. These findings suggest that the notion of prior information can be used to reveal thermodynamic features in quantum systems, thus pointing to a new connection between thermodynamic behavior and the concept of information.

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The connection between thermodynamics and the concept of information is one of the most subtle analogies in our physical theories. It has played a central role in the exorcism of Maxwell’s demon [1]. It is also crucial to how we may understand and exploit quantum information [2–4]. To make nanodevices [5, 6] that are functional and useful, we need to understand their performance with regard to heat dissipation and optimal information processing. To model such systems, standard thermodynamic processes and heat cycles have been generalised using quantum systems as the working media [7]–[16]. It is well accepted that the maximal efficiency, \(\eta\), of quantum heat engines from a Bayesian perspective.

As a model of a heat engine, consider a quantum system with Hamiltonian \(H_1 = \sum_n \varepsilon_n^{(1)}|n\rangle\langle n|\), where energy eigenvalues \(\varepsilon_n^{(1)} = \varepsilon_n a_1\). The factor \(\varepsilon_n\) depends on the energy level \(n\) as well as other fixed parameters/ constants of the system; \(a_1\) is a controllable external parameter equivalent to say, the applied magnetic field for a spin-1/2 system. Other examples of this class are 1-d quantum harmonic oscillator (\(a_1\) equivalent to frequency) and a particle in 1-d box (\(a_1\) inversely proportional to the square of box-width). Initially, the quantum system is in thermal state \(\rho(a_1) = \sum_n p_n^{(1)}|n\rangle\langle n|\) at temperature \(T_1\) with its eigenvalues given by the canonical probabilities \(p_n^{(1)}\). The quantum analogue of a classical Otto cycle between two heat baths at temperatures \(T_1\) and \(T_2\) involves the following steps [14]: (i) the system is detached from the hot bath and made to undergo the first quantum adiabatic process, during which the system hamiltonian changes to \(H_2 = \sum_n \varepsilon_n^{(2)}|n\rangle\langle n|\), where \(\varepsilon_n^{(2)} = \varepsilon_n a_2\), without any transitions between the

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levels and so the system continues to occupy its initial state. For \( a_2 < a_1 \), this process is the analogue of an adiabatic expansion. The work done by the system in this stage is defined as the change in mean energy \( \mathcal{W}_1 = \text{Tr}(\rho(a_1)[H_2 - H_1]) \); (ii) the system with modified energy spectrum \( \varepsilon_n^{(2)} \) is brought in thermal contact with the cold bath and it achieves a thermal state \( \rho(a_2) = \sum_n p_n^{(2)} |n\rangle \langle n| \). The modified canonical probabilities \( p_n^{(2)} \) now correspond to temperature \( T_2 \). On average, heat rejected to the bath in this stage is defined as \( Q_2 = \text{Tr}(\rho(a_2) - \rho(a_1) | H_2 \rangle \langle H_1 \); (iii) the system is now detached from the cold bath and made to undergo a second quantum adiabatic process (compression) during which the Hamiltonian changes back to \( H_1 \). Work done on the system in this stage is \( \mathcal{W}_2 = \text{Tr}(\rho(a_2) | H_1 - H_2 \rangle \langle H_1 \); (iv) finally, the system is brought in thermal contact with the hot bath again. Heat is absorbed by the system in this stage whence it recovers its initial state and its temperature attains back the value \( T_1 \). The total work done on average in a cycle is calculated to be

\[
\mathcal{W} = \sum_n \left( \varepsilon_n^{(1)} - \varepsilon_n^{(2)} \right) \left( p_n^{(1)} - p_n^{(2)} \right),
\]

\[
= (a_1 - a_2) \sum_n \varepsilon_n \left( p_n^{(1)} - p_n^{(2)} \right) > 0.
\]

Similarly, heat exchanged with hot bath in stage (iv) is given by \( Q_1 = a_1 \sum_n \varepsilon_n \left( p_n^{(1)} - p_n^{(2)} \right) > 0 \). Heat exchanged by the system with the cold bath is \( Q_2 = \mathcal{W} - Q_1 < 0 \). The efficiency of the engine \( \eta = \mathcal{W}/Q_1 \), is given by

\[
\eta = 1 - \left( \frac{a_2}{a_1} \right).
\]

For convenience, we express \( \mathcal{W} \equiv \mathcal{W}(a_1, \eta) \), using Eq. (3). Consider an ensemble of such systems where now the value of parameter \( a_1 \) may vary from system to system. If the ensemble corresponds to an actual preparation according to a certain probability distribution \( \Pi(a_1) \), then the state of the system can be expressed as \( \hat{\rho} = \int \rho(a_1) \Pi(a_1) da_1 \). Each system in the ensemble is made to perform the quantum heat cycle described above, with a fixed efficiency \( \eta \). We wish to study the optimal characteristics of the average work, in particular the efficiency at which the work becomes optimal. Clearly, choice of the probability distribution \( \Pi(a_1) \) is expected to play a significant role in the conclusions. In the following, we analyse this problem by choosing a distribution \( \Pi(a_1) \) according to the prior information available and show that the efficiency at optimal work is closely associated with CA value.

For simplicity, we now consider a two-level system as our working medium, with \( \varepsilon_0 = 0 \) and \( \varepsilon_1 = 1 \), so that the initial energy levels are 0 and \( a_1 \). The work over a cycle in this case is

\[
\mathcal{W}(a_1, \eta) = a_1 \eta \left[ \frac{1}{1 + e^{a_1/T_1}} - \frac{1}{1 + e^{a_1(1-\eta)/T_2}} \right] > 0,
\]

where Boltzmann’s constant is put equal to unity. The average work with the initial state \( \hat{\rho} \) for a given \( \eta \), can be expressed as

\[
\overline{\mathcal{W}} = \int_{a_{\min}}^{a_{\max}} \mathcal{W}(a_1, \eta) \Pi(a_1) da_1.
\]

A central issue in Bayesian probability is to assign a unique prior distribution corresponding to a given prior information. If the only prior information about the continuous parameter \( a_1 \) is that it takes positive real values but otherwise we have complete ignorance about it, then Jeffreys has suggested the prior distribution \( \Pi(a_1) \propto 1/a_1 \) [26, 52], or in a finite range, \( \Pi(a_1) = [\ln (a_{\max}/a_{\min})]^{-1} (1/a_1) \), where \( a_{\min} \) and \( a_{\max} \) are the minimal and the maximal energy splitting achievable for the two-level system. For the above choice, we obtain

\[
\overline{\mathcal{W}} = \left[ \ln \left( \frac{a_{\max}}{a_{\min}} \right) \right]^{-1} \eta \left[ \frac{T_2}{1 - \eta} \ln \left( \frac{1 + e^{a_{\max}(1-\eta)/T_2}}{1 + e^{a_{\min}(1-\eta)/T_2}} \right) - T_1 \ln \left( \frac{1 + e^{a_{\max}/T_1}}{1 + e^{a_{\min}/T_1}} \right) \right].
\]

It can be seen that the average work \( \overline{\mathcal{W}} \) vanishes for \( \eta = 0 \) and \( \eta = \eta_c \). In between these values of \( \eta \), the average work exhibits a maximum. We look for the efficiency at which this work becomes maximal for the given range \( [a_{\min}, a_{\max}] \), by imposing the condition \( \partial \overline{\mathcal{W}} / \partial \eta = 0 \). Here we consider the limit of \( a_{\min} \to 0 \) which gives

\[
\frac{T_2}{(1 - \eta)^2} \ln \left[ \frac{1 + e^{a_{\max}(1-\eta)/T_2}}{2} \right] - T_1 \ln \left[ \frac{1 + e^{a_{\max}/T_1}}{2} \right] - \frac{\eta}{(1 - \eta)} \frac{a_{\max}}{1 + e^{-a_{\max}(1-\eta)/T_2}} = 0.
\]
The solution $\eta$ of this equation has been plotted against $a_{\text{max}}$ in Fig. 1. Interestingly, in the asymptotic limit of $a_{\text{max}} \gg T_1$, the above expression reduces to

$$T_1 - \frac{T_2}{(1 - \eta)^2} = 0,$$

which yields the efficiency at optimal work as $\eta = 1 - \sqrt{T_2/T_1}$, exactly the CA value. More significantly, the conclusion also holds in general i.e. for a working system with spectrum $\varepsilon_n = \varepsilon_n a_1$ and with Jeffreys’ prior. It is to be noted that in the asymptotic limits, the expression for average work (Eq. (6)) diverges. However, the limits are taken after the derivative of work is set equal to zero in order to obtain well-defined expressions for the efficiency.

![Figure 1: Efficiency versus $a_{\text{max}}$ using Eq. (7). The curves correspond to $T_2 = 1$ and $T_1$ taking values 2, 4, 6 respectively, from bottom to top. Apart from the approach to corresponding CA value at large $a_{\text{max}}$, it is also seen that the limit is approached slowly for larger temperature differences.](image)

It is conceivable that other choices of the prior may yield similar results. To study consequences of deviations from the above choice, we consider a class of prior distributions, $\Pi(a_1) = Na_1^{1-\gamma}$, defined in the range $[0, a_{\text{max}}]$, where $N = (1 - \gamma)/a_{\text{max}}^{1-\gamma}$ and $\gamma < 1$. Upon optimisation of the average work as defined in Eq. (5) over $\eta$, we get

$$\int_0^{a_{\text{max}}} \left[ \frac{(a_1)^{1-\gamma}}{1 + e^{a_1/T_1}} - \frac{(a_1)^{1-\gamma}}{1 + e^{a_1(1-\eta)/T_2}} \right] da_1 - \frac{\eta}{T_2} \int_0^{a_{\text{max}}} \frac{(a_1)^{2-\gamma} e^{a_1(1-\eta)/T_2}}{(1 + e^{a_1(1-\eta)/T_2})^2} da_1 = 0.$$  

(9)

In the limit $a_{\text{max}}$ becoming very large, the above integrals can be evaluated using the standard results [33]. Then the above equation is simplified to

$$(1 - \eta^*)^{3-\gamma} - (1 - \eta)\theta^{2-\gamma}\eta^* - \theta^{2-\gamma} = 0,$$

(10)

where $\theta = T_2/T_1$. Now as $\gamma \to 1$, the above equation reduces to Eq. (8) and so CA value is also a limiting value for this model. Interestingly, even for other allowed values of $\gamma$, the solution $\eta^*$ of Eq. (10) depends only on the ratio $\theta$, apart from the parameter $\gamma$. In particular, Laplace and Bayes have advocated a uniform prior to quantify the state of complete ignorance. For this case, we set $\gamma = 0$. Then the above equation becomes $(1 - \eta^*)^3 - (1 + \eta^*)\theta^2 = 0$, which has only one real solution given as

$$\eta^* = 1 + \frac{\theta^{4/3}}{3 \left(1 + \sqrt{1 + \frac{\theta^2}{27}}\right)^{1/3}} - \theta^{2/3} \left(1 + \sqrt{1 + \frac{\theta^2}{27}}\right)^{1/3}.$$  

(11)

This solution along with other numerical solutions of (10) for general $\gamma < 1$ are shown in Fig. 2. Remarkably, these curves stay very close to the CA value. However, at this point it is not possible to say in general what prior information may be quantified by the parameter $\gamma$. The curves in Fig. 2 are also closely similar to those observed in finite-time models at optimal power [22]. It is seen here that in the near-equilibrium regime, all the curves merge into each other and approach the CA value which is approximately $\eta_c/2$ in this limit. This can be shown as follows: taking $\theta$ to be
close to unity in the near-equilibrium case, $\eta_c = (1 - \theta)$ is close to zero. The efficiency $\eta^*$ being bounded from above by the Carnot value is thus small too. On using these facts in the expansion of Eq. (10), we get

$$\eta^* \approx \frac{\eta_c}{2} + \frac{(3 - \gamma)}{16} \eta_c^2 + O(\eta_c^3).$$

(12)

Thus we recover the linear term $\eta_c/2$ mentioned earlier. For general values of $\theta$, the CA value is a lower bound for the efficiency at optimal work when $0 < \gamma < 1$. So using posterior probabilities, a well defined expression for average work is obtained even if the prior is non-normalisable in the asymptotic limit. More generally, given the value of external parameter $a_1$ and assuming canonical probabilities $p(n|a_1)$ to find the system in $n$th state, we infer the probability $p(a_1|n)da_1$ about the value of $a_1$, if the system is actually found in the $n$th state. Remarkably, the work given by eq. (13) attains optimal value exactly at the CA efficiency, regardless of the value of $\gamma$ in the prior. Furthermore, the average work $W(\eta)$ shows the same dependence on efficiency $\eta$ as found for the classical Otto cycle in [18].

In conclusion, we have argued the emergence of CA value as the efficiency at optimal work in quantum heat engines within a Bayesian framework. This effect of incorporating Bayesian probabilities leading to classical thermodynamic
behavior in quantum systems has not been addressed before and may shed new light on the connection between information and thermodynamics. Due to current interest in small scale engines, the observation of similar curves (Fig. 2) as obtained in some recently proposed models of these engines, points to an interesting link between finite time models and our model based on the idea of prior information. Addressing these issues would hopefully lead to a broader perspective on the performance characteristics of small engines and also help to understand the limits of their performance based on principles of information.

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[15] If we start with the prior distribution $N/a^{-\gamma}$ defined in the range $[a_{min}, \infty]$, normalisable for $a > 1$, and solve in the asymptotic limit $a_{min} \to 0$, then CA value is an upper bound for optimal efficiency. This choice is also presented in Fig. 2 for $\gamma = 1.5$. 

\[ \int_0^\infty \frac{x^{1-\gamma}}{1 + e^{x/T}} \, dx = (1 - 2^{\gamma-1})T^{2-\gamma} \zeta(2-\gamma), \] 
for $\gamma < 2$ and where $\Gamma[\cdot]$ and $\zeta[\cdot]$ are the Gamma function and Riemann zeta functions, respectively.