Informative priors and the analogy between quantum and classical heat engines

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Abstract
When incomplete information about the control parameters is quantified as a prior distribution, a subtle connection emerges between quantum heat engines and their classical analogues. We study the quantum model where the uncertain parameters are the intrinsic energy scales and compare it with the classical models where the intermediate temperature is the uncertain parameter. The prior distribution quantifying the incomplete information has the form \( \pi(x) \propto 1/x \) in both the quantum and the classical models. The expected efficiency calculated in the near-equilibrium limit approaches the value of one third of Carnot efficiency.

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(Some figures may appear in color only in the online journal)

1. Introduction

Quantum heat engines (QHEs) are novel tools to study the underlying thermodynamic properties of quantum systems [1–8]. The working substance in a QHE is a few-level quantum system and can show interesting features such as quantum correlation, coherence and so on. So QHEs may show unexpected behavior [1, 2, 4] which is not possible in the classical models of heat engines. But all these models are consistent with the second law of thermodynamics. Recent studies [6, 8] showed that the expected behavior of certain models of QHE exhibit classical thermodynamic features which points out an interesting and novel connection between information and thermodynamics. In these models, the uncertain parameters are treated as in the Bayesian approach.

In the Bayesian approach to probability theory, prior distribution [9, 10], also known simply as a prior, quantifies the prior knowledge about the uncertain parameter(s). Usually, there is some information available even about the uncertain parameters, e.g. from the nature of the parameters or from the physics of the problem. The prior which makes use of this knowledge is also addressed as an informative prior.

So the right choice of the prior plays an important role in this approach.

In this paper, we discuss a quantum and a classical model of heat engine and estimate their performance. In the quantum model, we consider a pair of two-level systems with energy level spacings \( a_1 \) and \( a_2 \). Reservoirs associated with the respective systems are at temperatures \( T_1 \) and \( T_2 \). These intrinsic energy level spacings can be controlled externally e.g. through an external magnetic field. In the classical model, the pair of two-level systems is replaced by a pair of classical ideal gas systems.

In the quantum model, the unknown parameters are the energy level spacings of the two-level systems. But in the classical case, the uncertain parameter is the intermediate temperature. To assign the prior, we invoke different observers who satisfy a consistency criterion and thus arrive at the prior for the unknown parameter. These prior distributions are used to estimate the expected behavior of thermodynamic quantities. Finally, we compare the estimated values of the physical quantities obtained from the quantum and the classical models. The main objective of this paper is to show the equivalence of the expected behavior of quantum and classical models under certain conditions. Interestingly, the expected efficiencies are also related to the efficiencies...
The average work done in one cycle is \( W = Q_1 + Q_2 \). To complete the cycle, the two systems are brought again in thermal contact with their respective reservoirs. The operation of the machine as a heat engine implies \( W \geq 0 \) and \( Q_1 \geq 0 \), which is satisfied if
\[
\alpha_1(T_2/T_1) \leq \alpha_2 \leq \alpha_1.
\]

3. Prior distribution

Now consider a situation in which the temperatures of the reservoirs are given \( a \) priori such that \( T_1 > T_2 \), but the exact values of parameters \( \alpha_1 \) and \( \alpha_2 \) are uncertain. The prior information about these parameters may be summarized as follows.

- \( \alpha_1 \) and \( \alpha_2 \) represent the same physical quantity, i.e. the level spacing for system \( R \) and \( S \), respectively, and so they can only take positive real values.
- If the setup of \( R + S \) has to work as an engine, then the criterion in equation (6) must hold, whereby if one parameter is specified, then the range of the other parameter is constrained.

Apart from the above conditions, we assume to have no information about \( \alpha_1 \) and \( \alpha_2 \). The question we address in the following is: what can we then infer about the expected behavior of physical quantities for this heat engine? We have suggested a subjective or Bayesian approach to address this question [6, 8]. This implies that an uncertain parameter is assigned a prior distribution, which quantifies our preliminary expectation about the parameter to take a certain value. Thus the prior should be assigned by taking into account any prior information we possess about the parameters. For example, if \( \alpha_1 \) is specified, then the prior distribution for \( \alpha_2 \), \( \pi(\alpha_2|\alpha_1) \), is conditioned on the specified value of \( \alpha_1 \), and is defined in the range \( [\alpha_1, \alpha_2] \), where \( \alpha = T_2/T_1 \), because we know the setup works like an engine if we implement equation (6).

We denote the prior distribution function for our problem by \( \Pi(\alpha_1, \alpha_2) \). To assign the prior, it seems convenient to involve two observers \( A \) and \( B \), who wish to assign priors for \( \alpha_1 \) and \( \alpha_2 \). Based on the derivation given in [8], we find that the prior for each parameter is
\[
\Pi(\alpha_i) = \frac{1}{\ln(d_{\text{max}})} \frac{1}{\alpha_i},
\]
and the joint prior for the system acting as an engine is given by
\[
\Pi(\alpha_1, \alpha_2) = \frac{1}{\ln(\frac{1}{\alpha_1})} \frac{1}{\alpha_1} \frac{1}{\alpha_2}. \tag{8}
\]

4. Expected values of quantities

In this section, we use the priors assigned above to find expected values for various physical quantities related to the engine. The expected value of any physical quantity \( X \) which may be a function of \( \alpha_1 \) and \( \alpha_2 \) is defined as follows:
\[
\bar{X} = \int \int X \Pi(\alpha_1, \alpha_2) \, d\alpha_1 \, d\alpha_2. \tag{9}
\]
These expected values reflect the estimates by an observer who assigns the priors. In principle, there are two ways to calculate the expected value of some quantity which depends, in general, on the method used. The method by which the observer A applies the joint prior is based on the definition

$$\Pi(a_1, a_2) = \Pi(a_2 | a_1) \Pi(a_1),$$

(10)
i.e. the prior for \(a_1\) is assigned first, followed by \(\Pi(a_2 | a_1)\), which is the conditional distribution of \(a_2\) for a given value of \(a_1\). On the other hand, observer B applies

$$\Pi(a_1, a_2) = \Pi(a_1 | a_2) \Pi(a_2),$$

(11)
whereby the prior for \(a_2\) is assigned first and \(\Pi(a_1 | a_2)\) represents the conditional distribution of \(a_1\) for a given value of \(a_2\).

4.1. Internal energy

We calculate the expected values of internal energies for systems \(R\) and \(S\). These values can then be used to find the expected work per cycle, heat exchanged and so on.

1. Initial state. For a given \(a_i\), the internal energy \(E_{\text{ini}}^{(i)}\) is given by equation (2). The expected initial energy is defined as

$$E_{\text{ini}}^{(i)} = \int_{a_{\text{min}}}^{a_{\text{max}}} E_{\text{ini}}^{(i)}(a_i) d\alpha_i,$$

(12)
where \(i = 1, 2\). Note that \(E_{\text{ini}}^{(i)}\) depends only on \(a_i\), so we need to average over the prior for \(a_i\) only. Using equations (2) and (7), we obtain

$$E_{\text{ini}}^{(i)} = \left[ \ln \left( \frac{a_{\text{max}}}{a_{\text{min}}} \right) \right]^{-1} \times \left( a_{\text{max}} - a_{\text{min}} \right) + T_i \ln \left( \frac{1 + e^{a_{\text{max}}/T_i}}{1 + e^{a_{\text{min}}/T_i}} \right).$$

(13)

2. Final state. In this case, the internal energy of \(R\) as well as \(S\) is a function of both \(a_1\) and \(a_2\) (see (3)) and so the expected values are obtained by averaging over the joint prior, \(\Pi(a_1, a_2)\). For instance, the expected final energy of system \(S\) (denoted by superscript (2)) as calculated by A is

$$E_{\text{fin}}^{(2)}(A) = \int \! \int E_{\text{fin}}^{(2)} \Pi(a_1 | a_2) \Pi(a_1) \, da_1 \, da_2$$

$$= K \int_{a_{\text{min}}}^{a_{\text{max}}} \frac{1}{(1 + e^{a_1/T_i}) a_1} \int_{a_{\text{ini}}}^{a_1} \frac{da_1}{a_1^{1/\theta}} \, da_2,$$

$$= K \left( 1 - \theta \right) \times \left[ (a_{\text{max}} - a_{\text{min}}) + T_i \ln \left( \frac{1 + e^{a_{\text{max}}/T_i}}{1 + e^{a_{\text{min}}/T_i}} \right) \right],$$

(14)
where \(K = [\ln(1/\theta) \ln(a_{\text{max}}/a_{\text{min}})]^{-1}\). Similarly as calculated by B, we have

$$E_{\text{fin}}^{(2)}(B) = \int \! \int E_{\text{fin}}^{(2)} \Pi(a_2 | a_1) \Pi(a_2) \, da_1 \, da_2$$

$$= K \int_{a_{\text{min}}}^{a_{\text{max}}} \frac{da_2}{(1 + e^{a_2/T_i}) a_2} \int_{a_{\text{ini}}}^{a_2} \frac{da_1}{a_1^{1/\theta}} \left( \frac{1}{a_1^{1/\theta}} \right),$$

(15)
which cannot be solved analytically.

Now in general, the expected final energies of \(S\), as given by equations (14) and (15) according to A and B, respectively, are not equal. One would expect that if the state of knowledge of \(A\) and \(B\) is similar, then they should expect the same value for a given quantity. (A similar feature is also observed in the expressions for the expected final energy of system \(R\).)

4.2. Asymptotic limit

As remarked above, observers \(A\) and \(B\) should arrive at similar estimates for physical quantities using their respective priors. This happens in the limit, \(a_{\text{min}} \ll T_2\) and \(a_{\text{max}} \gg T_1\). Then, equation (13) is approximated as

$$E_{\text{fin}}^{(i)} \approx \frac{\ln 2}{\ln(a_{\text{max}}/a_{\text{min}})} T_i.$$
and
\[ \overline{Q}_2 \approx \frac{\ln 2}{\nu_{\text{max}}} \left( 1 + \frac{(1 - \theta)}{\theta \ln \theta} \right) T_2. \]  
(21)

Now the expected work per cycle is defined as \( \overline{W} = \overline{Q}_1 + \overline{Q}_2 \). Thus the efficiency may be defined as \( \eta = 1 + \overline{Q}_2/\overline{Q}_1 \). Explicitly, using equations (20) and (21) we obtain
\[ \eta = 1 + \frac{\theta \ln \theta + (1 - \theta)}{\ln \theta + (1 - \theta)}. \]  
(22)

This is the efficiency at which the engine is expected to operate for a given \( \theta \). The above value is a function only of the ratio of the reservoir temperatures.

We note that the constant of proportionality in equations (16) and (17), which is \( \ln 2 \times (\ln(a_{\text{max}}/a_{\text{min}}))^{-1} \), can be related to heat capacity. The expected value of the initial heat capacity of system \( i \), defined as
\[ \overline{C}_i = \int_{a_{\text{min}}}^{a_{\text{max}}} C_i \Pi(a_i) da_i, \]  
(23)
where we know for a two-level system, the canonical heat capacity at constant volume is \( C_i = (a_i/T_i)^2(\exp(a_i/T_i))/(1 + \exp(a_i/T_i))^2 \).

In particular, for the asymptotic limit, the leading term yields
\[ \overline{C}_i \equiv \overline{C} \approx \frac{\ln 2}{\nu_{\text{max}}}. \]  
(24)

This value is independent of the temperature of the system and thus indicates an analogy with a constant heat capacity thermodynamic system.

Thus the requirement of consistency between the results of \( A \) and \( B \) implies, in an asymptotic limit, that the behavior expected from minimal prior information is the one which shows simple thermodynamic features such as constant heat capacity and equality of subsystem temperatures upon maximum work extraction.

5. The classical model

In this section, we discuss a classical model of the heat engine, within the subjective approach. Consider two thermodynamic systems at initial temperatures \( T_1 \) and \( T_2 \) (= \( T_1 \)), such that the heat capacity \( C \) can be assumed to be constant, i.e. the systems behave like classical ideal gases. Further consider the maximum work extraction by coupling the two systems to a reversible work source. This process preserves the total entropy, i.e. \( \Delta S = 0 \). Let us assume that at some stage, the temperatures of the systems are \( T_a \) and \( T_b \), respectively. Entropy conservation leads to
\[ T_b = \frac{T_1 T_2}{T_a}. \]  
(25)

The above equation relates \( T_b \) and \( T_a \), implying that given a value of one of them, the value of the other is fixed. The work \( W \) extracted from the system is given by the decrease in internal energy,
\[ W = C(T_1 + T_2 - T_a - T_b). \]  
(26)

Similarly, the heat absorbed from the initially hotter system will be
\[ Q_1 = C(T_1 - T_a). \]  
(27)

Now we consider the situation in which we have lack of information about the exact values of these intermediate temperatures \( T_a \) and \( T_b \). We want to estimate the properties of this engine, taking into account the prior information we have about the parameters. Now it is clear that we have to assign the prior either to \( T_a \) or \( T_b \), because the two parameters are related by equation (25). Imagine two observers \( A \) and \( B \) who respectively take \( T_a \) and \( T_b \), as the uncertain parameter for the considered thermodynamic process. Thus from the perspective of \( A \), the work is given by
\[ W = C \left( T_1 + T_2 - T_a - \frac{T_1 T_2}{T_a} \right), \]  
(28)
while from \( B \)'s point of view
\[ W = C \left( T_1 + T_2 - T_b - \frac{T_1 T_2}{T_b} \right). \]  
(29)

Further, we assume that \( A \) and \( B \) assign the same functional form for their priors and the range over which the parameters can take values is also the same. Thus probability distribution \( P \) for the temperatures \( T_a \) and \( T_b \) is defined in the range \([T_1, T_2]\). Now due to the constraint relating \( T_a \) and \( T_b \), the probabilities assigned to any pair of values related by equation (25) should be the same. This means that
\[ P(T_a) dT_a = P(T_b) dT_b. \]  
(30)

Using (25) and (30), we obtain
\[ P(T_a) = \frac{1}{\ln(1/\theta) T_a}, \]  
(31)

where \( \theta = T_2/T_1 \).

5.1. Estimated work and efficiency

The work estimated by \( A \) is defined as
\[ \langle W \rangle = \int_{T_1}^{T_2} W P(T_a) dT_a, \]  
(32)

where \( W \) is given by equation (28). Thus
\[ \langle W \rangle = C T_1 \left[ \frac{(1 + \theta) + 2(1 - \theta)}{\ln \theta} \right]. \]  
(33)

Similarly, the estimate for the heat absorbed is given by
\[ \langle Q_1 \rangle = C T_1 \left[ 1 + \frac{(1 - \theta)}{\ln \theta} \right]. \]  
(34)

The efficiency, \( \eta = \langle W \rangle/\langle Q_1 \rangle \), is given by
\[ \eta = 1 + \frac{\theta \ln \theta + (1 - \theta)}{\ln \theta + (1 - \theta)}. \]  
(35)

The observer \( B \) also arrives at the same estimates for work and efficiency. Now the expected values of intermediate temperatures calculated by \( A \) and \( B \) after the work extraction process are
\[ \langle T_a \rangle = \langle T_b \rangle = T_a \frac{(1 - \theta)}{\ln(1/\theta)}. \]  
(36)

Moreover, all these estimates are also the same as those derived from a QHE in the asymptotic limit in section 4.2.
6. Conclusions

We have analyzed the case of heat engines by assuming uncertainty in the exact values of the internal energy scales of the working medium. We have suggested the appropriate prior distributions for the uncertain parameters based on prior information. In the case of a quantum model, where the level spacings are the unknown parameters, the expected values of work, heat and efficiency are equivalent to the expected values calculated from the classical model, where the intermediate temperature is the unknown parameter. Moreover, in both the models, expected temperatures are equal at the end of work extraction. So the quantum model with two unknown parameters shows similar behavior as the classical model, with a single uncertain parameter. At this point, it is interesting to analyze a special case of the quantum model with a single unknown parameter. Such a kind of situation arises when the efficiency \( \eta = 1 - a_2/a_1 \) of the engine is given. This simplifies the problem to that of a single uncertain parameter, either \( a_1 \) or \( a_2 \). Introducing two observers as discussed in [8], we get the functional form of the prior as \( \pi(a_i) \propto 1/a_i \). We can then calculate the expected work per cycle. In the asymptotic limit, the expression for the expected work reduces to

\[
\bar{W} \approx C_{\eta} \left( T_1 - \frac{T_2}{(1 - \eta^2)} \right).
\]

(37)

Let us compare the above expression with its classical analogue. The classical model of the heat engine discussed in section 5 has an efficiency \( \eta = 1 - T_a/T_1 = 1 - T_3/T_5 \), when \( T_a \) and \( T_5 \) are specified. Substituting this efficiency into equations (28) and (29), we obtain the expression for work the same as the quantum case given in equation (37).

The efficiency at the maximum expected work (equation (37)) is equal to \( 1 - \sqrt{\theta} \), the well-known Curzon–Ahlborn efficiency [14]. In the near-equilibrium limit, this efficiency can be expanded as

\[
\eta^* \approx \frac{(1 - \theta)}{2} + \frac{(1 - \theta)^2}{8} + O(1 - \theta)^3.
\]

(38)

So this efficiency appears at the maximum value of the expected work in the asymptotic limit for the quantum model with an uncertain parameter as well as at the maximum work for the classical model without any uncertain parameter. This efficiency falls in a certain universality class [15, 16], where the leading term in the near-equilibrium expansion is half of the Carnot efficiency \( \eta_c \). At this point, it is interesting to analyze the near-equilibrium expansion of the efficiency expressed in equations (22) and (35):

\[
\eta^* \approx \frac{(1 - \theta)}{3} + \frac{(1 - \theta)^2}{9} + \frac{8(1 - \theta)^3}{135} + O[(1 - \theta)^4].
\]

(39)

This expected efficiency is obtained in two cases: from the quantum model where two parameters \( (a_1 \) and \( a_2 \)) are uncertain and from the classical model with a single uncertain parameter \( (T_a \) or \( T_5 \)). The leading term in the near equilibrium expansion of this efficiency is \( \eta_c/3 \) instead of \( \eta_c/2 \) observed in equation (38). As another example, the efficiency at the maximum power for an irreversible Brownian heat engine [17] when optimized over the load and barrier height is given by

\[
\eta^* = \frac{2(1 - \theta)^3}{3 - 29(1 + \ln \theta) - \theta^2}.
\]

(40)

Expanding this efficiency for the near-equilibrium regime, we obtain

\[
\eta^* \approx \frac{(1 - \theta)}{3} + \frac{(1 - \theta)^2}{9} + \frac{(1 - \theta)^3}{18} + O[(1 - \theta)^4].
\]

(41)

The similarity between equations (39) and (41) up to the second order suggests that there might be a new universality class which includes these efficiencies. In figure 1, the efficiencies given in (35) and (40) are plotted. To conclude, when all the unknown parameters are treated with prior probabilities, the expected behavior of the quantum model with two internal energy scales as the uncertain parameters is similar to the classical model with an intermediate temperature as the single uncertain parameter. Interestingly, the expected efficiency in both cases approaches the \( \eta_c/3 \) value in the near-equilibrium limit. Further, the analysis based on subjective treatment of the incomplete information suggests a new line of enquiry of a possible connection with optimal performance of the finite-time irreversible models of heat engines.

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