Quantum heat engines and nonequilibrium temperature

Ramandeep S. Johal
Department of Physics, Indian Institute of Science Education and Research Mohali,
Transit Campus: MGSIPA Complex, Sector 26, Chandigarh 160019, India
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I. INTRODUCTION

Consider the thermodynamic problem of work extraction \(^1\) \(^2\) from two systems at different temperatures \(T_1\) and \(T_2\) (let \(T_1 > T_2\)) by coupling them with a reversible work source. It is assumed that internal energy of each system is \(U_i = C_i T_i\), where \(C_i\) is independent of temperature. The process of work extraction stops when the two systems reach a common final temperature \(T_f\). Work performed is given by the difference of initial and final energies:

\[
W_0 = C_1 T_1 + C_2 T_2 - (C_1 + C_2) T_f. \tag{1}
\]

Now to extract maximal work, the process is assumed to be thermally isolated in which thermodynamic entropy of the total bipartite system is preserved. This criterion yields the value of the final temperature as

\[
T_f = (T_1)^{(1+\xi)/(1+\xi)} (T_2)^{1/(1+\xi)}, \quad \text{where} \quad \xi = C_1/C_2.
\]

One can discuss a cyclic process which proceeds in the following two steps: i) the two systems prepared as above and coupled to a reversible work source, are used to extract an amount of work given in Eq. (1) whence the systems reach a common final temperature; ii) the systems are then brought back to their initial states by separating them from the work source and making contact with thermal baths at \(T_1\) and \(T_2\) respectively. In the second step, the system 1 absorbs heat from the hotter bath and system 2 rejects some heat to the cold bath. The efficiency of this cyclic process is

\[
\eta(\xi, \theta) = 1 + \frac{1}{\xi} \frac{\theta - \theta^{1/(1+\xi)}}{\theta^{1/(1+\xi)}}, \tag{2}
\]

where \(\theta = T_2/T_1\). This system behaves very similar to a cycle discussed by Leff \(^3\) which is made up of a sequence of infinitesimal Carnot cycles and where both the heat source and the sink have a finite heat capacity.

The problem of work extraction has also been addressed from a quantum mechanical point of view \(^4\) \(^5\) \(^6\). Although the possibility of a quantum heat engine and validity of thermodynamic bounds has been recognised since 1950s \(^7\), the recent developments in nanotechnology and quantum information processing have contributed to enhanced interest in quantum thermodynamic machines \(^8\) \(^9\) \(^10\) \(^11\). Alongside, such models provide insight into fundamental questions about thermodynamics such as Maxwell’s demon and universality of the second law \(^8\) \(^11\) \(^12\). Many models employ few-level quantum systems as the working medium, such as quantum harmonic oscillators, spin-systems, particle-in-box and so on \(^13\) \(^14\) \(^15\) \(^16\) \(^17\). Usually the cycle is a quantum generalization of the well-known classical Carnot, Otto, Brayton heat engines which follow four-step cycles. In another class of models, instead of the two classical or macroscopic systems as discussed in the preceding paragraph, one can form a two-step engine using two quantum systems \(^6\). Recently, such a quantum heat engine employing two two-level systems (TLS) was discussed and implications of the optimization of work on the structure of the engine were highlighted \(^18\).

However, quantum engines being small systems, the validity of thermodynamic behaviour is not guaranteed. For instance, after work extraction in the latter class of models, the two systems may not reach mutual equilibrium. In this paper, we further discuss the two-step model for work extraction using two TLS, focusing on the final passive state (which is in general a nonequilibrium state) from a thermodynamic perspective. We define an effective temperature for this state and analyse its properties. The paper is organised as follows. In section II, we introduce the model of quantum heat engine. In section II A, the temperatures of subsystems are evaluated; the validity of thermodynamic definitions is enforced by deriving the specific heats of subsystems in section II B. Section III proposes a definition for effective temperature of the composite system, which is calculated explicitly in different regimes of parameter values. We also compare some of the other definitions in literature for effective temperature of nonequilibrium systems, in section IV. Concluding ideas are given in section V.

II. QUANTUM MODEL FOR WORK EXTRACTION

Consider two TLS labeled \(R\) and \(S\) with Hamiltonians \(H_R\) and \(H_S\), prepared in thermal states \(\rho_R\) and \(\rho_S\) corresponding to temperatures \(T_1\) and \(T_2\). The Hamiltonian of the total system is \(H = H_R \otimes I + I \otimes H_S\). The initial state of the composite system is \(\rho_{in} = \rho_R \otimes \rho_S\). The
eigenvalues of $H$ are \( \{0, a_2, a_1, a_1 + a_2\} \) given that energy eigenvalues of $H_R$ and $H_S$ are \((0, a_1)\) and \((0, a_2)\), respectively. The eigenvalues of the initial density matrix are \( \{r_1s_1, r_1s_2, r_2s_1, r_2s_2\} \). Here the probability to find each system in its excited state is

\[
\begin{align*}
    r_2 &= \frac{1}{1 + e^{a_1/T_1}}, \\
    s_2 &= \frac{1}{1 + e^{a_2/T_2}},
\end{align*}
\]  

(3)

with ground state probabilities being \( r_1 = (1 - r_2) \) and \( s_1 = (1 - s_2) \). We set Boltzmann constant \( k_B = 1 \).

The initial mean energy of the composite system is \( U = a_1r_2 + a_2s_2 \). Let us for concreteness choose, \( a_1 > a_2 \). Within the approach based on quantum thermodynamics, the process of work extraction is a unitary process which preserves not only the magnitude of the entropy but also all eigenvalues of the density matrix describing the state of the system. It has been shown in earlier works [4, 6, 18] that under such a process, the state which corresponds to a minimum value of the final energy is \( \rho_f = \rho_S \otimes \rho_R \), with eigenvalues \( \{r_1s_1, r_2s_1, r_1s_2, r_2s_2\} \).

Effectively, it means that the two systems exchange or swap their initial probability distributions in the final state. In other words, work performed is maximum if \( U' = a_1s_2 + a_2r_2 \) and is given by

\[
W(a_1, a_2) = U' - U = (a_1 - a_2)(s_2 - r_2). 
\]  

(4)

Net work is extracted if \( W < 0 \) which requires the following condition:

\[
s_2 < r_2 \implies \frac{T_1}{T_2} > \frac{a_1}{a_2}. 
\]  

(5)

The efficiency of this engine is \( \eta = 1 - \frac{a_2}{a_1} \), which is independent of temperature and its upper bound is Carnot value.

A. Temperatures of subsystems after work extraction

Now we study temperatures in the final state. After work, the mean energy of subsystem 1 is \( U_1' = a_1s_2 \), and \( U_2' = a_2r_2 \). Let us consider two such set-ups specified by the pair of energy parameters \( (a_1, a_2) \) and \( (a_1 + da_1, a_2 + da_2) \). Comparing the final states after work extraction, the change in energy of subsystem 1 is

\[
dU_1' = s_2da_1 + a_1\frac{ds_2}{da_2}da_2. 
\]  

(6)

We follow the standard interpretation of work as the change in mean energy due to shift in energy levels, at constant probabilities [10, 20, 21]. Similarly, heat is defined to be the change in mean energy when the energy levels stay fixed, but probability of occupation changes. Thus the heat contribution for system 1 is given by

\[
dQ_1' = a_1\frac{ds_2}{da_2}da_2. 
\]  

(7)

Similarly for subsystem 2, we have

\[
dQ_2' = a_2\frac{dr_2}{da_1}da_1. 
\]  

(8)

Let us now study entropy of each subsystem. In the initial state, the entropy of subsystems are given by

\[
S_1 = -(r_1 \ln r_1 + r_2 \ln r_2) \quad \text{and} \quad S_2 = -(s_1 \ln s_1 + s_2 \ln s_2) 
\]

respectively. After work, due to exchange of probabilities between the subsystems, we have \( S_1' = S_2, S_2' = S_1 \). Thus for subsystem, say 1, the change in entropy of the final state under a variation of the parameter \( a_2 \) is

\[
dS_1' = dS_2 = \frac{a_2 ds_2}{T_2} da_2. 
\]  

(9)

Now we evaluate the final temperature of system 1 as

\[
T_1' = \frac{dQ_1'}{dS_1} = T_2 \frac{a_1}{a_2}. 
\]  

(10)

Similarly, we obtain for system 2

\[
T_2' = T_1 \frac{a_2}{a_1}. 
\]  

(11)

These values of temperatures are precisely which may be obtained directly from the final probability distributions of the TLS, because a TLS can always be assigned an effective temperature.

Using Eq. \[5\], it can be seen that after work extraction, the hotter subsystem 1 cools down \( (T_1' < T_1) \), where as the relatively cold subsystem 2 now has a higher temperature \( (T_2' > T_2) \). Note that the sign of difference \( (T_1' - T_2') \) is not determined; it is possible to have \( (T_1' < T_2') \). But this does not violate the second law, because the condition \[5\] also ensures that energy flows from the hot to the cold system. Thus the change in energy of system 1, \( \Delta U_1 = a_1(s_2 - r_2) < 0 \) and the corresponding change in system 2 is \( \Delta U_2 = a_1(r_2 - s_2) > 0 \).

B. Heat capacity of subsystems

The canonical heat capacity of subsystem 1 in the final state is related to the fluctuations of energy in a well-known way [2]. However, heat capacity may also be evaluated as follows. Consider the final temperature as function of \( a_1 \) and \( a_2 \) (Eq. \[11\]). Then a change in temperature resulting from a variation in these parameters is

\[
dT_1' = \frac{T_2 da_1}{a_2} - \frac{a_1 T_2}{(a_2)^2} da_2. 
\]  

(13)

Then keeping \( a_1 \) fixed (which is equivalent to keeping volume of subsystem 1 fixed, because change in \( a_1 \) for subsystem 1 in the final state is interpreted as work, see
Thus for given reservoir temperatures \((T_1, T_2)\) the heat capacity (at constant volume) in the final state of system 1 is

\[
C_1' = \left(\frac{\partial U_1'}{\partial T_1}\right)_{a_1},
\]

\[
= C_2,
\]

where we have used the following identity

\[
\frac{dT_2}{da_2} = \frac{C_2 T_2}{(a_2)^2},
\]

Here \(C_2\) is the canonical heat capacity of the subsystem 2 in its initial state at temperature \(T_2\). Similarly, we get the result \(C_2' = C_1\). Thus upon swap-transformation, the specific heats of the two subsystems also get exchanged.

To recapitulate, the standard thermodynamic process in which two macroscopic bodies at different temperatures are coupled to a work source, the final temperatures of the two bodies are said to be equal. In the quantum framework, the subsystems in general do not reach mutual thermal equilibrium. In the next section, we ask: can the whole bipartite system be characterised by a global effective temperature in the final state, even though it is a nonequilibrium state with subsystems at different temperatures?

### III. 'Temperature' for the Bipartite System

For subsystem \(i\), we observed in the previous section that temperature can be defined thermodynamically. In this section, we extend the thermodynamic definition to the nonequilibrium final state of the composite system.

For convenience, we define \(a_2/a_1 = \nu\). So the final temperatures are rewritten as: \(T_1 = T_2/\nu\) and \(T_2' = T_1\nu\). Thus for given reservoir temperatures \((T_1, T_2)\), the final temperatures of subsystems is determined by a single parameter \(\nu\), which is also related to the efficiency of the engine \(\nu = 1 - \eta\). Consider different final and initial states which are characterized by the same parameter \(\nu\), but which may yield different amounts of work.

At a given value of \(\nu\), the changes in \(a_1\) and \(a_2\) are related as

\[
da_2 = \nu da_1.
\]

Thus the heat exchanged by system 1 in such a process can be rewritten from Eq. (17) as

\[
dQ_1' = a_1 \frac{ds_2}{da_2} \nu da_1
\]

\[
= a_2 \frac{ds_2}{da_2} da_1.
\]

Also, Eq. (8) yields \(dQ_2\). Then the total heat exchanged by bipartite system is \(dQ' = dQ_1' + dQ_2\).

Similarly, the von-Neumann entropy of the bipartite system is the sum of subsystem entropies, \(S = S_1' + S_2' = S_1 + S_2\), and the variation in total entropy is

\[
dS' = \left[\left(\frac{dS_1}{da_1}\right) + \nu \left(\frac{dS_2}{da_2}\right)\right] da_1,
\]

at a given \(\nu\), using Eq. (17). Then we define the effective temperature as the ratio of heat variation to the entropy variation, \(T = \frac{dQ'}{dS}\), yielding

\[
T = \frac{a_2 \left(\frac{ds_2}{da_2} + \frac{dr_2}{da_1}\right)}{(a_2)^2 \left(\frac{ds_2}{da_2} + \frac{dr_2}{da_1}\right)}.
\]

Using Eq. (16) and \(-\frac{dr_2}{da_1} = \frac{C_2 T_2}{(a_2)^2}\), we finally get

\[
T = \frac{C_2 T_1' + C_1 T_2'}{(C_1 + C_2)}.
\]

The above formula is the main result of the present paper. It resembles the thermodynamic expression if the two systems at temperatures \(T_1\) and \(T_2\) with constant heat capacities \(C_2\) and \(C_1\) respectively, come to a common temperature \(T\), without doing any work, (see Eq. (1)).

Now we evaluate the effective temperature for the case of two TLS, and discuss its features. The canonical heat capacity of a TLS is given by the well known expression

\[
C_i = \left(\frac{a_i}{T_i}\right)^2 \frac{\exp[a_i/T_i]}{(1 + \exp[a_i/T_i])^2}.
\]

We first discuss the limit when \(a_i/T_i = x \ll 1\). Then \(C_i(x) \sim x^2/4\) and the ratio \(C_1/C_2 \equiv \xi \sim (\theta/\nu)^2\). Thus the efficiency is given by \(\eta = 1 - \frac{\theta}{\sqrt{\xi}}\). The effective temperature in this regime is

\[
\frac{T}{T_1} = \frac{\sqrt{\xi}}{(1 + \xi)} (1 + \theta).
\]

At Carnot limit, \(\xi \rightarrow 1\) and \(T/T_1 = (1 + \theta)/2\). However, note that this formula holds in general also, because Carnot limit implies \(a_1/T_1 \rightarrow a_2/T_2\) and so \(C_1/C_2 \rightarrow 1\). Here the extracted work is vanishingly small and the final temperature is expected to be \((T_1 + T_2)/2\).

At the other extreme, for \(\xi \rightarrow \theta^2\), we have \(T/T_1 = (\theta + \xi)/(1 + \xi)\).

In other words, when \(a_2 \rightarrow a_1\), \(\mathcal{W} \rightarrow 0\) (see Eq. (1)). Then \(T_1' = T_2\) and \(T_2' = T_1\) in this limit. In this case, the effective temperature is simplified to

\[
\frac{T}{T_1} = \frac{(\theta + \xi)}{(1 + \xi)}.
\]

Finally, we make the following observations:

1) it is interesting to note that the effective temperature is a weighted average of the subsystem temperatures after work extraction.
follows from Eq. (21) that as well as the condition 
\[ \frac{\partial W}{\partial a_1} = 0 \] and 
\[ \frac{\partial W}{\partial a_2} = 0 \] determine optimal values \( a_1^* \) and \( a_2^* \) as well as the condition
\[ \frac{dr_2}{da_1} = \frac{ds_2}{da_2} \tag{26} \]
holds. So we have \( \nu^* = \sqrt{\theta/\xi} \), where now \( \xi^* \) is determined from using optimal values \( a_1^* \) and \( a_2^* \). Then it follows from Eq. (21) that
\[ T^* = \frac{2T_1' T_2'}{T_1 + T_2}. \tag{27} \]
This may be expressed as
\[ \frac{T^*}{T_1} = \frac{2\sqrt{\xi^*}}{1 + \sqrt{\theta}}. \tag{28} \]

iii) At the global maximum of work, the conditions \( \frac{\partial W}{\partial a_1} = 0 \) and \( \frac{\partial W}{\partial a_2} = 0 \) determine optimal values \( a_1^* \) and \( a_2^* \) as well as the condition
\[ \frac{dr_2}{da_1} = \frac{ds_2}{da_2} \tag{26} \]
holds. So we have \( \nu^* = \sqrt{\theta/\xi} \), where now \( \xi^* \) is determined from using optimal values \( a_1^* \) and \( a_2^* \). Then it follows from Eq. (21) that
\[ T^* = \frac{2T_1' T_2'}{T_1 + T_2}. \tag{27} \]
This may be expressed as
\[ \frac{T^*}{T_1} = \frac{2\sqrt{\xi^*}}{1 + \sqrt{\theta}}. \tag{28} \]

iv) Fig. 1 shows the behaviour of subsystem and effective temperatures as function of efficiency. Particularly, \( T \) shows a nonmonotonic trend. For a given value of \( \eta \), \( T \) in Fig. 1 corresponds to that engine set-up which yields the maximum work. From numerical calculations, it is observed that the temperature has a minimum at an efficiency which is bounded from below by Curzon-Ahlborn value.

\[ T = \frac{1}{\frac{1}{T_1} + \frac{1}{T_2}} \]

\[ T' = \frac{1}{\frac{1}{T_1'} + \frac{1}{T_2'}} \]

FIG. 1: For \( T_2 = 1 \) and \( T_1 = 9 \), the subsystem temperatures \( T_1', T_2' \) and the effective temperature \( T \) of the composite system evaluated at maximum work corresponding to a given efficiency. \( T \) is given by a weighted average over the subsystem temperatures and so its curve lies in between the curves for subsystem temperatures. All the three temperatures are equal at Curzon-Ahlborn efficiency.

IV. EFFECTIVE TEMPERATURES: A COMPARISON

The definition of nonequilibrium temperature is not unique for a given situation and one can envisage different definitions. We compare with our definition two other definitions of the effective temperature from literature, that are relevant to our system. The first candidate is the spectral temperature \( \eta \). This definition depends only on the energy probability distribution and the energy spectrum of the system and is applicable even for nonequilibrium situations. Thus for a non-degenerate spectrum, the inverse of spectral temperature is defined to be
\[ \frac{1}{T_s} = - \left( 1 - \frac{P_0 + P_M}{2} \right)^{-1} \sum_{i=1}^{M} \left( \frac{P_i + P_{i-1}}{2} \right) \ln P_i - \ln P_{i-1}, \tag{29} \]
where Boltzmann’s constant has been set to unity. \( P_i \) is the probability to occupy a level with energy \( E_i \) and index for the levels ranges from 0 (ground state) to \( M \). For our case of two TLS in the finite state after work extraction, using the values \( \{ E_i \} = \{ 0, a_2, a_1, a_1 + a_2 \} \) and \( \{ P_i \} = \{ r_1 s_1, r_2 s_1, r_1 s_2, r_2 s_2 \} \), the (inverse) spectral temperature is explicitly given by
\[ \frac{1}{T_s} = \frac{1}{T_1} \left( \frac{\nu - \theta}{(\nu - \nu^2)} x + \frac{1}{T_2} \right), \tag{30} \]
where \( x = (r_1 + s_1 - 2r_1 s_1) \). The special cases include: Carnot limit, when \( \nu \to \theta \) and so \( T_s = (1 + x)T'_2 \); when \( \nu \to 0 \), \( T_s \to 0 \). Finally, for CA efficiency \( (\nu = \sqrt{\theta}) \), the spectral temperature is equal to the subsystems’ temperature. In general, the behaviour of \( T_s \) as shown in Fig. 2 is quite different from the proposed definition.

FIG. 2: Comparison between other definitions of nonequilibrium temperatures for \( T_2 = 1 \) and \( T_1 = 9 \). \( T \) is same as in Fig.1 while \( T' \) denotes the spectral temperature and \( T_\nu \), the contact temperature, as defined in section IV. Inset shows the enlarged region around the point where all three temperatures are equal, which is at \( \eta = 1 - \sqrt{\theta} = 0.6667 \).

The second definition we consider is also called as the contact temperature \( (T_c) \). If a general nonequilibrium system whose different parts may be at different local temperatures, is brought in contact with such a heat bath, that some parts of the system give heat to the
latter and some absorb heat from it, so that the net heat transferred between the system and the bath is zero, then the temperature of that bath defines \( T \). \[23\] In other words, energy conservation holds for the system and different parts of it come to a common temperature equal to that of the heat bath. Thus for two TLS, we impose that the total mean energy calculated with canonical distributions for each TLS, corresponding to a temperature \( T_c \), is equal to the final mean energy \( U' = a_1s_2 + a_2p_2 \). The temperature obtained numerically is depicted in Fig. 2. The behaviour of the contact temperature is closer to the proposed definition in regions where subsystem temperatures are equal or nearly to each other. However, towards the extreme values of the engine efficiency, the two temperatures take on different values.

V. CONCLUSIONS

The notion of temperature is well understood in the domain of equilibrium thermodynamics. However, its extension to nonequilibrium situations is non-trivial. See for example \[24\] for a review of effective temperatures in nonequilibrium situations. In this paper, we have discussed a quantum heat engine in which two TLS prepared in different thermal states, undergo a unitary thermally isolated process and deliver work to an external work source. The final state of the two-TLS system is passive (i.e. no further work can be extracted from it) but a nonequilibrium state where each subsystem may have a different local temperature. We have proposed a thermodynamic definition to calculate effective temperature of the composite system in its final state. The obtained formula is very similar to the one expected on thermodynamic grounds. The proposed definition is compared with the spectral temperature, which seems to have a widely different behaviour. The other definition called contact temperature appears to have some semblence to our definition. All the three definitions converge for mutual equilibrium, but at Carnot limit or the vanishing efficiency they differ from each other significantly. Future experiments on measurement of temperatures in such systems may decide between the different definitions. Finally, it will be interesting to extend these ideas to more elaborate models such as involving entanglement between the TLS \[23\]. It is hoped that the present analysis will help to understand thermodynamic behaviour revealed by quantum heat engines.

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