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Quantum heat engines and nonequilibrium temperature

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A pair of two-level systems initially prepared in different thermal states and coupled to an external reversible work source do not in general reach a common temperature at the end of a unitary work extraction process. We define an effective temperature for the final nonequilibrium but passive state of the bipartite quantum system and analyze its properties.

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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 $T_f = (T_1)^{\xi/(1+\xi)} (T_2)^{1/(1+\xi)}$, where $\xi = C_1/C_2$.

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

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

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 [4–6]. Although the possibility of a quantum heat engine and validity of thermodynamic bounds has been recognized since the 1950s [7], the recent developments in nanotechnology and quantum information processing have contributed to enhanced interest in quantum thermodynamic machines [8,9]. Alongside, such models provide insight into fundamental questions about thermodynamics such as Maxwell's demon and universality of the second law [10–12]. Many models employ few-level quantum systems as the working medium, such as quantum harmonic oscillators, spin-systems, particle-in-box and so on [13–18]. 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 [19].

However, quantum engines being small systems, the validity of thermodynamic behavior 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 analyze its properties. The paper is organized as follows. In Sec. II, we introduce the model of quantum heat engine. In Sec. II A, the temperatures of subsystems are evaluated; the validity of thermodynamic definitions is enforced by deriving the specific heats of subsystems in Sec. 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 Sec. IV. Concluding ideas are given in Sec. 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 ρ_R and ρ_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 $\rho_{\text{in}} = \rho_R \otimes \rho_S$. 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 $\{r_1 s_1, r_1 s_2, r_2 s_1, r_2 s_2\}$. Here the probability to find each system in its excited state is

$$r_2 = \frac{1}{1 + e^{a_1/T_1}}, \quad s_2 = \frac{1}{1 + e^{a_2/T_2}}, \tag{3}$$

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 $U = a_1 r_2 + a_2 s_2$. 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 [4,6,19] 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 $\{r_1 s_1, r_2 s_1, r_1 s_2, r_2 s_2\}$. 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 $U' = a_1 s_2 + a_2 r_2$ and is given by

$$\mathcal{W}(a_1, a_2) = U' - U = (a_1 - a_2)(s_2 - r_2). \tag{4}$$

Net work is extracted if $\mathcal{W} < 0$ which requires the following condition:

$$s_2 < r_2 \Rightarrow \frac{T_1}{T_2} > \frac{a_1}{a_2}. \tag{5}$$

The efficiency of this engine is $\eta = 1 - a_2/a_1$, 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 $U_1' = a_1 s_2$, and $U_2' = a_2 r_2$. Let us consider two such setups 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

$$dU_1' = s_2 da_1 + a_1 \frac{ds_2}{da_2} da_2. \tag{6}$$

We follow the standard interpretation of work as the change in mean energy due to shift in energy levels at constant probabilities [16,20,21]. 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

$$dQ_1' = a_1 \frac{ds_2}{da_2} da_2. \tag{7}$$

Similarly for subsystem 2, we have

$$dQ_2' = a_2 \frac{dr_2}{da_1} da_1. \tag{8}$$

Let us now study entropy of each subsystem. In the initial state, the entropies of subsystems are given by $S_1 = -(r_1 \ln r_1 + r_2 \ln r_2)$ and $S_2 = -(s_1 \ln s_1 + s_2 \ln s_2)$, 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

$$dS_1' = dS_2 \tag{9}$$

$$= \frac{a_2}{T_2} \frac{ds_2}{da_2} da_2. \tag{10}$$

Now we evaluate the final temperature of system 1 as

$$T_1' \equiv \frac{dQ_1'}{dS_1'} = T_2 \frac{a_1}{a_2}. \tag{11}$$

Similarly, we obtain for system 2

$$T_2' = T_1 \frac{a_2}{a_1}. \tag{12}$$

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 $(T_1' < T_1)$, whereas 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 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

$$dT_1' = \frac{T_2}{a_2} da_1 - \frac{a_1 T_2}{(a_2)^2} da_2. \tag{13}$$

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 Eq. (6)], the heat capacity (at constant volume) in the final state of system 1 is

$$C_1' = \left(\frac{\partial U_1'}{\partial T_1'} \right)_{a_1} \tag{14}$$

$$= C_2, \tag{15}$$

where we have used the following identity:

$$-\frac{ds_2}{da_2} = \frac{C_2 T_2}{(a_2)^2}. \tag{16}$$

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 become equal. In the quantum framework, the subsystems in general do not reach mutual thermal equilibrium. In the next section, we ask the following: can the whole bipartite system be characterized 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 are determined by a single parameter ν, 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 ν but which may yield different amounts of work.

At a given value of ν, the changes in a_1 and a_2 are related as

$$da_2=\nu da_1. \tag{17}$$

Thus, the heat exchanged by system 1 in such a process can be rewritten from Eq. (7) as

$$dQ_1'=a_1\frac{ds_2}{da_2}\nu da_1 \tag{18}$$

$$=a_2\frac{ds_2}{da_2}da_1. \tag{19}$$

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

$$dS'=\left[\left(\frac{dS_1}{da_1}\right)+\nu\left(\frac{dS_2}{da_2}\right)\right]da_1, \tag{20}$$

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

$$T=\frac{a_2\left(\frac{ds_2}{da_2}+\frac{dr_2}{da_1}\right)}{\left(\frac{(a_2)^2}{a_1T_2}\frac{ds_2}{da_2}+\frac{a_1}{T_1}\frac{dr_2}{da_1}\right)}. \tag{21}$$

Using Eq. (16) and $-dr_2/da_1=C_1T_1/(a_1)^2$, we finally get

$$T=\frac{C_2T_1'+C_1T_2'}{(C_1+C_2)}. \tag{22}$$

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

$$C_i=\left(\frac{a_i}{T_i}\right)^2\frac{\exp[a_i/T_i]}{(1+\exp[a_i/T_i])^2}. \tag{23}$$

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

$$\frac{T}{T_1}=\frac{\sqrt{\xi}}{(1+\xi)}(1+\theta). \tag{24}$$

At Carnot limit, $\xi\to 1$ and $T/T_1=(1+\theta)/2$. However, note that this formula holds in general also, because Carnot limit implies $a_1/T_1\to a_2/T_2$ and so $C_1/C_2\to 1$. 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 $\xi\to\theta^2$, we have $T/T_1=(\theta+\theta^2)/(1+\theta^2)$.

In other words, when $a_2\to a_1$, $\mathcal{W}\to 0$ [see Eq. (4)]. Then $T_1'=T_2$ and $T_2'=T_1$ in this limit. In this case, the effective temperature is simplified to

$$\frac{T}{T_1}=\frac{(\theta+\xi)}{(1+\xi)}. \tag{25}$$

Finally, we make the following observations:

(i) It is interesting to note that the effective temperature is a weighted average of the subsystem temperatures after work extraction.

(ii) The overall temperature is the same as the subsystem temperature when the latter are also equal to each other. This corresponds to $\nu=\sqrt{\theta}$, which implies the well-known Curzon-Ahlborn efficiency [22].

(iii) At the global maximum of work, the conditions $\partial\mathcal{W}/\partial a_1=0$ and $\partial\mathcal{W}/\partial a_2=0$ 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 ξ^* 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

$$\frac{T^*}{T_1}=\frac{2\sqrt{\xi^*}}{(1+\xi^*)}\sqrt{\theta}. \tag{28}$$

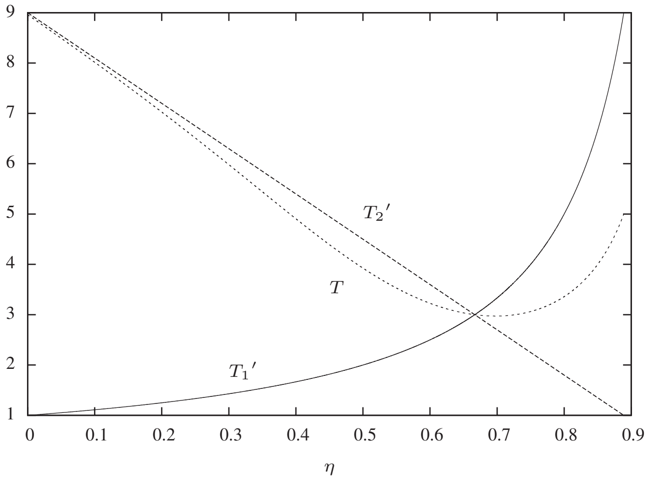

FIG. 1. For $T_2=1$ and $T_1=9$, the subsystem temperatures T_1', T_2' and the effective temperature T of the composite system evaluated at maximum work corresponding to a given efficiency. T is given by a weighted average over the subsystem temperatures and so its curve lies in between the curves for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

(iv) Figure 1 shows the behavior of subsystem and effective temperatures as function of efficiency. Particularly, T shows a nonmonotonic trend. For a given value of η, T in Fig. 1 corresponds to that engine setup 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.

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 [9]. 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 nondegenerate spectrum, the inverse of spectral temperature is defined to be

$$\frac{1}{T_s} = -\left(1 - \frac{P_0 + P_M}{2}\right)^{-1} \sum_{i=1}^{M} \left(\frac{P_i + P_{i-1}}{2}\right) \frac{\ln P_i - \ln P_{i-1}}{E_i - E_{i-1}}, \tag{29}$$

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 final state after work extraction, using the values $\{E_i\} \equiv \{0, a_2, a_1, a_1 + a_2\}$ and $\{P_i\} \equiv \{r_1 s_1, r_2 s_1, r_1 s_2, r_2 s_2\}$, the (inverse) spectral temperature is explicitly given by

$$\frac{1}{T_s} = \frac{1}{T_1'} \frac{(\nu - \theta)}{(\nu - \nu^2)} \frac{x}{(1+x)} + \frac{1}{T_2'} \frac{1}{(1+x)}, \tag{30}$$

where $x = (r_1 + s_1 - 2 r_1 s_1)$. The special cases include the following: Carnot limit, when $\nu \rightarrow \theta$ and so $T_s = (1+x) T_2'$; when

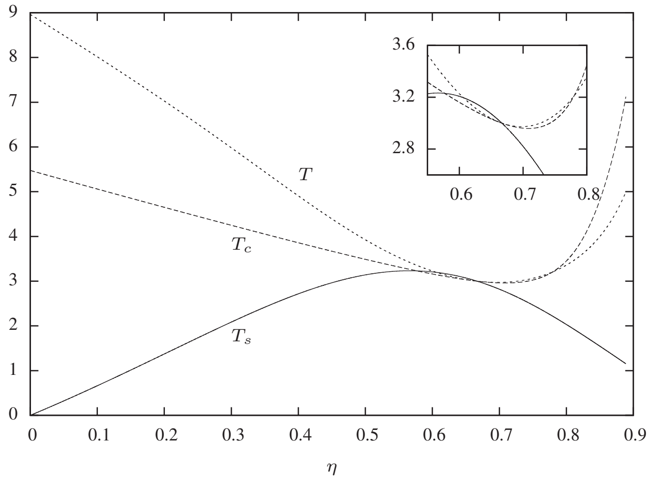

FIG. 2. Comparison between other definitions of nonequilibrium temperatures for $T_2=1$ and $T_1=9$. T is same as in Fig. 1 while T_s denotes the spectral temperature and T_c, the contact temperature, as defined in Sec. IV. The inset shows the enlarged region around the point where all three temperatures are equal, which is at $\eta = 1 - \sqrt{\theta} = 0.6667$.

$\nu \rightarrow 0$, $T_s \rightarrow 0$. Finally, for CA efficiency ($\nu = \sqrt{\theta}$), the spectral temperature is equal to the subsystems' temperature. In general, the behavior of T_s as shown in Fig. 2 is quite different from the proposed definition.

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_c [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 $U' = a_1 s_2 + a_2 r_2$. The temperature obtained numerically is depicted in Fig. 2. The behavior of the contact temperature is closer to the proposed definition in regions where subsystem temperatures are equal or nearly to each other. However, toward 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 nontrivial. 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 behavior. The other definition called contact temperature appears to have some semblance 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 [25]. It is hoped that the present analysis will help to understand thermodynamic behavior revealed by quantum heat engines.

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