

The Second Law, Maxwell's Demon, and Work Derivable from Quantum Heat Engines

Tien D. Kieu*

Centre for Atom Optics and Ultrafast Spectroscopy, Swinburne University of Technology, Hawthorn 3122, Australia
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With a class of quantum heat engines which consists of two-energy-eigenstate systems undergoing, respectively, quantum adiabatic processes and energy exchanges with heat baths at different stages of a cycle, we are able to clarify some important aspects of the second law of thermodynamics. The quantum heat engines also offer a practical way, as an alternative to Szilard's engine, to physically realize Maxwell's demon. While respecting the second law on the average, they are also capable of extracting more work from the heat baths than is otherwise possible in thermal equilibrium.

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Present technology allows for the probing and realization of quantum mechanical systems of mesoscopic and even macroscopic sizes, which can also be restricted to a relatively small number of energy states. It is thus important to study these quantum systems directly in relation to the second law of thermodynamics, which has been applicable to composite systems. We pursue this path below without assuming *for the systems* anything extra and beyond the principles of quantum mechanics [1]. Our study is part of a growing body of investigations into quantum heat engines [3–8]. Explicitly, the only principles we need are those of the Schrödinger equation, the Born probability interpretation of the wave functions, and the von Neumann measurement postulate [9]. In particular, we do not exclude, but make full use of, any exceptional initial conditions, as long as they are realizable physically. However, without a better understanding of the emergence of classicality from quantum mechanics, we have to assume the thermal equilibrium Gibbs distributions *for the heat baths* which are coupled to the quantum systems. This assumption is *extra* to those of quantum mechanics.

The expectation value of the measured energy of a quantum system is $U = \langle E \rangle = \sum_i p_i E_i$, in which E_i are the energy levels and p_i are the corresponding occupation probabilities. Infinitesimally,

$$dU = \sum_i (E_i dp_i + p_i dE_i), \quad (1)$$

from which we make the following identifications for infinitesimal heat transferred dQ and work done dW ,

$$dQ := \sum_i E_i dp_i; \quad dW := \sum_i p_i dE_i. \quad (2)$$

Thus, Eq. (1) is just an expression of the first law, $dU = dQ + dW$. These identifications concur with the fact that work done on or by a system can be performed only through a change in the generalized coordinates of the system, which in turn gives rise to a change in the distribution of the energy levels [10].

Our quantum heat engines are just two-level quantum systems, which are the quantum version of the Otto engines [7]. (They are readily extendable to systems of many discrete energy levels.) They could be realized with coherent macroscopic quantum systems like, for instance, a Bose-Einstein condensate confined to the bottom two-energy levels of a trapping potential. The exact cyclicity is enforced to ensure that upon completing a cycle all the output products of the engines are clearly displayed without any hidden effect.

A cycle of the quantum heat engine has four stages.

(1) *Stage 1.*—The system has the probability $1 - p_u^{(1)}(0)$ in the lower state *prior* to some kind of contact with a heat bath at temperature T_1 . After some contact time τ_1 , the system achieves a probability $p_u^{(1)}(\tau_1)$ to gain some energy from the heat bath to jump up an energy gap of Δ_1 to be in the upper state. Only heat is transferred in this stage to yield a change in the occupation probabilities.

(2) *Stage 2.*—The system is then isolated from the heat bath and undergoes a quantum adiabatic expansion to reduce the energy gap from Δ_1 to a smaller value Δ_2 . The probability in the upper state is maintained throughout (provided the expansion rate is sufficiently slow according to the quantum adiabatic theorem [11]); an amount of work is thus performed *by* the system, but no heat is transferred.

(3) *Stage 3.*—The system, with a probability $p_u^{(2)}(0)$ being in the upper state, is brought into some kind of contact with another heat bath at temperature T_2 for some time τ_2 until it gains a probability $1 - p_u^{(2)}(\tau_2)$ to release some energy to the bath and jump down the gap Δ_2 to be in the lower state.

(4) *Stage 4.*—The system is removed from the heat bath and undergoes a quantum adiabatic contraction to increase the energy gap from Δ_2 back to the larger value Δ_1 . An amount of work is performed *on* the system.

Note that we need not and have not assigned any temperature to the quantum system; all the temperatures are properties of the heat baths, which are assumed to be in the Gibbs state. However, in the operation above, the

absorption and release of energy in stages 1 and 3 occur neither definitely nor even deterministically. Quantum mechanics tells us that they can happen only probabilistically, and the probabilities that such transitions take place depend on the details of the interactions with and some intrinsic properties (namely, the temperatures) of the heat baths. The cyclicity of the heat engines then puts a constraint on the probabilities, $p_u^{(1)}(0) = p_u^{(2)}(\tau_2)$ and $p_u^{(2)}(0) = p_u^{(1)}(\tau_1)$. The net work done by our quantum heat engines in the two quantum adiabatic passages in stages 2 and 4 is, from (2), given that $\Delta_1 > \Delta_2$,

$$\Delta W = (p_u^{(1)}(\tau_1) - p_u^{(2)}(\tau_2))(\Delta_2 - \Delta_1). \quad (3)$$

If the system is allowed to thermalize with the heat baths in stages 1 and 3, the thermal equilibrium probabilities, for $i = 1, 2$,

$$\tilde{p}_u^{(i)} = 1/[1 + \exp(\Delta_i/kT_i)], \quad (4)$$

are to be used in (3). These probabilities are definitely *nonzero*. Thus, even in the case of ($T_1 \leq T_2$) there *exist*, even with a small probability $\tilde{p}_u^{(1)}(1 - \tilde{p}_u^{(2)})$, cycles in which the transitions described in stages 1 and 3 above actually take place. (The probability, however, diminishes exponentially for n_c consecutive cycles, $[\tilde{p}_u^{(1)}(1 - \tilde{p}_u^{(2)})]^{n_c}$, in all of which the system performs net work on the environment.) As a result, there *are* certain cycles whose sole result is the absorption of heat from a reservoir and the conversion of this heat into work, of the amount $(\Delta_1 - \Delta_2)$. This amounts to a violation of the Kelvin-Planck statement of the second law due to the explicit probabilistic nature of quantum mechanical processes. This violation, however, occurs only randomly, with some small probability, and thus is not exploitable.

However, there exists a sure way to *always* extract work, to the amount of $(\Delta_1 - \Delta_2)$, in each completed “cycle.” In order to eliminate the probabilistic uncertainty, we prepare the system to be in the lower state prior to stage 1; we make an energy measurement after stage 1 and let the engine continue to stage 2 only *if* the measurement result confirms that the system is in the upper state; and then we make another measurement after stage 3 and let the engine continue to stage 4 only *if* the measurement result confirms that the system is in the lower state. All this can be carried out even for the case $T_1 \leq T_2$ to extract, in a controllable manner, some work which would have been otherwise prohibited by the second law. This apparent violation of the second law is analogous to that of Szilard’s one-atom engine and is nothing but the result of an act of Maxwell’s demon [12]. Our quantum heat engines can thus provide a feasible and quantum way to realize Maxwell’s demon in a different way to Szilard’s engine. Indeed, the condition of strict cyclicity of each engine’s cycle is broken here. After each cycle the measurement apparatus, being a Maxwell’s demon, has already registered the results which are

needed to determine the *next* stages of the engine’s operation. In this way, there are extra effects and changes to the register/memory of the apparatus, even if we assume that the quantum measurement steps themselves cost no energy and leave no net effect anywhere else. To remove these remnants in order to restore the strict cyclicity, we would need to bring the register back to its initial condition by erasing any information obtained in the cycles, either by resetting its bits or by thermalizing the register with some heat bath. For whichever way, extra effects are inevitable, namely, an amount of heat of at least $kT \ln 2$ is released per bit erased. The second law is thus saved [13]. More extensive discussions and debates on these issues can be found in the literature [12].

Despite the random quantum mechanical violation, the second law is upheld on the average. The work that can be performed *by* our engines in thermal equilibrium when and only when, as can be seen from (3), $p_u^{(1)}(\tau_1) > p_u^{(2)}(\tau_2)$, and thus when and only when, from (4),

$$T_1 > T_2(\Delta_1/\Delta_2). \quad (5)$$

The expressions (3) and (5) (which were also derived in a more specific context in [14]) not only confirm the broad validity of the second law but also refine the law further in specifying how much T_1 needs to be larger than T_2 before some work can be extracted. In other words, *work cannot be extracted, on the average, even when T_1 is greater than T_2 but less than $T_2(\Delta_1/\Delta_2)$* , in contradistinction to the classical necessary condition that T_1 needs only to be larger than T_2 . (However, for Carnot’s engines—see [7]—the ratio of successive energy gaps involved tends to one.)

The efficiency of our engines is [15]

$$\eta_q = \Delta W/Q_{\text{in}} = (1 - \Delta_2/\Delta_1), \quad (6)$$

which is *independent* of heat bath temperatures and is the maximum available within the law of quantum mechanics. This also serves as the upper bound, with appropriate Δ_1 and Δ_2 , of the efficiency of any heat engine, including Carnot’s engines, because the work performed by our heat engines through their quantum adiabatic processes is the maximum that can be extracted [17]. The efficiency of Carnot’s engines, $\eta_C = 1 - T_2/T_1$, can be derived from (6) through an infinite number of infinitesimal quantum adiabatic processes [7].

We present next a modification of the quantum heat engines which can better the work derivation than that available from thermal equilibrium. A modified cycle also has four stages, of which stage 2 and stage 4 remain the same as described previously, whereas stages 1 and 3 are replaced, respectively, by the following.

(1) *Stage 1'*.—The system is entered to a single-mode cavity which is tuned to match the energy gap Δ_1 of the system and which is in thermal equilibrium with a heat bath at temperature T_1 . The thermal distribution for the

cavity mode is given by (7) below. After some time interval τ_1 , the system is removed from the cavity.

(2) *Stage 3'*.—Like stage 1' above but with temperature T_2 and smaller energy gap Δ_2 . After some time τ_2 , the system departs the cavity for stage 4.

In each of the cavities so described, the state of the system satisfies the Schrödinger equation for a single two-level atom interacting with a single-mode field which has

the thermal probability $P_n(T_i)$ to find exactly n photons of frequency Δ_i/h in the cavity at temperature T_i ,

$$P_n(T_i) = \frac{1}{1 + \bar{n}_i} \left(\frac{\bar{n}_i}{1 + \bar{n}_i} \right)^n, \quad (7)$$

where \bar{n}_i is the thermal average boson number, $\bar{n}_i = 1/(e^{\Delta_i/kT_i} - 1)$. The *exact* solution of this Schrödinger equation is given in [18], from which we arrive at

$$p_u^{(i)}(t) = \frac{(1 + 2\bar{n}_i)p_u^{(i)}(0) - \bar{n}_i}{(1 + \bar{n}_i)} \sum_{n=0}^{\infty} P_n(T_i) \cos^2(\Omega_n t) + \frac{\bar{n}_i(1 - p_u^{(i)}(0))}{1 + \bar{n}_i}, \quad (8)$$

where $\Omega_n = g\sqrt{n+1}$ and g is the coupling constant between the system and the cavity mode. From (8) we can derive the bounds of the probability $p_u^{(i)}(t)$ in terms of the initial probability and temperature,

$$\begin{aligned} p_u^{(i)}(t) &\in [p_u^{(i)}(0), \bar{n}_i(1 - p_u^{(i)}(0))/(1 + \bar{n}_i)], & \text{for } p_u^{(i)}(0) \in [0, \bar{n}_i/(1 + 2\bar{n}_i)]; \\ p_u^{(i)}(t) &\in [\bar{n}_i(1 - p_u^{(i)}(0))/(1 + \bar{n}_i), p_u^{(i)}(0)], & \text{for } p_u^{(i)}(0) \in [\bar{n}_i/(1 + 2\bar{n}_i), 1]. \end{aligned} \quad (9)$$

Figure 1 depicts these bounds. The probability at any subsequent time is only accessible in the bounded, dark triangular areas, each of which corresponds to a different temperature, on the two sides of the diagonal. For the cavity in contact with the heat bath at T_1 , we want to have the exit probability to be greater (the greater, the better) than the initial probability, $p_u^{(1)}(\tau_1) > p_u^{(1)}(0) = p_u^{(2)}(\tau_2)$; thus we need to consider only the lower area for this temperature. Reversely, for the cavity in contact with the heat bath at T_2 , we want to have the exit probability to be smaller (the smaller, the better) than the initial probability, $p_u^{(2)}(\tau_2) < p_u^{(2)}(0) = p_u^{(1)}(\tau_1)$; hence we need to consider only the upper area for this temperature. Thus, Fig. 1 combines the two heat baths in which the upper area comes from T_1 and the lower from T_2 , with $T_1 = T_2(\Delta_1/\Delta_2)$. The coordinate of a point A in the lower area of Fig. 1 is $(p_u^{(2)}(0), p_u^{(2)}(\tau_2))$, representing an exit probability less than the entry one at the cavity with temperature T_2 . The corresponding point at temperature

T_1 must have, by requirement of cyclicity, the coordinate $(p_u^{(1)}(0), p_u^{(1)}(\tau_1)) = (p_u^{(2)}(\tau_2), p_u^{(2)}(0))$, which thus is the reflection of the point A across the diagonal. However, it is clearly seen that for $T_1 \leq T_2(\Delta_1/\Delta_2)$ this reflection is *not* in the accessible upper area. We then conclude that at these temperatures, even with T_1 greater than T_2 by a factor (Δ_1/Δ_2) , the quantum heat engines *cannot* do work *on the average*. Thus, we have once again confirmed the second law that, *on the average*, no process is possible whose sole result is the transfer of heat from a cooler to a hotter body, with or without a production of work. But we have also clarified the degrees of coolness and hotness in terms of the quantum energy gaps involved before such a process is possible; namely, we must have, as a *necessary* but not sufficient condition, $T_1 > T_2(\Delta_1/\Delta_2)$ as in (5).

The perfect agreement between this specific result derived from the quantum dynamical bounds (9) with the general result (5) derived from statistical mechanics is quite remarkable—but is yet to be fully understood and hence deserved further investigation elsewhere. We speculate that such agreement is not accidental but is a consequence of the Gibbs distributions assumed for the heat baths in both derivations; and it should thus be independent of specific details of the dynamics.

Figure 2 combines the cases T_2 and $T_1 > T_2(\Delta_1/\Delta_2)$ in which there is some overlap between the areas above the diagonal and thus makes possible the production of some work, ΔW_{cav} . If and when we choose to operate with a point below the thermal equilibrium line in the lower area (for T_2) such that its reflection across the diagonal is above the thermal equilibrium line in the upper area (for T_1) as shown in the figure, we can derive more work than the case of thermal equilibrium, ΔW_{th} . This is because the net work done is proportional to the difference in probabilities as shown in (3). Here $|\Delta W_{\text{cav}}|$ is greater than $|\Delta W_{\text{th}}|$ because the vertical distance between point A and its reflection in Fig. 2 is greater than the vertical distance between the two horizontal lines, which represent the two thermal equilibria.

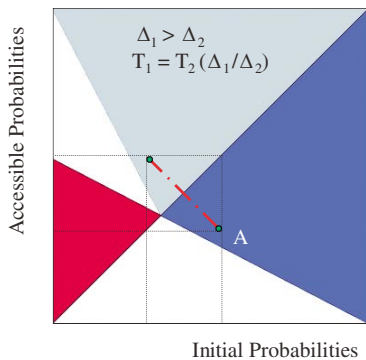


FIG. 1 (color online). For the cavity in contact with a heat sink at T_2 , the accessible probability at all times, given a particular initial probability, is bounded in the area under the diagonal, with its reflection shown in gray above the diagonal. The other bounded area above the diagonal is for the cavity in contact with a heat bath at $T_1 = T_2(\Delta_1/\Delta_2)$.

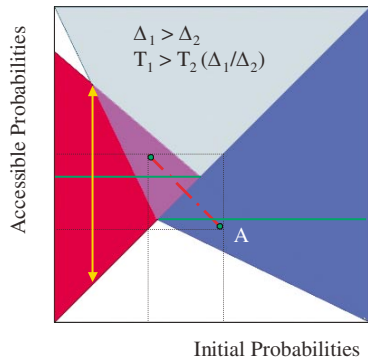


FIG. 2 (color online). Similar to Fig. 1 but this time with $T_1 > T_2(\Delta_1/\Delta_2) > T_2$. The maximum work can be extracted in a single cycle is proportional to the length of the vertical double arrow.

In summary, by interpreting work and heat, but without introducing entropy directly, in the quantum domain and by applying this interpretation to the simplest quantum systems of two levels, we have not only confirmed the broad validity of the second law but also been able to clarify and refine its various aspects. On the one hand, the second law is seen to be valid *on the average* in the broad sense. On the other hand, explicitly because of the probabilistic nature of quantum mechanics, there do exist physical processes which can violate certain classical statements of the second law. (Such violation, which can be observed in some cycles of our two-level heat engine, may not be observable in any single cycle for a system that consists of many subsystems, because the averaging effects over the subsystems already occur in *each* cycle for the composite system.) However, such violation occurs only randomly and can thus be neither exploitable nor able to be harnessed. This confirmation of the second law is in accordance with the fact that, while we can treat the quantum heat engines purely and entirely as quantum mechanical systems, we still have to assume the Gibbs distributions *for the heat baths* involved. Such distributions can be derived [17] only with non-quantum-mechanical assumptions, which ignore any quantum entanglement within the heat baths. Indeed, it has been shown that [19,20] the law of entropy increase is a mathematical consequence of the initial states being in such general equilibrium distributions. This illustrates and highlights the connection between the second law to the unsolved problems of emergence of classicality, of quantum measurement, and of decoherence, all of which are central to quantum mechanics. Only until some further progress can be made on these problems, the classicality of the heat baths will have to be assumed and remain in the assumption of the Maxwell-Boltzmann-Gibbs thermal equilibrium distributions.

We have also clarified the degree of temperature difference (5), in terms of the quantum energy gaps involved, between the heat baths before any work can be extracted. We have also shown how to extract more work

from the heat baths than otherwise possible with thermal equilibrium. Note that such an operation is subject to the bounds given in (9), which then, as can be seen through their depiction in the figures, ensure that we stay within the second law. Note also that this is not an operation of Maxwell's demon because the information about the time intervals τ_1 and τ_2 is fixed and forms an integrated part of the modified engines. This information, being common to *all* cycles, need not and should not be erased after each cycle. Finally, our class of quantum heat engines can readily offer a feasible way to physically realize Maxwell's demon, in a way different from Szilard's engine but also through the acts of quantum measurement and information erasure.

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*Electronic address: kieu@swin.edu.au

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