



Quantum coherence and Carnot engines

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Abstract

A four-level atom is used to model recently proposed quantum systems that have challenged the fundamental principles of thermodynamics. The simplicity of our system should help evaluate those challenges.

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1. Introduction

In the last few years examples have been provided in which quantum coherence has been translated into work. This applies in varying degrees to Refs. [1–7]. In this article, we simplify such exploitation so as to focus on its essential features.

The motive for simplicity is clear. Historically, apparent contradictions to the second law were often hidden behind technicalities. In our attempts to understand the schemes referred to above, we found that they involved techniques of condensed matter physics, statistical mechanics, quantum optics and more. Some of these techniques carry

with them approximations, so that an exhaustive check requires considerable expertise. Nevertheless, even our simple example has subtleties that truly come with the territory: in particular, the work/heat distinction.

We first present a degenerate two-state system in contact with a single heat bath and evaluate both the work available from coherence and the cost of purifying to recover coherence. Next we consider a two-level system which has a radiative transition between these levels and which is in contact with a single heat bath. We then suppose that a single object is described by a Hilbert space that is the product of those of the two foregoing systems. This object is led through a Carnot cycle, like that in Ref. [1], in which it radiates but is restored to its original state. Despite being in contact with a single heat bath, the system seems to perform net

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positive work. A feature of our example is that for the purpose of getting work, what replaces the low temperature reservoir is *information*. The efficiency of our cycle is less than unity. Nevertheless, it at first appears that the net change in entropy of the universe is *negative*. We discuss where a missed entropy contribution enters. Finally, in an appendix we show that obtaining work from information is already (in a well-known way) present in classical thermodynamics.

2. Two-state system

Let A and B be degenerate quantum states of a system, to be called an “atom”. They form symmetric and antisymmetric combinations, P and M :

$$\begin{aligned} |P\rangle &= \frac{1}{\sqrt{2}}[|A\rangle + |B\rangle] \quad (\text{“plus”}), \\ |M\rangle &= \frac{1}{\sqrt{2}}[|A\rangle - |B\rangle] \quad (\text{“minus”}). \end{aligned} \quad (1)$$

There is a heat bath or reservoir, R , at temperature T that can be brought into contact with them. Take units with Boltzmann’s constant, k_B , unity and define $\beta \equiv 1/T$. R allows transitions between the states. We ignore the in-principle level-splitting due to this coupling, assuming it to be much smaller than the energy level changes now to be considered. We do not attempt to model R [8]. Thus, in the absence of other influences, the energy of all the four states (A, B, P, M) is the same. We take this energy to be zero.

An external object, to be called a “magnet,” will be assumed to couple to the atom when it is in M , but not when it is in P . Its role is that of a piston. We do not flesh out our model to the point where it involves bona fide magnetic fields. This fictive magnet can be brought to various distances from the atom. When it is far away, the coupling energy to M is zero; as it gets closer we assume the coupling energy increases without limit. With distance measured by “ r_M ,” there is some function $E_M(r_M)$, with $E_M(\infty) = 0$ and $E_M(0) = \infty$. The actual r_M -dependence is unimportant.

Assume that initially the atom is in P , and not connected to R . Since M is unoccupied it costs nothing to bring the magnet close. Quantum coherence matters, since it is only because of the phase relation between A and B that the magnet can approach with no change in energy and thus no force.

Now couple to the heat bath. For r_M ever so slightly positive, $E_M < \infty$, and the state M is occupied with non-zero probability. There is therefore a force *pushing* on the magnet, since moving the magnet farther away decreases its coupling energy. Energy flows, to and from R , will be analyzed, but the overall picture is that in the course of the process the system is doing work on the magnet, only possible by virtue of its initial coherence.

We will calculate the work available due to this coherence. But we also calculate the work needed to recreate the initial coherent state. There will be no free lunch. Coherence is converted to work with the help of R ; nevertheless, producing coherence costs the same amount of work.

3. Extracting work in the two-state system

Work is extracted from coherence with the following two-step process:

1. Withdraw magnet; heat bath uncoupled

Let the magnet be at r_M such that $E_M(r_M) = E$. Then M is occupied with a probability

$$P_M = y/Z \quad \text{with } y \equiv e^{-\beta E} \text{ and } Z \equiv 1 + y. \quad (2)$$

The expected internal energy U of the system is

$$U = \langle \text{Internal Energy} \rangle = yE/Z. \quad (3)$$

Moving the magnet farther changes E_M to $E - dE$. Due to the coupling, the magnet can be thought of as being in a field of potential energy. The field, and hence the system, has done work on the magnet in the amount

$$dW = P_M dE = y dE/Z. \quad (4)$$

2. Couple to heat bath; keep magnet fixed

With the energy lowered in step 1, level occupations are distorted. Coupling to R restores

them to their proper values, as given in Eq. (2), with $E \rightarrow E - dE$. This restoration requires heat flow in the amount

$$dU = d\frac{yE}{Z} = \frac{y dE}{(1+y)^2} [1+y - E\beta]. \quad (5)$$

Perform these two steps many times, until $r_M \rightarrow \infty$ and the magnetic coupling energy is zero (and the system is equal parts P and M). The total work performed by the system is

$$\begin{aligned} W &= \int P_M dE = \int \frac{y}{1+y} dE \\ &= \int \frac{y}{1+y} \left(\frac{-1}{\beta} \right) \frac{dy}{y} = \frac{1}{\beta} \log 2, \end{aligned} \quad (6)$$

where the limits on the range of E correspond to $0 \leq y \leq 1$. The total heat transfer can be calculated by integrating Eq. (5), or, more simply, directly from Eq. (3). By Eq. (3), U is zero both for infinite and zero energy. This implies that although energy passes in both directions, the net heat transfer is zero. [Eq. (5) implies that at early stages heat goes from R to the system, and later, when the change in occupancy is less important than the change in energy, it goes back to R .]

Two conclusions follow: (1) Work in the amount $T \log 2$ is extracted, based on coherence. (2) Although the heat bath is essential for the coupling and for intermediate energy bookkeeping, there is no *net* heat transfer.

To complete a Carnot cycle we must restore the system to its initial state, P . We do not know a better way to do this than the process just described, run backwards. No profit. No loss. No contradictions.

4. Two-state system with radiation

Consider a different system. It will later be combined with that of Sections 2 and 3. This system, also to be called an atom, has two states, U (up) and D (down). It is in contact with a different heat bath, R' , also at temperature T , and can radiate, emitting a photon and dropping from U to D . Let D have energy 0 and U have energy ε . The occupations of upper and lower states are

respectively $x/(1+x)$ and $1/(1+x)$, with $x \equiv \exp(-\beta\varepsilon)$. When a photon is emitted by this atom, is its energy to be considered heat or work?

The work/heat distinction is one of the profound issues of thermodynamics; without it there is no Second Law. In a previous publication we have studied the definition of *macroscopic* that is implicit in this distinction [9], but for now it is not necessary to probe so deeply. We adopt the standard perspective that work is energy without entropy. This means that the energy is stored in one or a small number of degrees of freedom. One can also think of work as energy at infinite temperature. In the well-known example of a three-level maser acting as a heat engine [10], the authors only ascribe work to the radiated photon when it is emitted coherently, with the system functioning as a maser. Another situation where a photon's energy is work is when it goes off into the vacuum with no chance of return, and no possibility that other photons enter via the channel by which this one left. This "vacuum" acts as a zero-temperature reservoir. If you are in contact with a zero-temperature reservoir then your heat can be considered work, since the Carnot efficiency is unity.

Scully's one-temperature work source [1] has a further subtlety. The maser cavity that accepts radiation acts as a one-way channel because only excited atoms are exposed to the cavity. If unexcited atoms were to enter the cavity, they could absorb energy, and Scully's scheme would fail. Thus, the fact that these photons provide work arises from *information* that you have about the beam entering the cavity. The one-way passage of energy *to* the cavity does not arise because the cavity has zero temperature (its temperature is essentially irrelevant), but because of what we know about the system state. This sorting of states is accomplished by what one might call a Stern–Gerlach–Maxwell demon [1]. (Regarding measurement, see Ref. [11].)

5. Four-state system

We combine the systems so far studied into a two degree of freedom atom. The full state is

specified by pairs of labels; one is for U vs. D , the other for A vs. B (or P vs. M). The $A/B/P/M$ coordinate will be called “ r ” and the U/D coordinate “ q .” The r coordinate will be used to sort for the q state, very much as the position is used in Ref. [1]. R and R' are both heat baths at temperature T , but affect q and r in different ways.

Initially r is in P and the system is in contact with R' . See Fig. 1. This heat bath does not facilitate $A \leftrightarrow B$ (or $P \leftrightarrow M$) transitions. The radiation channel (to the external world) is not open and the four possible states have the following probabilities:

$$\begin{aligned} \Pr(|PU\rangle) &= \frac{x}{1+x}, & \Pr(|PD\rangle) &= \frac{1}{1+x}, \\ \Pr(|MU\rangle) &= 0, & \Pr(|MD\rangle) &= 0. \end{aligned} \tag{7}$$

Next, contact with R' is broken and the system is sorted according to q as follows. An operator that exchanges $|PU\rangle$ and $|MU\rangle$, while leaving the other two states unchanged, is unitary. Call this operator \mathcal{S} and assume that it possesses a physical realization [12]. Since $|MU\rangle$ was unoccupied, the exchange gives $|MU\rangle$ probability $x/(1+x)$. Following Ref. [1], we assume that the P/M distinction determines whether, the atom passes through a cavity, a cavity in which U -state atoms always radiate (inducing excitation in the radiation field). The cavity, in which D -state atoms could actually absorb radiation, thus acts as a

one-way channel by virtue of the selection of what enters it, despite its not being at zero temperature. The work extracted in this way is $W = \epsilon x/(1+x)$. After passage through the cavity (and excitation of the cavity state, no photon emission, so far) the atom’s wave function is a superposition of $|PD\rangle$ and $|MD\rangle$. However, do not forget that it is now entangled with the electromagnetic field of the cavity, so it would be more accurate to write these states as $|PD, n\rangle$ and $|MD, n+1\rangle$ where n is the initial number of photons in the cavity.

As above, this is not a Carnot cycle until we have restored the initial condition. This can be done by the procedure of Section 3. We assume the magnet implements a measurement, presumably because we notice whether or not a force is being exerted on it [13]. After purification by R and the magnet, the system is no longer entangled with the cavity and is entirely in the state $|PD\rangle$, and could be reconnected to the heat bath for another cycle.

5.1. Net work

Since the work needed to purify is $(1/\beta)\log 2$, and this is applied with probability $x/(1+x)$, the net work is

$$\begin{aligned} W_{\text{net}} &= \frac{\epsilon x}{1+x} - \frac{1}{\beta} \frac{x}{1+x} \log 2 \\ &= -\frac{1}{\beta} \frac{x}{1+x} (\log x + \log 2) \end{aligned} \tag{8}$$

(using $x = \exp(-\beta\epsilon)$). This quantity can take both signs, and is maximal (and positive) for $x_{\text{max}} \approx 0.1572$ [so that $E_{\text{max}} = (-1/\beta)\log x_{\text{max}} \approx (1/\beta)1.8503$]. The maximal net work is easily seen to be $W_{\text{net}} = (1/\beta)x_{\text{max}}$.

5.2. Efficiency

The efficiency of this system is less than unity. The “work out” comes from photons, while “work in” is required for the purification process. Efficiency is given by net work, divided

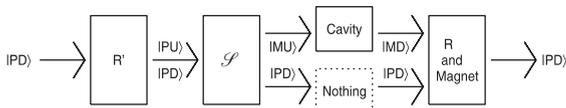


Fig. 1. A full cycle, from $|PD\rangle$ to $|PD\rangle$. Heat is supplied by the reservoir R' , and raises a fraction of the atoms to the U state. The device \mathcal{S} distinguishes between U and D states, and in particular changes the state $|PU\rangle$ to $|MU\rangle$ and sends those atoms into the cavity. Work is extracted from them, and when they exit the cavity they are in the state $|MD\rangle$. Work is then supplied in the “ R and Magnet” stage for purification, but no net heat is transferred. R and R' are at the same temperature, T . Although it is convenient to use the terminology, “these atoms go here, those go there,” the discussion actually applies to the density matrix of a single atom.

by heat, namely

$$\eta = \frac{W_{\text{net}}}{\text{heat in}} = \frac{-\frac{1}{\beta} \frac{x}{1+x} \log(2x)}{-\frac{1}{\beta} \frac{x}{1+x} \log(x)} = 1 + \frac{\log 2}{\log x} = 1 - \frac{T}{\varepsilon} \log 2. \quad (9)$$

This quantity approaches one for decreasing T and increasing ε , but the profit is small in this limit.

6. Significance—and a turnabout

It appears that we have obtained work from a system in contact with a single temperature. There is no need for a low-temperature reservoir, since the operation of the one-way channel is accomplished through the use of information.

6.1. Entropy

By the second law of thermodynamics the total entropy of the universe should increase or remain constant. In the course of one cycle our system returns to its original state ($|PD\rangle$). Therefore, the entropy of everything else should increase or remain constant.

The work created in the cavity equals the energy lost by R' . Per atom, that heat thus equals the radiation energy, which is work, and is $x\varepsilon/(1+x)$. The reduction of energy in R' means a decrease of entropy (of the universe)

$$(\Delta S)_{\text{due to heat bath}} = -\frac{\Delta Q}{T} = -\beta\varepsilon \frac{x}{1+x}. \quad (10)$$

The work however could only be done by virtue of information we had concerning the r -state. (The “wrong”-state component of the wave function must not enter the cavity.) The amount of this information is $\log 2$, as evidenced by the fact that purifying the atom to recover the original state costs $T \log 2$. Since the purification only need be applied to atoms that decay, for a large collection of atoms, the per atom entropy cost is $[x/(1+x)] \log 2$.

If this information cost and $(\Delta S)_{\text{due to heat bath}}$ are the only entropy changes, then overall

$$\begin{aligned} (\Delta S)_{\text{Total}} &= -\frac{\Delta Q}{T} + \frac{x}{1+x} \log 2 \\ &= [-\beta\varepsilon + \log 2] \frac{x}{1+x}. \end{aligned} \quad (11)$$

Up to a sign and factor of T , this is our previously calculated W_{net} . Since for appropriate ε that was strictly positive, for those same values $(\Delta S)_{\text{Total}}$ will be strictly negative. *This contradicts the Second Law of Thermodynamics.*

6.2. Resolution

Where has an entropy contribution been missed?

6.2.1. Photons

Consider the entropy of the created photon. We have called it work, but one can also take the matter-of-fact perspective that photons in a thermal distribution have entropy equal to about $3.6k_B$ per photon, irrespective of energy [14].

Even if correct, this does not resolve our dilemma. The total entropy change can be negative if ε is large enough.

6.2.2. The unitary preparation $P \leftrightarrow M$

It is natural for suspicion to fall on the glibly implemented unitary transformation, \mathcal{S} , that changed the quantum label P to M if and only if the q coordinate was in the state U . [See the discussion following Eq. (7).] In Ref. [1] this transformation is done by the Stern–Gerlach apparatus. Our suspicions are aroused because Eq. (11) balances a term independent of ε (the information term) with one that manifestly does depend on ε . And it is the ε -dependent term that is negative. So to get rid of this it would seem that manipulations on the atom when it is in the excited state are the place to look. The purification, after the cavity, only involves atoms in D . The creation of the (PM) - U correlation by \mathcal{S} however should involve (in a quantum description) a Hamiltonian that connects states of order ε apart.

Although this is a candidate, and the Hamiltonian does connect such states, we do not see why

that is necessarily reflected in the entropy. Presumably, a no-entropy assertion should be accompanied by a working model, but we do not attempt this, since an entropy source is identified below.

6.2.3. Purification using a magnet and heat bath

The mischief is in the purification. After the atom has passed the cavity stage (whether it interacted with the cavity or not) there is a *mixture* consisting of P and M quantum states. Our cost-of-purification estimate has been $\log 2[x/(1+x)]$, representing the “log 2” cost of changing M to P , multiplied by the fraction of M states. However, there is a flaw in this reasoning.

First consider the entropy of this mixture from an information perspective. There is probability x/Z of being in the state M [here $Z = 1 + x$ and $x = \exp(-\beta\varepsilon)$], and probability $1/Z$ of being in P . As in the classical theory this has entropy

$$\begin{aligned} S_{\text{mixing}} &= -\sum p \log p \\ &= -\frac{1}{Z} \left[x \log \frac{x}{Z} + \log \frac{1}{Z} \right]. \end{aligned} \quad (12)$$

Our entropy-decrease problem arises for large ε , corresponding to small x , for which Eq. (12) takes the form

$$\begin{aligned} S_{\text{mixing}} &= -\frac{1}{1+x} \log x + \log(1+x) \\ &\approx -x \log x = \beta\varepsilon \exp(-\beta\varepsilon). \end{aligned} \quad (13)$$

Comparing this to Eq. (11), this clearly has the possibility of resolving our dilemma.

The solution lies in R . We calculated the cost of changing M to P , assuming that bringing the magnet to the proximity of the atom will gradually force M states to turn into P 's. But recall from Section 3 that this can only be accomplished by repeatedly exposing the system to a heat bath that mixes A and B (equivalently, M and P) states. But this will *also* allow some of the P states to turn (partially) into M 's. Thus there is either a way to distinguish these states before purifying, which one would estimate must cost at least S_{mixing} , or one must do the process for *all* atoms, in which case the $x/(1+x)$ multiplying the $\log 2$ in Eq. (11) must be removed and a full $\log 2$ be added to

the entropy cost. The latter procedure leaves the total entropy positive for all $\beta\varepsilon$ values (a numerical fact).

6.3. Work reconsidered

The cost of purification, taking into consideration the last argument of Section 6.2.3, must include the cost either of separation of P and M post-cavity, or else the cost of purifying all atoms. Let us evaluate the situation for the latter approach (we leave the possibility of clever separation open—it might reduce estimates, but not change the conclusion). Once the heat bath is allowed to operate on P states, they will acquire M components and the expenditure of $T \log 2$ will be required for the entire collection of atoms. This will mean that the *net* work is just proportional (with an opposite sign) to the entropy, hence, for the net work, negative.

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Appendix A. Relation to “ordinary” thermodynamics

As emphasized by Brillouin [15], *information* can be used to make positive the sum $-Q/T + S$, where the S can be entirely due to information. This is why there should be no in-principle objection to the idea that the sorting that takes place prior to radiation (in Scully's example [1] as well as our own) can lead to work, despite the fact that only one ambient temperature exists.

As a classical example, consider osmotic pressure. Let a container be divided into two parts, on one side is a mixture of gases A and B , on the other only A . Both are at the same pressure and temperature; they are in contact with a heat bath at fixed temperature (same for both). Suppose the solid partition is replaced (with neither work nor

heat transfer) by a semi-permeable membrane that allows only the passage of B , not A . Then B atoms will develop an essentially one-way flow (for a while at least), increasing the pressure on the formerly A -only side. This pressure can perform work. The net effect is that heat from the reservoir is converted to work, with no temperature differential. The key is information. As the B 's become more evenly distributed, the entropy of the system increases. Alternatively, restoring the initial state would recover lost information, *and* would require work.

Appendix B. Another perspective

In the approach of Ref. [16] to non-equilibrium statistical mechanics, a one-way transition, as postulated in this article, is problematic. The context is stochastic dynamics. One works with transitions between possibly coarse-grained states, x , each of which has an entropy-weight, representing (the log of) the number of microstates associated with x . If R_{xy} is the transition probability from y to x , then the stationary distribution, $p_0(x)$, absent external forces (a closed system), satisfies detailed balance, $R_{xy}p_0(y) = R_{yx}p_0(x)$. The intrinsic entropy of x is $\log p_0(x)$. External forces correspond to contact with reservoirs and induce processes in which a detailed balance-like relation holds, but which includes reservoir entropy. With a reservoir at temperature T , an energy transfer Q induces a finite entropy transfer $|Q/T|$, as usual. The entropy of the reservoir changes by this amount. Therefore there can be no one-way transition, $\forall xy, R_{xy} \neq 0 \Leftrightarrow R_{yx} \neq 0$. For a *nearly* one-way transition, either the final entropy is nearly zero or the temperature is nearly zero. For a conventional reservoir, the former is not possible and one-way transitions can only be in the direction of zero temperature (this could be the vacuum for radiation). The other possibility is zero entropy, which corresponds to a work transition.

With this perspective, consider the one-way transition in the cavity in our process. If we consider the photon energy to be heat, we must take the cavity to be at zero temperature.

Alternatively, the cavity state may be considered to have zero entropy, in that all photons are in a single microscopic state.

Appendix C. Coherence, entropy and scattering

Much of the discussion of quantum mechanics and the second law centers around the use of phase information as a source of work. A recent calculation [17] shows another statistical mechanics/thermodynamic side of coherence.

Ref. [17] reports a surprising feature of wave packet evolution that takes place when unequal mass particles scatter. Start from Gaussian wave packets, and assume that the spread of the packet stabilizes. Then a collection of mixed-mass particles will evolve so that the wave packet spreads; σ^2 are related to corresponding particle masses, m , by $m\sigma^2 \sim \text{const}$. Moreover, if the wave packet was not quite Gaussian, the calculation suggests that it will tend to lose non-Gaussian components. Finally, it turns out that when $m\sigma^2 \sim \text{const}$, and the wave function is Gaussian, there is *no* kinematic entanglement. By this I refer to the fact that after a scattering, the coordinates of the colliding particles are intertwined, and even if the collision has but a single outcome, momentum conservation alone suggests—but apparently does not require—entanglement. I will not go into details, but I will mention a thermodynamic aspect of these results with emphasis on the role of entropy.

The calculation (in Ref. [17]) goes from pre- to post-scattering wave functions. Remarkably (and which has long been known), if one is not close to a resonance, the wave packet retains its shape, even if many possible outcomes (e.g., scattering angles) are possible. In general, after a scattering, by momentum conservation, one obtains an entangled wave function, so for the *next* scattering of, say, particle #1, one needs to trace out over the coordinates of #2. Obviously this is a loss of information—an entropy increase. It follows that convergence to the $m\sigma^2 \sim \text{const}$ limit, which is a limit in which there is *no* entanglement, represents a *maximization of entropy* (von Neumann entropy). As such we are seeing a kind of equilibration, not of energy (well, that too), but of a purely

quantum mechanical property, the wave function spread. This is happily consistent with the theme that coherence is a property meriting a role in thermodynamics. Note too that the condition $m\sigma^2 \sim \text{const}$ is reminiscent of classical equipartition, and now the connection is seen to be even closer: both represent entropy maximization. In Ref. [17] there is the implicit assumption that on successive scatterings there is no memory of phase relations; this recalls the Boltzmann *Stosszahlansatz* (molecular chaos assumption).

Checking the conclusions of Ref. [17] experimentally would have implications beyond those of that article. A positive result would confirm that wave functions tend toward coherent states as well as the issue of the stabilization of wave packet spreads. In Ref. [18] is a discussion of the experimental measurability of σ .

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