

A short note on passivity, complete passivity and virtual temperatures

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We give a simple and intuitive proof that the only states which are completely passive, i.e. those states from which work cannot be extracted even with infinitely many copies, are Gibbs states at positive temperatures. The proof makes use of the idea of virtual temperatures, i.e. the association of temperatures to transitions. We show that (i) passive states are those where every transition is at a positive temperature, and (ii) completely passive states are those where every transition is at the same positive temperature.

INTRODUCTION

The notion of a passive state was introduced in the seminal work of Pusz and Woronowicz [1] as a characterisation of quantum states which cannot be processed to extract work. That is, given a state ρ with Hamiltonian H , we ask whether the average energy can be lowered by a unitary transformation on the system, which is otherwise isolated (which is equivalent to a cyclic Hamiltonian process¹). The change in average energy is denoted by W and given by

$$W = \max_U \text{tr} (H (\rho - U\rho U^\dagger)), \quad (1)$$

States for which $W = 0$, i.e. states from which no work can be extracted, are referred to as passive states. On the other hand, states for which $W > 0$ are termed active states, and contain extractable work.

It is possible to show that passivity can be re-expressed solely as a property of the state. Namely, a state ρ is passive if and only if it satisfies the following two properties:

- $[\rho, H] = 0$, i.e. the state is (block) diagonal in the energy eigenbasis of the Hamiltonian.
- $E_i > E_j$ implies $\lambda_i < \lambda_j$, where E_i, E_j are energy eigenvalues and λ_i and λ_j are the associated populations of the state ρ . That is, the population of levels is strictly decreasing as the energy increases.

In general one is not only interested in a single copy of a system, but in multiple copies that can be processed jointly. In particular, one may ask how much work can be extracted from n copies of a state. Crucially, the composition of passive systems may not remain passive, hence exhibiting a form of activation. That is, there exist situations where a unitary U acting on n copies of a system is able to lower the average energy of the total

system, whilst if one had access to only $n - 1$ copies of the system no such unitary exists. This then naturally leads to the question of what is the class of states which remain passive under composition, i.e. from which no work can be extracted even from an infinite number of copies. Such states are termed completely passive. The celebrated result of [1] is to show that the set of completely passive states is exactly equivalent to the set of thermal (or Gibbs) states

$$\rho = \frac{1}{Z} \exp(-\beta H), \quad (2)$$

where $Z = \text{tr}(\exp(-\beta H))$ is the partition function and $\beta = 1/k_B T$ is the inverse temperature. This result puts on firm grounds the notion of a heat bath in the form of an infinitely large Gibbs state, from which no work can be extracted. The importance of these results in the context of quantum thermodynamics has been highlighted, see for instance [3–7].

This result was originally proven in the context of C^* algebras and shortly afterwards translated into the framework of standard quantum mechanics by Lenard [2]. In both cases although the end result is intuitive, the proof of the result does not convey too much intuition. In particular, it is not explicit why it is that passive but not thermal states can be activated for work extraction.

In this short note we provide a simple and intuitive proof based upon the idea of associating temperatures to transitions. This is the idea behind the concept of virtual temperatures and virtual qubits introduced in [8], and further discussed in [9, 10]. Furthermore, our technique illustrates explicitly how work can be extracted from a sufficient number of copies of a passive but non-thermal state, hence giving an upper bound on the number of copies needed.

VIRTUAL TEMPERATURES

We start by discussing in more detail the idea of assigning a temperature to a transition. Consider a system ρ with Hamiltonian $H = \sum_k E_k |k\rangle\langle k|$ comprised

¹ i.e. we switch on a time-dependent interaction Hamiltonian $V(t)$ only during $0 \leq t \leq \tau$.

of d energy eigenstates $|k\rangle$, with energy eigenvalues E_k , and assume ρ is diagonal in this basis. In total there are $d(d-1)/2$ transitions between energy levels. Consider the transition between the energy states $|i\rangle$ and $|j\rangle$, and let us assume without loss of generality that the gap $E_i - E_j > 0$ ². Given populations λ_i and λ_j respectively, we associate a virtual inverse temperature β_v to the transition, given by

$$\beta_v = \frac{\log \lambda_j - \log \lambda_i}{E_i - E_j}, \quad (3)$$

which arises by identifying the ratio of the populations with the Boltzmann factor, $\lambda_i/\lambda_j = e^{-\beta_v(E_i - E_j)}$. First we note that in general the virtual inverse temperature defined this way need not be positive. In particular, whenever $\lambda_i > \lambda_j$, i.e. the transition has a population inversion, then the temperature will be negative. Second, the reason for calling this a virtual temperature is because by coupling an external system to this transition, one can prepare physical systems at the virtual temperature, i.e. it behaves in this respect like a real temperature [8].

It will also be important to us to understand how virtual temperatures transform under composition. To that end, consider now two systems. For the first system we consider the transition between states $|i\rangle_1$ and $|j\rangle_1$, with energy gap $\Delta_1 = E_i - E_j$, populations λ_i and λ_j and virtual inverse temperature β_v^1 . Likewise for the second system we consider transitions between the states $|i'\rangle_2$ and $|j'\rangle_2$, with gap $\Delta_2 = E_{i'} - E_{j'}$, populations $\lambda_{i'}$, $\lambda_{j'}$ and virtual temperature β_v^2 .

Now, the joint system features 2 non-trivial transitions (i) between the pair of levels $|i\rangle_1|j'\rangle_2$ and $|j\rangle_1|i'\rangle_2$, and (ii) between $|i\rangle_1|i'\rangle_2$ and $|j\rangle_1|j'\rangle_2$. For case (i), the population of the first level is $\lambda_i\lambda_{j'}$, the second $\lambda_j\lambda_{i'}$, and the gap is $\tilde{\Delta} = \Delta_2 - \Delta_1$ (where we have assumed without loss of generality that $\Delta_2 > \Delta_1$). From (3) the inverse virtual temperature $\tilde{\beta}_v$ of the composed transition is given by

$$\begin{aligned} \tilde{\beta}_v &= \frac{\log(\lambda_i\lambda_{j'}) - \log(\lambda_j\lambda_{i'})}{\Delta_2 - \Delta_1} \\ &= \frac{(\log \lambda_{j'} - \log \lambda_{i'}) - (\log \lambda_j - \log \lambda_i)}{\Delta_2 - \Delta_1} \\ &= \frac{\beta_v^2\Delta_2 - \beta_v^1\Delta_1}{\Delta_2 - \Delta_1} \end{aligned} \quad (4)$$

where we have used equation (3) in the final step. Note that we obtain the same expression in the case $\Delta_1 > \Delta_2$ (i.e. the formula is insensitive to the sign of the gap). For case (ii) the populations are now $\lambda_i\lambda_{i'}$ and $\lambda_j\lambda_{j'}$, gap is $\tilde{\Delta}' = \Delta_2 + \Delta_1$, and a similar analysis shows that the

inverse virtual temperature $\tilde{\beta}'_v$ of the transition is given by

$$\tilde{\beta}'_v = \frac{\beta_v^2\Delta_2 + \beta_v^1\Delta_1}{\Delta_2 + \Delta_1} \quad (5)$$

Hence we see that the inverse virtual temperatures compose linearly in both cases. Finally, we note that $\tilde{\beta}'_v$ is always in between the composed temperatures β_v^1 and β_v^2 , while $\tilde{\beta}_v$ is in fact always larger than the biggest or smaller than the smallest temperature.

PASSIVITY

The notions introduced above will now allow us to re-express the notion of passivity in simple terms. Specifically the second requirement for a state to be passive, i.e. that $E_i > E_j$ implies $\lambda_i < \lambda_j$, is rephrased in the language of virtual temperatures as saying that the virtual temperature of every transition is positive. On the contrary, if the state has one or more negative virtual temperatures, work can be extracted by exploiting the associated population inversion.

COMPLETE PASSIVITY

We have seen above that passive states are those where every transition is at a positive temperature. We are now going to show that completely passive states are those where every transition is at the same positive temperature. The proof works by showing that whenever a system has two (or more) transitions at different virtual temperatures, then by composing sufficiently many copies, the combined system always has a transition at a negative temperature, and is therefore not passive.

Consider again a system ρ with d levels and consider first a transition between states $|i\rangle$ and $|j\rangle$, with gap $\Delta_1 = E_i - E_j$ and virtual inverse temperature β_v^1 . Let us consider n copies of ρ , and the same transition in each system. Now, by applying the composition rule (5) $n-1$ times, it is straightforward to see that the joint system has a transition between the states $|i\rangle^{\otimes n}$ and $|j\rangle^{\otimes n}$ with gap $n\Delta_1$ and the same virtual inverse temperature β_v^1 . Similarly, consider another transition of ρ between the states $|i'\rangle$ and $|j'\rangle$, with gap $\Delta_2 = E_{i'} - E_{j'}$ and virtual inverse temperature $\beta_v^2 > \beta_v^1$, without loss of generality. Now consider another k copies of ρ . Exactly as above, the joint system has a transition between the states $|i'\rangle^{\otimes k}$ and $|j'\rangle^{\otimes k}$ with gap $k\Delta_2$ and the virtual inverse temperature β_v^2 .

Finally, for the $n+k$ copies of ρ together, consider the transition between the states $|i\rangle^{\otimes n} \otimes |j'\rangle^{\otimes k}$ and $|j\rangle^{\otimes n} \otimes |i'\rangle^{\otimes k}$. This transition has an energy gap of $n\Delta_1 - k\Delta_2$, and from the composition rule (4), it has

² We do not define virtual temperatures for degenerate transitions. Since no work can ever be extracted from such transitions we will never need such a concept.

the inverse virtual temperature

$$\beta_v = \frac{\beta_v^1 n \Delta_1 - \beta_v^2 k \Delta_2}{n \Delta_1 - k \Delta_2} \quad (6)$$

Now, since $\beta_v^2 > \beta_v^1$, i.e. the two transitions are at different virtual temperatures, then it is always possible to find a negative β_v , by choosing an appropriate number of copies n and k such that the numerator of (6) is negative, whilst the denominator is positive. In particular, choosing

$$\frac{\Delta_2}{\Delta_1} < \frac{n}{k} < \frac{\Delta_2 \beta_v^2}{\Delta_1 \beta_v^1} \quad (7)$$

ensures that $\beta_v < 0$. Thus, any passive state with two virtual temperatures is not completely passive. The only possibility for a completely passive state is thus one containing only a single virtual temperature, which is precisely the defining property of a thermal state.

Finally, it is worth noting that (7) provides a sufficient condition for finitely many copies of a state to become non-passive: One has to find the smallest number $n + k$ such that (7) is satisfied for any possible pair of virtual temperatures in the system.

CONCLUSIONS

In summary, we have presented what we believe is a simply and insightful alternative proof that the only completely passive states are thermal states. The only notion that our proof relies upon is the association of virtual temperatures to transitions in a system via Gibbs weights, and can be simply stated as the only completely passive states are those which contain a single virtual temperature. To show this we proved that every passive but not completely passive state has the property that

upon composition one can find a transition at a negative virtual temperature, from which work can then be extracted.

This statement is intuitive from the perspective of thermal machines, where having access to two baths at differing temperatures is all that is required to build a work extracting machine.

Acknowledgements. We acknowledge financial support from the Swiss National Science Foundation (grant PP00P2_138917) and an EU Marie Curie COFUND action (ICFOnest).

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