Towards experimentally-friendly single shot thermodynamic operations

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(Dated: November 26, 2014)

I. INTRODUCTION

Thermodynamics, one of the most successful ans solid branch of physics, had it boom in the XIX century, mostly due to Carnot, the "father of thermodynamics", who studied heat engines to help France win the Napoleonic Wars, followed by the development of foundametals of thermodynamics and statistical thermodynamics by, for example, Rudolf Clausius, William Thomson, Ludwig Boltzmann, J. Willard Gibbs and Max Planck [1]. Nowadays, thermodynamical phenomenons are common and crucial to our everyday life, even we do not always realize it. Heat engines are "hearts" of many devices, like cars or trains that are used in transport; refrigerators and freezers allow us to store food effectively. Also, we observe effects of thermalization/equilibration commonly, e.g., our hot coffees and teas get cold fast and beers warm even faster. Thermodynamics has been developed to deal with macroscopic objects, i.e., composed of many particles, but it was also sucessfully applied to situations that surpass its original domain like black holes.

But now, with the emergence, both theoretical and experimental, of quantum and nano devices, like quantum and nano engines [2–5], thermodynamics has it second boom, namely there is a renewed interest in foundations of thermodynamics from the quantum point of view and describing thermal properties of objects composed of singel particles (see, for example, [6–16]), especially in the single shot scenario. The motivation to study thermodynamic laws for the single shot scenario, rather than the asymptotic scenario commonly used in thermodynamics, ăis the issue of thermodynamics of single microscopic systems, where the average over many events may not be a relevant description, as opposed to macroscopic systems, or to many identical copies of microscopic systems. In single shot thermodynamics one assumes a single copy of the system and access to a heat bath. One then asks: what are possible transformations of the systemă given a thermodynamically motivated class of operations. There are two approaches to answer this. The first, detailed approach, follows the spirit of Pusz and Woronowicz [17] formulation of second law where detailed control over the heat bath is assumed. This approach leads to a class of Thermal operations introduced in [18] that has been applied in [19], where the authors cast thermodynamics as a resurce theory [20–22] obtaining limitations for an amount of work that can be extracted from a system and transitions between states diagonal in energy basis. Thermal operations have been also apllied to obtain laws of thermodynamics [23], general state-to-state transformations [24] and many other results, for example, [25–28]. In contrast, there also exists approach that follows a more traditional and experimentaly-friendly route [29–31], where we have arbitrary control only on the system, while the heat bath is accessed in a very limited way, e.g. through weak coupling. Most crude approach is that the system can only fully thermalize. One can also consider partial thermalization [3], i.e. initially in a state ρ_0 becomes thermalized withăprobability p and remains intact with probability $1 - p$, i.e. $\rho_1 = p\tau + (1 - p)\rho_0$. Surprisingly, both approaches give the same limitations to the amount of work that can be drawn from a system that was initially out of equilibrium with the heat bath [19, 30].ă

At the end, let us report here that one can also use other frameworks in quantum thermodynamics that are based on averages to obtain some limitations [32–35].

II. THERMAL OPERATIONS

Let us start with recalling how thermodynamics can be viewed as a resource theory [18–21]. It allows to exploit some mathematical machinery from information theory, for example, from single-shot information theory, where one does not have access to copies of independent and identically distributed bits of information. Namely, one considers some class of operations, and then asks how much of some resource can be used to perform the desired task and how this resorce can be manipulated. In the case of thermodynamics, it is viewed as a theory involving state transformations in the presence of a thermal bath.

We want to obtain limitations, that's why we demand to precisely account for all sources of energy in our setup, and to model that, as the class of possible operations, we will use, Thermal operations, introduced in [18].
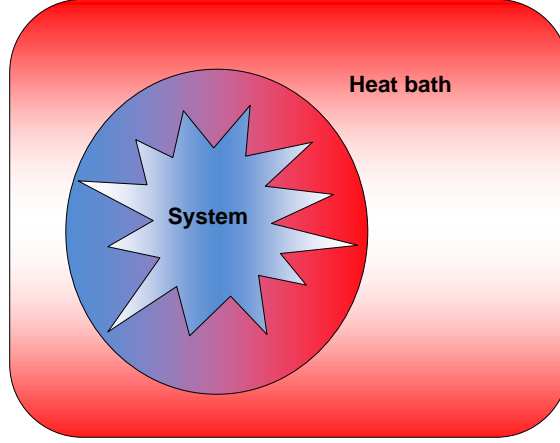
FIG. 1: **(Color online)** Briefly speaking, one considers a system S (blue star) in a quantum state with a fixed Hamiltonian H_S, in contact with the heat bath R (red rectangle) in a Gibbs state τ_R (possibly many copies of it) acting as a free resource, some interactions (red-white circle) between them, and try to determine possible state transitions, assuming that all operations are energy-conserving. The energy spectrum of the bath is highly degenerated (small or no degeneracy drastically reduce the set of Thermal operations) and together with the energy of the bath will tend to infinity. We also make an usual assumption that the bath is much larger than the system.

This choice has a physical motivation, since all fundamental processes are (as far as we know) energy conserving. Formally, under Thermal operations one can (see also, Fig. 1 for a short overview ans assumptions)

1. Bring in an arbitrary system in a Gibbs state with temperature T (free resource).

2. Remove (discard) any system.

3. Apply a unitary that commutes with the total Hamiltonian.

Mathematically, the class of Thermal operations on a system with (ρ_S, H_S) can be viewed as

$$(\rho_S, H_S) \mapsto (\mathrm{Tr}_R[U\left(\rho_S \otimes \tau_R^{\otimes n}\right)U^\dagger], H_S) = (\sigma_S, H_S) \tag{II.1}$$

where $\tau_R = e^{-\beta H_R}/Z_R$ is the thermal state of the reservoir for some reservoir Hamiltonian H_R at inverse temperature β, ρ_S and σ_S are some initial and final states from H_S. The class is generated by the unitaries U (which act on the system, bath, interactions...) which obey the energy conservation condition

$$[U, H_S + H_R + H_I] = 0, \tag{II.2}$$

where H_I is the term that describes interactions, a clock, a work system and other object under consideration besides the system and bath.

As a remark, let us notice that one can derive laws of thermodynamics under Thermal operations, the first allowed operation gives the zeroth law [23], the commutation relation stands for first law (energy conservation) [19] and the unitarity (conservation of information) results in second law(s) [23]. The third law can also be obtained in this framework [36].

At the end, let us mention that the assumption that a Gibbs state is the only possible free resource is very important. Allowance of other states acting as a resource would lead to the situation where there are simply no real limitations on possible transformations - every transformation is possible and there is no room for obtaining any bounds [23].

III. COARSE OPERATIONS

An explicit example of **how** the implementation of such a thermal process would proceed are given in [30] (in a form that is less "paranoidal" than Thermal operations). He considers a three-step process on the system with

initial (diagonal) distribution q_n for each energy E_n of the initial Hamiltonian H_S. Starting with each initial energy level E_n, he considers:

1) Level transformations, i.e. $E_n \mapsto E'_n$ where $E_n, n = 0, 1, ..., d$ are eigenvalues of H_S with $\dim \mathcal{H}_S = d$, and E'_n are eigenvalues of H'_S. H'_S is chosen such that the distribution q_n is its thermal distribution at inverse temperature β, i.e. $q_n = \frac{e^{-\beta E'_n}}{Z'}$. Here $Z' = \sum_n e^{-\beta E'_n}$ is the thermal partition function of H'_S.

2) Thermalisation, i.e. $E'_n \mapsto \{E'_m\}_{m=0}^{d-1}$ with transfer probability $p_{m|n} = \frac{e^{-\beta E'_m}}{Z'}$ (i.e. independent of initial level).

3) ITR = thermal distribution ($q_n = p'_n$) for H'_S is transferred to thermal distribution (p_n) for H_S through a sequence of infinitesimally small level transformations and thermalizations, i.e. for $j = 0, ..., N-1$, $E^j_{m_j} \mapsto E^{j+1}_{m_j} \mapsto \{E^{j+1}_{m_{j+1}}\}_{m_{j+1}=0}^{d-1}$. Here $E^0 = E'$ and $E^N = E$.

Ahberg identifies that during step 1) the work extracted is $W^1(n) = -(E'_n - E_n)$ for each level n and step 2) does not involve any work. For step 3) Ahberg argues in Appendix C that the (non-averaged) work probability distribution for the work during an ITR peaks increasingly sharply at ΔF in the limit of $N \to \infty$ where N is the number of discretisation steps of the path, see (C5). There is no explicit proof though, so we provide the proof.

IV. CREATION OF NON-EQUILIBRIUM STATES

Just as one can draw work from a state which is out of equilibrium from the rest of the thermal bath, it is also possible to perform the reverse process to create a state from the thermal bath by adding work. The amount of work needed for it can be quantify in terms of the max-relative entropy and such an expression has been obtained in in [19]. Here, we show that the same expression can be easily obtained adapting the formalism from [30]. The goal is to start from a Gibbs state and by adding work, transform it to a desired state. In the spirit of [30], it can be done like

$$(\rho^\beta, H, p_i) \xrightarrow{\text{ITR}} (\sigma_S, H', p'_i) \xrightarrow{\text{LT}} (\sigma_S, H, p_i), \tag{IV.1}$$

where ρ^β is an initial state, the Gibbs state for a Hamiltonian H that we change to a state σ_S that is Gibbs for H' by ITR; in the last step we separate energy levels by LT to obtain the desired state σ_S. The amount of work needed in the ITR step is equal to the free energy difference ΔF between two equilibrium states, when in the LT step is equal to the maximum energy difference between particular levels from the latter and former states. In total it gives $W = \Delta F + \max_i(E_i - E'_i) = kT D_{\max}(\sigma || \rho^\beta)$, where p_i and q_i are thermal probabilities (eigenvalues) for Hamiltonians H' and H defined as $p_i = \frac{e^{-\beta E_i}}{Z}$ and $q_i = \frac{e^{-\beta E'_i}}{Z'}$; Z, Z' are the partition functions, and we apply a natural logarithm to the both sides of expressions for thermal probabilities to obtain E_i, E'_i, i.e., energies of i-th energy levels of states ρ_S and σ_S respectively (for qubits, the ground (g) and excited (e) level).

V. WORK-FREE TRANSFORMATIONS - THERMO-CASCADES

In [19], the authors have shown that when one has two states ρ and σ that has the same β-order and ρ thermo-majorizes σ, i.e, cummulative curve of ρ is above that of σ on a thermo-diagram, then one can transform the former state into the latter for free ($W = 0$) under Thermal operations, so no work is needed for such a state transition. We are going to show now, that the same happens for coarse operations, just by mixing the initial state with the Gibbs state. The result is valid both for trivial (zero) and non-trivial Hamiltonians.

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