Limits to catalysis in quantum thermodynamics

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Quantum thermodynamics is a research field that aims at fleshing out the ultimate limits of thermodynamic processes in the deep quantum regime. A complete picture of quantum thermodynamics allows for catalysts, i.e., systems facilitating state transformations while remaining essentially intact in their state, very much reminding of catalysts in chemical reactions. In this work, we present a comprehensive analysis of the power and limitation of such thermal catalysis. Specifically, we provide a family of optimal catalysts that can be returned with minimal trace distance error after facilitating a state transformation process. To incorporate the genuine physical role of a catalyst, we identify very significant restrictions on arbitrary state transformations under dimension or mean energy bounds, using methods of convex relaxations. We discuss the implication of these findings on possible thermodynamic state transformations in the quantum regime.

I. INTRODUCTION

In chemical reactions, it is common that a certain reaction should in principle be allowed, but in reality cannot take place (or occurs at extremely low rates) because of the presence of some large energy barrier. Fortunately, the situation is sometimes redeemed by the presence of certain chemical substances, referred to as catalysts, which effectively lower the energy barrier across the transformation. That is to say, catalysts significantly increase the reaction rates. Importantly, these catalysts can remain unchanged after the occurrence of the reaction, and hence a small amount of catalytic substance could be used repeatedly and is sufficient to facilitate the chemical reaction of interest.

The basic principles of chemical reactions are governed by thermodynamic considerations such as the second law. There have specifically been a number of recent advances in the quest of understanding the fundamental laws of thermodynamics [1-8]. These efforts are especially focused on the quantum nano-regime, where finite size effects and quantum coherences are becoming increasingly relevant. One particularly insightful approach is to cast thermodynamics as a resource theory [2,5,7,8], reminding of notions in entanglement theory [2,11]. In this framework, thermodynamics can be seen as the theory that describes conditions for state transformation $\rho \rightarrow \sigma$ from some quantum state to another under thermal operations (TO). The notion of TO means allowing for the full set of global unitaries which are energy preserving in the presence of some thermal bath. This is a healthy and fruitful standpoint, and allows the application of many concepts and powerful tools derived from information theory [12-14].

In the context of thermal operations, catalysts emerge as ancillary systems that facilitate state transformation processes: there are cases where $\rho \rightarrow \sigma$ is not possible, but there exists a state $\omega_C$ such that $\omega_C \otimes \rho \rightarrow \omega_C \otimes \sigma$ is possible. The metaphor of catalysis is appropriate indeed: This implies that by using such a catalyst $\omega_C$, one is enabled to perform the thermodynamic transformation $\rho \rightarrow \sigma$, while returning the catalyst back in its exact original form. This is called exact catalysis. The inclusion of catalyst states in thermal operations serve as an important step in an eventual complete picture of quantum thermodynamics; it allows us to describe thermodynamic transformations in the full picture, where the system is interacting with experimental apparatus, for example a clock system. Furthermore, it has been shown that one can obtain necessary and sufficient conditions for exact catalysis in terms of a whole family of generalised free energies [1]. The ordinary second law of ever-decreasing free energy is but the constraint on one of these free energies.

 Naturally, for physically realistic scenarios inexact catalysis is anticipated, where the catalyst is returned except for a slight degradation. However, rather surprisingly, it has been shown [1] that at least in some cases, the conditions for catalytic transformations are highly non-robust against small errors induced in the catalyst. The form of the second law thus depends crucially on the measure used to quantify inexactness. In particular, if inexactness is defined in terms of small trace distance, then there is no second law at all: for any $\epsilon > 0$ one could pick any two states $\rho$ and $\sigma$, and starting from $\omega_C \otimes \rho$, get $\epsilon$-close in terms of trace distance to $\omega_C \otimes \sigma$ via thermal operations. We refer to this effect as thermal embezzling: Here one observes that instead of merely catalysing the reaction, energy/purity has possibly been extracted from the catalyst and used to facilitate thermodynamic transformations, while leaving the catalyst state arbitrarily close to being intact [15]. On physical grounds, such a setting seems implausible, even though it is formally legitimate. A clarification of this puzzle seems very much warranted.

Argued formally, a first hint towards a resolution may be provided by looking at how the error depends on the system size. Naturally, the trace distance error $\epsilon$ depends on the dimension of the catalyst states $\dim(\omega_C) = n$; nevertheless one can find examples of catalysts where $\epsilon \rightarrow 0$ as $n$ approaches infinity. While examples show that in principle thermal embezzling may occur [1], hardly anything else is known otherwise. Indeed, it would be interesting to understand the crucial properties that distinguish between a catalyst and an active reactant in thermodynamics. From a physical perspective, it