PhD project
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Quantum thermodynamics of non-equilibrium Green's functions

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Project summary

Non-equilibrium Green's functions (NEGFs) is a widely used tool for describing transport across nanoscale junctions and devices. However, its quantum thermodynamic properties have so far been largely unexplored. In fact, most of the developments for transport have been done using the notion of Lindblad master equations. The goal of this project is to fill in this gap and contribute towards the development of quantum thermodynamics of NEGFs. To accomplish this, we shall focus on linear bosonic systems coupled to multiple reservoirs, for which the tools of Gaussian quantum mechanics can be exploited. After establishing the basic NEGFs for this scenario, we shall first study relevant examples, specially in the fields of quantum optics and ultra-cold atoms in optical lattices. Afterwards, we move towards the development of a self-consistent thermodynamic theory capable of describing NEGFs in this scenario. Of particular interest to us will be the role of system-environment correlations, as quantified by information-theoretic measures, in driving the system away from equilibrium. The distinctions and similarities between NEGFs and Lindblad master equations will also be explored.

1 Introduction

The main goal of quantum thermodynamics is to extend the first and second laws of thermodynamics to scenarios prone to quantum effects. This would in principle allow one to exploit information theoretic resources such as entanglement and coherence, to perform thermodynamic tasks that would otherwise be impossible in the classical realm. The formulation of the laws of thermodynamics is an ongoing process and depends heavily on the type of scenario under consideration. Of particular importance to this PhD project is the quantum transport scenario, where an arbitrary quantum system is coupled to two or more reservoirs kept at different temperatures. In this case, after some initial transients, the system will eventually relax towards a non-equilibrium steady-state (NESS) characterized by the existence of finite currents between the different baths.

The formulation of the laws of thermodynamics in this case has seen substantial progress in recent years. This progress relies on the realization that, unlike classical systems, in the quantum realm the coupling to the heat bath is not universal, but depends both on the internal structure of the bath as well as the type of system-bath interaction. This marks a fundamental difference between quantum and classical thermodynamics. As a consequence, even within a given scenario, multiple types of descriptions are still possible. For instance, substantial progress has been made in the so called "local vs. global dilemma", which refers to which kind of Lindblad master equation more adequately models a NESS scenario [1–5]. This is, in fact, an area of research in which Prof. Landi has been actively involved in past years [6–10].

In condensed matter physics, on the other hand, transport problems have long been studied using the concept of non-equilibrium Green's functions (NEGFs) [11]. They offer a versatile way of computing transport coefficients across junctions, which can be readily extended to multi-terminal setups and other scenarios of interest to experimental condensed matter physics. While master equations work with density matrices, NEGFs deal with operators in the Heisenberg picture. This is advantageous for computing currents across multi-terminal systems, but is not as useful to study information theoretic properties such as entanglement between system and environment. The reconciliation between NEGFs and thermodynamics is thus a quite new and largely unexplored subject [12–14].

The goal of this project is to contribute towards the formulation of the laws of thermodynamics for NEGFs in the NESS scenario. To this end, we shall depart from the usual approach in condensed matter physics, which focuses on fermionic transport, and consider instead bosonic systems coupled to multiple baths. The reason for this is two-fold. First, it will allow us to explore a vast set of tools developed by the quantum optics and quantum information community on light-atom interactions [15], input-output theory [16] and Gaussian quantum dynamics [17]. Second, bosonic systems are of interest to a series of new applications involving transport in the booming field of ultra-cold atoms [18, 19], which we plan to explore in this project.

Contextualization

In our group we currently have multiple branches of research within the field of quantum thermodynamics and quantum transport. This includes also the interface with different fields, such as quantum thermometry and dissipative quantum phase transitions. However, the core research topic in our research is the construction of thermodynamic rules for quantum systems. This project falls precisely within this goal and should, therefore contribute to our overall understanding of thermodynamics in the quantum regime.

Academic contributions of this project

This PhD project is quite timely, focusing on a problem that has seen a surge of interest in recent years [2, 4, 7, 10]. It should therefore help to bring the student towards the forefront of this research field. To aid in this task, the project will count with the collaboration of several researchers from Brazil and abroad. In particular, we mention Profs. John Goold from Trinity College Dublin, Nicola Lo Gullo from Turku University in Finland and Caio Lewenkopf from UFRJ. It will also count with the support of Prof. Luis Gregório Dias, from IFUSP, who is a specialist in transport problems in condensed matter.

Scientific impact

This project will help to draw attention in Brazil to the important fields of quantum thermodynamics and ultra-cold atoms, which are among the fastest growing communities in physics. Moreover, it will help to strengthen the collaboration between members of the SPIN off QuBIT of quantum information scientists in the state of São Paulo, which will take place through bimonthly meetings.

The progress of the project will be measured primarily by publications in high impact journals such as Physical Review Letters , Nature quantum information, New Journal of Physics and Quantum. All papers will also be accessible on arXiv, and computational libraries will be made available in institutional repositories. The student will be encouraged to participate in international conferences and present talks, as well as to visit other universities to disseminate results of the project. We also recognize the importance of actively publicizing our research on blogs such as `spinoffqubit.info` and *quantum Rio*, as well as social media pages such as "Quantum Information and Quantum Computer Scientists of the World Unite", "Quantum Correlations" and "Quantum Thermodynamics".

2 Objectives and methodology

We now move on to describe the specific goals that will be pursued in this PhD project, together with the methodology with which they shall be approached. The objectives will be divided into three sections. The first (A) consists of bibliographical reviews that the student will have to learn in order to acquaint himself with the basic principles of NESSs, NEGFs, master equations and Gaussian quantum dynamics. The second (B) contains a series of toy models which Mr. Comar will study in order to gain acquaintance with the tools involved in bosonic transport. Finally, the third section (C) contains the routes towards the development of the laws of thermodynamics for bosonic NEGFs.

A. Bibliographical review and basic tools

A.1 **Non-equilibrium Green's functions (NEGF) and quantum Langevin equations:** Within the context of bosonic systems, there is a deep overlap between NEGFs and quantum Langevin equations. As the first bibliographical review, the student will learn about these two topics by studying famous textbooks in the subject [11, 15, 16].

A.2 **Connection between NEGF and quantum Lindblad equations:** There are only a handful of papers dealing with the connection between NEGFs and Lindblad master equations. In particular, we mention Refs. [2, 4], which the student will study in detail. Some of the authors of these papers are collaborators of Prof. Landi and have already offered to help Mr. Comar with any difficulties that may arise during his studies.

A.3 **Foundations of quantum thermodynamics:** Finally, Mr. Comar will also study quantum thermodynamics, in particular Refs. [6,7,20] by Prof. Landi. This will help him get acquainted with the main challenges regarding the first and second laws of thermodynamics. Of particular importance is Ref. [7] which discusses how to reconcile thermodynamics with local master equations.

B. Applications of bosonic NEGFs

In order to gain acquaintance with the basic features of NEGFs, Mr. Comar will study a series of toy models that capture the main features of the problem. Among them, we mention:

B.1 **Transport through a one-dimensional tight-binding chain:** This is essentially a bosonic extension of Ref. [2]. It can also be directly compared with the local and global approaches studied in [8]. We shall also exploit different spectral densities; e.g. Lorentzians.

B.2 **Transport involving squeezing:** As a first extension, one can consider the situation where squeezing terms are added to the system or the baths. This can be matched with recent developments on the thermodynamics of radiation squeezing [21, 22]. It will also allow one to develop Onsager's theory for the joint transport of heat and squeezing.

B.3 **Self-consistent baths (Büttiker probes):** This corresponds to modified reservoirs which add noise to the system, but not energy. They are often used as a tool to induce diffusive transport in an otherwise ballistic system. A version of this has recently been studied in Ref. [10] for Lindblad master equations. The extensions to NEGFs seem like an interesting as well as timely application.

B.4 **Linear response theory for the NESS:** Linear response theory has recently been extended to Lindblad master equations featuring arbitrary steady-states [23]. As another application, one may study the extension of linear response to the bosonic NEGFs.

C. Quantum thermodynamics of NEGFs

Finally, having gained familiarity through toy models, Mr. Comar will move on to develop the thermodynamics of NEGFs. This will be based on the following steps:

C.1 **Entropy production from system-environment correlations:** The theory of entropy production can be developed starting from the correlations developed between system and environment, as first put forth in Ref. [24]. The advantage of bosonic systems is that these correlations, quantified by the mutual information [25], can be computed easily using the tools of Gaussian quantum information [17, 26]. This was used recently in Ref. [27] and will also benefit from some of the techniques recently developed in our group [28].

C.2 **Additivity of noise channels:** A key question, first put forth in [2], is that in reality the presence of multiple environments is not additive. This is not at all obvious within Lindblad master equations, but appears naturally in NEGFs. The thermodynamic consequences of this, however, have so far not been explored.

C.3 **Connection with input-output theory:** The NESS within the NEGF scenario can be viewed as an input-output process, where signals are transmitted from one bath to another, with the system functioning as a scattering center [16]. The thermodynamics of input-output still remains entirely unexplored, although some progress has already been made in fermionic systems [14].

C.4 **Phase-space measures of irreversibility:** Finally, Mr. Comar will expand on the results of Refs. [10, 29] and discuss phase-space formulations of the entropy production problem. This will allow for the identification of irreversible currents in phase space which are ultimately responsible for the emergence of irreversibility. This also relates to the idea of exact dilations, as first put forth in [30], which will also be useful in this context.

3 Summary

To summarize, in this PhD research project we propose to investigate the thermodynamics of non-equilibirum Green's functions. This research proposal is both timely and ambitious. It combines tools and concepts from the fields of statistical mechanics, condensed matter and quantum information theory. And has the potential to lead to publications in high impact scientific journals.

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