Centre for
Theoretical Atomic, Molecular and Optical Physics
CTAMOP
Queen's University Belfast

Ph.D. Project 2020-2023

Machine learning approach to non-equilibrium quantum thermodynamics

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State of the art and motivations

Quantum mechanics is the framework for the description of the microscopic world. The physical behaviour of atoms, molecules and weak electromagnetic field are predicted with outstanding accuracy by the quantum formalism. This formidable framework is expected to break down, or become irrelevant, at scales that go beyond the size of a few atoms and for systems endowed with a very large number of degrees of freedom [1]: Any quantum system is continuously monitored by its environment and gets correlated to it. In this way, the environment depletes any quantum feature in the state of the system, driving it to a merely classical description. Such a process, which is termed QtC transition, is believed to become increasingly relevant with the complexity of the system, intended as its mass, size, and/or number of individual constituents [1]. How would such a QtC transition occur? Is there a threshold degree of complexity that triggers the occurrence of such crossover? So far, only partial answers to these questions have been given. Their provocative nature is reinforced by the fact that strong quantum features can be observed in systems that, for their number of degrees of freedom or size, can be considered as truly "complex". Systems such as superconducting ones, ion crystals, cold atoms, and massive mechanical oscillators [2–5], to name a few cases, are used to investigate quantum phenomena at scales beyond any microscopic description. These examples challenge the conjecture that large and complex systems should behave classically and justify the need for an exploration of quantum effects in systems that are complex and open to environmental effects.

This project will go beyond the approach currently used to investigate the QtC transition and address the thermodynamic implications of emergent quantum effects in non-equilibrium large-scale systems. The rationale behind such an approach is that thermodynamics encompasses both many-body features and the interaction with environments. It is thus a well-motivated methodological candidate for the study of the QtC crossover. Moreover, the dynamical nature of the QtC transition demands an approach that addresses dynamics explicitly. Studying non-equilibrium physics will thus lead to new understanding. Although the link between thermodynamics and quantum mechanics has always been intimate, key advances have only been recently made. These include attempts at defining heat, work, and temperature at the micro/nano-scale; the derivation of the laws of thermodynamics using an ab initio quantum mechanical approach, and the establishment of a link between thermodynamics and entanglement; the proposal of schemes for work-extraction from a single bath through quantum coherences; the formulation of quantum fluctuation relations; the design of microscopic quantum machines. This project will be different from such endeavours as it will address the non-equilibrium thermodynamic behaviour of open mesoscopic systems with the aim of understanding the phenomenology behind the QtC crossover. From the entirely new assessment of thermodynamic through large-scale quantum systems, this project will lead to new understanding on such a foundational issue.

In the past decades, various machine learning tools have been developed by data analysts to extract relevant information from confusing data sets — including principal component analysis (PCA), artificial neural networks, and variational autoencoders. Some of these methods provide a roadmap for how to reduce a complex data set to a lower dimension to reveal the sometimes hidden, simplified structures that often underlie it. For example, PCA can construct optimal low-rank approximations from the spectral decomposition of a data matrix. Other methods can be trained on given data, labelled using certain properties of interest, to then classify unseen new data; and others can even discover without supervision new properties of a system.

Quantum physical systems are particularly complex and, recently, various machine learning techniques developed in the context of classical data analysis have been deployed by researchers in quantum technologies to help our understanding of "quantum data" [**?**, **?**] — namely, classical data emerging from measurements on quantum systems.

Objectives & Methodology

The project is built to achieve the following objectives:

Objective (1) To demonstrate that the irreversible thermodynamic entropy produced in non-equilibrium processes allows for the refined characterisation of the QtC transition in open complex quantum systems.

Objective (2) To design thermodynamic machines based on open complex quantum settings, whose working principles are enhanced by qmachine learning techniques.

Objective (1) will put the information carried by thermodynamic quantities such as work, heat, and irreversible entropy at the core of the studies on the QtC transition. Irreversible entropy, in particular, is very sensitive to quantum features in the state of a system. The thermodynamic irreversible entropy of a system exposed to the effect of a strong environment maintains features that are distinctively different from any fully classical calculation, thus showing its enhanced sensitivity to "non-classicality". It can thus be used to accurately pinpoint the occurrence of QtC crossover in complex quantum systems. Objectives (2) will impact on the current experimental activities in out-of-equilibrium quantum systems, inspiring a new generation of experiments focused on non-equilibrium quantum thermodynamics (NEQT). It will build upon the knowledge generated by tackling Objective (1) to underpin the design of machines (quantum engines, refrigerators, and motors) operating explicitly out of equilibrium (thus generating non-zero power) and in open-system conditions. The efficiency of such devices will then be optimised using techniques for machine learning, benchmarked by comparison with optimal control and shortcuts to adiabaticity.

Collaborations

The project will involve interactions with long-term international collaborators of the supervisors, including experimentalists. Those are recognised experts in the field of quantum information science, and collaborations with them will be of clear benefit. A strong and regular interaction with Dr. A. Ferraro and G De Chiara at Queen's University Belfast is expected.

Required skills

The interested student will have a passionate and inquisitive approach toward mathematics and physics. A good knowledge of Quantum Theory and Mathematical Methods of Physics is required. Advanced computing skills are not required, although the student will become familiar with tools such as Mathematica, Matlab, Python.

Further information

The student will be a member of the Quantum Technology group at Queen's University Belfast and will participate to its activities (group meetings, seminars, meetings with guest scientists) and it is expected the participation at international conferences and schools.

Further information can be requested by contacting Prof Paternostro m.paternostro@qub.ac.uk.

References

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[3] S. Ulm et al., Nat. Commun. 4, 2290 (2013).

[4] H. Ritsch et al., Rev. Mod. Phys. 85, 553 (2013).

[5] M. Aspelmeyer et al., Rev. Mod. Phys. 86, 1391 (2014)..