Research agenda of Quantum Resources Group

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I. MOTIVATION AND THE GENERAL GOAL

Recent progress in experimental control over noisy intermediate-scale quantum (NISQ) systems [1] may soon bring the advent of new technologies, whose operation will be based on purely quantum effects and that will be able to overcome current limitations of electromechanical systems and information processors [2]. From a theoretical point of view, the first step to achieve this is to identify which components of quantum theory can provide such an advantage. In other words, we need to recognise what actually constitutes quantum resources. Of course, this will strongly depend on the type of tasks we want to perform, e.g. quantum entanglement [3] is a useful resource for secure communication through the use of E91 protocol [4]; but it is not sufficient for universal quantum computing, as families of circuits generating highly entangled states can be simulated on classical computers via Gottesman-Knill theorem [5]. Once the relevant resources are identified, the next step is to characterise them. Informally this corresponds to translating qualitative statements like "entanglement is a useful cryptographic resource" to quantitative ones like "entangled state A is five times better than B, because it allows one to securely communicate five times more bits". More formally, characterisation requires one to understand when different resources can be interconverted and how efficiently this can be done, which is captured by the mathematical framework of resource theories [6, 7]. Finally, there is also the third essential step: finding optimal ways to experimentally implement protocols exhibiting quantum advantage, while taking into account realistic constraints.

The general goal of the Quantum Resources Group is to develop a theoretical framework underpinning quantum technologies, with a particular focus on quantum computing and quantum thermodynamics, by investigating all three aspects of quantum resource theories: identification, characterisation and implementation. These research goals will be pursued by realising three objectives, described more precisely below, and the specific research tasks will include:

- **Goal 1 – Identification:** investigating possibilities for quantum advantage within thermodynamic scenarios and finding operational interpretations for coherence resources.
- **Goal 2 – Characterisation:** determining the constraints for manipulating magic states and developing quantitative methods to characterise thermodynamic irreversibility.
- **Goal 3 – Implementation:** constructing experimentally feasible protocols for probing quantum thermodynamic phenomena and devising classical simulation algorithms for the certification and verification of the NISQ devises.

II. RESEARCH OBJECTIVES

A. *Objective 1: A unified framework for classical simulations of quantum circuits*

It is of foremost importance, both from the foundational and technological point of view, to understand what components of the quantum theory are responsible for quantum supremacy [8], i.e. the potential ability of quantum computers to solve problems that cannot be solved efficiently on classical machines. One of the most promising ways to achieve this is to identify sub-theories of the quantum theory that can be efficiently simulated on classical computers. The first result of this kind was the celebrated Gottesman-Knill theorem, which states that the stabiliser sub-theory, where one is restricted to state preparation and measurements in the computational basis and evolution according to Clifford gates, can be simulated in such a way [5]. Moreover, the addition of a single type of a pure "magic" (non-stabiliser) state allows one to promote this classically simulable sub-theory to universal quantum computing [9]. Due to magic state distillation protocols one can also convert mixed non-stabiliser states to a pure magic state, and the rate of this conversion can be related to the amount of quantum computing resource present in a state [10]. In other words, this yields a way to quantify how useful a given quantum state is in promoting classically simulable computation to universal quantum computation. These initial results were later extended by devising efficient simulation schemes for quantum circuits with positive Wigner representation [11, 12]. Independently, classical algorithms have been developed to simulate matchgate circuits [13, 14], and it was shown that these can also be promoted to universality by the addition of the SWAP gate [15].

More recently, mathematical tools have been developed not only to separate classically simulable sub-theories from universal quantum computing, but also to quantify the amount of overhead needed to simulate circuits that include resource magic states. In Ref. [16] the authors developed Monte Carlo sampling techniques that allow one to estimate the probabilities of outcomes of a quantum circuit, with the run-time growing with the total negativity of the circuit, thus highlighting the role of negativity as a measure of quantum computational resources. The next step was to remove all "quantumness" from the circuit and transfer it to the initial magic states of ancillary systems through gadgetisation of quantum gates [9]. Employing this, the aforementioned sampling techniques and the stabiliser decomposition of ancillary magic states, algorithms simulating universal quantum circuits were designed with the overhead scaling with the stabiliser rank [17, 18] and the robustness of magic [19]. Alternative Pauli decomposition was also considered providing complementary results [20].

Although the above classical algorithms differ in details, one can observe that they nevertheless all operate on the same underlying principle. First, identify the free sub-theory, e.g. Clifford circuits, matchgates or Gaussian operations, and a gate that promotes it to universality. Then, find a gadgetisation of this gate and thus rewrite any universal circuit as a free circuit with additional ancillary resource states. Finally, decompose the resource states into a combination of (exponentially many) free elements, use Monte Carlo sampling techniques to sample a subset of these, and propagate them efficiently through the free circuit. I believe that this three-step algorithm not only provides a very promising direction to unify many known simulation schemes, thus deepening our understanding of the nature of quantum computing, but also provides a clear way to develop novel simulation algorithms. Each of the three steps described above can be optimised independently. In particular, to optimise steps 1 and 2, one would need to have a better handle on how to quantify and manipulate magic states, which could be achieved by studying the interconversion problem within the resource theory of magic [21]. While in step 3 one would need to identify possible sets of free elements that magic states can be decomposed into (e.g. mixed and pure state stabiliser state decompositions, but also decompositions into elements that are not states, like Pauli decomposition [20]), and find optimal decompositions that would minimise the simulation overhead.

Specific research tasks:

1) Developing a unified scheme for classical simulation of universal quantum circuits based on a three-step algorithm: identifying free sub-theory, gadgetizing all quantum resources, sampling and propagating the free elements taken from optimal magic state decomposition (Goal 3 – Implementation).
2) Devising novel algorithms with improved run-time scaling by employing alternative free element decompositions, especially the decomposition into pure free states. Implementing these algorithms on classical computers and employing them to certify and verify NISQ devices [1] (Goal 3 – Implementation).
3) Investigating the interconversion problem for the resource theory of magic states, with a particular focus on asymptotic interconversion and magic distillation (Goal 2 – Characterisation).

B. Objective 2: Feasibility and quantum advantage of quantum thermodynamic protocols

Thermodynamics is one of the most versatile physical theories, finding applications in almost all fields of science, from cosmology and astrophysics to chemistry and the theory of computation. Its strength comes from the fact that it provides a universal framework that uses statistical tools to study physical phenomena in the so-called thermodynamic limit, i.e. when the number of involved systems is very large. However, our increasing ability to manipulate and control systems at smaller and smaller scales allows us to build novel nanodevices [22–24], displaying quantum-mechanical properties like coherence or entanglement, which cannot be properly captured within the traditional framework. Therefore, in order to understand the thermodynamic properties of such devices, from the early 2000s a novel approach to quantum thermodynamics, strongly based on mathematical tools from the field of quantum information theory, has been developed [25–28]. As a result, a resource-theoretic framework has been established that uses information-theoretic notions to describe thermodynamics of single quantum systems [29].

One of the main aims of the Quantum Resources Group within Objective 2 is to bring the abstract resource theory of quantum thermodynamics closer to actual physical applications. Most of the current results have a very fundamental character, telling us whether a given transformation is possible in principle. The problem is that in many cases optimal transformation protocols require a very fine control over the transformed systems and their interactions with the environment. We will work towards extending this theory so that it does not only characterise fundamental constraints of physical processes, but also faithfully describes the limitations arising in realistic experimental scenarios. This way the predictions of resource theories could be tested experimentally, which is a necessary condition for a theory to play an active role in developing future quantum technologies. I believe that the first steps towards this direction, aligned with Goal 3 – Implementation, should include abandoning the commonly studied idealised scenarios, stemming from simplifying assumptions of asymptotic limit, adiabatic control and memoryless interactions with the environment. In my previous research I have already started building a framework capable of addressing these issues [30–33], and Quantum Resources Group will work further on expanding the potential of resource-theoretic formalism to capture finite-size, finite-time and finite-memory effects.

A parallel aim within Objective 2 is to investigate possibilities for real quantum advantage within thermodynamics, analogous to quantum supremacy in the computational field [8]. The results I have obtained so far are among the first to have captured the quantumness of thermodynamic processing, explained how it can be seen as a hybrid resource theory of athermality and asymmetry, and linked thermodynamic considerations to the concept of quantum reference frames [34, 35]. Although these kind of results are essential for describing quantum phenomena in thermodynamics, they mainly provide mathematical tools required to pursue Goal 1: identifying thermodynamic protocols whose performance cannot be explained within classical theory, e.g. the reversed direction of heat flow due to quantum entanglement [36] that has been very recently probed experimentally [24]. Thus, Quantum Resources group will focus on studying the limitations of stochastic-thermodynamic models, and more generally classical hidden variable models, in explaining the behaviour of quantum heat machines.

Specific research tasks:

1) Investigating the potential to experimentally probe the recently predicted resource resonance phenomenon [33] through the analysis of the performance of heat engines in a more traditional framework that is closer to experiment (e.g. Hamiltonian control and thermalisation model from Ref. [37]), with a particular focus on conditions for which the resonance is predicted (Goal 3 – Implementation). Search for the resonance phenomenon within the resource theory of U(1) asymmetry in order to extend the formalism of thermodynamics beyond the thermodynamic limit [31] to states with coherence (Goal 2 – Characterisation).
2) Exploring the capabilities of resource-theoretic formalism under the restrictions of limited control due to access only to transformations that could be implemented experimentally, e.g. local Hamiltonian control [38] and partial thermalisations [39] or coarse-grained operations (Goal 3 – Implementation). Assessment and quantification of the role of memory (creating correlations with the bath) in performing optimal thermodynamic transformations (Goal 2 – Characterisation).
3) Devising quantum thermodynamic protocols with improved performance compared to their classical counterparts: employing coherence to increase power output [40] or decrease runtime of thermodynamic processes; reduction of work fluctuations; exploiting entanglement to bend the thermodynamic arrow of time and reduce irreversible dissipation [36] (Goal 1 – Identification).

C. Objective 3: Operational resource theory of coherence

Arguably, what underlies all quantum resources, from computational to cryptographic ones, is the quantum principle of superposition, i.e. the wave-like feature of quantum states that allows them to interfere constructively or destructively, thus exhibiting coherent behaviour. Thus, a quantitative framework allowing one to assess how coherent a given state or process is would constitute an invaluable tool to study the power of quantum theory to overcome classical constraints. Such a tool has indeed been developed by constructing the resource theory of coherence [41–43]. During the recent years this field has driven a lot of attention and flourished [44], with many important results on manipulating coherence being established, e.g. finding conditions on single-shot pure state transformations under incoherent operations [45] or deriving optimal interconversion rate for coherence resources in the asymptotic limit [46]. Moreover, the framework has also been extended to study coherent properties of quantum channels, e.g. by introducing the coherence power of a map [47, 48], or by employing the Choi-Jamiołkowski isomorphism [49, 50].

However, what seems to be missing in this explosion of interest around the resource theory of coherence is its operational meaning and the role played in particular quantum protocols. We could say that while the problems within Goal 2 –

Characterization have been scrutinised in detail, not much work has been done to achieve the other two goals. Concerning Goal 3 – Implementation, the allowed sets of transformations, like incoherent operations [42], have been mostly defined in an axiomatic way, and thus their relation to real physical constraints is usually not clear. Although some works pointed out the relation with conservation laws and superselection rules [51], and thus physically motivated the use of covariant channels and the resource theory of asymmetry [52] to study coherence, the progress along this direction garnered limited attention (especially when compared to the axiomatic formulation). And when it comes to Goal 1 – Identification, the usefulness of coherence in phase-estimation protocols has been studied [53], but the full analysis of the role coherence plays in different quantum protocols and under various constraints has yet to be performed. These could include communication scenarios with quantum reference frames [54], optimal implementations of quantum channels [55], or avoiding dissipation while inducing a fixed energy transfer.

Specific research tasks:

1) Determine physical constraints under which coherence monotones become operationally meaningful in communication, computation or thermodynamic scenarios (Goal 1 – Identification). Exploring the interplay between coherence and other resource theories [56] (Goal 2 – Characterisation).
2) Sharpen our foundational and operational understanding of coherence measures for quantum channels [49] by studying the structural differences between classical stochastic dynamics and open quantum dynamics (Goal 1 – Identification).
3) Investigating the interplay of coherence and memory in state interconversion processes [30] (Goal 2 – Characterisation). Finding limitations on Markovian hidden variable models and studying conditions under which Markovian processes employing quantum coherence can overcome them (Goal 1 – Identification).

III. ORGANISATION OF WORK AND COLLABORATIONS

Quantum Resources Group will consist of seven people: project leader, supporting scientist (50% employment), two post-doctoral researchers, two PhD students and a Master student. The group will operate within a wider TEAM-NET project whose duration is set to 48 months. Both PhD students will be employed for the full period of 48 months and it is planned that the research of one PhD student will be devoted to Objective 1, while the other one will focus on Objectives 2 and/or 3. Post-doctoral researchers, employed for the period of 24 months, with a possible extension by 12 or 24 months, are expected to take part in all research activities of the group. However, it is assumed that one of them will have a stronger expertise in quantum algorithms, simulations and computing, while the other in open quantum systems, quantum information and resource theories. Two Master students, each employed for 24 months, will work on smaller problems within Objectives 1-3, while learning the necessary analytical and computational skills and getting research experience. The supporting scientist will help with the supervision of the students and will work on one chosen Objective.

The group will closely collaborate, especially when it comes to realising Objective 1, with the other three research groups forming the TEAM-NET consortium. These are: Quantum Computing Group at the Center for Theoretical Physics of the Polish Academy of Sciences in Warsaw led by Michał Oszmaniec, Quantum Machine Learning Group at the Institute of Theoretical and Applied Informatics of the Polish Academy of Sciences in Gliwice led by Zbigniew Puchała, and Quantum Error Correction Group at the Jagiellonian University in Kraków led by Erik Aurell. Moreover, the research along the directions within Objective 3 will be supported by the TEAM-NET consortium leader, Karol Życzkowski from the Jagiellonian University, and work on Objective 2 will be performed in cooperation with the researchers from the International Centre for Theory of Quantum Technologies at the University of Gdańsk.

Concerning international collaborators, Tasks 1 and 2 of Objective 1 will be followed in close partnership with Hakop Pashayan from University of Sydney, the author of the original Monte Carlo sampling technique underlying the classical algorithm for simulating quantum circuits. Tasks 2 and 3 of Objective 2 and Task 3 of Objective 3 will be investigated in collaboration with Matteo Lostaglio from ICFO Barcelona, an emerging leader in the field of quantum thermodynamics. Task 1 of Objective 2 and Task 1 of Objective 3 will be pursued together with Marco Tomamichel from University of Technology Sydney, a well-established quantum information theorist. Further potential collaborators include David Jennings from University of Leeds (Objectives 1-3) and Christopher Chubb from University of Sherbrooke (Task 3 of Objective 1).

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