PhD Project
"Quantum algorithms for thermal equilibrium"
Supervisor: Álvaro Martín Alhambra

Introduction:

We are currently at the dawn of the age of synthetic quantum matter, in which various kinds of quantum computing and simulation platforms are at a crucial stage of development. Fast experimental developments promise to set numerous scientific breakthroughs within their reach of in the coming years.

However, we still have not fully understood the computational power of these news devices, and we have not fully elucidated the problems that they most naturally help us solve. It is widely believed that one of the more promising near term avenues is the exploration of quantum many-body physics. This is being done through the development of "quantum simulators", which will be able to reproduce the physics of a plethora of complex models. This is particularly interesting because large quantum systems are generally very hard to simulate by standard computers, and we are currently reaching the stage in which these new devices are able to probe regimes provably beyond our numerical capabilities.

This now begs the question: what is the range of physical settings that we are able to reliable and efficiently probe with quantum devices? This can be answered within the theory of quantum algorithms. With it, we can construct abstract models of the types of schemes and protocols that are in principle possible to implement.

In this project, we focus on one of the most pressing questions along these lines: that of studying thermal equilibrium with quantum computers. The key task we want to be able to do is to prepare Gibbs states on a quantum computer. This, in contrast to the simulation of unitary dynamics, is significantly less developed, even if it widely considered as a crucial problem, due to two complementary reasons:

1. The first is that the Gibbs state, representing thermal equilibrium, is one of the most ubiquitous states of matter: it appears whenever there are couplings to an external environment, such as radiation or phonon fields. As such, their generation in quantum computers is necessary in order to solve a great variety of important physical problems.

2. Beyond the obvious physical importance, these states are also relevant from a computational perspective. In particular, sampling from Gibbs distributions is a subroutine in various quantum algorithms, such as those solving optimization problems.

Academic background:

Prospective candidates must have completed a masters degree on a subject related to the project, or be expectd to complete it in the near future. The project offers a certain degree of flexibility in terms of backgrounds. However, we expect that succeful candidates have experience in the form of masters or final-year undergrad courses, and/or master or bachelor thesis, in topics along the lines of:

-Quantum computing and quantum algorithms
-Quantum information theory
-Mathematical physics
-Condensed matter theory

Programming experience is valuable but not required.

Expected scientific activities:

While the project is motivated on a high level by technological developments, it is of a fundamental and theoretical character, aiming at elucidating the near term and future capabilities of quantum simulators and quantum computers beyond specific architectures or implementations. The project has a markedly mathematical nature, and will involve using tools and ideas from theoretical quantum computing. As such, the methodology is theoretical in nature, and our results will be for the most part in the form of lemmas and theorems which imply guarantees on the performance, reliability and runtime of the algorithms. This type of mathematical rigour is typically needed to make grounded complexity-theoretic statements, such as placing a specific problem in a given complexity class. The types of frameworks we will work with are:

-Mathematical physics tools to analyze many-body thermal equilibrium, including new models of quantum thermalization.

-Theory of quantum algorithms: we will use well established frameworks for quantum algorithm design, which allows us to systematically construct schemes with provable bounds on the runtimes and resources involved.

-Quantum information theory: Important ideas such as the mutual information, and the conditional mutual information , which allow us to systematically characterize the nature of the correlations among the constituents of the many body system.

Our algorithms will be useful as part of explorations of the physics of strongly coupled quantum many-body systems. They will also potentially be an important subroutine of other important quantum algorithms, for various tasks such as optimization. By devising efficient methods to prepare Gibbs states, we will:

-Be enlarging the sets of quantum simulation experiments that can happen at finite temperature, also with rigorous guarantees showing that thermal physics is really what we are seeing in the measurements.

-Bring new computational capabilities to the field of quantum simulators. These algorithms will ultimately serves as part of the toolkit for simulating many quantum systems, which ultimately is expected to unlock breakthroughs in many fields of science such as material or drug design, as well as chemistry.

-Beyond enabling quantitative explorations, we also envision a path for new ways of understanding physics based on complexity theory. The progressive characterization of quantum phenomena in informational and computational terms repeatedly appears very useful within the practice of physics, and this project will further confirm that idea.

The project includes funds for an international research stay within the second half of the PhD project, as well as funds for attending conferences and summer schools.

Research group and center:

The PhD candidate will join the doctoral program of the Institute of Theoretical Physics (IFT) UAM/CSIC, which can be considered a reference in Spain. It complements and extends the prestigious “Master in Theoretical Physics” of the Department of Theoretical Physics of the UAM, in collaboration with the IFT. This program has been recognized with the prestigious Quality Mention by the Ministry of Education and Science. The Theoretical Physics Doctorate program has received this award since its first call in the 2003-2004 academic year.

The doctoral project will be carried out within the "Quantum Information and Quantum Matter" group of the Institute of Theoretical Physics. In addition to the main supervisor, the group has 4 other permanent members, as well as numerous postdocs and students. It is a dynamic group with many young members working on a variety of related topics.

The student is expected to participate in the activities of the group and the institute at large, such as regular seminars, group meetings and colloquia. They will also be encouraged to participate in the range of outreach activities promoted at the IFT.

Relevant references:

[1] C. Rouze, D. S. Franca, and Á. M. Alhambra, «Efficient thermalization and universal quantum computing with quantum gibbs samplers," https://doi.org/10.48550/arXiv.2403.12691 2024
[2] C.-F. Chen, M. J. Kastoryano, and A. Gilyén, «An efficient and exact noncommutative quantum Gibbs sampler». arXiv, 15 de noviembre de 2023. doi: 10.48550/arXiv.2311.09207.
[3] Á. M. Alhambra, «Quantum many-body systems in thermal equilibrium», *PRX Quantum*, vol. 4, n.o 4, p. 040201, nov. 2023, doi: 10.1103/PRXQuantum.4.040201.
[4] Á. M. Alhambra, J. I. Cirac, «Locally accurate tensor networks for thermal states and time evolution», *PRX Quantum*, vol. 2, n.o 4, p. 040331, nov. 2021, doi: 10.1103/PRXQuantum.2.040331.

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