Simulating Quantum Complex Many-body systems with quantum computations

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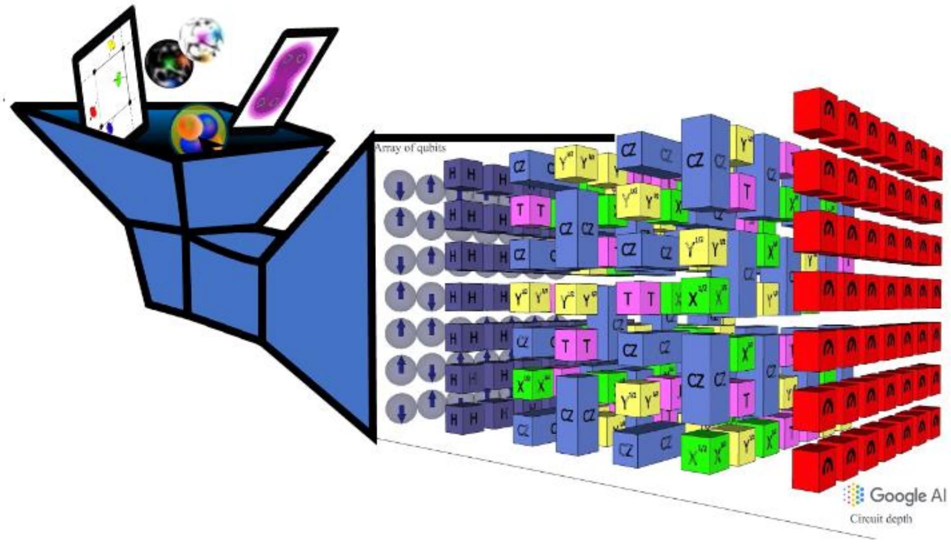
This prospective is part of the QC2I project objectives.

Abstract:

With recent advances in quantum computer prototypes, the field of quantum computing is gaining momentum towards real applicability. This disruptive technology opens new perspectives for the quantum simulation of complex systems. The aim of the project is to use state-of-the-art progresses in this field to simulate atomic nuclei and more generally complex quantum many-body systems. Such systems appear for instance in atomic physics, condensed matter, nuclear and particle physics as well as in quantum chemistry. Regarding nuclear systems, nuclei, that are made of fermions interacting strongly with each other, enter into the class of complex quantum systems that could hardly be treated exactly on classical computers when the number of nucleons increases. Exact ab-initio methods can describe only a few percent of the atomic nuclear chart. Quantum computers might potentially surpass this barrier. In this project, we propose to use the nuclear many-body problem as a strong test for quantum devices and quantum algorithms. This will pave the way to future applications in nuclear physics, and our feedback will further support future developments in the field of quantum computing (a schematic view of the project's goals is shown below).

Note that the present document is adapted from an ANR submitted in 2021 and was also discussed within the "Atelier de Physique Théorique" 7-8 June 2021.



Introduction:

The development of real-world quantum computers is now progressing rapidly, with several international companies racing towards building prototypes with an increasing number of qubits. This intense international competition is contributing to rapid advances in both technological and fundamental research. Overall, this field is experiencing a boost on a global scale with parallel developments of new hardware and new programming methods *[Nielsen, 2000]*. Quantum devices have entered the NISQ (Noisy Intermediate-Scale Quantum) *[Preskill, 2018]* era, i.e., non-trivial calculations are possible but noise and stability limit the size of quantum circuits that can be executed reliably. Despite these difficulties, scientists in different fields start to seriously consider quantum computers as a disruptive technology that opens new horizons.

Quantum simulations for many-body systems in condensed matter, chemistry, atomic physics, and nuclear physics may potentially bring us to address so-called 'Grand Challenge' problems, i.e. problems that cannot be tackled using classical computation. In particular, quantum computing (QC) may provide the possibility to work with Hilbert space dimensionalities that are exponentially larger than those accessible with classical computers, thus overcoming the limitations that are currently preventing the exact theoretical many-body description of large and complex systems. First concrete steps in this direction have been made in the past few years in quantum chemistry and condensed matter *[McArdle, 2020; Bauer, 2020]*.

The QC2I project of the IN2P3 started on January 2020, aiming to introduce to QC the High Energy and Nuclear Physics French community and to explore possible applications of QC for our research domains. One important activity in this project is the application of quantum technology in the context of the nuclear many-body problem, with three specific objectives:

(i) Test the pertinence of state-of-art algorithms and methods, mainly developed in other fields, in nuclear physics applications;
(ii) Design new algorithms tailored to nuclear systems;
(iii) Investigate the possible feedback of nuclear-physics approaches to quantum simulations of other interacting many-body systems.

These objectives will be achieved by combining our accumulated expertise in the nuclear many-body problem with the latest advances in quantum algorithms. On the hardware side, the project will make use of the new experimental (real devices) and theoretical (emulators) tools that are emerging in the QC field. The project will be a stringent test of their viability for future applications and will contribute to future improvements of the QC science together with opening new horizons in nuclear physics.

State of art:

First proof-of-principle calculations were performed in chemistry *[O'Malley, 2016, McArdle, 2020; Bauer, 2020]* and in nuclear physics *[Dumitrescu, 2018; Lu, 2019]*. A variety of emerging quantum technologies are becoming now available or under development like small trappedion systems, cold-atom systems, annealing devices as well as superconducting quantum devices. These new hardware progress allow to perform pioneering calculations on quantum computers. In this context, intensive efforts are now devoted, especially in the US laboratories, to explore the potentialities of quantum computers for nuclear or particle physics problems *[Cloet, 2019]*. So far, only very few applications have been made in the nuclear many-body problem and many questions remain open. Nuclear systems have specific features, like the number of constituents that varies from very few to several hundreds, the strong interaction between nucleons or the importance of symmetry breaking leading to superfluidity and/or shape coexistence. How these physical properties can be encoded efficiently on quantum computer, especially in the NISQ period, is an important challenge that might contribute globally to the treatment of complex quantum system by quantum devices.

Proposed Methodology:

The objective of the project is to explore in a more systematic way the new opportunities offered by quantum computers for mesoscopic many-body systems with a focus on atomic nuclei. Our strategy is to systematically address each step depicted in the generic circuit of Figure 1.

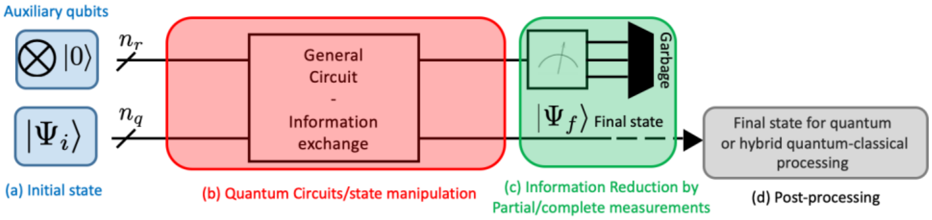


Fig 1*: Schematic view of a generic quantum circuits. The different steps are (a) Initial state preparation, (b) state processing by performing quantum operations, (c) measurement leading to final state and (d) state post-processing (adapted from [Lacroix, 2020]).*

We propose the following working plan:

(a) Initial state preparation and Hamiltonian encoding: Firstly, one of the crucial aspects to treat accurately the many-body systems is to prepare a many-body state. Nucleons are fermions that can be mapped to qubits *[McArdle, 2020]*; recently, a Hartree-Fock (HF) state was prepared on a real device *[Google, 2020].* Such HF states are crude approximations, unable to grasp correlations in strongly interacting systems. We plan to explore several methods to construct strongly entangled states beyond HF. A first step in that direction was made by us in Ref. *[Lacroix, 2020],* using symmetry breaking/restoration encoded on a QC. This direction will be pursued in the project with validation on other symmetries and real devices. In parallel, we will explore alternative methods based on coupled-cluster and Similarity Renormalization Group. In general, specific circuits need to be invented and used in step (b).

(b) Quantum state manipulation/evolution: following the leitmotiv that one of the primary applications of QC is the description of complex quantum system themselves that could not be described by classical computers, the core of the project will be devoted to the description of static and dynamical properties of many-body systems with QC. Once the methodology to set up many-body states with various degree of correlations are prepared in step (a), these states can be used in a second step for further quantum manipulations. In the first part of the project, we would like to test current algorithms based on unitary quantum evolution both used to extract energy spectra and to perform real-time evolutions. The aim will be to qualify these algorithms for tackling the nuclear many-body problem and so identify specific aspects that need to be improved. We expect to develop nuclear-physics adapted versions of existing methods and/or new quantum algorithms. Besides this global preliminary study, we plan to work on more specific problems:

Some of the main aspects on which we will focus are:

- We will study the possibility to encode Green Functions (GF) on a quantum computer *[Endo, 2020].* Green functions are indeed among the most powerful approaches used nowadays in classical computers for many-body nuclear ab-initio approaches *[Soma, 2020]* but become prohibitive as the number of particles increase. QC can potentially surpass present limitations.
- An important aspect in nuclei is the non-perturbative nature of the problem due both the strong interaction and the occurrence of spontaneous symmetry breaking. A typical example is the onset of superfluity in nuclei. In the project, we will explore the possible exact treatment of such problems in QC with the motivation (i) to demonstrate that QC is a promising technology for near term study to simulate problems that cannot be performed on classical computers (ii) to describe superfluidity on QC as an archetype of symmetry-breaking problem that is important in many areas of physics.
- We will explore the potential of quantum machine learning (QML) *[Biamonte, 2017, Albash 2018]* as an alternative to standard machine learning to address complex many-body problems. In many situations, we face the difficulty of an explosion of the Hilbert space or of extremely potential energy landscapes. The use of QML in this context will be studied.

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