Minicolloque n° PMQ30 **Poster**

Quantum simulation of bulk materials with Rydberg atoms device

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Finding the exact ground state of a highly correlated condensed matter system would be a real asset to understand some of its physical properties. Density functional theory is so far the state-of-the-art numerical method to find the ground state energy of alloys and complex systems. However, the result of this numerical method is only an approximation of the real ground state and it might not be efficient to grasp complex phenomena such as the para-magnetism of austenitic steels used in particular in industrial applications [1].

A new approach to overcome the limitation of the current simulation methods relies on quantum simulation applied to quantum chemistry and condensed matter to simulate materials in [1]. In particular, a hybrid variational approach combining quantum hardware with classical optimization, the variational quantum Eigen solver (VQE) [3] method, is being actively explored. However, so far, most of the results with this approach use Digital Quantum Simulation (DQS) [2]. The digital approach is challenging to implement experimentally, as most of hardwares are still too noisy. Consequently, DQS remains limited to very small systems. It is therefore interesting to investigate how far one can push the approach using the Noisy Intermediate Scale Devices already available [4]. This requires relying on an analog quantum simulation approach, as opposed to the universal digital quantum simulation. Here one has to use the Hamiltonian naturally implemented by the device.

The main purpose of this poster presentation is to introduce new methods to simulate chemistry and condensed matter physics by using analog quantum simulation and VQE on a particular quantum simulator based on arrays of Ryberg atoms, as developed in several labs and in the startup Pasqal [5]. We will benchmark this approach on the simple problem of finding the ground state of the H_2 molecule, using the various resource Hamiltonians (Ising and XY) available in the Rydberg platform, and including typical experimental imperfections and constraints. I will also discuss the limitations of these methods and the results we can expect in the near future.

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