QUANTUM COMPUTING FOR QUANTUM CHEMISTRY

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Résumé:
In quantum computing, solving the electronic structure problem from quantum chemistry is considered one of the most promising applications. Today, lots of efforts are devoted to the development of quantum algorithms in the hope that one day we will be able to access a high-level description of molecular properties at a speed greater than that of any classical computer. But tackling such complex problems with today's quantum devices requires caution, as experimental platforms are still in their infancy and suffer from significant constraints. Until quantum computers are more stable, we will have to adapt our vision of algorithm development.

In this introductory talk, I will describe the state-of-the-art in quantum algorithms for solving the electronic structure problem. Particular attention will be paid to the Variational Quantum Eigensolver: a hybrid classical-quantum method originally developed to target the ground state of molecules. I will then present an extension of this method called SA-OO-VQE[1] that I have recently developed to describe multiple electronic states (ground and excited). Finally, I will discuss some further developments I have made to allow access to nuclear gradients and non-adiabatic couplings[2], which represent key ingredients in the implementation of numerical quantum dynamics simulations.

Références:
1. Yalouz, S., et al. Quantum Sci. Technol., 2021, 6(2), 024004.
2. Yalouz, S., et al. J. Chem. Theory Comput. 2022, 18, 2, 776–794