Simulating molecular properties on a quantum computer

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Résumé

The increase in computational power together with theoretical method developments have played a significant role in our understanding of matter over the last decades. However, technological progress is now threatened by the predicted death of Moore's law and new strategies have to emerge.
Indeed, the modeling of molecules and materials requires to solve the electronic structure problem, which scales exponentially with the system size. Nowadays, workarounds to this exponential wall problem are the use of truncated wavefunction-based correlation methods, Kohn-Sham density functional theory or Monte Carlo techniques. Unfortunately, large complex systems having strong multiconfigurational character remain challenging either in terms of computational cost or accuracy. Alternatively, quantum embedding theories have been proposed and allow to partition the system such that only the most active part (fragment) is treated by a high-level method, while the rest of the system (environment) is treated by a low-level method. However and despite promising results, the (sometimes drastic) decrease in the size of the Hilbert space in embedding approaches comes with a decrease in accuracy, and they still scale exponentially with the size of the fragment. Therefore, only small fragments can be considered and large complex systems remain intractable on a classical computer. That is when quantum computing enters into the game. Quantum computers promise an exponential speed-up to solve the electronic structure problem, such that modeling chemical reactions and complicated molecular systems has been proposed as the "killer application" of a future quantum computer. In this talk, I will introduce the concept of quantum computing and the two main algorithms developed to extract the ground- (and eventually excited-) state energy, namely the quantum phase estimation and the variational quantum eigensolver. Finally, I will discuss our recent work on determining molecular properties on a quantum computer from the calculation of energy derivatives.

Mots-Clés: Quantum Computing, Quantum Phase Estimation, Variational Quantum Eigensolver, Exponential speedup

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