Towards Quantum Chemistry on Quantum Computers

Seminar

Monday, November 18, 2024

3:00 – 4:00 p.m.

Beaupre Center, Room 105

Several unsolved challenges in quantum-level computational chemistry require accurate and scalable approaches to solve the strong electron correlation problem for molecules and materials. Current and upcoming quantum computers provide immense opportunities to advance quantum chemistry by sidestepping the steep scaling of accurate methods for such problems. On the other hand, quantum chemistry is expected to be one of the first areas where quantum computers can demonstrate a clear and useful advantage over classical computers. Many algorithms are proposed for the key tasks in quantum chemistry, namely finding accurate molecular ground and excited states of a time-independent molecular Hamiltonian. At the same time, there are several challenges before these devices can assist research in chemical sciences. I will outline the research problem, recent developments in this exciting new field and some of the major theoretical challenges that need to be resolved in the future. Further, I will discuss our latest developments, particularly, the pulse-level variational molecular simulation algorithm (ctrl-VQE) and a new molecular excited-state method (q-sc-EOM) aimed at near-term and early fault-tolerant quantum computing.

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Fall 2024 Seminar Series

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