Hardware-Efficient Quantum Simulation of Strongly Correlated Molecules and Materials with Reconfigurable Atom Arrays

S Ostermann[1]

[1]*Department of Physics, Harvard University, Cambridge MA, USA*
Contact Email: stefanostermann@g.harvard.edu

Simulations of quantum chemistry and quantum materials are believed to be among the most important potential applications of quantum information processors. As such, realizing practical quantum advantage for problems such as the accurate calculation of electronic properties is a key milestone, which has yet to be achieved. In this talk, I will introduce a simulation framework to analyze molecules and materials with strong correlations that can be approximated by model Hamiltonians on a programmable quantum simulator. Specifically, we propose a method to simulate the dynamics of spin Hamiltonians in a hardware-efficient manner, using reconfigurable neutral atom arrays and multi-qubit entangling operations. We show that these tools enable Floquet engineering of many realistic systems, which include bi-quadratic and higher-order terms. We present a suite of algorithms for extracting detailed spectral information from time-dynamics, through snapshot measurements and ancilla-assisted control, enabling the efficient evaluation of quantities relevant to quantum chemistry and materials science such as excitation energies and finite-temperature susceptibilities. Moreover, our approach can efficiently integrate state-of-the-art classical and quantum methods to prepare low-energy variational states and to initialize the dynamics. As an example, we show how this method can be used to compute chemically-relevant properties of polynuclear transition metal catalysts and 1D magnetic materials.