COMPUTATIONAL RESEARCH in BOSTON and BEYOND SEMINAR

Programmable Simulations of Molecules and Materials with Reconfigurable Quantum Processors

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ABSTRACT:

Simulations of quantum chemistry and quantum materials are believed to be among the most important potential applications of quantum information processors, but realizing practical quantum advantage for such problems is challenging. Here, we introduce a simulation framework for strongly correlated quantum systems that can be represented by model spin Hamiltonians. Our approach leverages reconfigurable qubit architectures to programmably simulate real-time dynamics and introduces an algorithm for extracting chemically relevant spectral properties via classical co-processing of quantum measurement results. We develop a digital-analog simulation toolbox for efficient Hamiltonian time evolution utilizing digital Floquet engineering and hardware-optimized multi-qubit operations to accurately realize complex spin-spin interactions, and as an example present an implementation proposal based on Rydberg atom arrays. Then, we show how detailed spectral information can be extracted from these dynamics through snapshot measurements and single-ancilla control, enabling the evaluation of excitation energies and finite-temperature susceptibilities from a single-dataset. To illustrate the approach, we show how this method can be used to compute key properties of a polynuclear transition-metal catalyst and 2D magnetic materials.

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