Quantum Simulation of Molecules and Materials with present-day 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. We introduce a simulation framework for strongly correlated quantum systems that can be represented by model spin Hamiltonians. Our approach [1] 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 and other relevant chemical 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.

References

[1] Maskara N, Ostermann S, Shee J, Kalinowski M, Gomez AM, Bravo RA, Wang DS, Krylov AI, Yao NY, Head-Gordon M, Lukin MD. Programmable Simulations of Molecules and Materials with Reconfigurable Quantum Processors. arXiv:2312.02265.

Figures

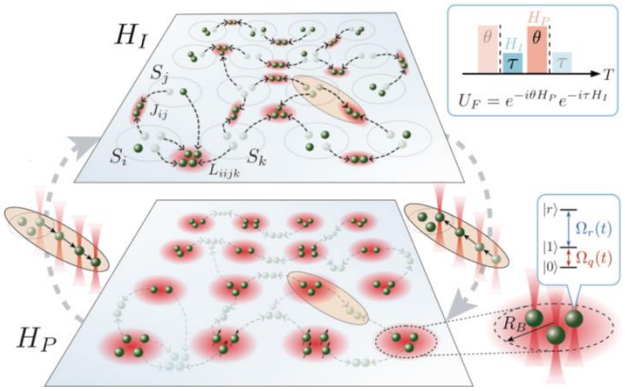

Figure 1: Hardware-efficient protocol for programmable simulation of generic spin Hamiltonian is based on applying sequences of interactions between non-overlapping few-qubit groups, moving atoms in between. This implementation of a complex spin model is using a dynamical projection approach where spin-S variables are encoded in the collective spin of a cluster of 2S qubits: interactions between spins are generated by evolving pairs of qubits from each cluster under an interaction Hamiltonian and then dynamically projected into the symmetric encoding space. This protocol can be realized in any reconfigurable quantum processor.