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Calculating the many-body density of states on a digital quantum computer

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Quantum statistical mechanics allows us to extract thermodynamic information from a microscopic description of a many-body system. A key step is the calculation of the density of states, from which the partition function and all finite-temperature equilibrium thermodynamic quantities can be calculated. In this work, we devise and implement a quantum algorithm to perform an estimation of the density of states on a digital quantum computer which is inspired by the kernel polynomial method. Classically, the kernel polynomial method allows us to sample spectral functions via a Chebyshev polynomial expansion. Our algorithm computes moments of the expansion on quantum hardware using a combination of random-state preparation for stochastic trace evaluation and a controlled unitary operator. We use our algorithm to estimate the density of states of a nonintegrable Hamiltonian on the Quantinuum H1-1 trapped ion chip for a controlled register of 18 qubits. This not only represents a state-of-the-art calculation of thermal properties of a many-body system on quantum hardware, but also exploits the controlled unitary evolution of a many-qubit register on an unprecedented scale.

Abstract category

Quantum Simulations

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