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Accelerating Quantum Chemistry Simulations on Quantum Computers with Signal Processing

davide.castaldo@phys.chem.ethz.ch Quantum phase estimation (QPE) is a flagship algorithm for quantum simulation on fault-tolerant quantum computers. However, recent resource estimates[1] suggest that surpassing classical simulation techniques requires millions of gates and hundreds of logical qubits. Consequently, significant effort is being devoted to developing QPE-like algorithms that could demonstrate practical quantum advantage on early fault-tolerant quantum computers—i.e., devices with error correction but a limited number of qubits[2] . A promising approach to reducing QPE's computational cost lies in recognizing that it estimates molecular energies by sampling the autocorrelation function in the time domain and performing a Fourier transform. This connection to signal recovery has recently inspired several methods for computing eigenvalues of quantum Hamiltonians using shallower QPE circuits[3–5]. Speeding up computation requires minimizing three key factors: (i) the total number of sampled points, (ii) the number of measurements per sampled point of the autocorrelation function, and (iii) the total length of the acquired signal. We adapt recent results from prolate Fourier theory[6] to design a quantum algorithm that simultaneously estimates ground and excited state energies while significantly shortening the total length of the sampled signal. At the same time, it demonstrates robustness to shot noise[7] . We perform a numerical analysis in both weak and strong correlation regimes, providing evidence that the algorithm achieves optimal (Heisenberg) scaling. Finally, we explore how the quality of the initial input state affects the accuracy of the estimates, suggesting that these improvements could lead to a practical quantum advantage.

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