Optimised Fermion-Qubit Encodings for Quantum Simulation with Reduced Circuit Depth

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Abstract

Simulation of fermionic Hamiltonians with gate-based quantum computers requires the selection of an encoding from fermionic operators to quantum gates, the most widely used being the Jordan-Wigner transform. Many alternative encodings exist, with quantum circuits and simulation results being sensitive to choice of encoding, device connectivity and Hamiltonian characteristics. Non-stochastic optimisation of the ternary tree class of encodings to date has targeted either the device or Hamiltonian. We develop a deterministic method which optimises ternary tree encodings without changing the underlying tree structure. This enables reduction in Pauli-weight without ancillae or additional swap-gate overhead. We demonstrate this method for a variety of encodings, including those which are derived from the qubit connectivity graph of a quantum computer. Across a suite of standard encoding methods applied to water in STO-3G basis, including Jordan-Wigner, our method reduces qDRIFT circuit depths on average by 27.7% and 26.0% for untranspiled and transpiled circuits respectively.

References

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2. Miller et al., PRXQuantum, 4 (2023), 030314
3. Liu et al., IEEE International Symposium on HPCA, (2025), 143-157
4. Li et al., Chinese Phys. Lett., 42 100001

Figures

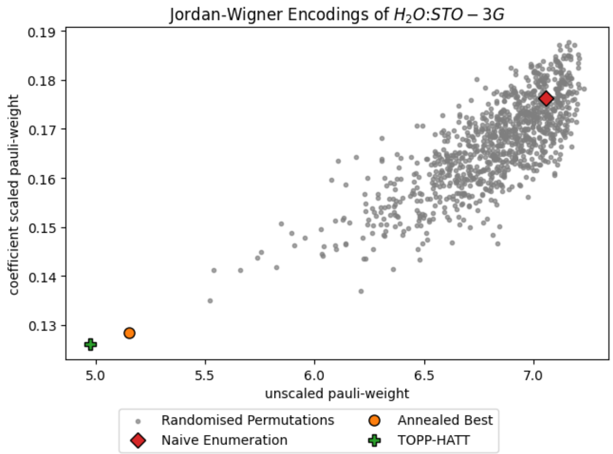

Figure 1: Pauli-Weight and Coefficent-Pauli-Weight of enumerations of the Jordan-Wigner encoding of H2O (STO-3G).

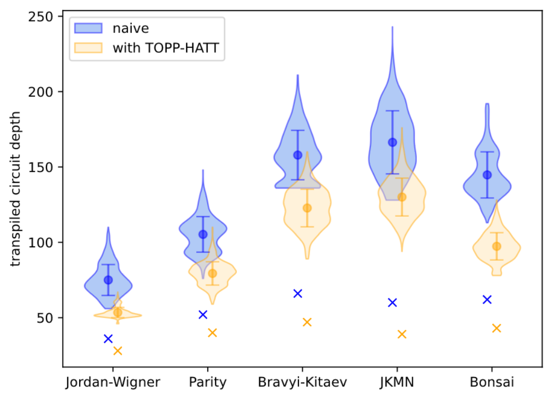

Figure 2: Reduction in qDRIFT circuit depth (t=0.001) for various encodings of H2O (STO-3G).