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Fast Partitioning of Pauli Strings into Commuting Families for Optimal Expectation Value Measurements of Dense Operators

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The Pauli strings appearing in the decomposition of an operator can be can be grouped into commuting families, reducing the number of quantum circuits needed to measure the expectation value of the operator. We detail an algorithm to completely partition the full set of Pauli strings acting on any number of qubits into the minimal number of sets of commuting families, and we provide python code to perform the partitioning. The partitioning method scales linearly with the size of the set of Pauli strings and it naturally provides a fast method of diagonalizing the commuting families with quantum gates. We provide a package that integrates the partitioning into Qiskit, and use this to benchmark the algorithm with dense Hamiltonians, such as those that arise in matrix quantum mechanics models, on IBM hardware. We demonstrate computational speedups close to the theoretical limit of $(3/2)^m$ relative to qubit-wise commuting groupings, for $m = 2, \ldots, 6$ qubits.

Topical area

Quantum Computing and Quantum Information

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