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Optimizing Qubit Resources for Quantum Chemistry Simulations in Second Quantization on a Quantum Computer NIKOLAJ MOLL, ANDREAS FUHRER, PETER STAAR, IVANO TAVERNELLI, IBM Research - Zurich — Quantum chemistry simulations on a quantum computer suffer from the overhead needed for encoding the fermionic problem in a bosonic system of qubits. By exploiting the block diagonality of a fermionic Hamiltonian, we show that the number of required qubits can be reduced by a factor of two or more. There is no need to go into the basis of the Hilbert space for this reduction because all operations can be performed in the operator space. The scheme is conceived as a pre-computational step that would be performed on a classical computer prior to the actual quantum simulation. We apply this scheme to reduce the number of qubits necessary to simulate both the Hamiltonian of the two-site Fermi-Hubbard model and the hydrogen molecule. Both quantum systems can then be simulated with a two-qubit quantum computer.

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