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Optimization schemes for reduction of many-body terms for quantum computations with fermions PANAGIOTIS KL. BARKOUTSOS, NIKOLAJ MOLL, PETER W.J. STAAR, ANDREAS FUHRER, STEFAN FILIPP, IBM Research Zurich, MATTHIAS TROYER, Institute for Theoretical Physics, ETH Zurich and Quantum Architectures and Computation Group, Microsoft Research, IVANO TAVERNELLI, IBM Research Zurich — Many-body fermionic quantum calculations performed on an analog quantum computer suffer from the existence of k-local terms, which represent interactions among more than two qubits. These originate from the application of Jordan-Wigner transformation for fermion-to-qubit map, to the electronic Hamiltonians in second quantization form. Existing solutions to this problems rely on the use of perturbation theory via Hamiltonian gadgets. The main obstacle associated to this technique is the introduction of large coupling constants, which are several orders of magnitude larger than the terms in the unperturbed physical Hamiltonian. To improve on it, we propose a new optimization scheme, that unfolds the k-local terms into a linear combination of 2-local terms in the enlarged Hilbert space, built as a tensor product between the physical and ancilla space. The optimization procedure ensures that the physical properties of the new Hamiltonian (eigenspectrum and density matrices) remain the same as in the original, while keeping all coupling constants comparable in size, making it better suited for an experimental quantum computer implementation.

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