Applications of Cartan Decomposition in Quantum Dynamics Simulation

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Abstract: The goal of quantum dynamics simulation is to accurately calculate the time-evolution operator of a given Hamiltonian. Our proposed method is based on the Cartan decomposition of the Lie algebra generated by the Hamiltonian, which splits the Lie algebra into two parts: a maximal abelian subalgebra (MASA) and a complementary subspace. The key idea of our method is to dynamically represent the time-evolution operator in terms of the MASA and the complementary subspace, such that the killing form, which is a measure of the exact decomposition, remains satisfied. This allows us to decompose the Hamiltonian evolution into smaller steps, which can be implemented using a series of quantum gates. Compared to other simulation methods, such as product formulas, our algorithm drastically improves simulation precision while using fewer quantum gates. In addition to providing exact circuits for a broad set of spin and fermionic models, our algorithm also provides broad analytic and numerical insight into optimal Hamiltonian simulations.