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Beyond S_2 : Generalized Higher-Order Product Formulae

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Quantum simulation of molecular Hamiltonians represents one of the most promising applications of quantum computing. At the heart of most quantum simulation algorithms lies the fundamental challenge of decomposing the evolution operator e^{-iHt} for a composite Hamiltonian $H = X + Y$ into a sequence of implementable quantum gates. Product formulae, also known as Trotter-Suzuki decompositions, provide a direct and practical approach to this problem by approximating the full evolution as a product of exponentials of individual Hamiltonian terms.

The systematic construction of high-order product formulae has been extensively studied, with fractal methods providing a general framework for achieving arbitrary accuracy orders. However, these approaches suffer from rapidly growing gate counts, making them impractical for near-term quantum devices. Recent advances have shown that numerically optimized product formulae can dramatically outperform their analytical counterparts.

A common assumption for constructing higher-order product formulae is that they are products of S_2 (second-order Trotter-Suzuki decompositions) operators. In this work, we search for formulae without this constraint, enlarging the solution space with additional free parameters while potentially reducing the total number of required exponentials. In this approach, we systematically derive order conditions from Baker-Campbell-Hausdorff (BCH) expansions in a chosen basis for the evolution operator, yielding systems of nonlinear equations that we solve using numerical root-finding methods. Our fourth-order formula achieves a 79% reduction in eigenvalue error while using fewer exponentials than existing methods. For sixth-order, our formula achieves a 50% reduction in eigenvalue error with a comparable number of exponentials to state-of-the-art approaches. These results show that exploring the enlarged parameter spaces combined with advanced numerical optimization can help us find better product formulae for Hamiltonian simulation, particularly relevant for early fault-tolerant quantum computers, where gate count remains critical.

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