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Quantum Algorithms for Hamiltonian Simulation with Unbounded Operators

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ABSTRACT

Recent years have witnessed tremendous progress in developing and analyzing quantum algorithms for quantum dynamics simulation of bounded operators (Hamiltonian simulation). However, many scientific and engineering problems require the efficient treatment of unbounded operators, which frequently arise due to the discretization of differential operators. Such applications include molecular dynamics, electronic structure theory, quantum control and quantum differential equations solver. We will introduce some recent advances in quantum algorithms for efficient unbounded Hamiltonian simulation, including Trotter type splitting and the quantum highly oscillatory protocol (qHOP) in the interaction picture. The latter yields a surprising superconvergence result for regular potentials.