Abstract

The main objectives of this thesis are to develop scalable quantum circuits for unitary matrices that describe the evolution of many-body quantum systems. Specifically, a quantum neural network-based framework is proposed to approximate any target unitary for n-qubit systems, and a circuit representation for the exponentials of scaled Pauli strings is established and used to propose scalable quantum circuit simulations of various Hamiltonians on near-term quantum devices. Furthermore, a discrete-time three-state quantum walk model for Cayley graphs is introduced, along with its corresponding quantum circuit model using elementary qutrit gates. The circuit complexity of the proposed quantum circuit models is explored, and various noise models are considered to investigate the performance of the proposed circuit simulations on near-term quantum computers.

First, we develop a parametric representation of unitary matrices of dimension d with the introduction of a new unitary Hermitian basis for the algebra of $d \times d$ complex matrices. Then, we adopt a Lie group theoretic approach to create an optimization algorithm for approximating any target unitary matrix using this parametric representation. Consequently, these results are employed to propose a new unitary Hermitian basis for the algebra of $2^n \times 2^n$ complex matrices, called the Standard Recursive Block Basis which serves as an alternative to the Pauli-string basis and is used to develop an optimization-based approximation algorithm for a scalable quantum neural network representation of a target unitary for n-qubit systems. Next, we develop a scalable quantum circuit representation of the exponentials of scaled Pauli strings, which is applied to execute circuit simulations of several one-dimensional Hamiltonians on near-term quantum computers, utilizing the first-order Suzuki-Trotter formula. These Hamiltonians include 2-sparse Hamiltonians, Ising Hamiltonians, and time-independent and time-dependent Random Field Heisenberg Hamiltonians, and Transverse Magnetic Random Field Quantum Ising Hamiltonians.

Besides, we introduce discrete-time three-state quantum walk models on Cayley graphs corresponding to Dihedral groups, using parametric coin operators known as generalized Grover coins. We analytically derive the periodicity of these walks and demonstrate that Grover walks on Cayley graphs corresponding to Dihedral groups do not exhibit periodicity properties, unlike Grover walks on other graphs documented in the literature. Numerical simulations show that the walker tends to localize at the initial position for a wide range of parameters of the coin operator, depending on the choice of initial coin states. We then develop qutrit quantum circuit models for simulating these quantum walks on Cayley graphs defined by Dihedral groups and the additive group of integers modulo a positive integer. These circuit models are scalable and are constructed using elementary qutrit quantum gates, such as single qutrit rotation gates, the qutrit-X gate, and two-qutrit controlled gates.

Keywords : Parameterized quantum circuits, special unitary matrices, Hamiltonian, Suzuki-Trotter product formula, quantum walks, Cayley graphs, periodicity,

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