Quantum Solver of PDEs by Triangle Quantum Circuits

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In this paper we discuss the utilization of quantum computing techniques, specifically the Variational Quantum Eigensolver (VQE) with Parameterized Quantum Circuits (PQCs), to solve linear and nonlinear partial differential equations (PDEs). The proposed approach involves transforming PDEs into matrix eigenvalue problems using the finite difference method and optimizing parameters within the VQE framework to approximate the ground state energy of the PDEs. The key technology to solve partial differential equations (PDEs) is using parameterized quantum circuits tailored from triangle qubit channels. These circuits play a crucial role in variational quantum eigensolvers (VQEs) by enabling the computation of objective functions through quantum measurements and subsequent classical optimization algorithms. The triangle blocks are applied to construct a universal ansatz.

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I. INTRODUCTION

To solve linear and nonlinear partial differential equations (PDEs), we discuss a solution that is going to apply quantum computing techniques, specifically the variational quantum eigensolvers (VQEs) with triangle quantum circuits. The proposed approach involves transforming PDEs into matrix eigenvalue problems using the finite difference method and optimizing parameters within the VQE framework to approximate the ground state energy of the PDEs. The key technology to solve Partial Differential Equations (PDEs) applies circuits of triangle blocks as universal ansatz. These circuits play a crucial role in VQEs by enabling the computation of objective functions through quantum measurements and classical optimization algorithms.

II. SOLUTION

A. Partial Differential Equation (PDE)

A Partial Differential Equation (PDE) is an equation of dependent variables and their partial derivatives. To solve a Partial Differential Equation (PDE), we first transform it into a matrix eigenvalue problem using the Finite Difference Method (FDM). Next, in constructing a Variational Quantum Eigensolver (VQE), we create an ansatz and a trial wave function using Parameterized Quantum Circuits (PQCs). Additionally, we define the corresponding Hamiltonian for the problem at hand. Finally, we optimize the parameters within the VQE to approximate the ground state energy.

B. Finite Difference Method (FDM)

Finite Difference Method (FDM) is a method of converting continuous partial differential equations into discrete algebraic equations. Its basic idea is to divide the domain of partial differential equations into a set of grid points, and then replace the partial derivatives with differential approximations to obtain a linear or nonlinear algebraic equation system. If a partial differential equation is an eigenvalue problem, then the finite difference method can reduce it to a matrix eigenvalue problem. Specific steps are as follows:

First, determine the form of the partial differential equation, such as $Lu = \lambda u$ where L is a linear differential operator, u is the unknown function, and λ is the eigenvalue. Secondly, choose a

suitable grid division, for example $x_i = i\Delta x$, $i = 0, 1, \ldots, N-1$, where Δx is the grid spacing , N is the number of grid points. Thirdly, replace the partial derivatives with a difference approximation, e.g.

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

where u_i is an approximation of $u(x_i)$. Fourthly, substitute the difference approximation into the partial differential equation to obtain a system of algebraic equations, such as

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = \lambda u_i, \;\; i = 1, 2, \ldots, N-1$$

where u_0 and u_N are boundary conditions. Finally, write the algebraic equations in matrix form, such as

$$\mathbf{Au} = \lambda \mathbf{u}$$

where $\mathbf{A}$ is a $N-1 \times N-1$ matrix, $\mathbf{u}$ is a $N-1$ dimensional vector, λ is the eigenvalue.

C. Variational Quantum Eigensolver (VQE)

Variational Quantum Eigensolver is a method that uses a quantum-classical hybrid algorithm to solve matrix eigenvalues and eigenvectors. It is mainly used to solve the ground state and low excited state of quantum systems, and has broad application prospects in partial differential equetions.

The concept of VQE is to first select a trial wave function containing parameters $|\psi(\theta)\rangle = U(\theta)|\psi_0\rangle$ where the initial parameter is θ_0, $U(\theta)$ is a quantum circuit containing parameters, and $|\psi_0\rangle$ is a reference state. Then use a quantum computer to measure $|\psi(\theta)\rangle$. The energy expectation is $C(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$ where H is the matrix to be solved. Finally, use the classic optimizer to update the parameters $\theta_0 \to \theta_1$, and iterate until convergence.

D. Hamiltonian Matrix

The Hamiltonian is an operator that describes the energy of a physical system. To find the Hamiltonian of a partial differential equation, one way is to transform the partial differential equation into an eigenvalue problem $H\psi = E\psi$, where H is the Hamiltonian, ψ is the wave function and E is the energy. In this way, the form of the Hamiltonian can be determined based on the form

of the eigenvalue problem. For example, to convert an Euler equation into a Hamilton equation for VQE, we can work follow these steps:

- First, identify the Lagrangian function $L(q,\dot{q},t)$ of the system, where q is the generalized coordinate, $\dot{q}$ is the generalized velocity, and t is the time. The Euler equation is derived from the principle of stationary action, which states that

$$\delta S = \delta \int_{t_1}^{t_2} L(q,\dot{q},t)dt = 0$$

  where S is the action and δ denotes the variation.

- Second, define the generalized momentum p as $p = \frac{\partial L}{\partial \dot{q}}$ and use it to eliminate $\dot{q}$ from the Lagrangian function. This gives the Hamiltonian function $H(q,p,t)$, which is defined as

$$H(q,p,t) = p\dot{q} - L(q,\dot{q},t)$$

  where $\dot{q}$ is expressed in terms of q, p, and t using the definition of p.

- Third, derive the Hamilton equations, which are the equations that take the place of the Euler equation in the Hamiltonian formalism. The Hamilton equations are given by

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \ \frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

  where q and p are treated as independent variables.

- Fourth, use the Hamilton equations to solve for the dynamics of the system, or find the stationary points of the Hamiltonian function, depending on the problem at hand. For VQE, we are interested in finding the minimum eigenvalue and the corresponding eigenvector of the Hamiltonian function, which represent the ground state energy and the ground state wavefunction of the quantum system, respectively.

It's important to note that the specifics of the Hamiltonian matrix, such as its size and structure, depend on the particular system and its degrees of freedom. The steps outlined above provide a general framework for obtaining the Hamiltonian matrix from the Euler equations in a Lagrangian formulation.

E. Parameterized Quantum Circuit (PQC)

PQC is the abbreviation of Parameterized Quantum Circuit. It is a quantum circuit composed of a series of quantum gates containing parameters, which can be used to implement tasks such as quantum machine learning and quantum optimization. The advantage of PQC is that parameters can be adjusted based on data or objective functions to achieve optimal performance. Nielsen and Chuang [10]

The core of VQE is to use a PQC to construct a trial wave function, then use a quantum computer to measure the energy expectation of the wave function, and then use a classical optimizer to update the parameters until convergence. The steps to use PQC in VQE are as follows:

First, select a Hamiltonian matrix H. Secondly, select a quantum circuit $U(\theta)$ with parameters, such as a layered quantum circuit. Thirdly, select a reference state $|\psi_0\rangle$, such as an all-zero state or a Hartree-Fock state. Then, use PQC to act on the reference state to obtain a trial wave function $|\psi(\theta)\rangle = U(\theta)|\psi_0\rangle$ where θ is the parameter vector. Then, use a quantum computer to measure the energy expectation of the trial wave function $C(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$ and use it as the objective function . Finally, use the classic optimizer to update the parameters θ so that the objective function reaches the minimum value, thereby obtaining the minimum eigenvalue of the matrix and the corresponding eigenvector.

F. Trial Wave Function and Ansatz

The trial wave function is a function used to approximate the exact wave function. It usually contains some adjustable parameters and can be used to solve eigenvalue problems in quantum mechanics. Variational is a method that uses the variational principle to construct trial wave functions. Its basic idea is to first assume a trial wave function with parameters $|\psi(\theta)\rangle$, and then calculate its energy expectation

$$E(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$$

A universal ansatz is a type of parameterized quantum circuit (PQC) that can approximate any quantum state or unitary transformation, up to a certain accuracy. A universal ansatz is useful for quantum machine learning, quantum optimization, and quantum simulation tasks. It typically consists of a sequence of layers, each containing some parameterized single-qubit and multi-qubit gates, such as $R_y(\theta)$ and CNOT. A universal ansatz can be optimized by adjusting the parameters to

minimize a cost function, such as the energy expectation, the loss function, or the reward function. Tilly *et al.* [12],Cerezo *et al.* [2].

In order to optimize the parameter θ in PQC, we need to use a classic optimizer, such as gradient descent method, Newton method, etc., to minimize an objective function, such as expected energy, loss function, reward function, etc. The general steps for optimizing the parameter θ in PQC are as follows:

- First, select a suitable objective function, such as solving the ground state energy of the quantum system, the loss function for training the quantum neural network, the reward function for performing quantum reinforcement learning, etc.

- Secondly, select a suitable optimizer, such as gradient descent method or Newton method, as well as some optimization parameters, such as learning rate, momentum, decay rate, etc.

- Thirdly, a quantum computer is used to perform PQC to obtain the output results of the quantum circuit, such as wave function, probability distribution, action selection, etc. Then, a classical computer is used to calculate the value of the objective function and the gradient of the objective function to the parameter theta, such as using the finite difference method.

- Finally, the optimizer is used to update the parameters so that the objective function reaches the minimum value, thereby obtaining the optimal PQC.

III. TRIANGLE QUBIT CIRCUITS

A. Channel-State Duality

Channel-state duality (CSD) refers to the one-to-one correspondence between quantum channels and bipartite quantum states Choi [3], allowing the use of quantum states to study channels and vice versa through the Choi-Jamiołkowski isomorphism. Araújo [1] This duality enables the representation of unital channels by Bell diagonal states, where the probabilities of the Bell diagonal state correspond to the canonical parameters of the unital channel. Jiang, Luo, and Fu [6] Bell diagonal states, which are probabilistic mixtures of Bell states, play a crucial role in this correspondence
.

B. Triangle Qubit Channel

The triangle qubit channel is a type of unital qubit channel that described by real Bloch representation diag$(1,\lambda_1,\lambda_2,\lambda_3)$ where real functions $\lambda_{1,2,3} \in \mathbf{R}$ are determined by real parameters α,β, and $\gamma \in \mathbf{R}$, forming a triangle on the unit circle. This channel is characterized by the probabilities q_{00},q_{01},q_{10}, and q_{11}, which satisfy specific identities involving cosine functions of (α,β,γ). The triangle qubit channel can be utilized in various quantum computing applications . Li [7]

C. Triangle Qubit Circuit

The parameterized quantum circuit of a triangle qubit channel involves a probability generator circuit called *Triangle Block* that is used to generate the probabilities associated with the channel. This circuit may be followed by additional components such as Hardmard and CNOT gates to manipulate the quantum states accordingly Gårding *et al.* [5], Li [8].

In the triangle block circuit below, $R_y(\theta)$ is a single-qubit rotating gate that can rotate the quantum state along the y-axis. The advantage of $R_y(\theta)$ is that it can be rotated at any angle around the y-axis, thereby achieving any transformation of the quantum state.

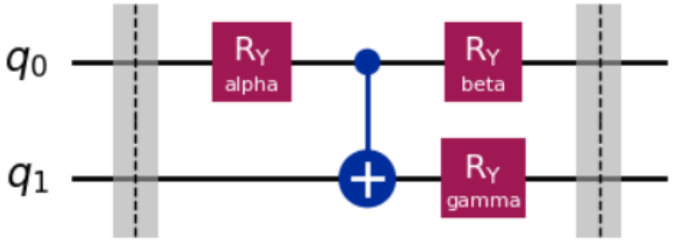

FIG. 1. **Triangle Block.** The three phase gates $R_y(\alpha),R_y(\beta),R_y(\gamma)$ and the CNOT gate generate parameterized probability distributions of triangle block (Gårding *et al.* [5], Li [8]).

A hierarchically structured quantum circuit is a quantum circuit composed of multiple identical layers, each layer containing some parameterized quantum gates, such as triangle blocks. Hierarchical structured quantum circuits can be used to implement tasks such as quantum machine learning and quantum optimization with variational quantum eigensolver (VQE). An example schematic diagram of a hierarchically structured quantum circuit is as follows:

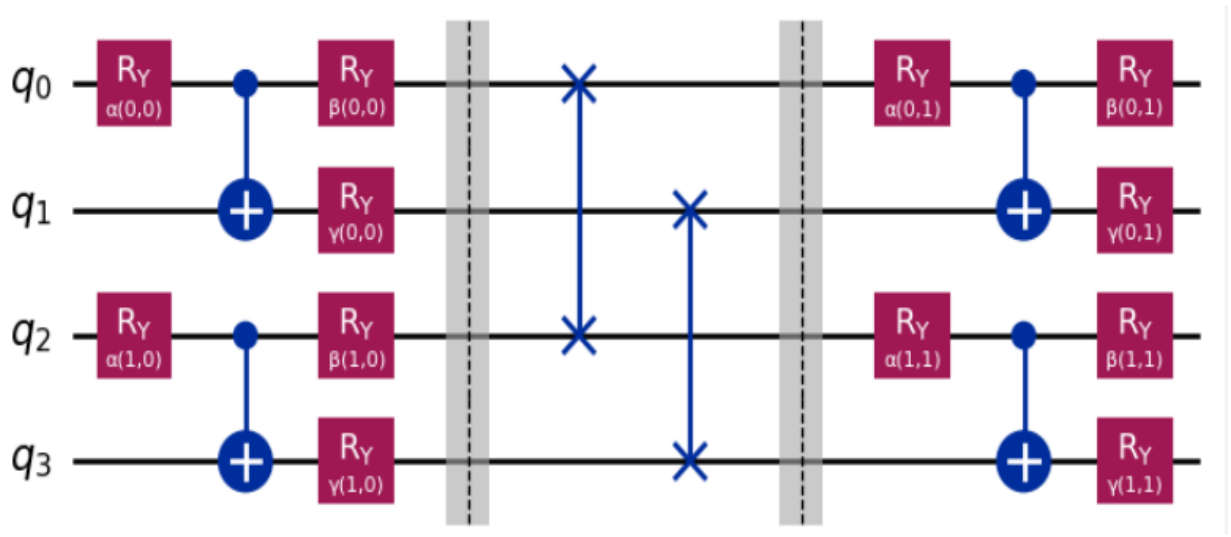

FIG. 2. **Four Qubit Universal Ansatz by Triangle Blocks and Swap Gates.** The first part is two triangle blocks. The second part consists of two swap gates to swap dual qubits. The third part also includes two triangle blocks.

IV. IMPLEMENTATION

A. Universal Ansatz

The universal ansatz is a type of parameterized quantum circuit (PQC) that can approximate any quantum state or unitary transformation, up to a certain accuracy. We can construct a universal ansatz by triangle blocks with parameterized probability distribution and other gates forming a parameterized quantum circuit.

A Variational Quantum Eigensolver (VQE) with four triangle blocks can be implemented using open-source quantum frameworks like Qiskit[11] or Cirq[4] to implement the universal ansatz. An example curve of a 4x4 Hamilitonian matrix is displayed below.

V. CONCLUSION AND OUTLOOK

The approacho of VQE by triangle block has several key strengths. It leverages the concept of Channel-State Duality (CSD), which establishes an one-to-one correspondence between quantum channels and bipartite quantum states, facilitating the study of channels using quantum states and vice versa. It also utilizes Bell diagonal states, mixtures of Bell states, to effectively represent

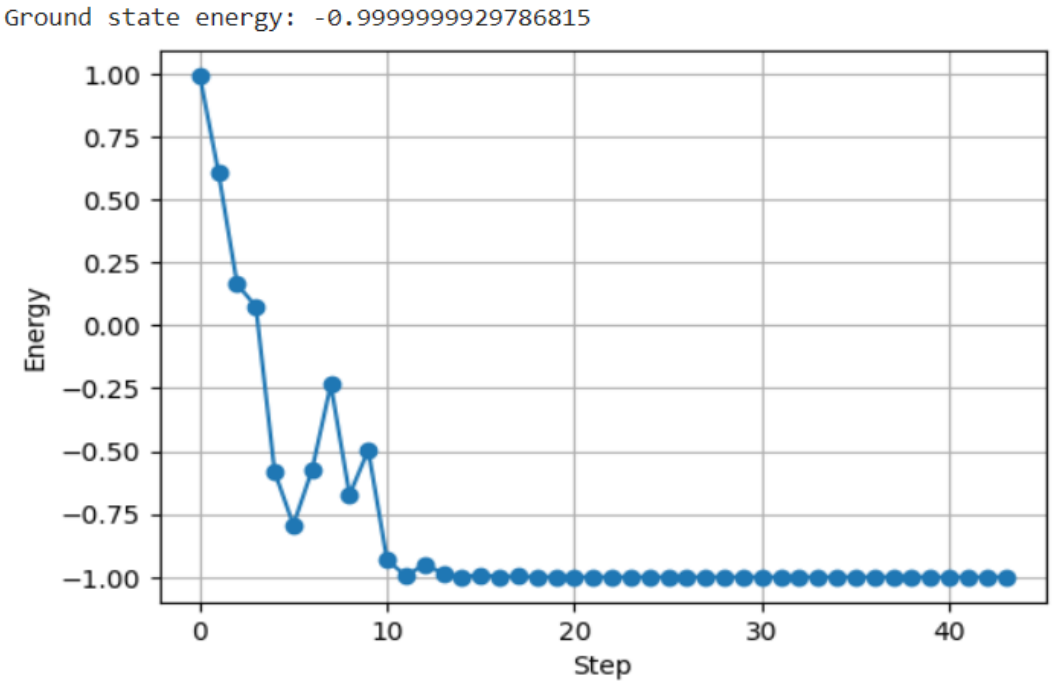

FIG. 3. **A Variational Quantum Eigensolver (VQE) by Triangle Qubit Blocks.** This curve describes a variational quantum eigensolver by using the parameterized quantum circuit of triangle qubit blocks with a given Hamiltonian matrix. It shows the process to arrive the ground state energy.

unital channels, with their canonical parameters corresponding to the probabilities of the unital channel. This provides a clear representation of quantum operations. Furthermore, triangle quantum channels are represented as completely positive and trace-preserving linear maps, ensuring the preservation of positivity and the trace of the density matrix, thus offering a robust description of quantum channels and their actions on quantum states.

The probability distribution of triangle qubit channels can be determined based on specific parameters, providing a clear understanding of the probabilities associated with different outcomes, which is crucial for designing quantum circuits and implementing quantum algorithms.

To elevate the solution and make it industrially relevant, several potential steps could be undertaken. These include

- Implementing advanced optimization techniques like hybrid classical-quantum optimization algorithms to efficiently fine-tune the parameters of variational quantum circuits for enhanced performance.

- Integration of triangle quantum channels and parameterized quantum circuits into quantum

machine learning frameworks could be explored to harness quantum computing capabilities for machine learning tasks.

- Strategies to boost the solution's scalability by optimizing resource allocation and circuit design for larger-scale quantum computations could be developed.
- Rigorous validation and benchmarking of the solution using quantum simulators and actual quantum hardware could be conducted to evaluate its performance, reliability, and scalability in real-world industrial applications.

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