The effective Hamiltonian method to cover the absence of quantum entanglement caused by monolayer ansatz

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I. INTRODUCTION

The anti-ferromagnetic Heisenberg model of the multi-dimensional lattice is the simplest and most useful model to investigate the physical properties of anti-ferromagnetic materials. If the lattice has triangular bond structures between the two atomic sites, especially, a spin frustration, the quantum phenomenon of high degrees of energy degeneration, occurs and is well investigated theoretically to find out the novel condensed matter phases such as a quantum spin liquid state. Although it is ideal to investigate the quantum state of the atomic site number $N \simeq 10^{24}$ of the Hamiltonian of the Heisenberg model, it is difficult to promote the exact diagonalization even if using the quantum computer (QC).

In such a case, the variational approach for optimizing the wave function is useful. In particular, variational quantum eigensolver (VQE), one of the variational methods based on quantum algorithms, reduces the computational complexity within the polynomial order. Nevertheless, covering the 10^{24} sites by using the present quantum devices is the remaining issue. In addition, because of the structural constraint of the devices, we may not avoid representing the entanglement between two nearest neighbor sites by using a few CNOT gates, which causes the circuit depth coming to be in exponential order. In the viewpoint of quantum error, the exponential order of the circuit depth is not practical, so that we usually approximate the VQE ansatz within constant depth by neglecting such local entanglement. It is important for us to cover the global and local entanglement of the total system which cannot be included by the constraint of the number of qubits and ansatz of the VQE caused by the constraint of the quantum device, respectively.

We present novel and innovative methodologies to overcome the two difficulties in the contest. The absence of the representability of the ansatz is covered by updating to the effective Hamiltonian from the old Hamiltonian by taking unitary transformation respecting the VQE ansatz after optimizing the variational parameters. Under the assumption that the optimized ansatz should be a convenient unitary transformation in the block diagonalization to obtain the ground state energy, we think that the local entangled state is well described while reducing the depth of CNOT by performing block diagonalization many times. By exchanging the representation of the Hamiltonian, we successfully make the constant depth ansatz which estimates ground state energy with high precision, corresponding to satisfying the system-size-scalability of the depth of the ansatz. By choosing the total z-spin equal to zero as the initial state of the VQE and making z-spin symmetry-protected ansatz for reducing optimization parameters, we finally result in $\leq$1% relative error from exact ground state energy by using fake-guadulupe.

II. THEORETICAL FOUNDATION

A. Ansatz

Including the Kagome lattice system, the antiferromagnetic Heisenberg model takes a stable configuration in terms of energy where neighboring sites are aligned with opposite spins. It is known that the z-axis direction of the total spin angular momentum in the ground state, including frustration systems, has an eigenstate of zero. Therefore, at the ansatz and initial guess stage, we decided to design it to close in an eigenstate where the z-axis direction of the total spin angular momentum becomes zero. In a 2-qubit system, a unitary transformation that conserves the spin angular momentum in the z-axis direction is described as follows (the gate shown in FIG.1).

$$u(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\theta & -\sin 2\theta & 0 \\ 0 & \sin 2\theta & \cos 2\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{1}$$

However, we have imposed the condition that the eigenstates are represented by real vectors. Additionally, we chose $|010101010101\rangle$ as the initial state. By placing the unitary transformation $u(\theta)$ in a stripe pattern between all 2-qubits,

a layered gate is created to describe the entangled state. The gate in one layer is shown in the following diagram FIG.2.

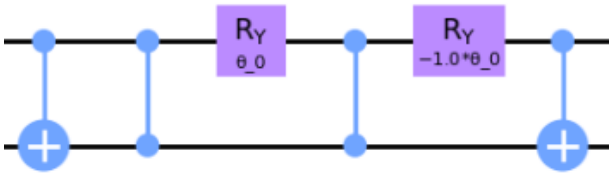

FIG. 1. The 2qubit-gate for operating Eq.(1)

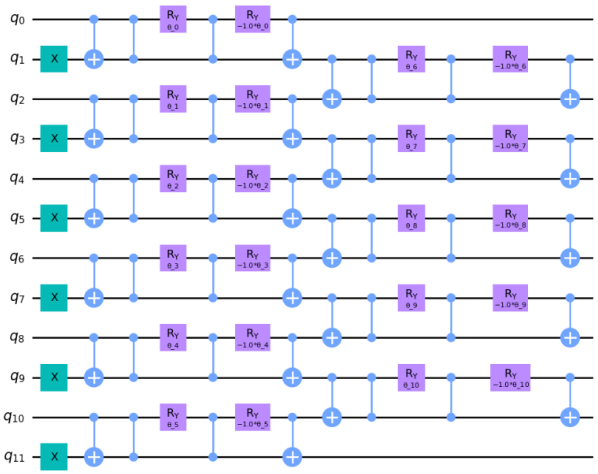

FIG. 2. The initial state and monolayer ansatz for present method in using 12 full qubits.

B. Apdate to the effective Hamiltonian

Usually, to describe an entangled state, an ansatz is stacked in multiple layers. However, as the system size increases, the number of layers required to obtain a wave function that is close to the exact one increases as well. From the perspective of errors, increasing the depth is not necessarily desirable. Therefore, to avoid increasing the error without increasing the number of layers, we adopt an approach of updating the Hamiltonian by applying a unitary transformation to it in each layer. Let the parameter set for the Nth layer be $\vec{\theta}_N$ and the unitary transformation that describes the ansatz be $U(\vec{\theta}_N)$. Then, the energy is given by:

$$E = \langle\psi| U^\dagger(\vec{\theta}_N)...U^\dagger(\vec{\theta}_2)U^\dagger(\vec{\theta}_1)HU(\vec{\theta}_1)U(\vec{\theta}_2)...U(\vec{\theta}_N)|\psi\rangle \tag{2}$$

$$H_j = U^\dagger(f(\vec{\theta}_j))H_{j-1}U(f(\vec{\theta}_j)) \tag{3}$$

and define the update of the Hamiltonian using the following procedure.

1) Define the effective Hamiltonian H_j at the jth iteration, with $j = 0$ being the initial Hamiltonian H.
2) Run the VQE with ansatz consisting of one layer of U to optimize the parameters $\vec{\theta}j$.
3) Obtain the jth effective Hamiltonian Hj using the following equation:

$$H_j = U^\dagger(f(\vec{\theta}j))H_{j-1}U(f(\vec{\theta}_j)) \tag{4}$$

where $f(\vec{\theta}_j)$ is a multivariable function defined as follows:

$$[f(\vec{\theta}j)]_m = \begin{cases} \frac{\pi}{2} \ (\frac{\pi}{4} < [\vec{\theta}_j]_m < \frac{3}{4}\pi) \\ \pi \ (\frac{3}{4}\pi < [\vec{\theta}_j]_m < \frac{5}{4}\pi) \\ \frac{3}{2}\pi \ (\frac{5}{4}\pi < [\vec{\theta}_j]_m < \frac{7}{4}\pi) \\ 0 \ (\frac{7}{4}\pi < [\vec{\theta}_j]_m < 2\pi, 0 < [\vec{\theta}_j]_m < \frac{1}{4}\pi) \end{cases} \tag{5}$$

The updated Hamiltonian H_j defined by this procedure is expressed as a summation of $3N$ types of Pauli strings. Thus, the computational complexity of the summation-up in VQE can be kept at $O(N)$ because the Pauli string of the Hamiltonian evaluated by VQE does not increase after the update.

4) Return to step 2) after step 3) and run the VQE with the updated Hamiltonian H_j.

In this iterative procedure, stop updating H_j when the upper limit is reached or the representation matrix of H_j returns to its previous state before the update, with $j = N$ being the stopping point. The lowest energy state obtained from the set of updated Hamiltonians $H_0, H_1, ..., H_N$ is then determined as the sought-after ground state. This ensures that the number of layers on the QC run by VQE remains constant, satisfying system-size scalability in the depth direction. Additionally, the Hamiltonian H_j is updated by a unitary transformation that characterizes the qubit number on the QC, and there is no reduction in matrix dimension. Therefore, this method does not introduce any approximation in updating H_j, eliminating concerns about the deterioration of approximation performance with increasing system size, and satisfying system-size scalability in that sense.

III. NUMERICAL RESULT

We present the results obtained for the ansatz which we prepared in fake-guadalupe. First, the VQE using the initial Hamiltonian, H_0, converged in 228 iterations on the 12-qubit device, as shown in FIG. 3. After updating H_1 based on Eqs. (4)-(5), the VQE iterations were performed starting from the 229th iteration. Finally, after 192 iterations, a converged solution was obtained, with a numerical solution within 1% of the exact ground-state energy of -18.0 for both the VQE using H_0 (-17.9979) and the VQE using H_1 (-17.9977) after updating. Since the exact solution was well described at the point of H_0, it was confirmed that the ansatz we set in this study was of high quality and the proposed update of H_1 was not necessary. Moreover, the Hamiltonian update method itself was confirmed to be free from approximation in terms of reproducing the ground-state energy, as it was able to reproduce the exact ground-state energy well even after updating.

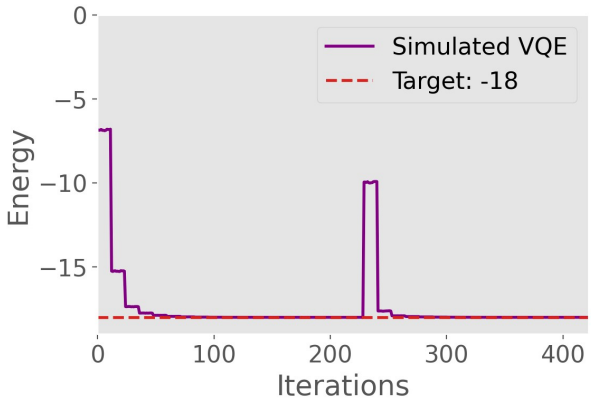

FIG. 3. The iteration cycle of VQE in using the ansatz shown in FIG.2

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FIG. 4. Our latest draft and notebook are stored here. Please refer to the latest version.