Variational Quantum Eigensolver For Kagome Lattice

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Abstract

Previous quantum algorithms for solving the round state of a given Hamiltonian H were based on adiabatic state preparation and Quantum Phase Estimation (QPE)[1], both of which have circuit depth requirements beyond those available in the Noisy Intermediate-Scale Quantum (NISQ) era. At the same time, the Variational Quantum Eigensolver (VQE)[2] shows a useful quantum advantage on NISQ devices because of its natural hardware compatibility. In this article, we first illustrate the way to use VQE to get the ground state and the k-th excited state of kagome lattice. After that, we classically simulate the noiseless VQE to find the ground state energy and the first few excited states of 20-site patch of the kagome lattice Heisenberg Antiferromagnet (HAFM) following the work by *Joris Kattem ölle and Jasper van Wezel*[3] and compare the result to the real ones. In the end of this article, we discuss the influence of different initial states to the final result.

Keywords: NISQ, VQE, kagome lattice, HAFM, HVA

I. Introduction

Though reseaching for decades, the property of Heisenberg antiferromagnet (HAFM) on the kagome lattice remain opaque, because of its geometrical frustration. To understand what's the geometrical frustration, we need first give out the Hamiltonian of the HAFM system:

$$H = \sum_{\langle i,j \rangle} \mathbf{S}^{(i)} \cdot \mathbf{S}^{(j)} \tag{1}$$

where, the symbol $\langle i, j \rangle$ means particle i and particle j are adjacent. It's obvious that to get the lowest energy, we can just let $\mathbf{S}^{(i)}$ and $\mathbf{S}^{(j)}$ opposite in direction so that each term in the equation (1) will take the minimum value. However, in the situation of kagome lattice (Fig.1), when the particle at A choose to be spin up and the particle at B choose to be spin down, then the particle at C will have no choice to choose to make its spin direction opposite to both A and B. It's actually what we called 'geometrical frustration'.

Classical approaches to solve this ground state problem include exact diagonalization of finite-size patches[4] and the density matrix renormalization group (DMRG) method[5]. However, all of the classical methods have some unavoidable disadvantages, for example by the inability to treat large patches (exact diagonalization), or the inability to describe highly entangled states (DMRG).

In this article, we will first introduce how to use VQE finding the ground state and excited states of a given system and the Hamiltonian Variational Ansatz (HVA)[6] in Sec.II. Then, we will show how to build a quantum circuit and make a Variational Quantum Eigensolver (VQE) in kagome lattice with 20 sites and the choice of initial states in Sec.III.

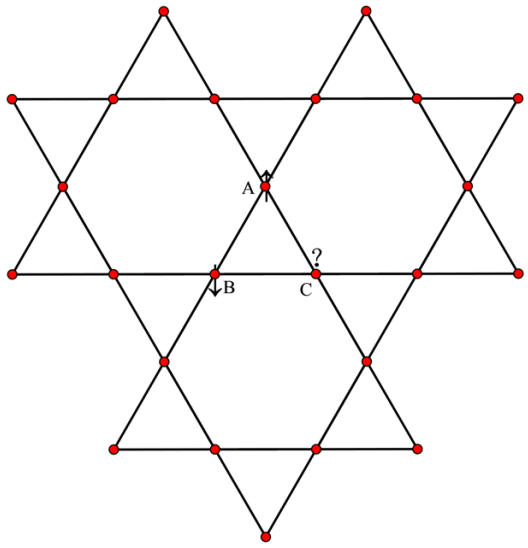

Fig 1: The construcion of kagome lattice

Data analysis will be given in Sec.IV, comparing the results got from VQE with the real ones. Finally, in Sec.V, we analyze whether the choices of the initial states will influence the final results of VQE.

II. Methods

A. VQE

1. VQE for the ground state

In this part, we will first give a detailed introduction about VQE and a theoretical prove why the smallest energy we got from VQE can be treated as the approximation of the system's ground state.

Consider a given system with its Hamiltonian $\hat{H}$ and HIlbert space $\mathcal{H}$. Suppose the Hamiltonian $\hat{H}$ has eigenstates $\{|n\rangle\}$ so that $\hat{H}|n\rangle = E_n|n\rangle$. For $\forall |\psi\rangle \in \mathcal{H}$, we can express it as: $|\psi\rangle = \sum_n C_n |n\rangle$. The energy measured by $|\psi\rangle$

$$\langle\psi|\hat{H}|\psi\rangle = \sum_n |C_n|^2 E_n \geq \sum_n |C_n|^2 E_g = E_g \qquad (2)$$

where, E_g is the ground energy state. Equation (2) tells us that whatever state you have, the measurement towards the Hamiltonian will never be smaller than the ground state energy. If we construct a subset of $\mathcal{H}$: $\{\psi(a), a \in A\}$, then equation (2) proves that:

$$E(a^*) = \langle\psi(a^*)|\hat{H}|\psi(a^*)\rangle = \underset{a\in A}{Min}\langle\psi(a)|\hat{H}|\psi(a)\rangle \qquad (3)$$

is the best variational approxiamation of the ground state energy in the range of our subset. and $|\psi(a^*)\rangle$ is the best variational approxiamation of the ground state.

For real quantum machine, we need to express the Hamiltonian as:

$$\hat{H} = \sum_{i=1}^{l} h_i \hat{H}_i \qquad (4)$$

where $\hat{H}_i$ are all Hermitian operators.

After having the basic knowledge about VQE, we also have to prepare the ansatz state so that the VQE can be applied on. To do this, a easy-prepared quantum initial state and quantum circuit to bring parameters in are both indispensible, we call them $|\psi_{init}\rangle$ and C. In real VQE, there's actually not only a parameter as what we'vw written in equation (3). In the remaining part of this article, we will use θ to imply all of the parameters used in the ansatz state $|\theta\rangle$.

VQE is actually a hybrid algorithm, where the quantum part measure the energy under the state $|\theta\rangle$ repeatedly and calculate the average value and the classical part optimize the concrete value of the parameters. The more detailed illustration of VQE is shown in Alg.1,

2. VQE for the excited states[7]

In the last section, we've introduced the way to use VQE to solve the ground state problem. It seems quite difficult to directly get the excited states of a given Hamiltonian using VQE. The main idea of constructing VQE for excited states is to change one of the original excited states into the ground state, and then to solve it as what have been done before.

Our method extends VQE to calculate the k-th

Algorithm 1: VQE proceeding pseudocode

Input: $|\psi_{init}\rangle$,$\hat{H}$

Output: The ground state energy approxiamtion E_g

$C(\theta)$ is randomly set at first;
while *The difference between the adjacent* $E(\theta) >$ *A given number* **do**
  $|\theta\rangle = C(\theta)\,|\psi_{init}\rangle$; //Prepare the ansatz state $|\theta\rangle$ using the HVA circuit
  $E(\theta) = \sum_i h_i \langle\theta|\,\hat{H}_i\,|\theta\rangle$; //Measure the energy under the state $|\theta\rangle$ repeatedly and calculate the average value. (As we are simulating on the classical computer, we actually do a inner product and save it here.)
  Using classical algorithm to update the value of θ (such as BFGS algorithm implemented in SciPy);
  Update the parameters in circuit $C(\theta)$;
$\theta = \theta^*$;$E(\theta) = E(\theta^*)$;
return θ^*, $E(\theta^*)$;

excited state by instead optimising the cost function:

$$F(\theta) = \langle\theta|\,\hat{H}\,|\theta\rangle + \sum_{i=0}^{k-1}\beta_i|\,\langle\theta|i\rangle\,|^2 \tag{5}$$

where $|i\rangle$ is the i-th excites state, $|0\rangle$ is the ground energy state, and $|\theta\rangle$ is the ansatz state for k-th excited state. For the second term in the formula, we need to choose sufficiently large parameter $\beta_0, \ldots, \beta_{k-1}$. It can be seen as minimising $E(\theta) = \langle\theta|\,\hat{H}\,|\theta\rangle$ with the constraint that $|\theta\rangle$ is orthogonal to the states $|0\rangle, \ldots, |k-1\rangle$. But how large the series of $\{\beta_i\}$ should be choosen so that the minimum of $F(\theta)$ can guarantee $|\theta\rangle$ goes to the k-th excited state and the energy $E(\theta) = \langle\theta|\,\hat{H}\,|\theta\rangle$ is the k-th excited state energy? To illustrate this problem, we can first rewrite the the equation (5) as:

$$\begin{aligned} F(\theta) &= \langle\theta|\,\hat{H}\,|\theta\rangle + \sum_{i=0}^{k-1}\beta_i\,\langle\theta|i\rangle\,\langle i|\theta\rangle \\ &= \langle\theta|\left(\sum_{i=0}^{n} E_i\,|i\rangle\,\langle i| + \sum_{i=0}^{k-1}\beta_i\,|i\rangle\,\langle i|\right)|\theta\rangle \\ &= \langle\theta|\,\hat{H}_k\,|\theta\rangle \end{aligned} \tag{6}$$

where,

$$\begin{aligned} \hat{H}_k &= \hat{H} + \sum_{i=0}^{k-1}\beta_i\,|i\rangle\,\langle i| \\ &= \sum_{i=k}^{n} E_i\,|i\rangle\,\langle i| + \sum_{i=0}^{k-1}(E_i+\beta_i)\,|i\rangle\,\langle i| \end{aligned} \tag{7}$$

Equation (6) and (7) tell us that when optimizing $F(\theta)$, we are actually finding the ground state of the effective Hamiltonian H_k. Therefore, if we choose the $\beta_i > E_k - E_i$, $i = 0, \ldots, k-1$, the ground state of H_k will be $|k\rangle$ and the VQE for the ground state can be applied to it. Since $E_k - E_i \leq E_k - E_0$, it will be sufficient to choose $\beta_i > E_k - E_0$.

B. Cyclic HVA[3]

In the Alg.1, we've already told that to prepare the ansatz state:

$$|\theta\rangle = C(\theta)\,|\psi_{init}\rangle \tag{8}$$

HVA circuit $C(\theta)$ is need to use. So, in this part, we are going to explain how to build the $C(\theta)$ theoretically. In general, we can express $C(\theta)$ as:

$$C(\theta) = \exp\left(-\mathrm{i}\theta_M H_{i_M}\right)\ldots\exp\left(-\mathrm{i}\theta_1 H_{i_1}\right) \tag{9}$$

where, the M parameters are formed by the time duration of the M evolutions. Many practical applications will let the circuit C consist of p cycles of a smaller circuit c, each time defined by the same sequence i of terms in the Hamiltonian. Every cycle gets its own set of m parameters. It is convenient to write θ as $\theta = (\theta_1, \ldots, \theta_p)$, with $\theta_j = (\theta_{j_1}, \ldots, \theta_{j_m})$. Then, a single cycle:

$$c(\theta_j) = \exp(-\mathrm{i}\theta_{j_m} H_{i_m}) \ldots \exp(-\mathrm{i}\theta_{j_2} H_{i_2}) \exp(-\mathrm{i}\theta_{j_1} H_{i_1}) \tag{10}$$

and so

$$|\theta\rangle = c(\theta_p) \ldots c(\theta_1) |\psi_{\text{init}}\rangle \tag{11}$$

We call this type of HVA the cyclic HVA. The cyclic HVA shows a close relation between static quantum simulation and dynamic quantum simulation; choosing $i = (1, \ldots, l)$ (or a permutation thereof) and $\theta_j = (t/p, \ldots, t/p)$ for all j , the cyclic HVA implements quantum time evolution for a target time t with p Trotter steps. In this way, the cyclic HVA can also mimic (but is more general than) adiabatic time evolution. In the case that no gap closes while adiabatically evolving from H_{init} to H , the HVA thus ensures that the ground state of H can in fact be prepared with the ansatz (but without guaranties on the required circuit depth). This formed the initial motivation for the HVA in VQEs.

III. Circuit

In this problem, we will use the cyclic HVA sllustrated in Sec.II.B. The Hamiltonian of the HAFM system to be solved has already been given in Sec.I:

$$H = \sum_{\langle i,j \rangle} \mathbf{S}^{(i)} \cdot \mathbf{S}^{(j)} \tag{1}$$

where, $\mathbf{S}^{(i)} = (X_i, Y_i, Z_i)^T /2$ with X_i, Y_i, Z_i the Pauli matrices acting on spin i only.

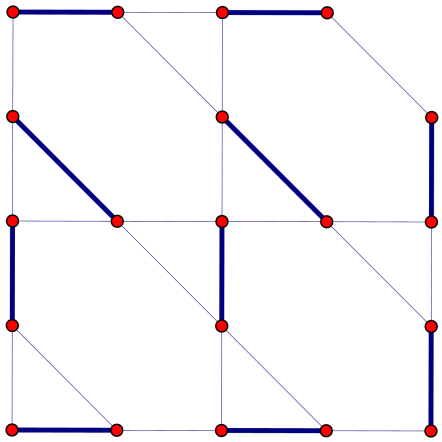

Fig 2: The quantum circuit of 20-site kagome lattice

According to the equation (9) and (10), we can similarly define the gate HEIS(α) as time evolution along a single term in the HAFM Hamiltonian:

$$\begin{aligned} \text{HEIS}(\alpha) &\equiv \mathrm{e}^{-\mathrm{i}\alpha/4} \mathrm{e}^{-\mathrm{i}\alpha \mathrm{S}^{(1)} \cdot \mathrm{S}^{(2)}} \\ &= \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\alpha/2} & 0 & 0 & 0 \\ 0 & \cos(\alpha/2) & -\mathrm{i}\sin(\alpha/2) & 0 \\ 0 & -\mathrm{i}\sin(\alpha/2) & \cos(\alpha/2) & 0 \\ 0 & 0 & 0 & \mathrm{e}^{-\mathrm{i}\alpha/2} \end{pmatrix} \end{aligned} \tag{12}$$

where, the first term $\mathrm{e}^{-\mathrm{i}\alpha/4}$ is just a phase transformation for the simplicity of the matrix representation. In a parametrized circuit, every instance of the HEIS gate gets its own parameter $\alpha = \theta_{jk}$.

Now, consider a 20-site kagome lattice (Fig2). Because there's interaction between each two adjacent qubits, there will be totally 30 terms in the Hamiltonian of the HAFM system (Eq.1). In the picture, spin-1/2 particles are placed on the vertices and the Heisenberg interaction is defined along the edges. Besides, the red dots represent qubits and the solid blue lines represent singlets. It can be seen from the picture that we choose 10 pairs of singlets as the initial states $|\psi_{init}\rangle$ of the 20-site kagome lattice. That's because the ground state of a single term in H is the singlet state, we consider this choice of the initial state will be close to the real ground state.

IV. Results

In the HVQE method, our simulation tests covered 5 systems, specific system organization is shown in Fig 3. Among these systems, the square lattice and the chain lattice were relatively simple ones while the kagome lattice will be our target test systems in simulated HVQE experiments.

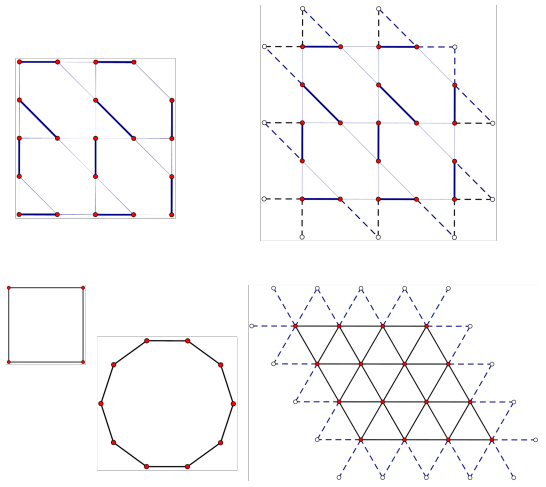

Fig 3: All simulated systems

The whole experiment system is implemented by classical computer simulation, in which we used 20/40-core Intel Xeon Gold 6248 CPUs for the simpler models such as square lattice and used NVIDIA DGX-2 V100/32G GPUs for the complex systems such as kagome lattice to accelerate the computing process.

In the experiment process, we first performed the sparse matrix eigenvalue decomposition using classical algorithm in SciPy package and use the results as ground truth. Then we used HVQE method to calculate the ground state energy, the first excited state energy and the second excited state energy in turn.

First, we calculated the ground state, first excited state and second excites state energies for all 5 systems with 1 layer of HVQE, which contain 30 parameters. CPU simulated results is as shown in Fig 4. In some simple systems like square lattice and chain lattice, our ground state energy is close to the ground truth calculated by classical methods. This result proved that we successfully implemented and simulated HVQE on classical computer CPUs. Some complicated systems like kagome lattice did have an extinct gap to ground truth, we continued on experiments with more layers and parameters to simulate kagome lattice system.

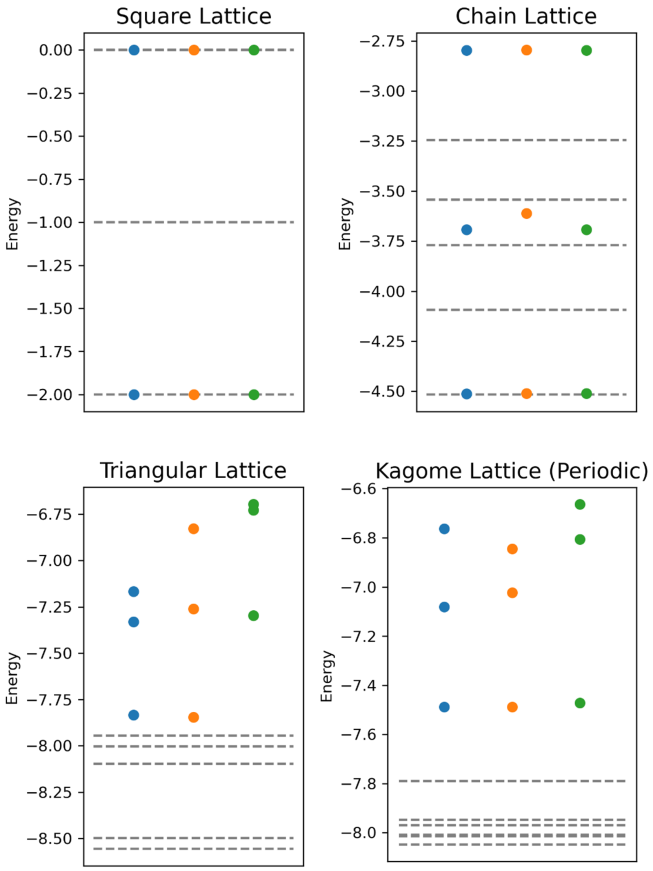

Fig 4: Simulation results for 4 systems with 30 parameters

In HVQE solving kagome lattice, we used a range of depth of layer to verify amount of parameters needed for accurately calculated ground and excited states energies. We tested 1, 4, 7 and 10 layers of HVQE with 3 repeats each, and experiments with no more than 4 layers were run on 40-core CPUs, while others on V100 GPUs. Simulation experiments results is shown in Fig 5. When more layers were used in simulating kagome lattice system, calculated ground state

energies and excited state energies were more closed to ground truth. Besides, for kagome system, we can easily to find that 7 layers of HVQE, contained 210 parameters, has enough accuracy for calculating the top 3 most stable system energies.

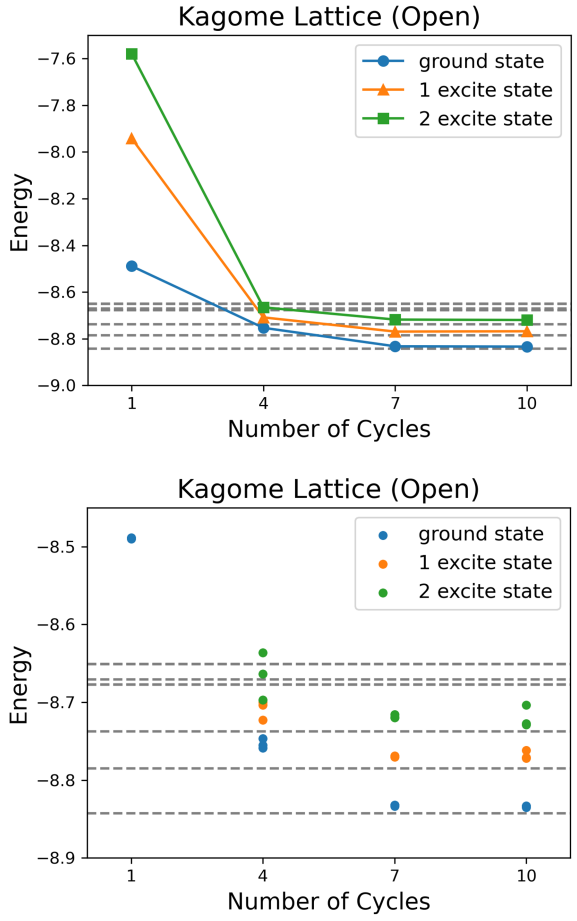

Fig 5: Simulation results for kagome lattice with different amount of parameters

To further verify our strategy for calculating excited system worked, we measured the part of the cost function to satisfy the orthogonal constrains. Using different large parameter β, we found out that using a β larger than 10 is enough to make this part of cost function to be closed to 0, which means our excited states is orthogonal to other more stable states.

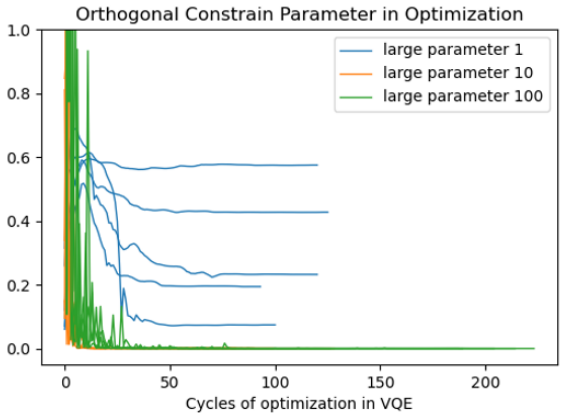

Fig 6: Evaluation of cost function orthogonal constrain part

V. Discussion

In addition to the above results, there exists something more interesting. The whole system, includes initial states, Hamiltonian, and circuits, possess an $SU(2)$ rotational symmetry.

In Kattemölle's article, he specifically explains how it works:[3]

The total spin operator is defined by $\mathbf{S^2} = \mathbf{S} \cdot \mathbf{S}$, with $\mathbf{S} = \sum_{i=1}^{n} \mathbf{S^{(i)}}$, and is related to the total spin quantum number S by $\mathbf{S^2} |\psi\rangle = S(S+1) |\psi\rangle$ for eigenstates $|\psi\rangle$ of $\mathbf{S^2}$. The total magnetization operator in the α-direction is defined as $\mathbf{S}_\alpha = \sum_{i=1}^{n} \left[\mathbf{S^{(i)}}\right]_\alpha$, and is related to the magnetization quantum number S_z by $\mathbf{S_z} |\psi\rangle = S_z |\psi\rangle$ for eigenstates $|\psi\rangle$ of $\mathbf{S_z}$. $\mathbf{S^2}$ and $\mathbf{S_z}$ commute, and are hence simultaneously diagonalizable. Acting with the laddar operator $\mathbf{S}_\pm = \mathbf{S_x} \pm i\, \mathbf{S_y}$ on a state with quantum number S_z raises (lowers) the S_z quantum number of that state with unity, for as long as the new value of S_z lays between $-S$ and S, and annihilates that state otherwise. The Hamiltonian, circuit and $|\psi_{init}\rangle \langle\psi_{init}|$ all commute with $\mathbf{S_x}$, $\mathbf{S_y}$ and $\mathbf{S_z}$ (and hence with $\mathbf{S^2}$ and $\mathbf{S}_\pm$), and therefore have a $SU(2)$ symmetry.

So the initial state $|\psi_{init}\rangle$ and the parameterized

state $|\theta\rangle$ have the same total spin quantum number S and the same total magnetization quantum number S_z. This reduces the search space of the VQE to the correct total spin sector.

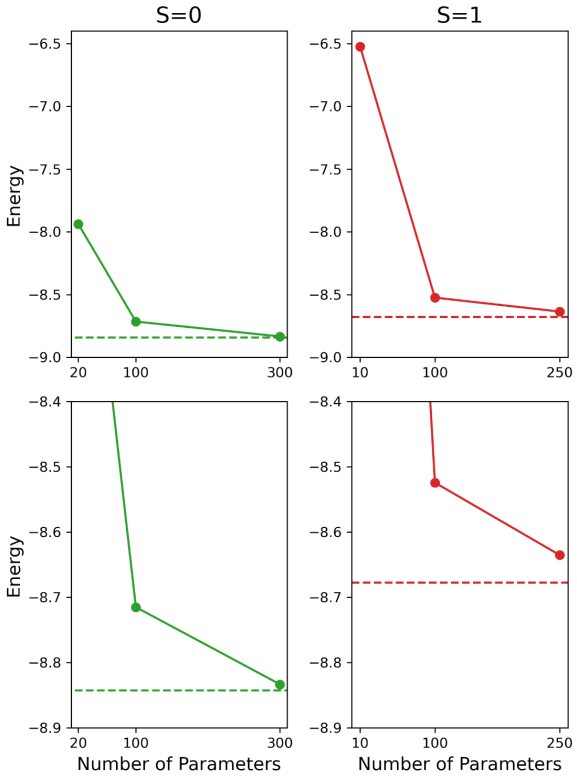

Fig 7: The different results between $S = 0$ and $S = 1$

In Fig 7, we showed the different results between $S = 0$(all singlet, red) and $S = 1$(only one triplet, green). Dashed lines represent the ground truth eigenenergy calculated by calssical method. The green one on the left has no degeneracy, while the red one on the right has there-fold degeneracy. Each dots represent a simulated result and the number of the parameters for simulation has been marked on it. Apparently as the number of the parameters increases, the ground energy computed by the VQE approachs the exact ground energy.

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Appendix A Initialization

For instance, the figure below is the initialized circuit of 6-size kagome lattice which is the smallest kagome lattice. The whole circuit is based on a quantum platform IBMQ. Please refer to the tutorial for the meanings of all symbols.

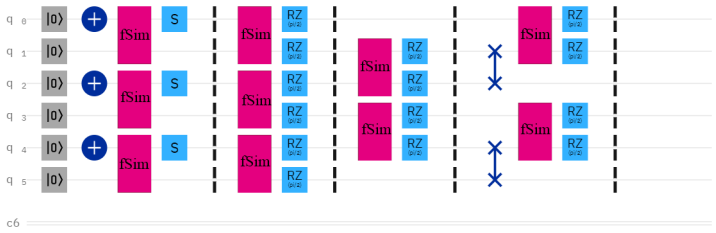

Fig 8: The initialized circuit of 6-size kagome lattice

Here we introduce a new two qubit gate:

$$\mathrm{fSim}(\theta,\Phi)=\begin{pmatrix}1&0&0&0\\0&\cos(\theta)&-\mathrm{i}\sin(\theta)&0\\0&-\mathrm{i}\sin(\theta)&\cos(\theta)&0\\0&0&0&\mathrm{e}^{-\mathrm{i}\Phi}\end{pmatrix} \tag{13}$$

At the APS 2019 conference, Google proposed a new parameterized 2-bit quantum gate, fSim gate, which may have higher computational performance than the standard CNOT or CZ gate in the fields of error correction, quantum advantage, quantum chemistry and quantum optimization algorithms. While Google's 54 bit quantum chip Sycamore is consist of fSim gates, we choose the fSim gate and single qubit gate to form the HEIS gate.

The relevant formulas are listed below:

$$\begin{aligned}\frac{|01\rangle-|10\rangle}{2}(singlet)&=\sqrt{Z}\,\mathrm{HEIS}(\pi/2)X\,|00\rangle\\&=\sqrt{Z}\,\mathrm{fSim}(\pi/4,0)X\,|00\rangle\end{aligned} \tag{14}$$

$$\mathrm{HEIS}(\alpha)=RZ_0(\alpha/2)RZ_1(\alpha/2)\,\mathrm{fSim}(\alpha/2,\alpha) \tag{15}$$

$$\mathrm{SWAP}=\sqrt{Z_0}\sqrt{Z_1}\,\mathrm{fSim}(\pi/2,\pi) \tag{16}$$