IBM Quantum Open Science Prize 2022 Writeup

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1 Kagome Lattice Cell Problem

The task is to find the Ground State Energy E_g of a Heisenberg Spin-1/2 system on a Kagome lattice unit cell with the lowest possible relative error of the measured state's energy expectation value with respect to the exact value. The measured ground state energy should be found on the 16-qubit ibmq_guadalupe device.

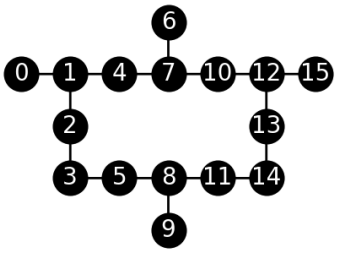

Figure 1: Layout of the 16-qubit ibm_guadalupe device

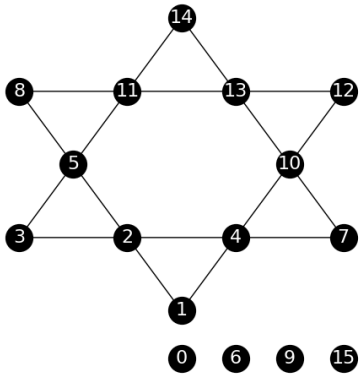

Figure 2: 12-site Kagome lattice unit cell with unused site labels in the cell

The 12-qubit Heisenberg model Hamiltonian is:

$$\hat{H} = \sum_{i,j} \left(\hat{X}_i \hat{X}_j + \hat{Y}_i \hat{Y}_j + \hat{Z}_i \hat{Z}_j \right) \tag{1}$$

For our submission, we have prepared 4 Jupyter notebooks, indexed 01 to 04, in which more detailed information can be found. Notebook 01 implements Section 2.1 of this writeup on our VQE ansatz and optimizer. Notebooks 02 and 03 implements the scale factor, and Notebook 04 puts it all together.

2 Outline of methods

Our main method of achieving the correct ground state energy comes from the method of rescaling, similar to that described in ref [1]. The scale factor is given as

$$f = \frac{\langle \hat{M} \rangle_{\text{noiseless}}}{\langle \hat{M} \rangle_{\text{hardware}}} \tag{2}$$

where $\hat{M}$ is an operator with an expectation value that should be easy to obtain classically. Our final ground state energy measurement can then be rescaled according to

$$E_g = f \langle 0 | U^\dagger(\theta) \, \hat{H} U(\theta) \, | 0 \rangle. \tag{3}$$

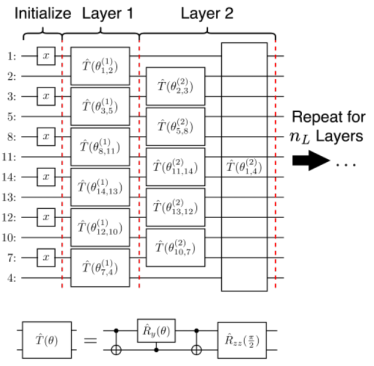

Figure 3: Excitation preserving ansatz consisting of CNOT, CRY, and ZZ gates. The number of layers can be set. From our results, only 4 layers of our ansatz is needed to find the ground state.

2.1 Choice of ansatz and optimizer

By considering the frustration of spins for each of the 6 triangles in the Kagome Lattice, we can observe that the ground state of the Kagome Hamiltonian consists of basis states with six spin ups and six spin downs. With Z2 symmetry (flipping up-spins and down-spins) and additional symmetry from rotating the graph and reassigning the qubits, the ground states consist of a combination of many of these possible basis states preserving the number of excitations.

The default excitation preserving ansatz in Qiskit decomposes to a long circuit that can be difficult to implement on the real backend. Following ref [2] and ref [3], we used an excitation preserving ansatz consisting of CRy, CNOT, and ZZ gates that decoposes into a much shorter circuit. The structure of our circuit can be seen in Fig 3.

Our classical optimizer of choice is RotoSolve [4]. RotoSolve is a gradient free optimizer that is able to find the local minimum of a variational parameter with 3 calls of the cost function. For RotoSolve to work optimally, the expectation value of our desired operator is required to be sinusoidal with respect to the variational parameter with a period of 2π.

While this is not the case for all the variational parameters in our ansatz, we have found that RotoSolve, without any modifications, is still able to converge to a minimum surprisingly quickly. RotoSolve also has the advantage of not having to fine tune any hyperparameters typical of gradient based optimizers. RotoSolve is also easier to implement as there is no dynamical changing of the ansatz during optimization, unlike RotoSelect, which changes the gates used in the ansatz during optimization. As we are not aware of any implementation of RotoSolve in Qiskit, we wrote an implementation to be used in our code.

We have selected 15 runs that have managed to minimize $\langle \hat{H} \rangle$ for submission. Due to queue issues on ibmq_guadalupe, these runs were done using 1000 shots on a simulator, and running the optimized parameters on the ibmq_qasm_simulator using Qiskit Runtime with a noise model queried from the ibmq_guadalupe backend.

Not all our runs are able to find the minimum, with some getting stuck in local minima. However, choosing the runs with the best minimum (even if they don't reach the ground state on the quantum hardware) should not pose an issue to our methods as the focus of our VQE implementation is to find the lowest cost function value, rather than an analysis of how well our ansatz and optimizer combination performs. Additional techniques in error mitigation and scaling can then be added on with the focus of obtaining the accurate energy value.

2.2 Scale factor

To maintain the spirit of the competition, and to make our methods more generalizable, we decided against using the provided ground state energy of Eq 1 as part of our scale factor. However, to accurately characterize the noise of the qubits we want to use, we would want an operator $\hat{M}$ that acts on the same 12 qubits and connections of the inner ring of the ibmq_guadalupe backend that we intend to use for our VQE.

We started off with a 2-qubit Hamiltonian with the same XX, YY, ZZ interactions as Eq 1. This results in a 4×4 matrix that is easily diagonalizable, with a ground state energy of -3.

2.2.1 Simple Hamiltonian

With our 2-qubit interaction, we construct two Hamiltonians:

$$\hat{\mathcal{G}}_1 = \sum_{\langle i,j \rangle \in \mathcal{G}_1} (X_i X_j + Y_i Y_j + Z_i Z_j) \text{ and } \hat{\mathcal{G}}_2 = \sum_{\langle i,j \rangle \in \mathcal{G}_2} (X_i X_j + Y_i Y_j + Z_i Z_j) \tag{4}$$

by applying our interactions to the two perfect matchings of the inner ring of ibmq_guadalupe, $\mathcal{G}_1$ and $\mathcal{G}_2$. The ground state of $\hat{\mathcal{G}}_i$ is easy to calculate as it is simply $6 \times (-3) = -18$, and we use the same ansatz and optimization method used to find our ground state to obtain the denominator in Eq 2. The scale factor, f, is then obtained from average over both Hamiltonians, $f = \frac{1}{2}\left(\frac{\langle \hat{\mathcal{G}}_1 \rangle_{\text{noiseless}}}{\langle \hat{\mathcal{G}}_1 \rangle_{\text{hardware}}} + \frac{\langle \hat{\mathcal{G}}_2 \rangle_{\text{noiseless}}}{\langle \hat{\mathcal{G}}_2 \rangle_{\text{hardware}}}\right)$.

Fifteen VQE runs were used to find the ground state of our simple Hamiltonian, and measured using ibmq_guadalupe, with each run producing a single f value for a total of 15 f values.

Due to queue related issues, $\langle \hat{\mathcal{G}}_1 \rangle_{\text{hardware}}$ was obtained using a noise model queried from ibmq_guadalupe and executed on the ibmq_qasm_simulator using Qiskit Runtime.

3 Results

Figure 4 shows the 15 runs that we have chosen for this submission reaching the targeted value of -18. Together with 15 scale factor values, we obtain a combination of $15 \times 15 = 225$ values of Eq 3. Figure 5 shows the distribution of these 225 estimated $\langle \hat{H} \rangle$, with a mean centered within the 1% bounds.

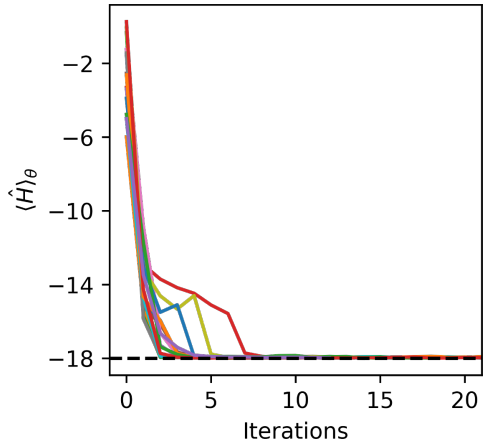

Figure 4: Plot of 15 optimization runs reaching the ground state using our ansatz with Roto-Solve. 4 layers of our ansatz and 1000 shots were used to estimate $\langle \hat{H} \rangle$.

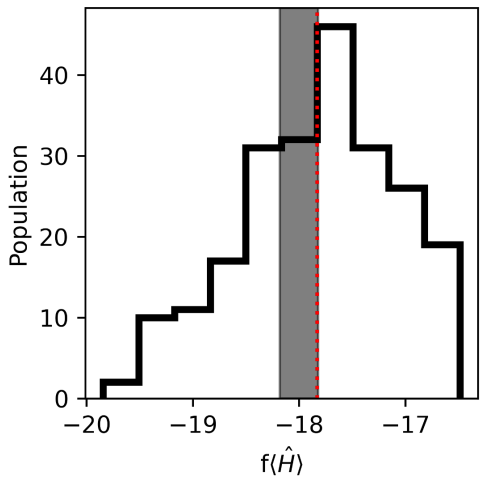

Figure 5: Distribution of 225 estimated $\langle \hat{H} \rangle$ values obtained after scaling.

4 Discussion and conclusion

Due to queue related issues, our results were obtained using 1000 shots on a simulator. However, we believe our results are unlikely to be compromised even if the optimization was carried out on a real backend. Noise within the backend when calculating $\langle \hat{H} \rangle$ will be reflected similarly when calculating $\langle \hat{\mathcal{G}} \rangle$, therefore adjusting the scale factor accordingly.

While noise in the device may change the optimization landscape unpredictably, RotoSolve's quick convergence allows for more VQE runs for data to be gathered in reasonable time, compared to optimizers where multiple hyperparameter values need to be tested.

Lastly, we would like to thank the judges for considering our submission in the challenge.

References

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[4] Mateusz Ostaszewski, Edward Grant, and Marcello Benedetti. Structure optimization for parameterized quantum circuits. *Quantum*, 5:391, 2021.