IBM Quantum Awards: Open Science Prize 2022 Submission: Calculating the highly frustrated ground state of a Heisenberg spin-1/2 model on a Kagome lattice using the Variational Quantum Eigensolver (VQE) algorithm

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Abstract

In order to prepare the highly frustrated ground state of the Heisenberg spin 1/2 model on a Kagome lattice using the VQE we found that one of the most important points is to design an appropiate ansatz for the VQE. We use a method based on the Hamiltonian Variational Ansatz. We prepare a state that is a known ground state of a known hamiltonian that we call H_0. After it we apply a time evolution that will evolve slowly to the desired hamiltonian H (the Hamiltonian of the Kagome lattice). Thanks to the adiabatic theorem if we achieve a sufficient slow time evolution we will arrive to the ground state of the final Hamiltonian. We parametrize the time evolution steps by trotterization.

1 Layout

We decided to use a layout designed for Heavy Hex device architectures, usable with the 16-qubit Guadalupe device, but also with larger Heavy Hex devices. The main idea is to map the device hexagons to the Kagome lattice hexagons, as they have the same kind of connectivity.

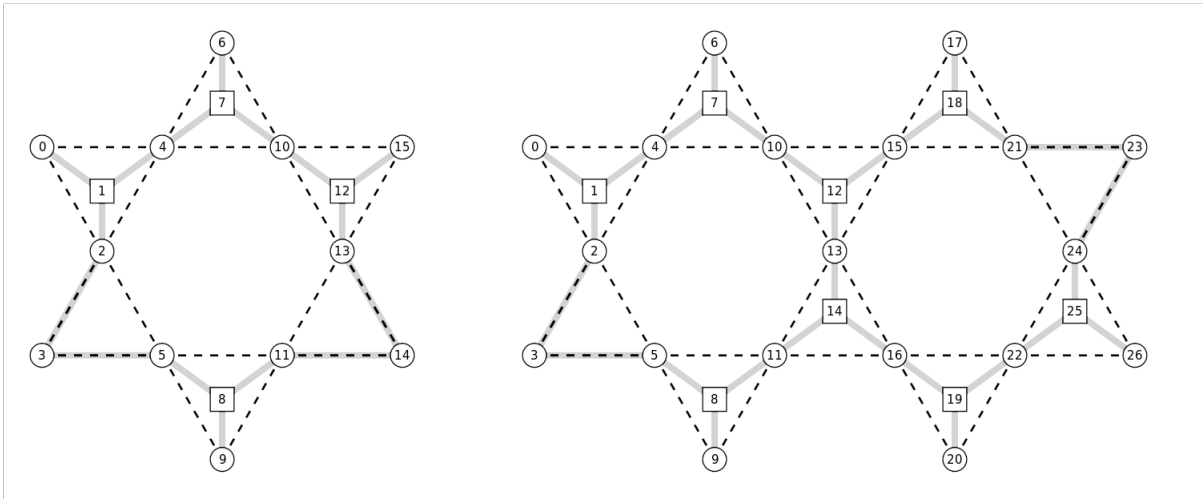

Figure 1: The layout we use to map the Kagome lattice to the IBMQ Guadalupe device (left). The same kind of layout that can be used for larger devices, here a 27-qubit Heavy Hex device such as IBMQ Cairo (right). Grey lines represent the connection between two device qubits. Dashed black lines represent the edges in the Kagome lattice. Circled vertices are device qubits that map directly to Kagome lattice vertices. Squared vertices are device qubits that we use as "control" qubits.

Most Kagome triangles map to a 4-qubit structure in the Heavy hex architectures (as shown in Fig.1). The central device qubit belongs to just one triangle and is used as a "control" qubit for error mitigation. The remaining three device qubits map directly to the Kagome triangle and may belong to other Kagome elements (triangle or hexagon). Due to the finite size of the physical devices, some Kagome triangles on the border map to a 3-device-qubit structure instead of a full 4-device-qubit structure, and do not have control qubits.

2 Hamiltonian Variational Ansatz

The XXX Kagome antiferromagnetic Heisenberg model Hamiltonian is

$$H = \sum_{\langle ij \rangle}^{N} X_i X_j + Y_i Y_j + Z_i Z_j$$

where the sum is over neighboring spins and X, Y, and Z are the usual Pauli matrices. This model has a canonical mapping to qubits: we assign one spin to each qubit.
Given a Hamiltonian H and ground state $|\psi_g\rangle$, according to the variational principle one can found an approximate ground state $|\tilde{\psi}_g\rangle \approx |\psi_g\rangle$. In order to find the approximate ground state $|\tilde{\psi}_g\rangle$, we start with a parameterized state called an ansatz $|\psi(\boldsymbol{\theta})\rangle$ where $\boldsymbol{\theta} \equiv (\theta_1, \theta_2, \dots)$ are the parameters. In theory, there is a combination of parameter values where the anstaz approximates the ground state $|\psi(\boldsymbol{\theta})\rangle \approx |\psi_g\rangle$, and those parameter values are optimized by many cycles of quantum and classical computing drive the ansatz toward the approximate ground state. The quantum computer computes the energy expectation value of Hamiltonian H acting on the the parameterized anstaz for a given set of parameter values

$$E(\boldsymbol{\theta}) = \langle \psi(\boldsymbol{\theta}) | H | \psi(\boldsymbol{\theta}) \rangle \ .$$

This is the cost function and the goal is to minimize it.
The Hamiltonian Variational ansatz [1] is based on the adiabatic theorem. We start with a ground state of an initial Hamiltonian H_0 and we evolve it under a time-dependent Hamiltonian $H(t)$ into the target Hamiltonian H. The time evolution can be implemented by trotterization, applying $e^{-iH_0\Lambda t}$ and $e^{-iH\lambda t}$.

2.1 Initial state and parametrization

The general idea is to choose an initial Hamiltonian that can be written as a sum of commutable edge Hamiltonians (i.e. edges that do not share vertices). In the case of a single cell unit of Kagome, we chose the six edges as shown in Fig. 2

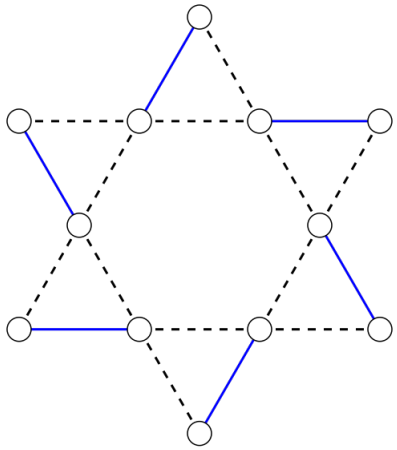

Figure 2: The 6 edges (blue) used for the initial Hamiltonian

By preparing each edge to the ground state of a single edge Hamiltonian, w can prepare a state that is a ground state of this Hamiltonian, as shown in Fig 3. When there is a control qubit, we chose a circuit that, in a noiseless environment, prepares the two Kagome edge vertices in the ground state for the Kagome edge Hamiltonian, and keep unchanged the value of the control qubit when its value is 0 before the circuit.
We chose to parameterized the circuit with R_z gates, in order to optimize the initial state in a noisy context.

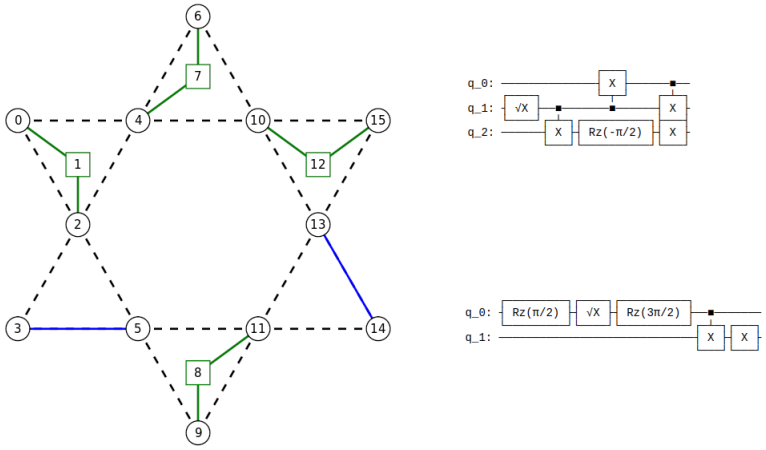

Figure 3: Left: in blue the edges than can be prepared in a ground state directly, in green where we use an additional control qubit. Top right: the basic circuit corresponding to the green edges when there is a control qubit (q_1). Bottom right: the basic circuit corresponding to the blue edges when there is no control qubit

2.2 Trotterization

For the case of a single cell unit of Kagome, the chosen initial state would be a ground state of the entire Hamiltonian in a noiseless environment, so we decided to drop the variational part corresponding to the trotterization from the initial Hamiltonian to the entire Hamiltonian. The ansatz consisting of the preparation of the initial state in a parameterized way is the ansatz that we used in the VQE.
However, in larger devices and with larger Kagome lattices, this may not be true. In more general cases, one can colour the edges of a Kagome lattice with four colours [2] such that there are not two consecutive edges of the same colour (Fig.4)

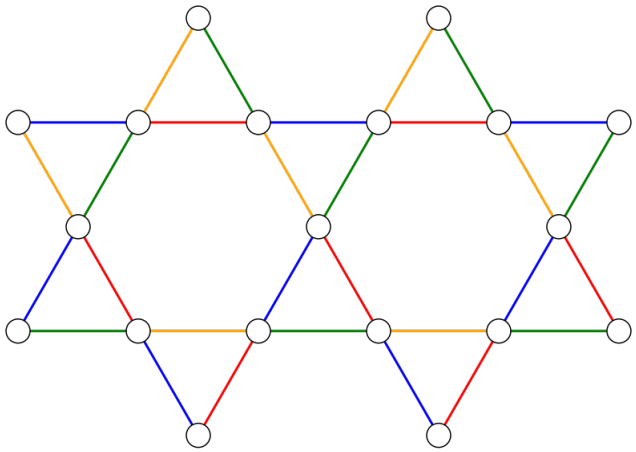

Figure 4: Colouring a 19-vertex Kagome lattice with four colours.

In this way, one can define

$$H = H_{blue} + H_{green} + H_{orange} + H_{red}$$

These four Hamiltonians do not conmute, but each one is separable by each edge, and thus one can found the

ground state easier. This yields the following parametrization:

$$U(\theta) = \Pi_{i=1}^{p} \left[e^{-i\theta_{i,0} H_0} \Pi_{j \in [3,2,1,5,4]} e^{-i\theta_{i,j} H_j} \right]$$

where $\Pi_{j \in [j_1,\ldots,j_n]} U_j = U_{j_1} \ldots U_{j_n}$ denotes the product ordering. This ansatz is called "per edge color" ansatz ([1]), since the decomposition of the Hamiltonian corresponds to an edge colouring for the lattice. Such an ansatz would be composed by an initial state (fixed or parameterized) that is the ground state of a known Hamiltonian, followed by the circuit implementing the trotterization steps.

3 Optimizer

We use a SPSA optimizer. For the case of a Kagome unit cell, we don't use a trotterization circuit but just an initial state preparation circuit that we chose to parameterize. The optimizer will look around the central parameters that would prepare a perfect ground state for the initial hamilonian in a noiseless environment.

4 Measurement and error mitigation

Our main contribution is the use of a custom estimator that use the control qubits (see the section 1). We use the qiskit sampler primitive and have design a custom estimator algorithm.

4.1 Measurement

The XXX Heisenberg hamiltonian for a Kagome lattice can be decomposed into 3 components: the X, the Y and the Z components. Each of these components is a sum of Pauli edge hamiltonians that commute the ones with the others, thus all the edge hamiltonians of a given component can be measured simultaneously. Thus, we decided to estimate each of the 3 components of the full hamiltonian separately, and have different circuits for each components.

4.2 Error mitigation

For each component (X, Y and Z) of the full hamiltonian, we use an error mitigation mechanism to estimate the expectation value. For reasons of readability and clarity, we will describe how it works with one control qubit, and then explain how it can be generalized for more control qubits.

4.2.1 Simple case of 1 control qubit

The aim of the control qubit is to get a better estimation of the expectation value, by detecting the errors occuring during the action of the quantum circuit (before the measurement part) and lowering their impact on the expectation value.
Before the measurement, the state of the system can be described by a density matrix ρ, and the expectation value for the hamiltonian H is $E(\rho) = tr(\rho H)$. Our main hypothesis is to decompose the expectation value as follows:

$$E(\rho) = \lambda_t E_t + \lambda_C \left(E_{\epsilon_0} + E_{\epsilon_1} \right)$$

with:

- E_t the targeted expectation value, which we believe will be closer to the theoretical energy measured if the circuit had no errors
- λ_t, λ_C probabilities such as $\lambda_t + 2\lambda_C = 1$
- E_{ϵ_1} the expectation value associated with measuring 1 for the control qubit with 100% probability in a perfect measuring system

- $E_{\epsilon_0} = E_{\epsilon_1} = E_\epsilon$ same expectation value as E_{ϵ_0}, but associated with measuring 0 for the control qubit.

Under this hypothesis and if there were no readout errors, when mesuring the circuit, we can estimate:

- λ_C: the probability of measuring 1 for the control qubit
- $\lambda_t + \lambda_C$: the probability of measuring 0 for the control qubit
- E_ϵ the expectation value of the hamiltonian when measuring 1 for the control qubit
- $(\lambda_t E_t + \lambda_C E_\epsilon) / (\lambda_t + \lambda_C)$ the expectation value of the hamiltonian when measuring 0 for the control qubit.

and derive an estimator of E_t:

$$\hat{E}_t = \frac{p_0 E_0 - p_1 E_1}{p_0 - p_1}$$

with p_0 and p_1 the frequency of obtaining 0 and 1 for the control qubit, and E_0 and E_1 the expectation values when we measure 0 and 1 for the control qubit.
In practice, to tackle the readout errors, we use two methods:

- the energies E_0 and E_1 are estimated with the twirled readout error extinction (T-REx) algorithm [3]
- we use a simple bayesian model for each control qubit taken individually, to estimate the probability of measuring a value for the control qubit whereas we would had measured another value if there were no readout errors.

4.2.2 Generalization for several control qubits

For the Kagome cell unit and under the ansatz that we used, we decided to take each triangle of the Kagome separately, and to estimate each triangle energy with the method described in section 4.2.1.
However, we believe that our method can be adapted to handle more general ansatzs in larger devices, when the triangles are more entangled than here. We also believe that the noise model used to define the "targeted" energy with a control qubit could be optimized during a calibration phase.

References

[1] Jan Lukas Bosse and Ashley Montanaro. Probing ground state properties of the kagome antiferromagnetic heisenberg model using the variational quantum eigensolver, 2021.

[2] Joris Kattemölle and Jasper van Wezel. Variational quantum eigensolver for the heisenberg antiferromagnet on the kagome lattice. *Physical Review B*, 106(21), December 2022.

[3] Ewout van den Berg, Zlatko K. Minev, and Kristan Temme. Model-free readout-error mitigation for quantum expectation values. *Physical Review A*, 105(3), mar 2022.