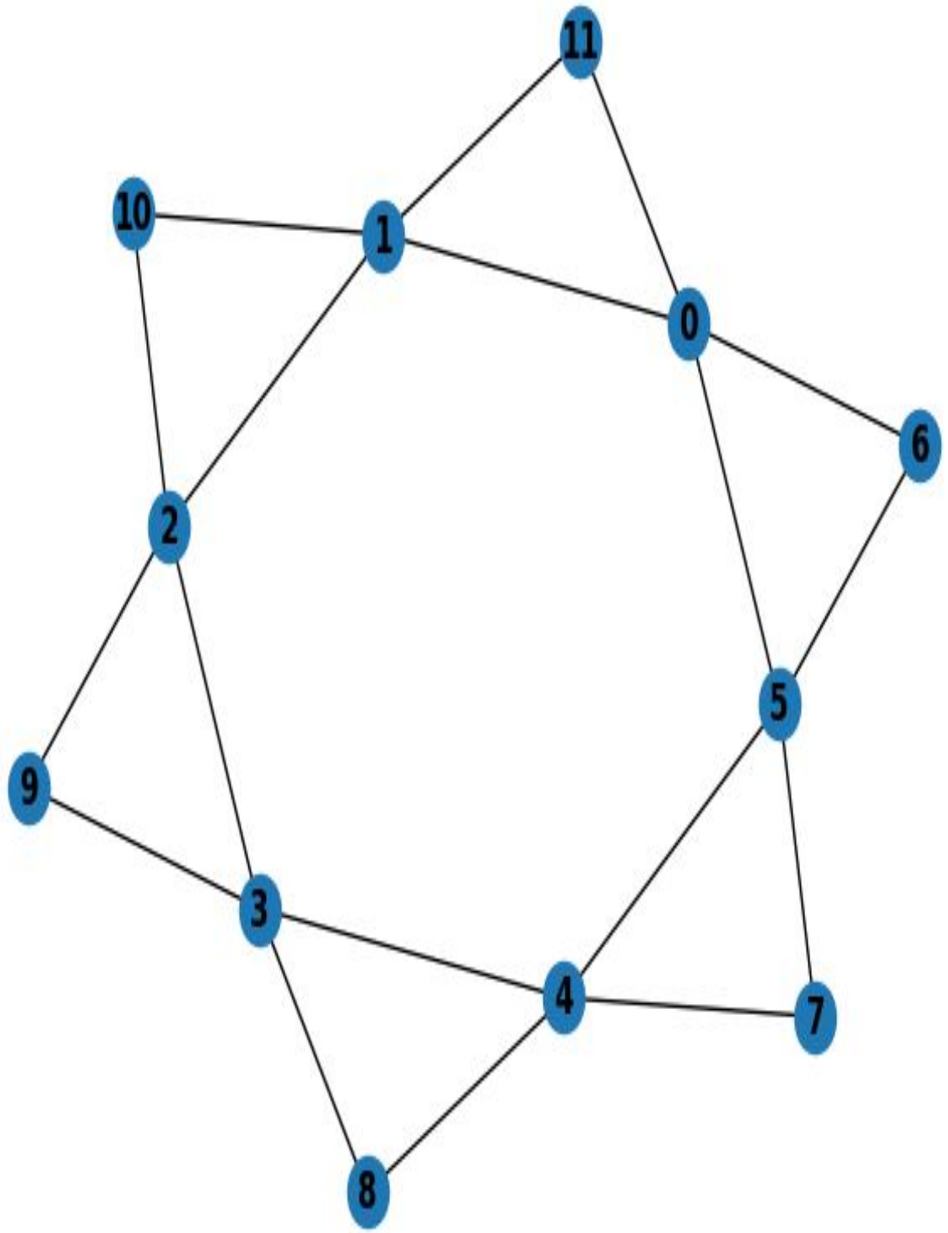

Graph optimization of the Kagome lattice unit cell

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The Variational Quantum Eigensolver Approach

1

Problem Definition

The Hamiltonian we have is the coupled 12 qubit hamiltonian for 1 single unit cell of the kagome graph. The hamiltonian can be time evolved for simulation of the hamiltonian by encoding the hamiltonian directly in the circuit. This has been demonstrated in Kattermole et al, using KVQE and CVQE methods.

2

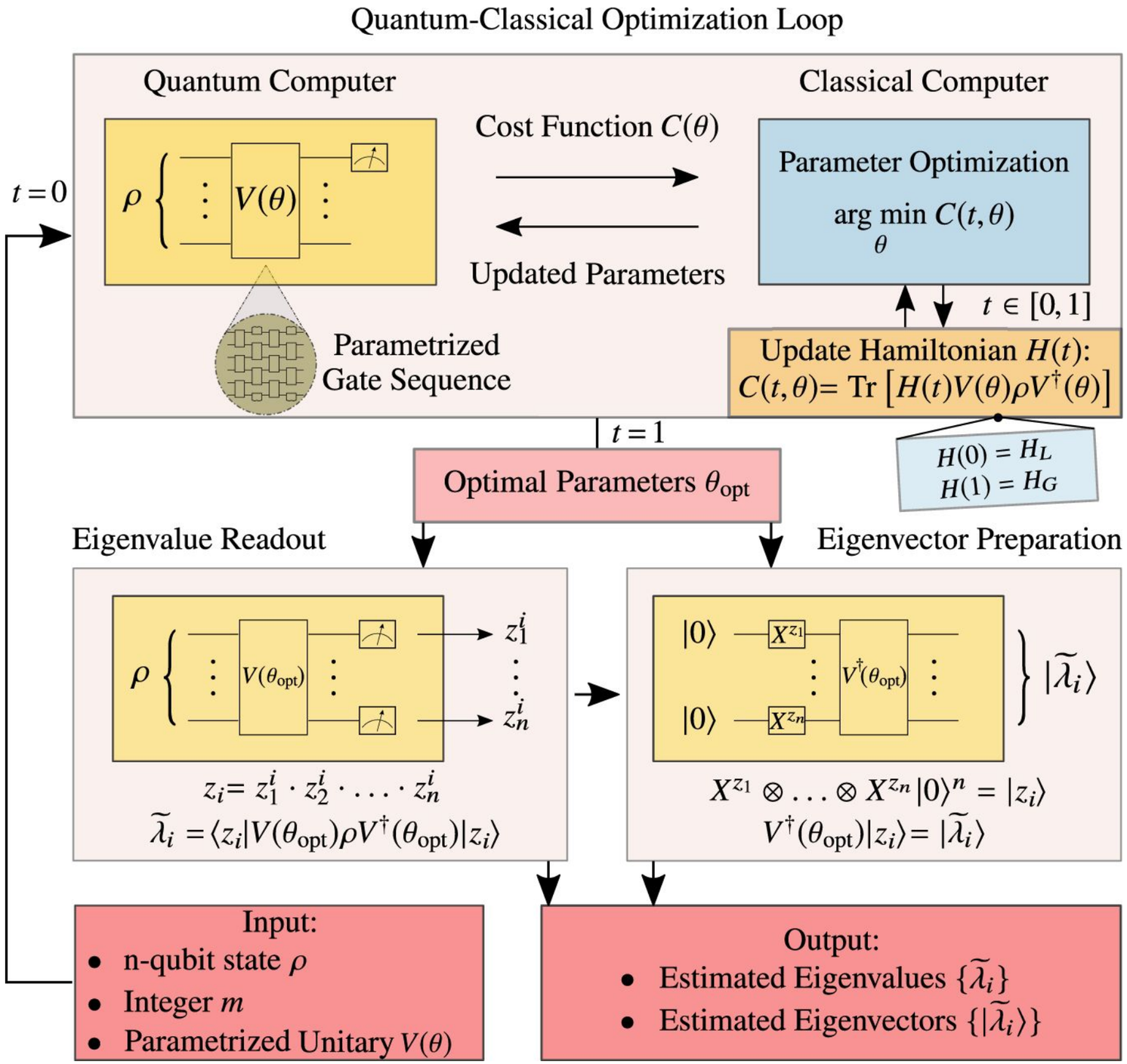
VQE Methodology

The VQE methodology like most QML algorithms tells us to assume a suitable ansatz and run it for a variational run to find the minimum energy of the

3

VQE Implementation

The VQE we have implemented uses Simplified Two design ansatz and the x,y,z coupled hamiltonian for the 12 qubit kagome graph.



The usual workflow of the VQE algorithm

- The goal is to variationally optimize our circuit to find the ground state of the ha
- In this case, we have a n dimensional hamiltonian with n entangled quantum qubits to show higher order correlations between them as tensor product networks.
- All of these are parameterized using pauli rotation gates and some initial parameters.
- This particular sequence is is run against a quantum computers to find the exact energy values of the hamiltonian which has its own potential energy function.
- The classical optimizer could be chosen to be anything.
- The cost function is given by the following expression below - $\langle \Psi(\theta) | H | \Psi(\theta) \rangle$

The usual workflow of the VQE algorithm (contd)

- The Hamiltonian potential curve is analyzed by the classical computer which classically optimizes the values spitted out by the quantum computer.
- This minimum state is reconsidered for the reiteration of the cost function value and continues till we set some amount of convergence tolerance and maximum epoch constraint.
- The values are updated using some fixed learning rate for the optimizer function.

Hamiltonian to qubit/ spin encoding

1

The encoding and conversion into an hamiltonian

The hamiltonian is a second quantized function which is usually described using creation and annihilation operators for many body systems. The hamiltonian can also be described using plain wave solutions. There needs to be a way to convert these hamiltonians into a form that the quantum computers can understand

2

Encoding for the quantum computer

The creation and annihilation operators have simple properties on the fock space of the quantum hamiltonian. These actions can be equated using the actions of trivial single qubit pauli basis operators. That is how the encoding must be done. But different systems require different architectures. Hamiltonian encoding is an active area of research.

3

Examples

Many Hamiltonians for which VQEs are proposed are fermionic. Examples include those in quantum chemistry and the Fermi-Hubbard model. For a VQE to solve for the ground state of a fermionic Hamiltonian, it first needs to be mapped to a spin Hamiltonian, for example, by the Jordan-Wigner, Bravyi-Kitaev or ternary-tree transformations. Fermion to spin maps either increase the nonlocality of terms in the Hamiltonian or introduce additional qubits, in any case leading to an overhead in quantum resources.

Workflow up until now

1

Visualizing the Kagome graph

We use the QAOA method to find the Hamiltonian for the graph state of the 12 qubit Kagome Hamiltonian, the frustrated antiferromagnetic model which behaves like a spin liquid at room temperatures.

2

Building the hamiltonian

The Kagome Hamiltonian is a Heisenberg chain in a star like 2d structure. For our analysis now we are using the single unit cell of the 12 qubit lattice instead of the infinitely long 2d chain for the same. The scaling is not really possible for a finite size computer. We will however explore a way to simulate a larger variable size of Heisenberg chains of the same orientation or better approximation.

3

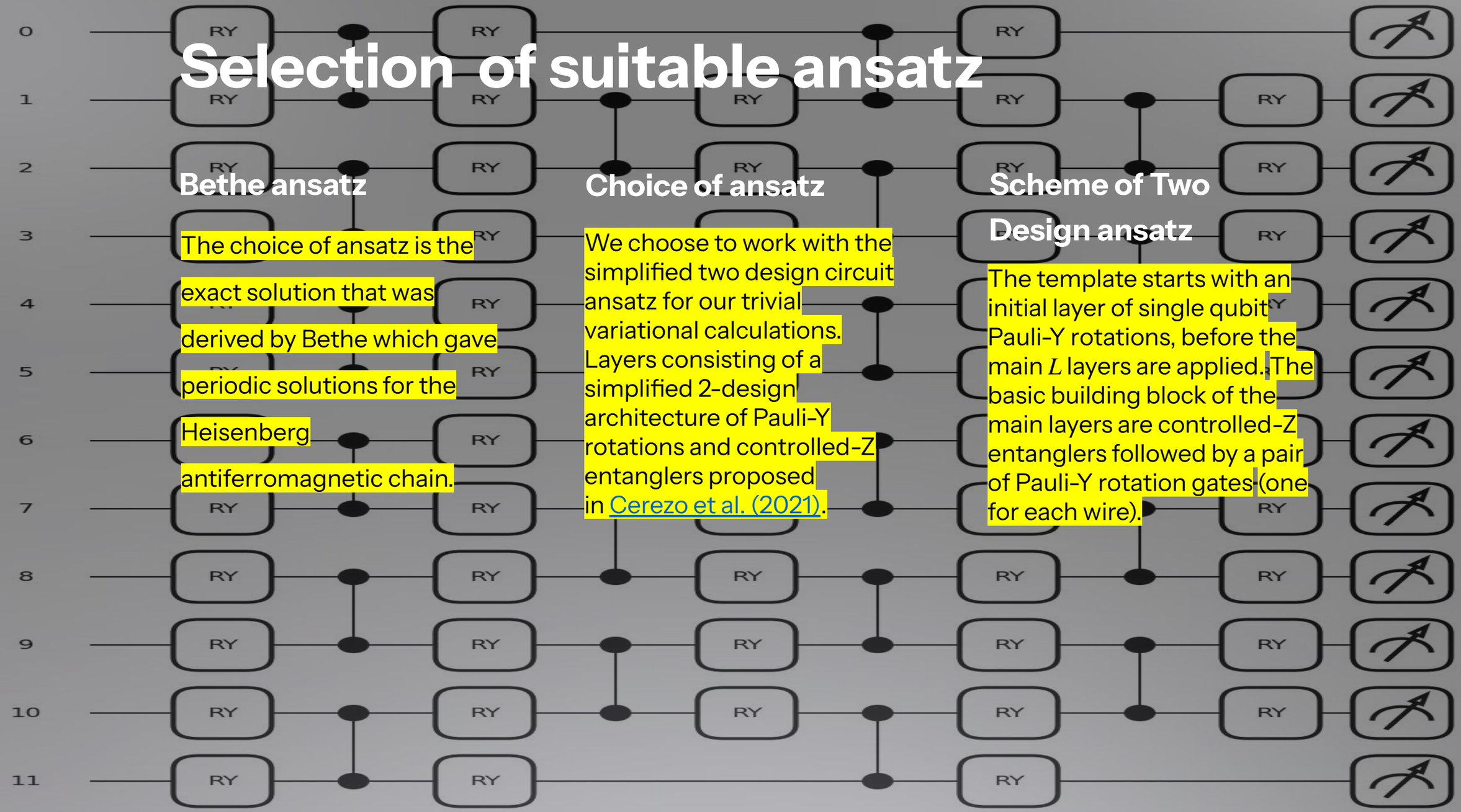
Spin interactions are trivial

The spin interactions between two lattice points are bounded by the laws of the spin operator commutation relations.

```
  (1.0) [X0 X1]
+ (1.0) [Y0 Y1]
+ (1.0) [Z0 Z1]
+ (1.0) [X0 X5]
+ (1.0) [Y0 Y5]
+ (1.0) [Z0 Z5]
+ (1.0) [X0 X6]
+ (1.0) [Y0 Y6]
+ (1.0) [Z0 Z6]
+ (1.0) [X0 X11]
+ (1.0) [Y0 Y11]
+ (1.0) [Z0 Z11]
+ (1.0) [X1 X2]
+ (1.0) [Y1 Y2]
+ (1.0) [Z1 Z2]
+ (1.0) [X1 X10]
+ (1.0) [Y1 Y10]
+ (1.0) [Z1 Z10]
+ (1.0) [X1 X11]
+ (1.0) [Y1 Y11]
+ (1.0) [Z1 Z11]
+ (1.0) [X2 X3]
+ (1.0) [Y2 Y3]
+ (1.0) [Z2 Z3]
+ (1.0) [X2 X9]
+ (1.0) [Y2 Y9]
+ (1.0) [Z2 Z9]
+ (1.0) [X2 X10]
+ (1.0) [Y2 Y10]
+ (1.0) [Z2 Z10]
+ (1.0) [X3 X4]
+ (1.0) [Y3 Y4]
+ (1.0) [Z3 Z4]
+ (1.0) [X3 X8]
+ (1.0) [Y3 Y8]
+ (1.0) [Z3 Z8]
+ (1.0) [X3 X9]
+ (1.0) [Y3 Y9]
+ (1.0) [Z3 Z9]
+ (1.0) [X4 X5]
+ (1.0) [Y4 Y5]
+ (1.0) [Z4 Z5]
+ (1.0) [X4 X7]
+ (1.0) [Y4 Y7]
+ (1.0) [Z4 Z7]
+ (1.0) [X4 X8]
+ (1.0) [Y4 Y8]
+ (1.0) [Z4 Z8]
+ (1.0) [X5 X6]
+ (1.0) [Y5 Y6]
+ (1.0) [Z5 Z6]
+ (1.0) [X5 X7]
+ (1.0) [Y5 Y7]
+ (1.0) [Z5 Z7]

Vector space dimension of the ansatz circuit :  12
```

Selection of suitable ansatz



Bethe ansatz

The choice of ansatz is the exact solution that was derived by Bethe which gave periodic solutions for the Heisenberg antiferromagnetic chain.

Choice of ansatz

We choose to work with the simplified two design circuit ansatz for our trivial variational calculations. Layers consisting of a simplified 2-design architecture of Pauli-Y rotations and controlled-Z entanglers proposed in Cerezo et al. (2021).

Scheme of Two Design ansatz

The template starts with an initial layer of single qubit Pauli-Y rotations, before the main L layers are applied. The basic building block of the main layers are controlled-Z entanglers followed by a pair of Pauli-Y rotation gates (one for each wire).

Variational Run

1

Parameter

The parameters chosen for our ansatz are all as per the choice of our simplified two design parameter requirement. All are initialized to 1.

2

Optimizer Choice

The optimizer that I am using is the SPSA optimizer which is a non classical optimizer run. This after a lot of trials with other optimizers turns out to have one of the best convergence rates.

3

Cost function and energy updated specifications

The Cost function is the usual cost function for VQE for our graphical hamiltonian of the kagome lattice. It is the expectation value of the parameterized ansatz state with respect to the graph hamiltonian build via trivial second order spin coupling interactions.

4

Specifications from the code

Energy optimization at 0 th step is : 0.7875308867384085

Energy optimization at 50 th step is : -8.410568789151908

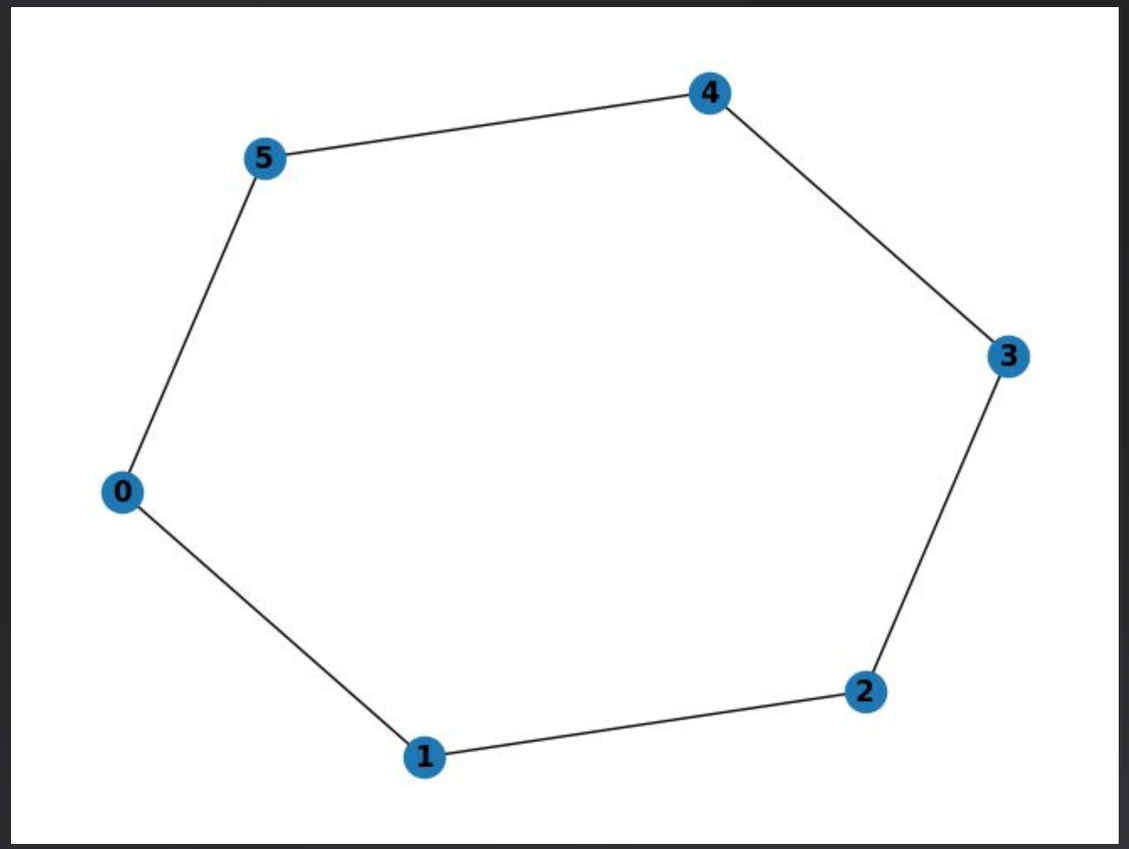
Energy optimization at 100 th step is : -9.760999322219002

Energy optimization at 150 th step is : -10.851608449219613

Energy optimization at final step is : -11.233433871078494

CPU times: total: 1min 26s Wall time: 54.5 s

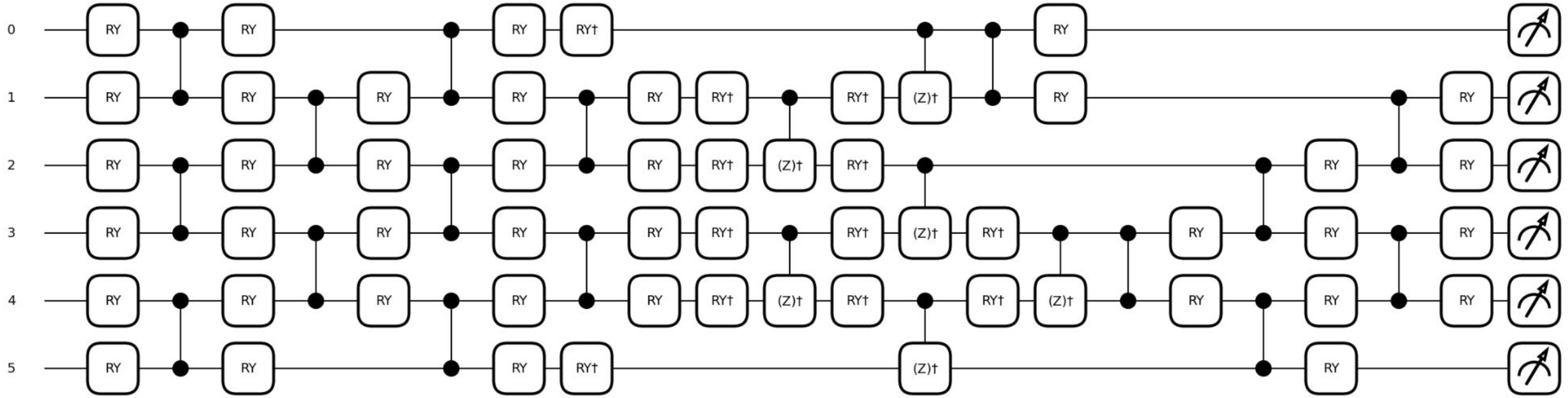
Hexagon hamiltonian



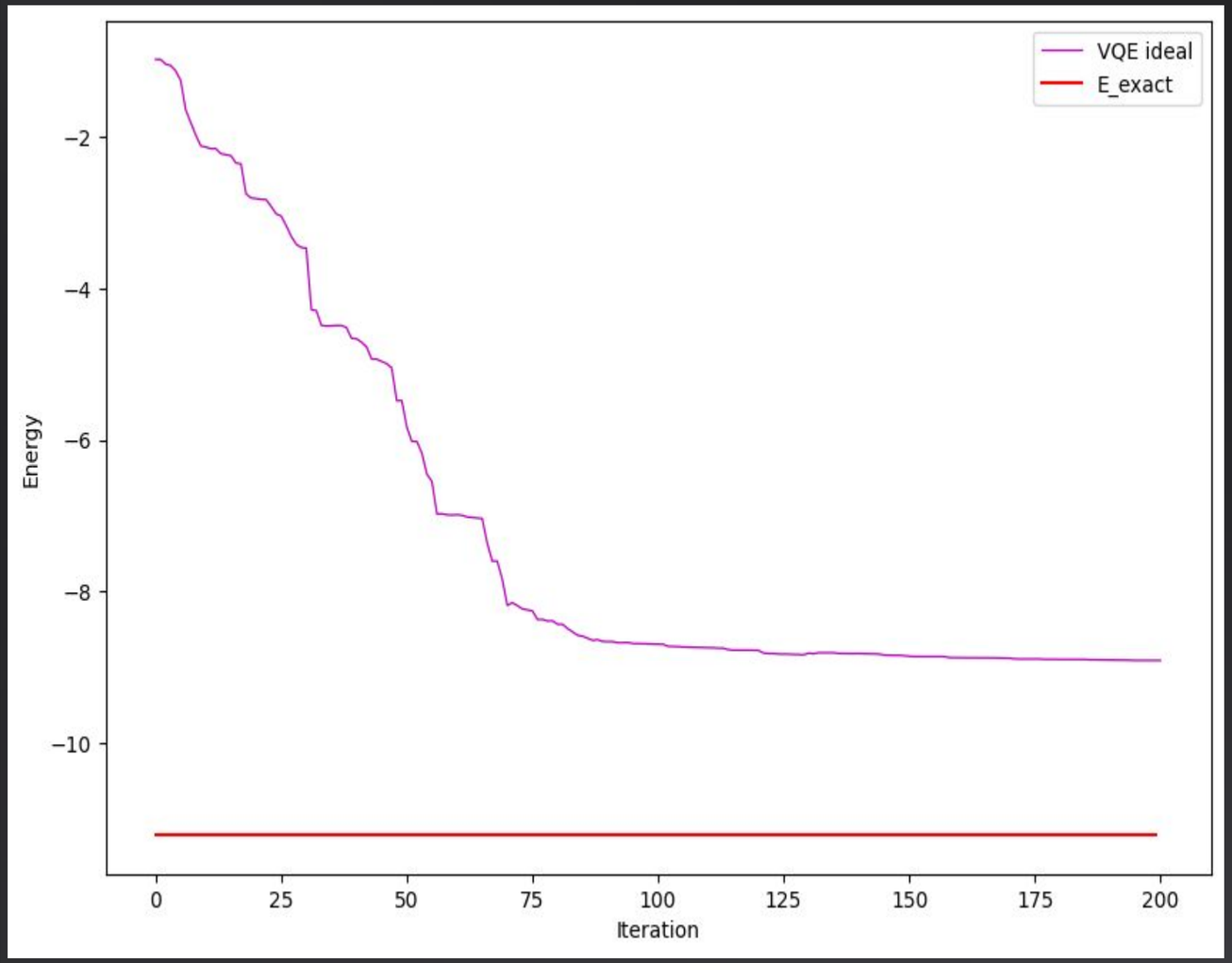
- Before going through with the final kagome lattice hamiltonian we will first optimize their constituents :- The hexagon and the triangle.
- The graph seen in the left is that of the hexagon lattice with spin spin interactions.
- The interactions of the spin hamiltonians are constrained by the edge vertex structure of the graph.
- The maximum order of coupling here is second order only.

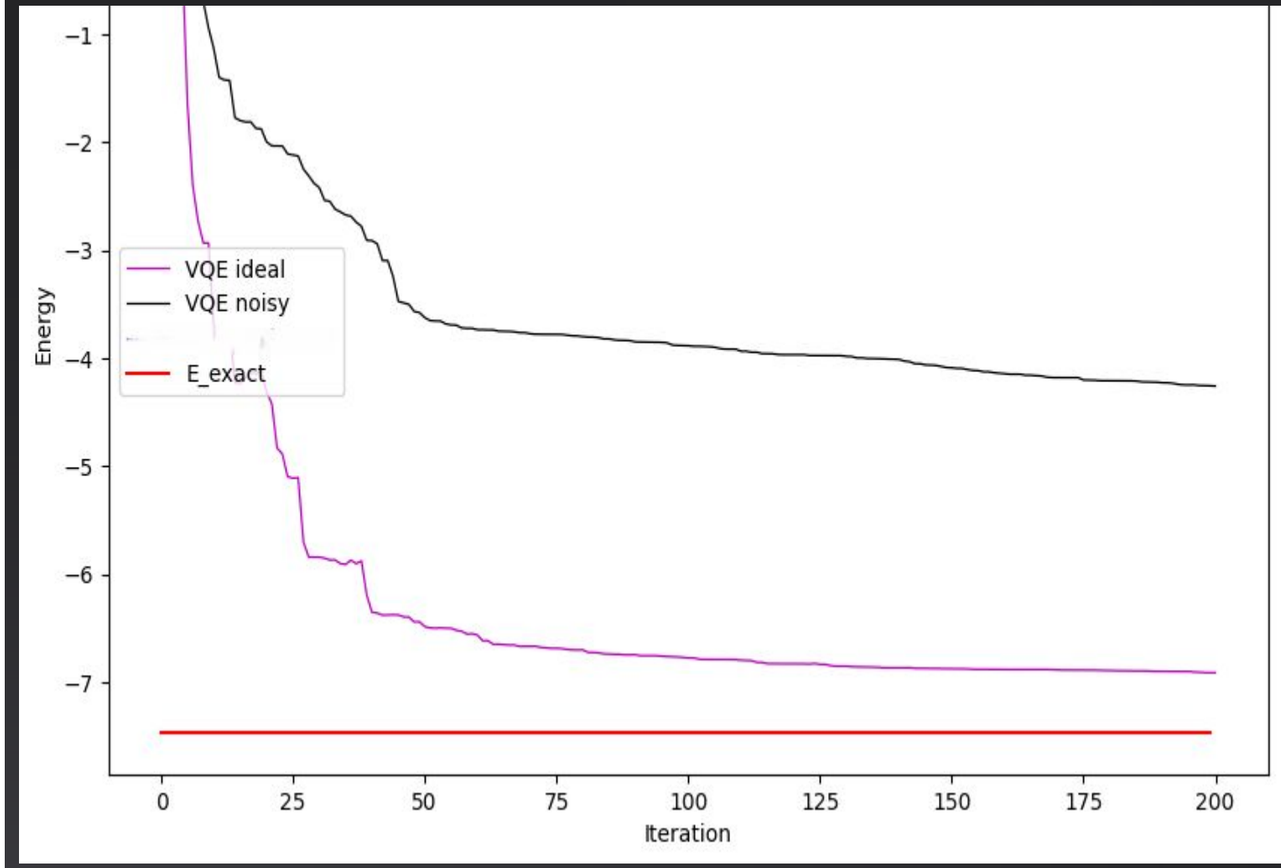
Hexagon circuit

- We have six qubits here and the initial ansatz is created using suitable entanglements and rotation gates.
- This ansatz will have some initial parameters and the same will be optimized as per the cost function and the vqe algorithm.

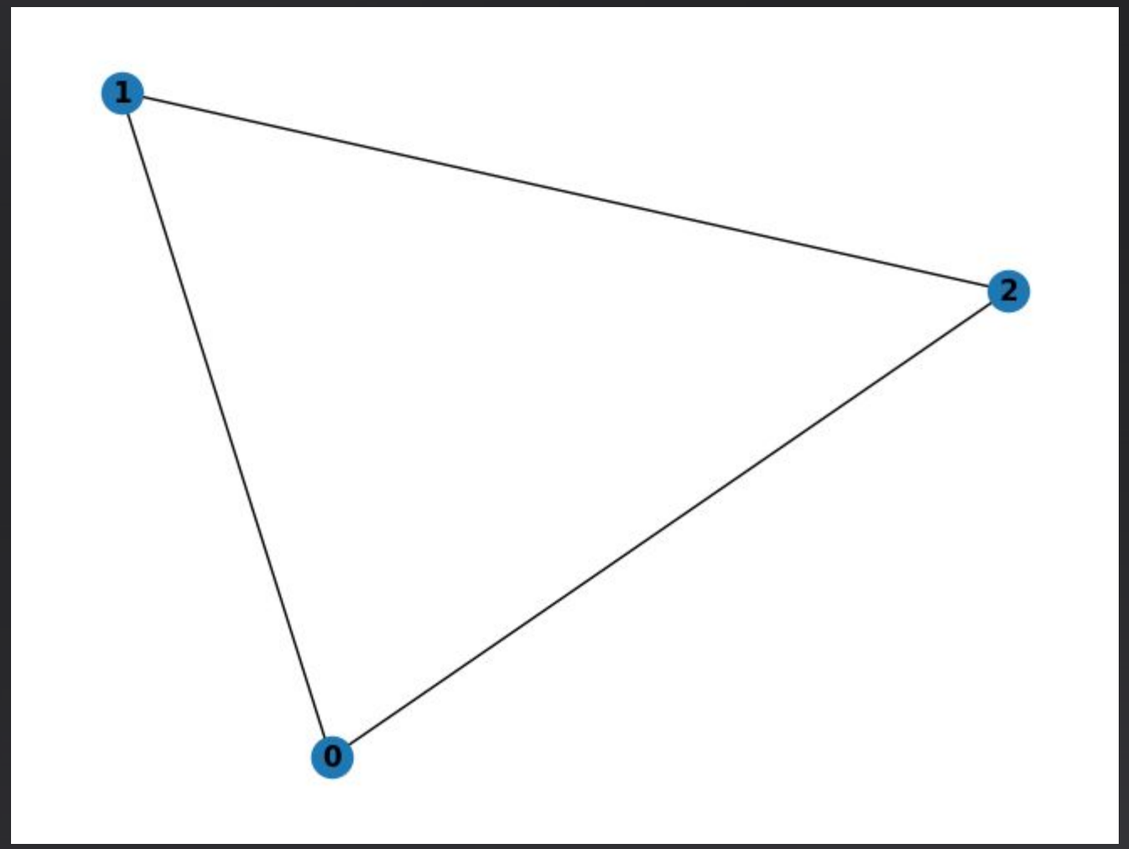


Optimization plots with and without noise





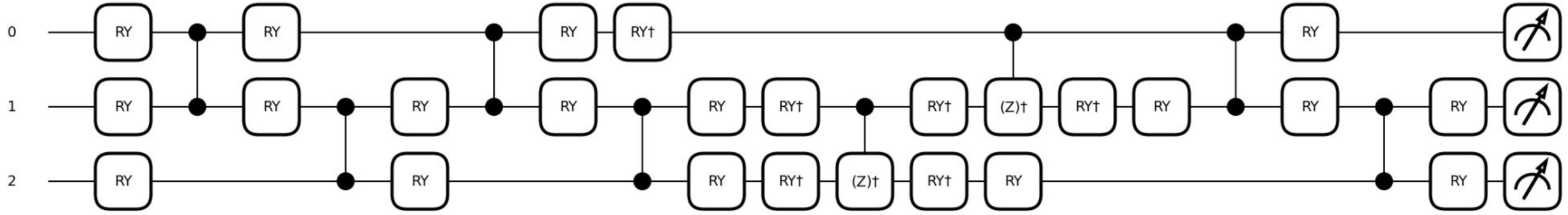
Triangle hamiltonian



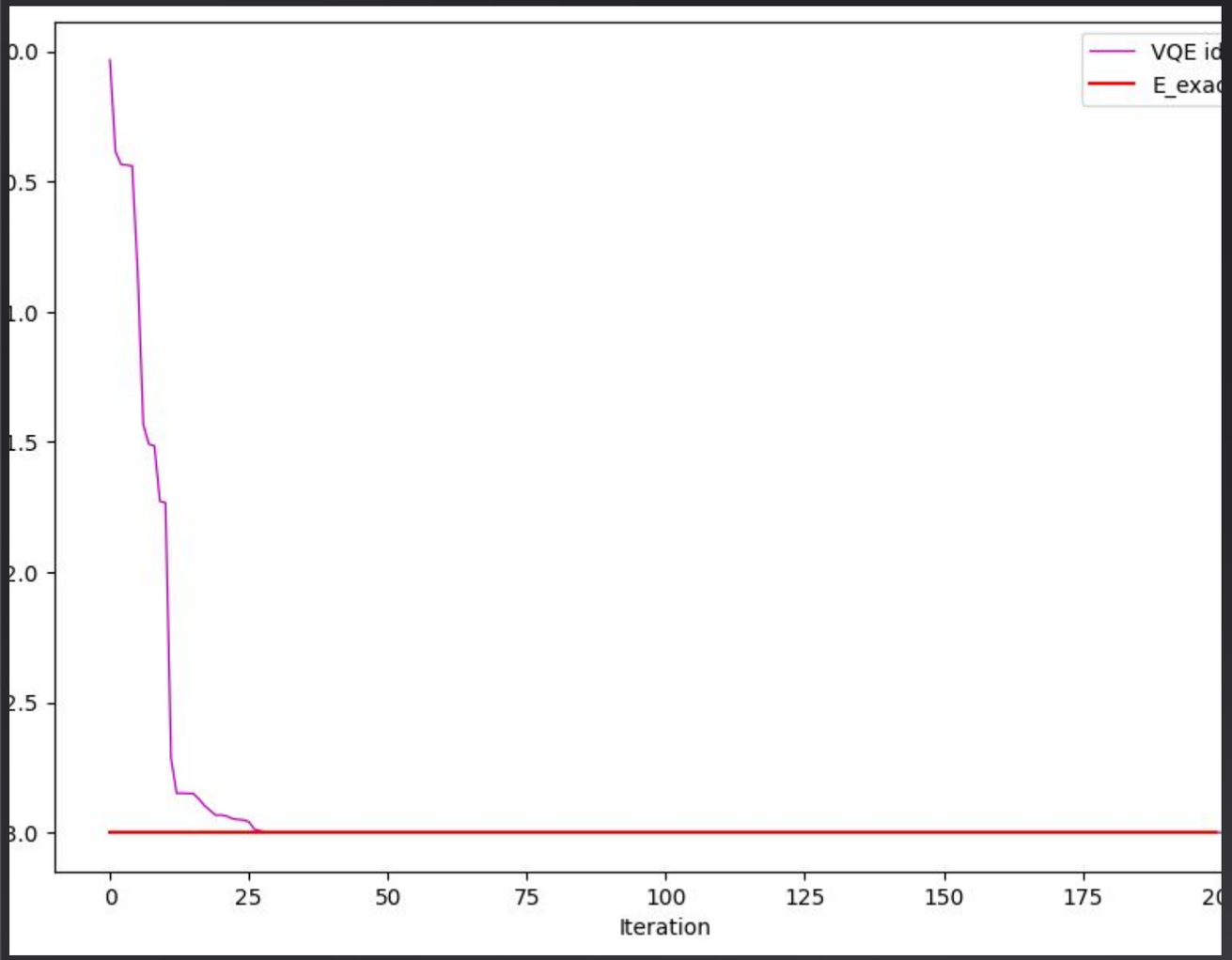
- Hamiltonian for the triangle is small and easy to interpret and hence we are showing it here explicitly.
- Ham : (1.0) [X0 X1] + (1.0) [Y0 Y1] + (1.0) [Z0 Z1] + (1.0) [X0 X2] + (1.0) [Y0 Y2] + (1.0) [Z0 Z2] + (1.0) [X1 X2] + (1.0) [Y1 Y2] + (1.0) [Z1 Z2]
- Vector space dimension: 3
- The triangle circuit is given below

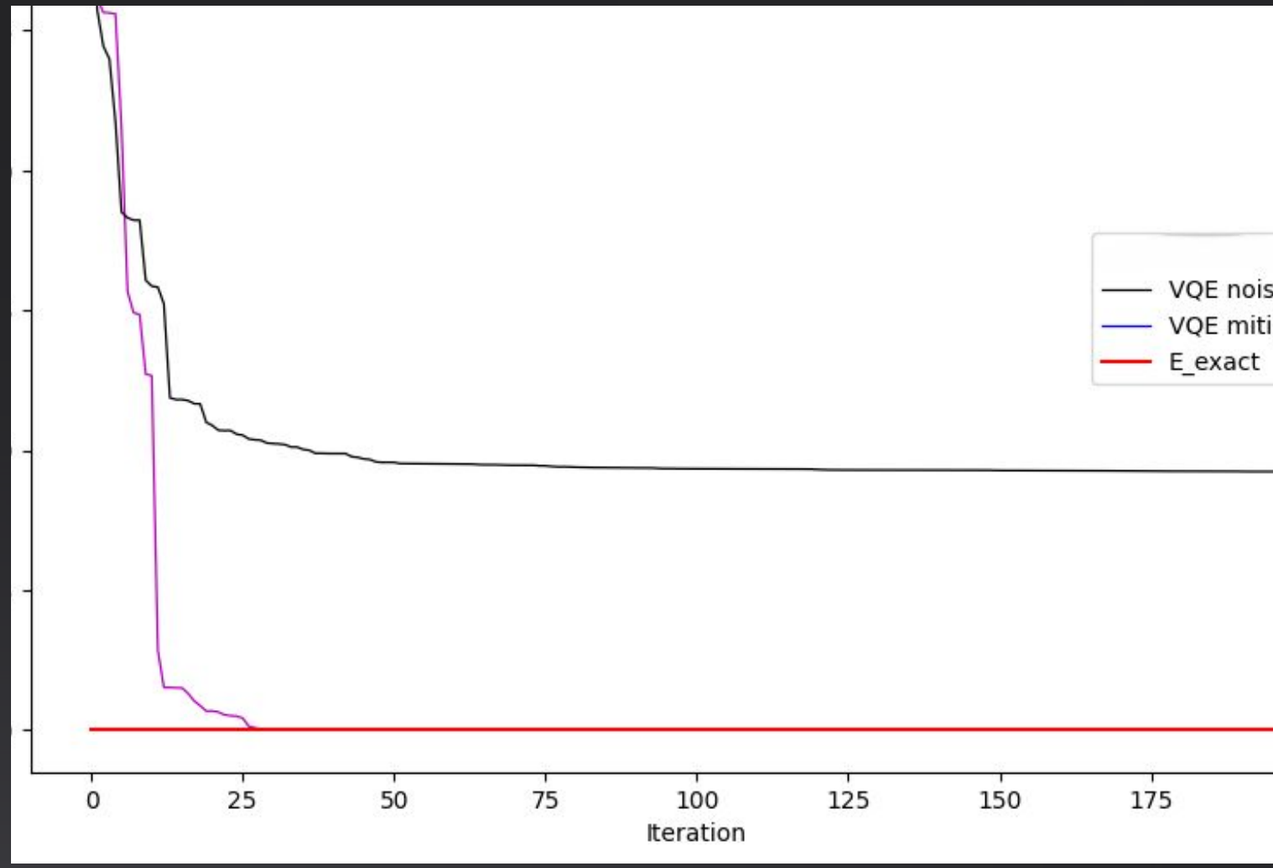
Triangle circuit

- We have three qubits here and the initial ansatz is created using suitable entanglements and rotation gates.
- This ansatz will have some initial parameters and the same will be optimized as per the cost function and the vqe algorithm.

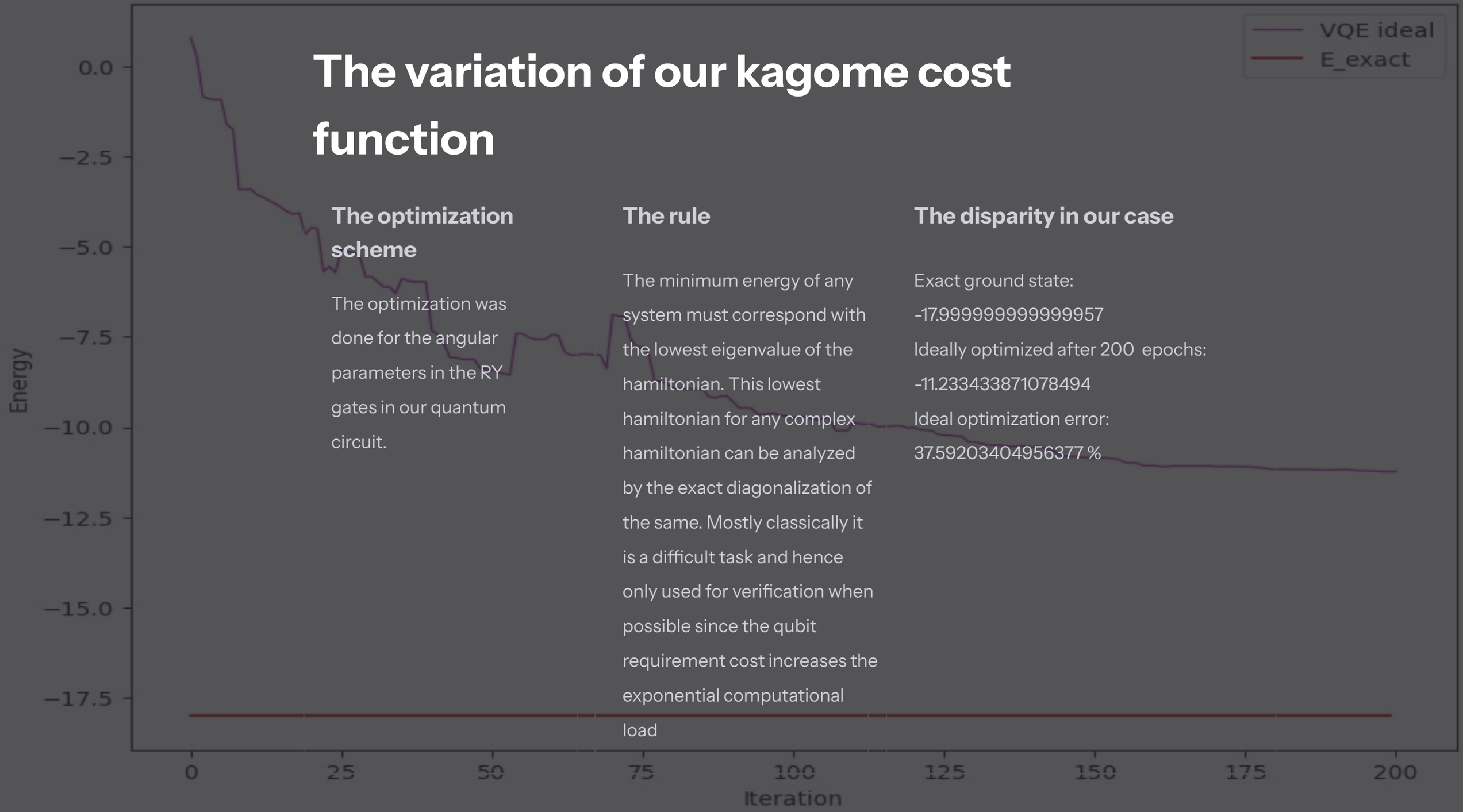


Optimization plots with and without noise





The variation of our kagome cost function



The optimization scheme

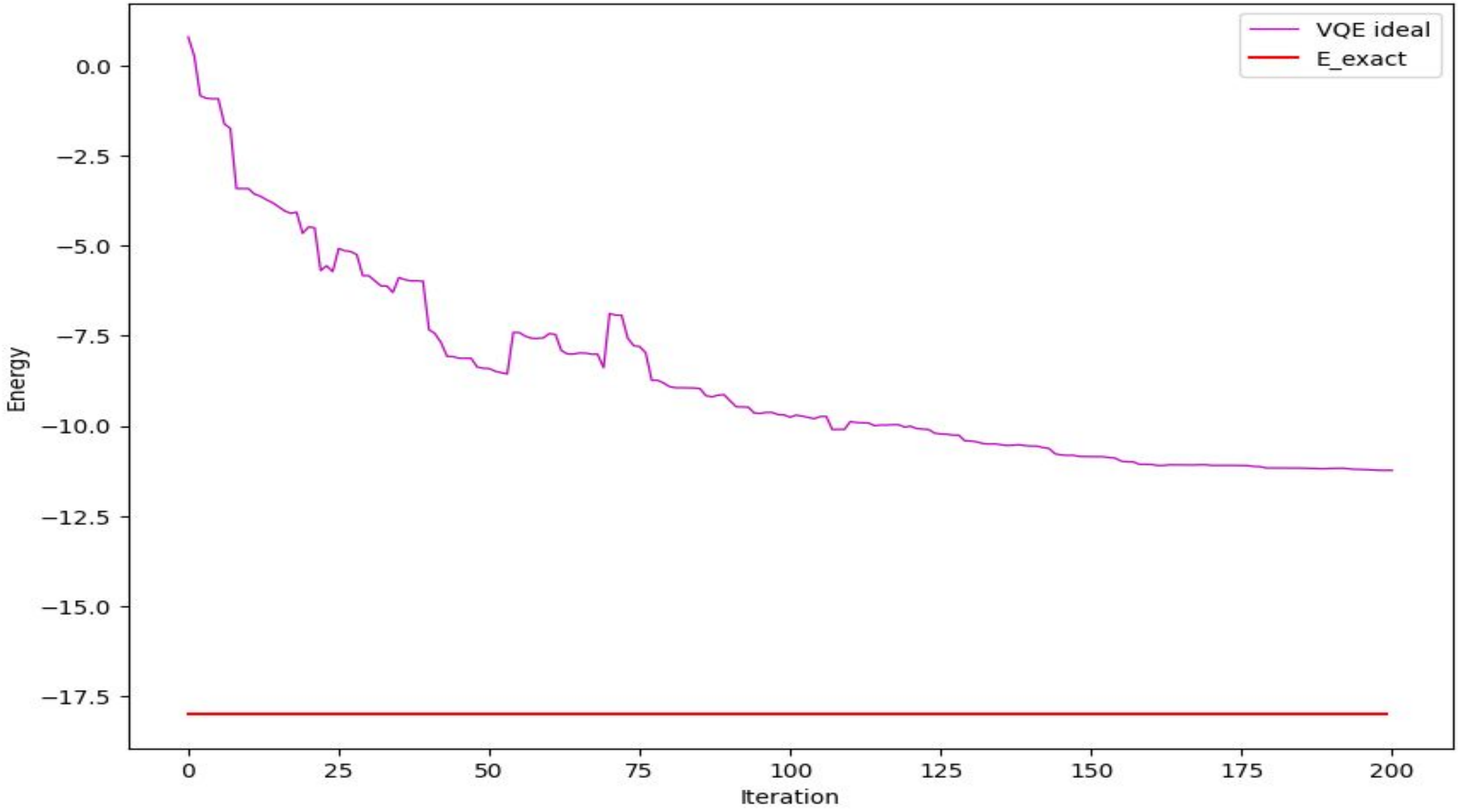
The optimization was done for the angular parameters in the RY gates in our quantum circuit.

The rule

The minimum energy of any system must correspond with the lowest eigenvalue of the hamiltonian. This lowest hamiltonian for any complex hamiltonian can be analyzed by the exact diagonalization of the same. Mostly classically it is a difficult task and hence only used for verification when possible since the qubit requirement cost increases the exponential computational load

The disparity in our case

Exact ground state:
-17.999999999999957
Ideally optimized after 200 epochs:
-11.233433871078494
Ideal optimization error:
37.59203404956377 %


VQE ideal
E_exact
0.0
−2.5
−5.0
−7.5
−10.0
−12.5
−15.0
−17.5
Energy
0
25
50
75
100
125
150
175
200
Iteration

Conclusion

Key Findings	- VQEs for the HAFM on the Kagome lattice show exponential decay of energies with circuit depth in the noiseless case. - Error mitigation techniques and technological improvements in error rates are necessary to achieve energies below the first excited state.
Future Outlook	- Theoretical and technological advancements are needed to realize a useful quantum advantage on near-term quantum devices. - The proposed 36-site VBC ground state can be used as the initial VQE state on quantum computers with a similar number of qubits.