Solving the Lipkin Model with VQE

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We have estimated the ground state energy of a 3×3, 4×4 and a 5×5 hamiltonian by using a variational quantum eigensolver. The method sees some success on the small cases, but fails when put against the larger ones.

I. INTRODUCTION

Many problems boils down to an eigenvalue problem. In quantum mechanical systems this holds especially true. But as Richard P. Feynman postulated in his paper *Simulating Physics with Computers* [1], to simulate quantum systems you would need a quantum computer. The problem arises with large quantum system, where keeping track of probabilities become impossible solely with upscaling and parallelism of classical computers.

In this article we will try to look at the possibility of using quantum computing as a tool to find eigenvalues of hamiltonians of quantum mechanical systems. Specifically we will look at the variational quantum eigensolver algorithm. We will however, slightly ironically, simulate these quantum computations with a classical computer, but will still hopefully gain some insight in the application of such an algorithm by doing so.

We are going to study three problems, each with increasing complexity: first we will diagonalize a symmetric Hamiltonian $H \in \mathbb{R}^{2\times 2}$. This will be used for comparison with the other two problems as well as a known correct soltuion for when we will implement a variational quantum eigensolver and use it to find the eigenvalues of the 2×2 Hamiltonian. Further we will extend the problem into a two-qubit basis, which would make the Hamiltonian $H \in \mathbb{R}^{4\times 4}$, and find the eigenvalues by standard solver as well as our implementation of a VQE. Finally we will look at the Lipkin model, where we study the model for cases $J = 1$ and $J = 2$, which has respectively a 3×3 and a 5×5 hamiltonian. These hamiltonians we will diagonalize as well with both standrard eigensolver and with a VQE.

II. THEORY

II.1. Standard Computational Basis

The standard computational basis consist of

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Higher many-body computational computational bases can be created by tensor product of the single-qubit ones:

$$|00\rangle = |0\rangle \otimes |0\rangle = [1, 0, 0, 0]^T \tag{1}$$

$$|10\rangle = |1\rangle \otimes |0\rangle = [0, 1, 0, 0]^T \tag{2}$$

$$|01\rangle = |0\rangle \otimes |1\rangle = [0, 0, 1, 0]^T \tag{3}$$

$$|11\rangle = |1\rangle \otimes |1\rangle = [0, 0, 0, 1]^T \tag{4}$$

II.2. The Pauli matrcies

The Pauli matrices are:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$Z = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

They have all the two eigenvalues $+1$ and -1 and their corresponding eigenvectors are:

$$\phi_{X+} = \frac{1}{sqrt2} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \phi_{X-} = \frac{1}{sqrt2} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\phi_{Y+} = \frac{1}{sqrt2} \begin{bmatrix} 1 \\ 1i \end{bmatrix}, \phi_{Y-} = \frac{1}{sqrt2} \begin{bmatrix} 1 \\ -i \end{bmatrix}$$

$$\phi_{Z+} = \frac{1}{sqrt2} \begin{bmatrix} 1 \\ 10 \end{bmatrix}, \phi_{Z-} = \frac{1}{sqrt2} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

II.3. The Born Rule

The Born rule says that the probability of measuring a state in the basis state i is:

$$P(\phi = i) = \langle i| \rho |i\rangle$$

,

where ρ is the density matrix of the state.

II.4. The von-Neumann entropy

The von-Neumann entropy is a way to quantify entanglement in a quantum state. For density matrix of the combined state A, B: $\rho_{A,B}$, we have the entropy:

$$S\left(A,B\right) = -Tr\left(\rho_{A,B}\log_2\left(\rho_{A,B}\right)\right)$$

II.5. The Bell State

The Bell state is the four maximally entangled 2-qubit states:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right)$$

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle - |11\rangle\right)$$

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right)$$

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right)$$

These states have the highest von-Neumann entropy, and an example of setting up and measuring one of these states can be found in this[2] jupyter notebook.

II.6. Hamiltonian as Pauli matrices

To rewrite a matrix as a linear combination of Pauli matrices in the 2×2 case would look like:

$$H = a_0 I + a_1 X + a_2 Y + a_3 Z$$

And in increasing the size of the matrix we can use the tensor product of the Pauli matrices instead.

$$H^{4\times4} = a_{00} II + a_{01} IX + ...a_{44} ZZ$$

The coefficients can be extracted by:

$$a_{AB} = \frac{1}{m} tr\left(\left(A \otimes B\right) H\right), \tag{5}$$

where m is the size of the matrix.

III. METHODS

III.1. Simulating a Quantum Circuit

To set up our quantum circuits we will use Qiskit [3] and for measurements we will use the average over 1 000 runs.

For the Pauli matrix form Hamiltonian we will make a quantum circuit where the first qubit represents the first Pauli operator of each string. For example, in:

$$H = aXII + bXZI + cZZZ,$$

The qubits would represent as:

$$q_1 = aX, bX, cZ$$

$$q_2 = aI, bZ, cZ$$

$$q_3 = aI, bI, cZ$$

Which will be done through basis transformation.

III.2. Measuring in the Pauli matrix basis

When measuring a state in Pauli matrix form we want to measure in the the strings different Pauli basis'. For example if we have the string:

$$X \otimes I \otimes Z,$$

we would want to measure the first qubit in the X's basis, the second in the standard basis and Z in it's basis. We then take the average value as:

$$\langle M \rangle = \frac{\lambda_1 n_{v_1} + \lambda_2 n_{v_2}}{n_{measured}},$$

where n_{v_1} and n_{v_2} are the number of times measured in the basis vector states for that Pauli operator and $n_{measured}$ is the number of times measured.

III.3. The Variational Quantum Eigensolver

For a Hamiltonian

$$H = a_{000} III + ... + a_{444} ZZZ,$$

we want to

1. setup three qubits and measure them in the different bases for each string.
2. setup the three qubits in a new state with scipy.optimize.minimize [4] method.
3. go back to 1 after a number of iterations.

The implementation of this can be found in the VQE jupyter notebook at github [5].

III.4. The $H \in \mathbb{R}^{2\times 2}$ hamiltonian

As our toy case we define the symmetric hamilitonian:

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}$$

Can be written as

$$H = H_0 + H,$$

where

$$H_0 = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix}$$

and

$$H_I = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix}$$

where the H_0 part is the non-interacting solution:

$$H_0 |0\rangle = E_1 |0\rangle$$

,

$$H_0 |1\rangle = E_2 |1\rangle$$

Rewriting H as a combination of Pauli matricies:

$$H_0 = \varepsilon I + \Sigma\sigma_x, \varepsilon = \frac{E_1 + E_2}{2}, \Sigma = \frac{E_1 - E_2}{2},$$

and

$$H_I = cI + \omega_z\sigma_z + \omega_x\sigma_x,$$

where

$$c = \frac{V_{11} + V_{22}}{2}, \omega_z = \frac{V_{11} - V_{22}}{2}, \omega_x = V_{12} = V_{21}.$$

And we let the hamiltonian depend on the strength parameter λ:

$$H = H_0 + \lambda H_I.$$

We set the parameters

$$E_1 = 0, E_2 = 4, V_{11} = -V_{22} = 3, V_{12} = V_{21}$$

We will then solve this eigenvalue problem with standard eigenvalue solvers as well as our implementation of VQE.

III.5. Two-Qubit System

This system is composed of two subsystem A, B, both with the standard computational basis. In this case our non-interacting part of the Hamiltonian define the eigenstates 1:

$$H_0 |00\rangle = \epsilon_{00} |00\rangle$$

$$H_0 |01\rangle = \epsilon_{01} |01\rangle$$

$$H_0 |10\rangle = \epsilon_{10} |10\rangle$$

$$H_0 |11\rangle = \epsilon_{11} |11\rangle$$

The interacting part is given by:

$$H_I = H_x\sigma_x \otimes \sigma_x + H_z\sigma_z \otimes \sigma_z,$$

where H_x and H_z are interaction strength parameters. We then have our final Hamiltonian:

$$H = \begin{bmatrix} \epsilon_{00} + H_z & 0 & 0 & H_x \\ 0 & \epsilon_{10} - H_z & H_x & 0 \\ 0 & H_x & \epsilon_{01} - H_z & 0 \\ H_x & 0 & 0 & \epsilon_{11} + H_z \end{bmatrix}$$

With the parameters

Hx = 2.0
Hz = 3.0
H0_energies = [0.0, 2.5, 6.5, 7.0]

We will find the eigenvalues of this Hamiltonian with both standard eigensolvers and our implementation of VQE.

III.6. The Lipkin Model

In second quantization the Hamiltonian is given by:

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{H}_1 + \hat{H}_2 \\ \hat{H}_0 &= \tfrac{1}{2}\varepsilon \textstyle\sum_{\sigma,p} \sigma a^\dagger_{\sigma,p} a_{\sigma,p} \\ \hat{H}_1 &= \tfrac{1}{2}V \textstyle\sum_{\sigma,p,p'} a^\dagger_{\sigma,p} a^\dagger_{\sigma,p'} a_{-\sigma,p'} a_{-\sigma,p} \\ \hat{H}_2 &= \tfrac{1}{2}W \textstyle\sum_{\sigma,p,p'} a^\dagger_{\sigma,p} a^\dagger_{-\sigma,p'} a_{\sigma,p'} a_{-\sigma,p} \end{aligned}$$

We define the quasi spin operator:

$$\hat{J}_+ = \sum_p a^\dagger_{p+} a_{p-}$$

$$\hat{J}_- = \sum_p a^\dagger_{p-} a_{p+}$$

$$\hat{J}_z = \frac{1}{2} \sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma}$$

$$\hat{J}^2 = J_+ J_- + J_z^2 - J_z$$

$$\hat{N} = \sum_{p\sigma} a^\dagger_{p\sigma} a_{p\sigma}.$$

And rewrite our Hamiltonian:

$$H_0 = \varepsilon J_z$$

$$H_1 = \frac{1}{2} V \left(J_+^2 + J_-^2 \right)$$

$$H_2 = \frac{1}{2} W \left(-N + J_+ J_- + J_- J_+ \right).$$

And end up with for $J = 1$ and set $W = 0$

$$H_{J=1} = \begin{bmatrix} -\varepsilon & 0 & -V \\ 0 & 0 & 0 \\ -V & 0 & \varepsilon \end{bmatrix}$$

And for the $J = 2$ case, with $W \neq 0$:

$$H_{J=2} = \begin{bmatrix} -2\epsilon & 0 & \sqrt{6}V & 0 & 0 \\ 0 & -\epsilon + 3W & 0 & 3V & 0 \\ \sqrt{6}V & 0 & 4W & 0 & \sqrt{6}V \\ 0 & 3V & 0 & \epsilon + 3W & 0 \\ 0 & 0 & \sqrt{6}V & 0 & 2\epsilon \end{bmatrix}$$

We can then rewrite these as a linear combination of Pauli matrices (padding it with zeros to make it a $2^n \times 2^n$ matrix):

$$H_{J=1} = \frac{\varepsilon}{2} (ZI + ZZ) - \frac{V}{2} (XI + IX)$$

And

$$\begin{aligned} H_{J=2} =& (-0.25\varepsilon + -0.5W) IZI + \\ & (0.25\varepsilon + -0.5W) IZZ + (-0.5\varepsilon + 1.25W) ZII + \\ & (-0.5\varepsilon - 0.25W) ZIZ + (-0.75\varepsilon - 0.5W) ZZI + \\ & (-0.25\varepsilon - 0.5W) ZZZ + (0.25\sqrt{6}V + 0.75V) IXI + \\ & (0.25\sqrt{6}V - 0.75V) IXZ + (0.25\sqrt{6}V) XXI + \\ & (0.25\sqrt{6}V) XXZ + (0.25\sqrt{6}V) YYI + \\ & (0.25\sqrt{6}V) YYZ + (0.25\sqrt{6}V + 0.75V) ZXI + \\ & (0.25\sqrt{6}V - 0.75V) ZXZ + 1.25W \cdot III + -0.25W \cdot IIZ \end{aligned} \tag{6}$$

A explenation of how we found the Pauli matrix form of $H_{J=2}$ can be found in appendix A.

IV. RESULTS AND DISCUSSION

IV.1. One qubit basis

For the one qubit basis we get the following result from the variational quantum eigensolver:

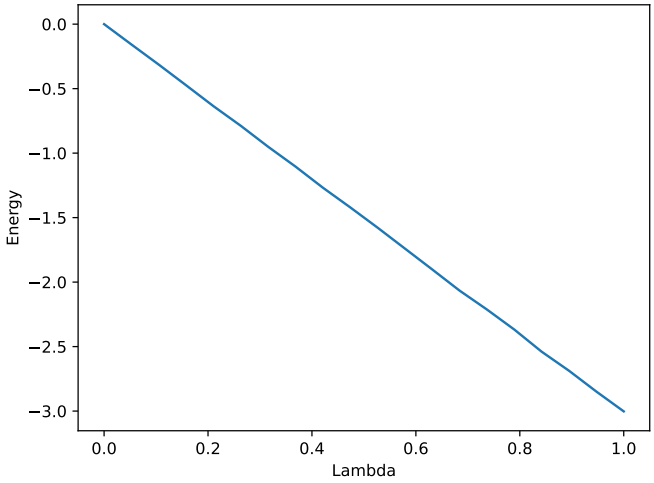

Figure 1: The estimated solution with VQE. Here we had $E_1 = 0$, $E_2 = 4$, $V_{11} = 3$, $V_{12} = 0.2$, $V_{21} = 0.2$, $V_{22} = -3$

We see that the ground state energy is zero when the there is no interaction strength, which would be a eigenstate of the non-interacting solution. As the interaction strength increases the ground state energy goes towards the lowest eigenstate of the interacting part, in this case -3.

IV.2. 2 qubit case

For the two qubit case we have the following true evolutions with respect to the interaction strengths H_x and H_z:

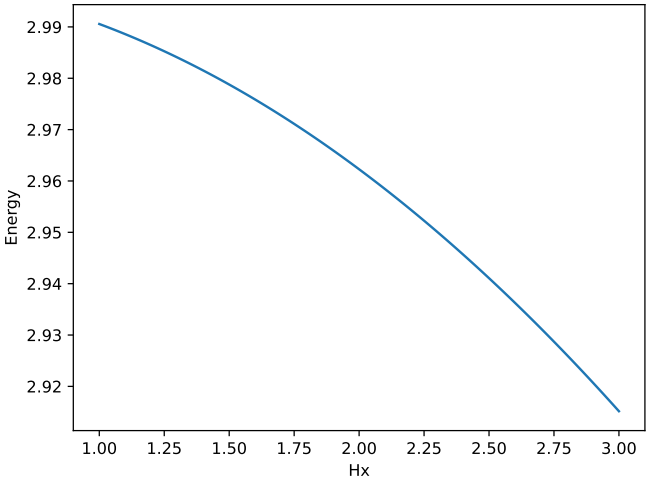

Figure 2: The evolution of the two qubit case with respect to the strength interaction parameter H_x.

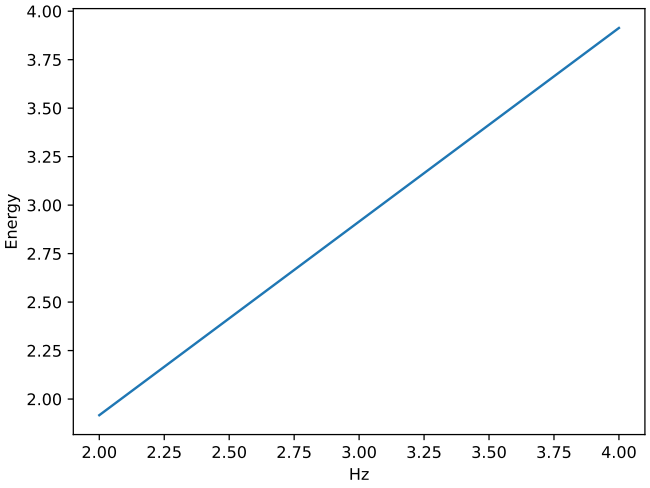

Figure 3: The evolution of the two qubit case with respect to the strength interaction parameter H_z.

We see that H_x has only a slight effect on the ground state energy, while it stays around H_z more or less. This is made clearer in the second plot 3 where we see the linear dependence on H_z. And the VQE estimations:

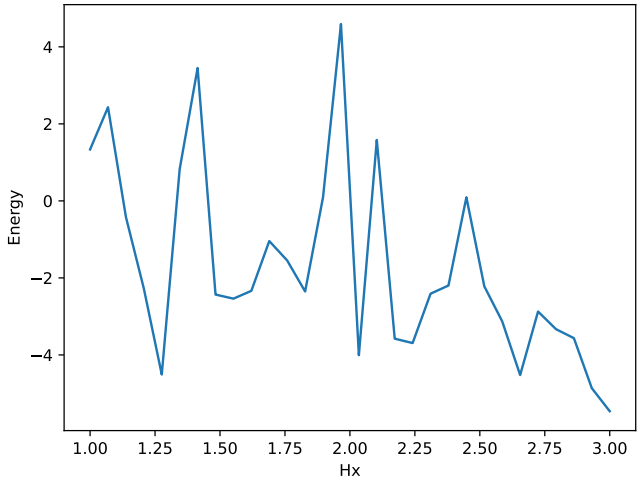

Figure 4: The estimated evolution of the two qubit case with respect to the strength interaction parameter H_x.

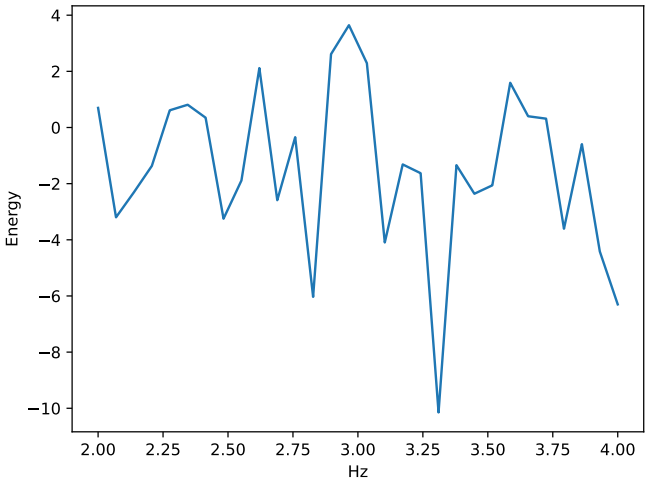

Figure 5: The estimated evolution of the two qubit case with respect to the strength interaction parameter H_z.

Here it is clear the variational quantum eigensolver doesn't have nearly enough accuracy to resemble the true evolutions at all.

IV.3. Lipkin Modell $J = 1$

For the Lipkin modell we have two scenarios, one where $J = 1$. Here we have the variables ε and V to look at, with the hamiltonian:

$$H_{J=1} = \begin{bmatrix} -\varepsilon & 0 & -V \\ 0 & 0 & 0 \\ -V & 0 & \varepsilon \end{bmatrix}$$

The true evolution of the ground state with respect to the two variables are shown in the following plots:

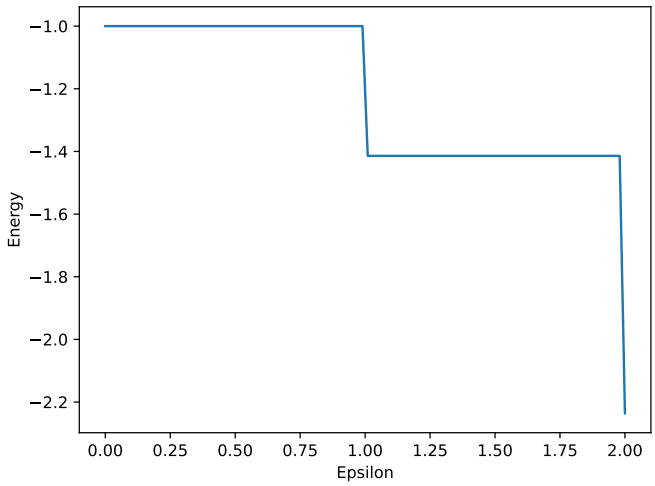

Figure 6: The true evolution of ε og the $J = 1$ lipkin modell ground state energy. $V = 1$ in this case

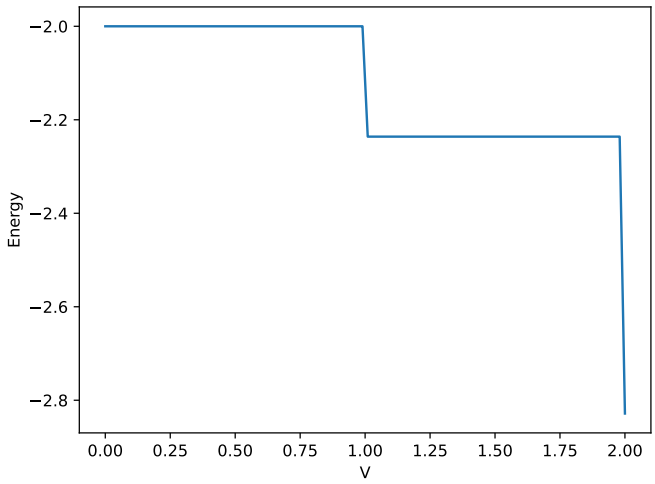

Figure 7: The true evolution of $J = 1$ og the $J = 1$ lipkin modell ground state energy. $\varepsilon = 1$ in this case.

We see here clear distinction in the ground state energy when either variable passes 1. This makes sense since the other variable is in each case constantly 1 such that when one of them goes higher than 1 they begin to dominate the lowest ground state energy, the non-interacting part ε against the interacting part V.

Following we have the VQE estimations:

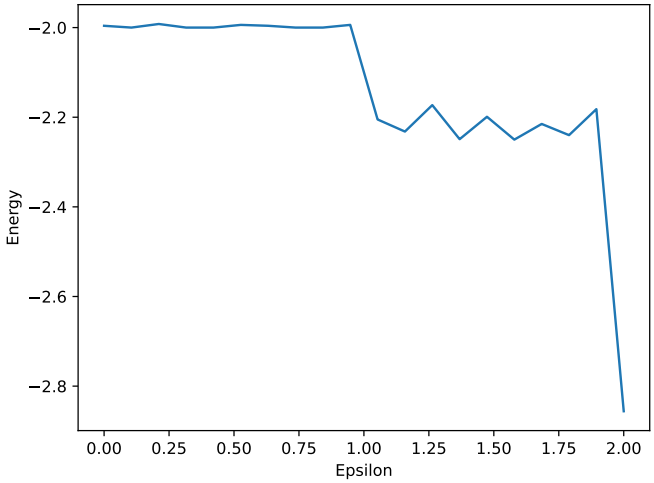

Figure 8: The VQE evolution of ε og the $J = 1$ lipkin modell ground state energy. $V = 1$ in this case

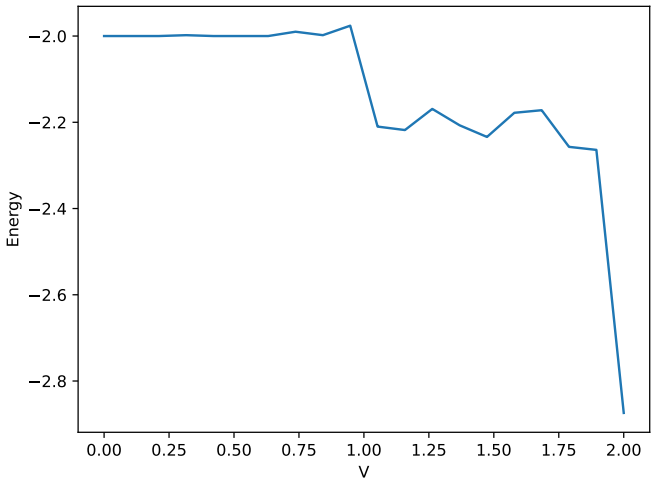

Figure 9: The VQE evolution of $J = 1$ og the $J = 1$ lipkin modell ground state energy. $\varepsilon = 1$ in this case.

The VQE clearly struggles a bit with accuracy, although it is clear that it follows the same general curve as the true solution in this case.

IV.4. Lipkin modell $J = 2$

For the $J = 2$ case we have the following true evolutions:

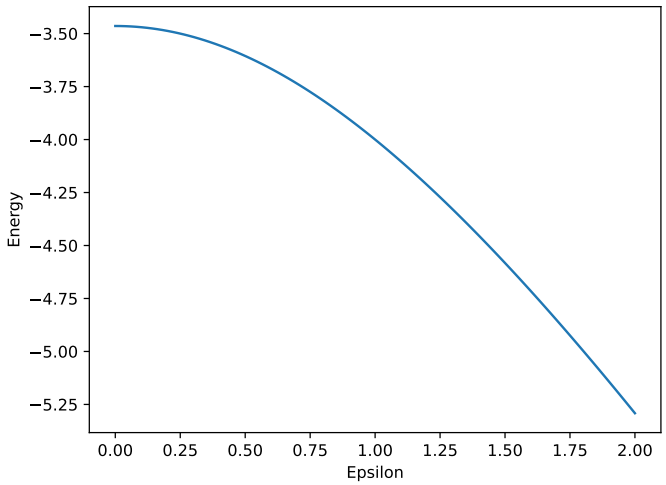

Figure 10: The true evolution of the ground state energy for the $J = 2$ Lipkin model wwith respect to ε.

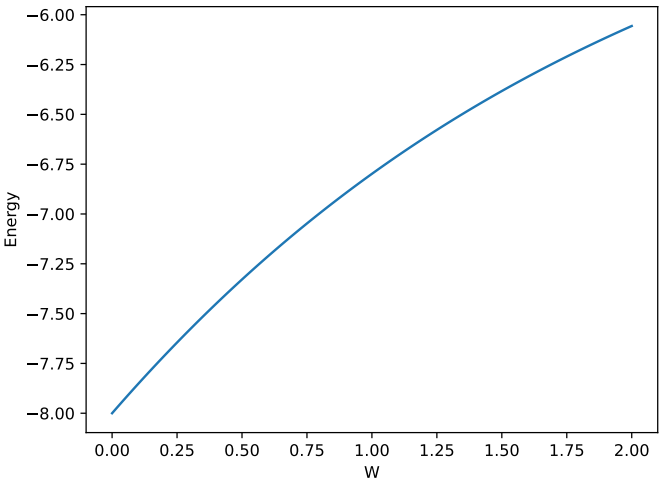

Figure 12: The true evolution of the ground state energy for the $J = 2$ Lipkin model wwith respect to W.

And the VQE managed to find these estimations:

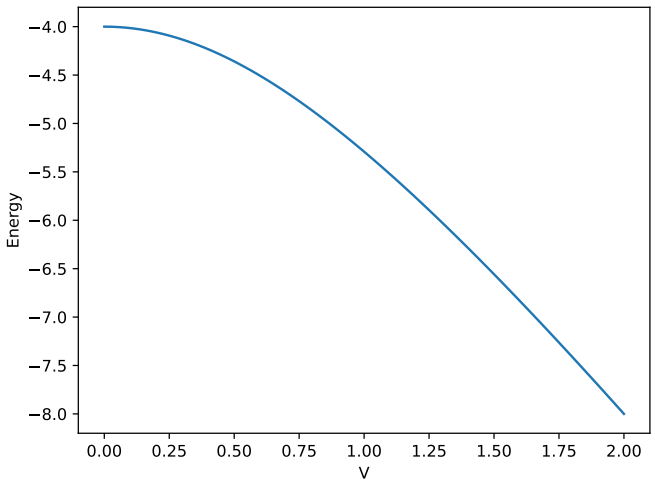

Figure 11: The true evolution of the ground state energy for the $J = 2$ Lipkin model wwith respect to V.

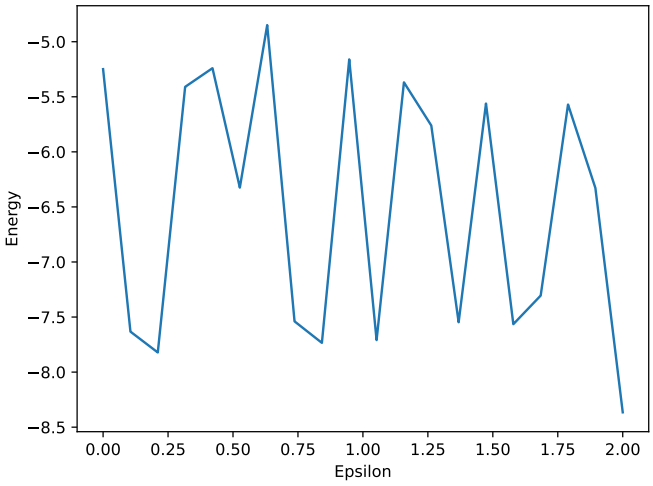

Figure 13: The VQE estimation of the evolution of the ground state energy of the $J = 2$ Lipkin model with respect to ε

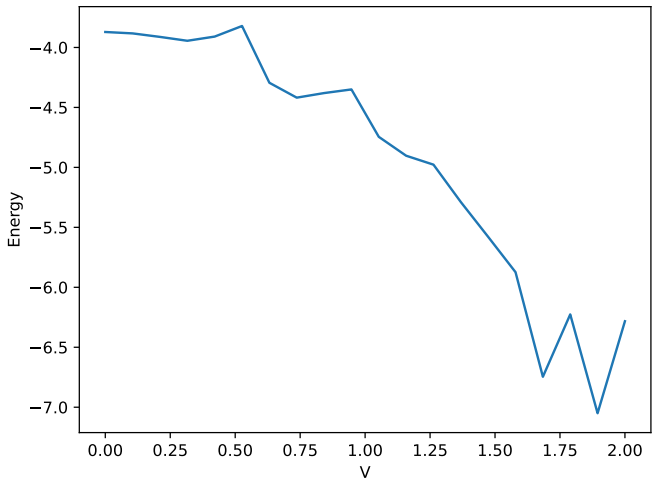

Figure 14: The VQE estimation of the evolution of the ground state energy of the $J = 2$ Lipkin model with respect to V

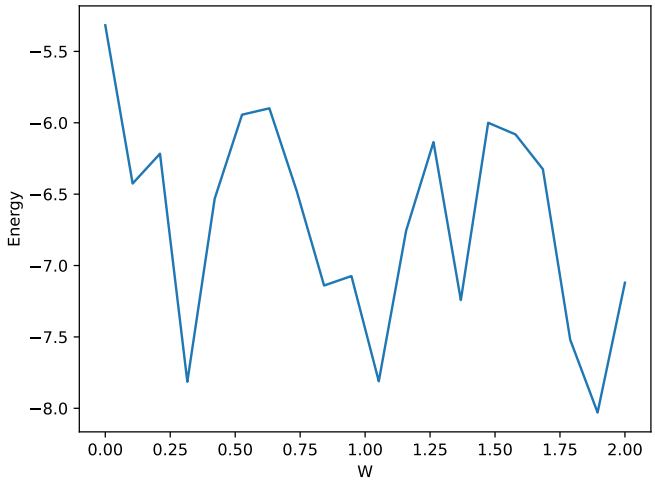

Figure 15: The VQE estimation of the evolution of the ground state energy of the $J = 2$ Lipkin model with respect to W

It is quite clearly that the VQE fails for both ε and W, although the estimation of V seems to work somewhat well. It is noteworthy that the VQE estimation for both ε and W is somewhat close to the starting and endpoint ground energy, but it seems like the uncertainty is in the same range as the difference between the two, so its quite hard to see any difference at all. The fact that the uncertainty changes for the different variables is surprising because the method of finding the ground state energy does not change. We think that it could be that the ground state energy becomes more sensitive to changes the qubit state (or in this case the angles Θ and Φ) with different ε or w, although that is hard to ascertain with current results.

V. CONCLUSION

In this article we looked at three hamiltonians and tried to estimate how their ground state energy evolves with respect to different interaction strenghts and non-interacting energies with a variational quantum eigensolver. First of we find that for the small cases of 3×3 hamiltonians we find that the VQE manages quite well to replicate the true solutions, but we see drastic uncertainties when looking at cases for 4×4 and 5×5 hamiltonians.

A. Finding the Pauli matrix form of $H_{J=2}$

To find the Pauli matrix form of the $H_{J=2}$ 6 equation, we used the formula for extracting the coefficient 5 by going through the exhaustive list of Pauli matrix tensor multiplication combinations. To do this we needed to slightly adjust the way we approached the Hamiltonian. First of we split it into the different variables:

$$H = H_a + H_b + H_c + H_d + H_f,$$

where

$$H_a = \varepsilon \begin{bmatrix} -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

$$H_b = \sqrt{6}V \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

$$H_c = 3W \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$H_d = 3V \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$H_f = 4W \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

By doing this we can find the Pauli matrix form for these matrices and combine them afterwards with their corresponding scalar. The code used to find these can be found on the github page [5]

[1] R. P. Feynman, "Simulating physics with computers," *International Journal of Theoretical Physics*, vol. 21, no. 6, pp. 467–488, Jun 1982. [Online]. Available: https://doi.org/10.1007/BF02650179

[2] H. [Breitenstein, "One qubit basis," 2023.

[3] "Qiskti," qiskit.org, accessed: 2023-04-05.

[4] "scipy.optimize.minimize," https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.minimize.html, [Accessed 16-May-2023].

[5] "Github," https://github.com/henrikbreitenstein/VQE.