# Task4_QoSF_Mentorship_Program

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September 2020

## 1 Problem Statement

Find the minimum eigenvalue of the following operator, using VQE-like circuits:

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

## 2 Formulation into VQE-like circuit

### 2.1 Step 1: Decomposition into Pauli Matrices

As is known, the Pauli operators form a complete orthogonal basis for the single qubit-operators, and their tensor products for larger Hilbert Spaces. Hence, as mentioned here we first need to decompose `U` into tensor products of the Pauli operators. This could be done manually, but we could instead simply take the trace of the product of the tensor products of the Pauli operators with `U`. Only the terms with a non-vanishing trace will be present in the decomposition. The remaining traces, when scaled by an appropriate value (that is dependent on the dimension of the Hilbert space), gives us the coefficients in the decomposition of the given operator. For a 2 qubit Hilbert space, this factor is $\frac{1}{4}$.
Here, only those traces that are non-vanishing are shown(`Z, X` and `Y` are the Pauli operators; `I` is the Identity matrix of dimension 4; `U` is the given operator):

$$\begin{aligned} ZZ &= Z \otimes Z \\ XX &= X \otimes X \\ YY &= Y \otimes Y \end{aligned}$$

$$\mathrm{Tr}[U(ZZ)] = 2$$

$$\mathrm{Tr}[U(XX)] = -2$$

$$\mathrm{Tr}[U(YY)] = -2$$

$$\mathrm{Tr}[U(I)] = 2$$

Using these, we can get the decomposition of the operator `U` as:

$$U = \frac{1}{2}(ZZ + I) - \frac{1}{2}(XX + YY) \tag{1}$$

## 2.2 Step 2:Determining the Ansatz

Arguably the most challenging part of creating a variational quantum eigensolver circuit, is to determine the ansatz required. This is done using knowledge of what the ground state of the given operator/Hamiltonian would look like, using symmetries or maybe even making assumptions of the same. Following a similar process, an attempt was made to understand the structure of the eigenstates of `U`.

Since it is only a 2 qubit matrix, it is very easy to understand what action it has on different states. The results of such a process are given below:

| `U` Takes... | To... |
|---|---|
| $\|00\rangle$ | $\|00\rangle$ |
| $\|01\rangle$ | $-\|10\rangle$ |
| $\|10\rangle$ | $-\|01\rangle$ |
| $\|11\rangle$ | $\|11\rangle$ |

Table 1: Operation of the given operator

From such a table it was easy to see that the Bell states were the eigenstates of this operator! So our ansatz should be such that it can actually achieve any bell state. But since a little more inspection actually gives the required eigenstate ($\frac{|01\rangle+|10\rangle}{\sqrt{2}}$) with an eigenvalue of -1, a variational circuit that can reach this state suffices. Such a ansatz was created and required only one variational parameter. Note that the ansatz given in the hint also does the same, but the first code made used a different ansatz, determined by using these properties. Both these ansatzes are drawn below.

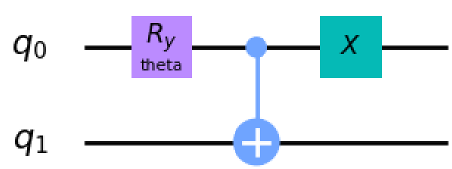


Figure 1: First ansatz with variational parameter in a Ry gate

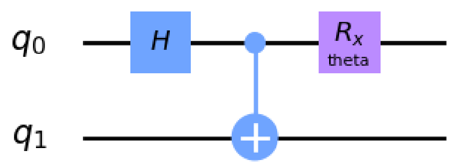


Figure 2: Second ansatz with variational parameter in a Rx gate

The first ansatz was derived by thinking of rotation on the Bloch sphere. The general circuit for generating the required bell state actually uses a Hadamard gate on the first qubit, followed by a CNOT with the first qubit as the control and the second as the target, and then a X gate on the first qubit. The Hadamard gate can be thought of as a rotation about the Y axis on the bloch sphere. Hence, to introduce a variational parameter, the first gate was made a Ry gate with $\theta$ as the variational parameter. Of course, the optimum value of $\theta$ would be where the Ry gate becomes a Hadamard, which is at $\frac{\pi}{2}$. This is the expected result, with an optimum value of -1 for the lowest eigenvalue.
After results were obtained from these single parameter VQE-like circuits, a VQE-like circuit with 2 parameters was also considered. This was obtained by observing that the second gate is as good as a rotation about the x-axis on the bloch sphere. Hence, the following circuit was also tried as an ansatz.

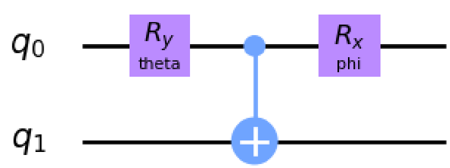


Figure 3: Third ansatz with 2 variational parameters

## 2.3 Step 3: Measurement in Z basis

Since most quantum devices allow us to measure only in the Z-basis directly, for measuring the expectation values of the Pauli operators other than the Z Pauli operator in the tensor decomposition, we need to somehow rotate the eigenvalues of these operators into that of the `ZZ` operator.
For this, first the eigenvalues and corresponding eigenvectors of the Pauli op-

erators present in the decomposition of `U` were found. After this operators, or rather in this case, gates were determined that could rotate these eigenvectors into the eigenvectors of the `ZZ` operator. The eigenvectors and the corresponding eigenevalues of the necessary operators are given in the following table.

| Operator | Eigenvector | Eigenvalue |
|---|---|---|
| ZZ | $\|00\rangle$ | +1 |
| | $\|01\rangle$ | -1 |
| | $\|10\rangle$ | -1 |
| | $\|11\rangle$ | +1 |
| XX | $\frac{\|00\rangle+\|11\rangle}{\sqrt{2}}$ | +1 |
| | $\frac{\|00\rangle-\|11\rangle}{\sqrt{2}}$ | -1 |
| | $\frac{\|01\rangle+\|10\rangle}{\sqrt{2}}$ | +1 |
| | $\frac{\|01\rangle-\|10\rangle}{\sqrt{2}}$ | -1 |
| YY | $\frac{\|00\rangle+\|11\rangle}{\sqrt{2}}$ | -1 |
| | $\frac{\|00\rangle-\|11\rangle}{\sqrt{2}}$ | +1 |
| | $\frac{\|01\rangle+\|10\rangle}{\sqrt{2}}$ | +1 |
| | $\frac{\|01\rangle-\|10\rangle}{\sqrt{2}}$ | -1 |

Table 2: Eigenvectors and Eigenvalues of the 2 qubit Pauli operators

A very interesting point to note here is that the eigenvectors of the `XX` and `YY` operators are the same! This means that these two operators commute, which in turn means we can find the expectation value of these operators simultaneously. This enables us to use just one circuit for measuring the expectation value of both of these circuits. Similar observations in larger dimensions can largely reduce execution time.

As can be seen, the eigenvectors of the `XX` and `YY` operators are just the Bell states again. So we want a circuit that takes the bell states to the eigenbasis of the `ZZ` operator. This is shown below, and was determined by taking the inverse circuit of the usual circuit for achieving the bell state of ($\frac{|00\rangle+|11\rangle}{\sqrt{2}}$) from $|00\rangle$.

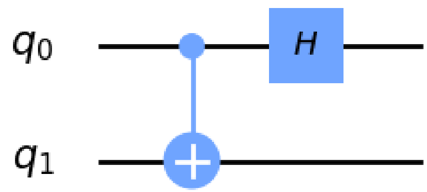


Figure 4: Gates to rotate XX and YY eigenvalues to ZZ eigenvalues

This circuit operates as given in the table below:

| Takes... | To... |
|---|---|
| $\frac{\|00\rangle+\|11\rangle}{\sqrt{2}}$ | $\|00\rangle$ |
| $\frac{\|00\rangle-\|11\rangle}{\sqrt{2}}$ | $\|10\rangle$ |
| $\frac{\|01\rangle+\|10\rangle}{\sqrt{2}}$ | $\|01\rangle$ |
| $\frac{\|01\rangle-\|10\rangle}{\sqrt{2}}$ | $\|11\rangle$ |

Table 3: Operation of the ”inverse bell” circuit

Using a combination of 3 and 4, we can determine the which measurements in the `ZZ` basis correspond to which eigenvalues. This is what the dictionary `qubit_2_eigenvalues` declared at the beginning of the code stores. A tabular form of the same is given below.

| Operator | Measurement in ZZ basis | Eigenvalue |
|---|---|---|
| ZZ | $\|00\rangle$ | +1 |
| | $\|01\rangle$ | -1 |
| | $\|10\rangle$ | -1 |
| | $\|11\rangle$ | +1 |
| XX | $\|00\rangle$ | +1 |
| | $\|01\rangle$ | -1 |
| | $\|10\rangle$ | +1 |
| | $\|11\rangle$ | -1 |
| YY | $\|00\rangle$ | -1 |
| | $\|01\rangle$ | +1 |
| | $\|10\rangle$ | +1 |
| | $\|11\rangle$ | -1 |

Table 4: "Eigenvectors" and Eigenvalues of the 2 qubit Pauli operators after measuring in ZZ basis

### 2.4 Step 4:Varying the Variational Parameter(s)

Although the question did not require us to use any optimisation algorithm, results using the `scipy.minimize` function, with the method specified as the argument to the function being `"Powell"`, are also demonstrated.

### 2.5 Final circuit

With these steps done, the final circuits required were determined. These are shown below with appropriate labels. Note that the circuits below are only for the 1st ansatz, with a variational `Ry` gate. The rest have similar looking circuits with the corresponding ansatz substituted.

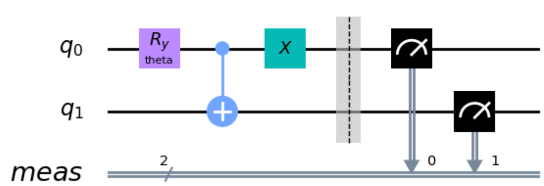


Figure 5: Circuit to measure the expectation of the ZZ component of the given operator

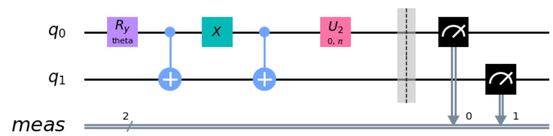


Figure 6: Circuit to measure the expectation of the XX, and YY, component of the given operator

# 3 Results

As expected, the minimum eigenvalue determined was -1. Results include both, using the `scipy.minimize` as well as just a simple search through the entire range of $\theta$. The latter gives a nice plot of the expectation versus the variational parameter and is shown below.

## 3.1 Using the "Ry" Ansatz

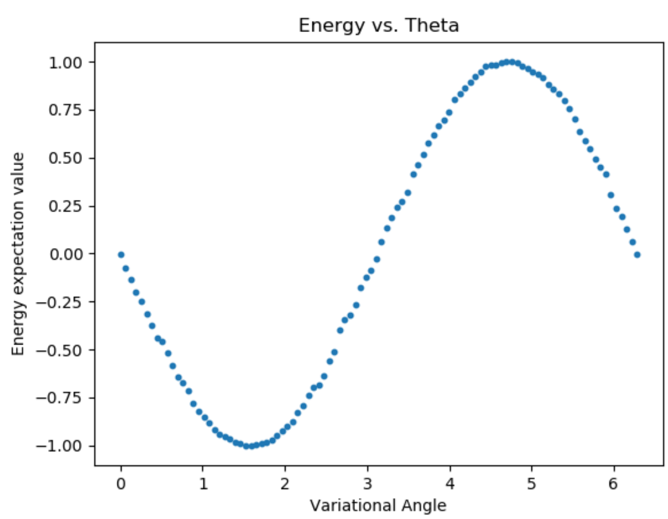


Figure 7: Energy vs $\theta$ with the Ry ansatz

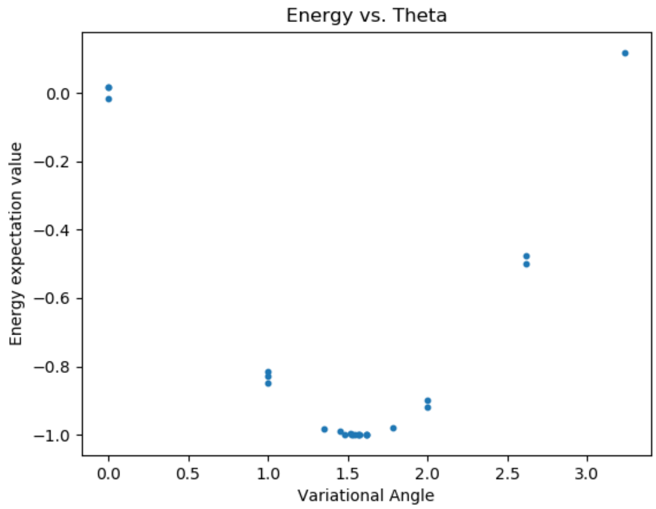


Figure 8: Energy vs $\theta$ with the Ry ansatz, using a minimiser

As can be seen, the minimum value of -1 is obtained at $\frac{\pi}{2}$. This is expected as the Hadamard gate is $\frac{\pi}{2}$ rotation around the Y axis. If we substitute the Hadamard gate instead of the Ry gate in the circuit, we will get the required bell state $\frac{|01\rangle+|10\rangle}{\sqrt{2}}$.

### 3.2 Using the Ansatz in the hint

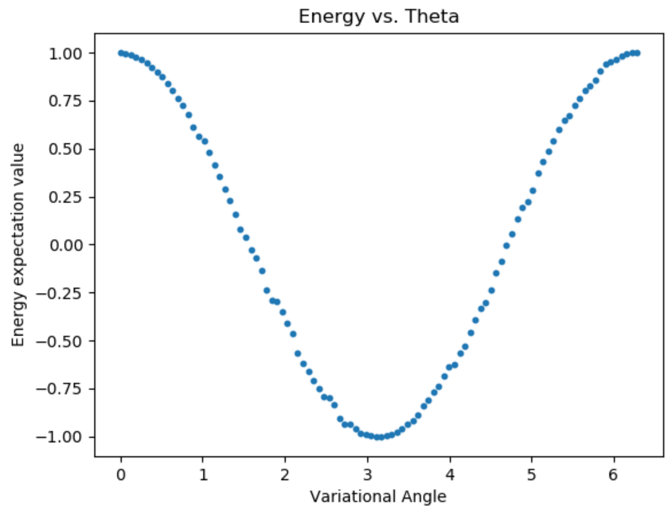


Figure 9: Energy vs $\theta$ with the Rx ansatz

As can be seen, the minimum value of -1 is obtained at $\pi$. Again, this is expected, as the X gate is $\pi$ rotation around the X axis. If we substitute the X gate instead of the Rx gate in the circuit, we will get the required bell state of $\frac{|01\rangle+|10\rangle}{\sqrt{2}}$.

### 3.3 Using two variational parameters

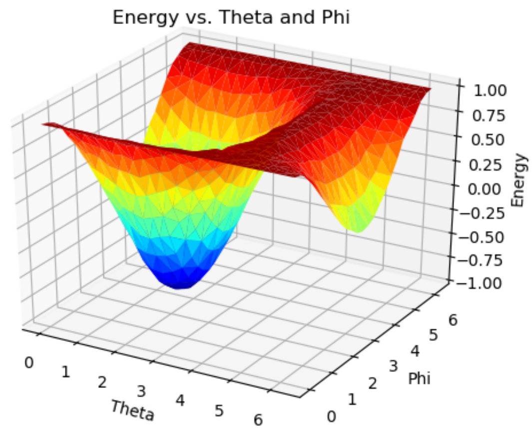


Figure 10: Energy vs $\theta$ and $\phi$

Exactly as expected, we get the minimum of -1 at the same values of $\theta$ and $\phi$ as from the individual circuits. Subsituting these values would again give us the Hadamard instead of the Ry gate and the X gate instead of the Rx gate.

# 4 Conclusion

Since the given operator was only a 2-qubit operator, it was easy to guess the ground state. But making such "ansatzes" for larger operators and Hamiltonians requires a deeper understanding of the nature of the operator and smart assumptions about the ground state. Key insights into the symmetries of the ground state are often helpful.
The VQE algorithm is a powerful one, which is extremely useful in the NISQ era. This problem, among the other 3 as well, introduced me to this topic, while also helping me gain some amount of coding experience for the same.