Ansatz

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Example:

We start with defining the Hamiltonian of of the molecular Hydgrogen.

$$H = g_0\mathbb{I} + g_1 Z_0 + g_2 Z_1 + g_3 Z_0 Z_1 + g_4 Y_0 Y_1 + g_5 X_0 X_1$$

Where: $\{X_i, Z_i, Y_i\}$ denote the Pauli matrices acting on the i-th qubit and the real scalars $\{g_\gamma\}$ are efficiently computable functions of the hydrogen-hydrogen bond length R.

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathbb{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$g_0\mathbb{I} = \begin{bmatrix} g_0 & 0 & 0 & 0 \\ 0 & g_0 & 0 & 0 \\ 0 & 0 & g_0 & 0 \\ 0 & 0 & 0 & g_0 \end{bmatrix}, \quad g_1 Z_0 = \begin{bmatrix} g_1 & 0 & 0 & 0 \\ 0 & g_1 & 0 & 0 \\ 0 & 0 & -g_1 & 0 \\ 0 & 0 & 0 & -g_1 \end{bmatrix}, \quad g_2 Z_1 = \begin{bmatrix} g_2 & 0 & 0 & 0 \\ 0 & -g_2 & 0 & 0 \\ 0 & 0 & g_2 & 0 \\ 0 & 0 & 0 & -g_2 \end{bmatrix},$$

$$g_3 Z_0 Z_1 = \begin{bmatrix} g_3 & 0 & 0 & 0 \\ 0 & -g_3 & 0 & 0 \\ 0 & 0 & -g_3 & 0 \\ 0 & 0 & 0 & g_3 \end{bmatrix}, \quad g_4 Y_0 Y_1 = \begin{bmatrix} 0 & 0 & 0 & -g4 \\ 0 & 0 & g4 & 0 \\ 0 & g4 & 0 & 0 \\ -g4 & 0 & 0 & 0 \end{bmatrix}, \quad g_5 X_0 X_1 = \begin{bmatrix} 0 & 0 & 0 & g5 \\ 0 & 0 & g5 & 0 \\ 0 & g5 & 0 & 0 \\ g5 & 0 & 0 & 0 \end{bmatrix}$$

$$H = \begin{bmatrix} g_0 + g_1 + g_2 + g_3 & 0 & 0 & g_5 - g_4 \\ 0 & g_0 + g_1 - g_2 - g_3 & g_5 + g_4 & 0 \\ 0 & g_5 + g_4 & g_0 - g_1 + g_2 - g_3 & 0 \\ g_5 - g_4 & 0 & 0 & g_0 - g_1 - g_2 + g_3 \end{bmatrix}$$

Decomposing the UCCSD ansatz

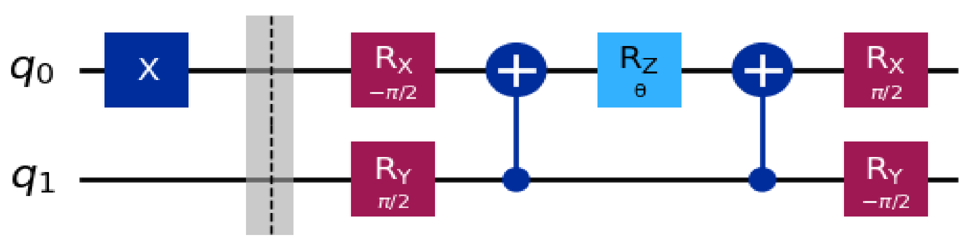
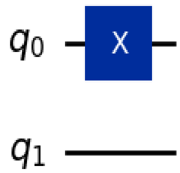


Figure 1: The UCCSD ansatz for the Hydrogen molecule.

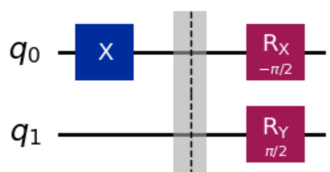
- Reference state $|10\rangle$



$$(X \otimes I) \cdot (|0\rangle \otimes |0\rangle) = |10\rangle$$

$$\left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right) \cdot \left(\begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

- Apply parameterized ansatz



$$\left(R_x(\frac{-\pi}{2}) \otimes R_y(\frac{\pi}{2})\right) \cdot |10\rangle$$

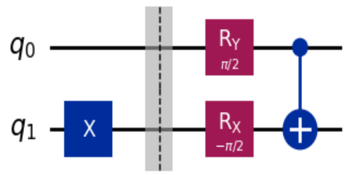
$$R_x(\frac{-\pi}{2}) = e^{-iX(\frac{-\pi}{4})} = \begin{bmatrix} \cos(\frac{-\pi}{4}) & -i\sin(\frac{-\pi}{4}) \\ -i\sin(\frac{-\pi}{4}) & \cos(-\frac{\pi}{4}) \end{bmatrix} = \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{i\sqrt{2}}{2} \\ \frac{i\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}$$

$$R_y(\frac{\pi}{2}) = e^{-iY(\frac{\pi}{4})} = \begin{bmatrix} \cos(\frac{\pi}{4}) & -\sin(\frac{\pi}{4}) \\ \sin(\frac{\pi}{4}) & \cos(\frac{\pi}{4}) \end{bmatrix} = \begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\left(R_x(\frac{-\pi}{2}) \otimes R_y(\frac{\pi}{2})\right) = \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{i\sqrt{2}}{2} \\ \frac{i\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix} \otimes \begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{-1}{2} & \frac{i}{2} & \frac{-i}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{i}{2} & \frac{i}{2} \\ \frac{i}{2} & \frac{-i}{2} & \frac{1}{2} & \frac{-1}{2} \\ \frac{i}{2} & \frac{i}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

$$\left(R_x(\frac{-\pi}{2}) \otimes R_y(\frac{\pi}{2})\right) \cdot |10\rangle = \begin{bmatrix} \frac{1}{2} & \frac{-1}{2} & \frac{i}{2} & \frac{-i}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{i}{2} & \frac{i}{2} \\ \frac{i}{2} & \frac{-i}{2} & \frac{1}{2} & \frac{-1}{2} \\ \frac{i}{2} & \frac{i}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{i}{2} \\ \frac{i}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$$

The first CNOT (entanglement)



$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} \frac{i}{2} \\ \frac{i}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} \frac{i}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{i}{2} \end{bmatrix}$$

The Z_θ rotation gate:

$$Z_\theta = e^{-iZ(\frac{\theta}{2})} = \begin{bmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{bmatrix}$$

$$(Z_\theta \otimes I) \cdot \begin{bmatrix} \frac{i}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{i}{2} \end{bmatrix} = \begin{bmatrix} e^{-i\frac{\theta}{2}} & 0 & 0 & 0 \\ 0 & e^{-i\frac{\theta}{2}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\theta}{2}} & 0 \\ 0 & 0 & 0 & e^{i\frac{\theta}{2}} \end{bmatrix} \cdot \begin{bmatrix} \frac{i}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{i}{2} \end{bmatrix} = \begin{bmatrix} \frac{\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} - i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} + i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \\ \frac{-\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \end{bmatrix}$$

The second CNOT (entanglement)

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} \frac{\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} - i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} + i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \\ \frac{-\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \end{bmatrix} = \begin{bmatrix} \frac{\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{-\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} + i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} - i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \end{bmatrix}$$

The final rotation gates:

$$\left(R_x(\frac{\pi}{2}) \otimes R_y(\frac{-\pi}{2})\right) \cdot \begin{bmatrix} \frac{\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{-\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} + i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} - i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \end{bmatrix}$$

$$= \left(\begin{bmatrix} \cos\left(\frac{\pi}{4}\right) & -i\sin\left(\frac{\pi}{4}\right) \\ -i\sin\left(\frac{\pi}{4}\right) & \cos\left(\frac{\pi}{4}\right) \end{bmatrix} \otimes \begin{bmatrix} \cos\left(\frac{-\pi}{4}\right) & -\sin\left(\frac{-\pi}{4}\right) \\ \sin\left(\frac{-\pi}{4}\right) & \cos\left(\frac{-\pi}{4}\right) \end{bmatrix} \right) \cdot \begin{bmatrix} \frac{\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{-\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} + i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} - i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \end{bmatrix}$$

$$= \left(\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \otimes \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \right) \cdot \begin{bmatrix} \frac{\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{-\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} + i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} - i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{-i}{2} & \frac{-i}{2} \\ \frac{-1}{2} & \frac{1}{2} & \frac{i}{2} & \frac{-i}{2} \\ \frac{-i}{2} & \frac{-i}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{i}{2} & \frac{-i}{2} & \frac{-1}{2} & \frac{1}{2} \end{bmatrix} \cdot \begin{bmatrix} \frac{\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{-\sin\left(\frac{\theta}{2}\right)}{2} + i\frac{\cos\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} + i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \\ \frac{\cos\left(\frac{\theta}{2}\right)}{2} - i\frac{\sin\left(\frac{\theta}{2}\right)}{2} \end{bmatrix} = \begin{bmatrix} 0 \\ -\sin(\frac{\theta}{2}) \\ \cos(\frac{\theta}{2}) \\ 0 \end{bmatrix} = |\phi(\vec{\theta})\rangle = -\sin\left(\frac{\theta}{2}\right)|01\rangle + \cos\left(\frac{\theta}{2}\right)|10\rangle \quad (1)$$

***Note: the first qubit is the left most bit.**

- The expectation value (Quantum Tomography): Using many measurements on identically prepared systems to get mean values of the some complete set of observables to reconstruct an estimate of the state. Quantum Tomography works to determine the state prior to the measurements.

In this case, our state we want to reconstruct is $|\phi(\vec{\theta})\rangle$.
Starting with the denstiy matrix:

$$\rho = |\phi(\vec{\theta})\rangle\langle\phi(\vec{\theta})|$$

The general two qubits wavefunction can be written as:

$$|\phi\rangle = a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle$$

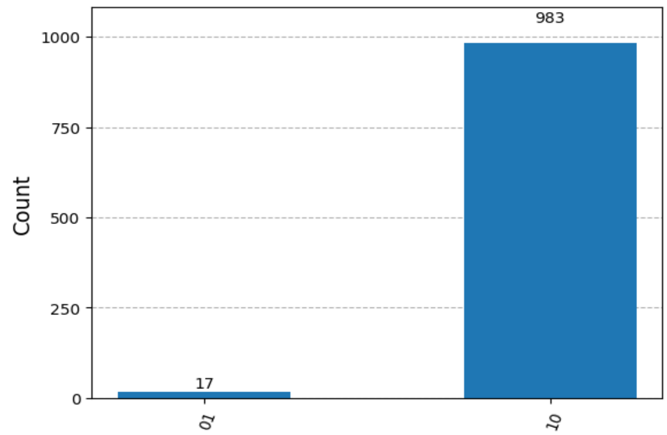
Where $a_{ij} \in \mathbb{C}$, and $\sum_{i,j}|a_{ij}|^2 = 1$. For our case, we have:

$$|\phi(\vec{\theta})\rangle = -\sin\left(\frac{\theta}{2}\right)|01\rangle + \cos\left(\frac{\theta}{2}\right)|10\rangle$$

Where: $a_{00} = 0, a_{01} = -\sin\left(\frac{\theta}{2}\right), a_{10} = \cos\left(\frac{\theta}{2}\right), a_{11} = 0$, the goal is to reconstruct a_{01} and a_{10}. To achieve this, we need to make measurement in different basis. (X, Y, Z).

To be countinue...

- Alternatively, using Bell Measurement to reconstruct the trial wavefunction with the parameter $\theta \approx -3.37$, getting the expectation after 1000 measurements:



From the figure, we have see there is 1.7% of $|01\rangle$ and 98.3% of $|10\rangle$.

$$\sqrt{98.3\%}|01\rangle + \sqrt{1.7\%}|10\rangle = |\phi(\vec{\theta})\rangle$$
$$\pm 0.99|01\rangle \pm 0.13|10\rangle = |\phi(\vec{\theta})\rangle$$

To determine the sign of our trial wavefunction, we can use Bell measurements. We can measures any state which is an superposition of $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ in the Bell basis.

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$
$$|\Phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$
$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$
$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

By combining a CNOT gate followed by a Hadamard gate, we can measure the state in the Bell basis.

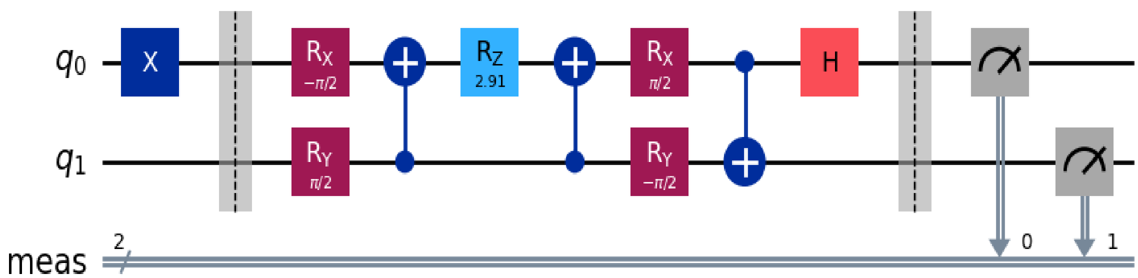
$$U|\Phi^+\rangle = |00\rangle$$
$$U|\Phi^-\rangle = |01\rangle$$
$$U|\Psi^+\rangle = |10\rangle$$
$$U|\Psi^-\rangle = |11\rangle$$

Where $U_{Bell} = (H \otimes I) \cdot \text{CNOT}(0, 1)$

$$U_{Bell} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \end{bmatrix}$$

Applying the U_{Bell} on $\begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix}$

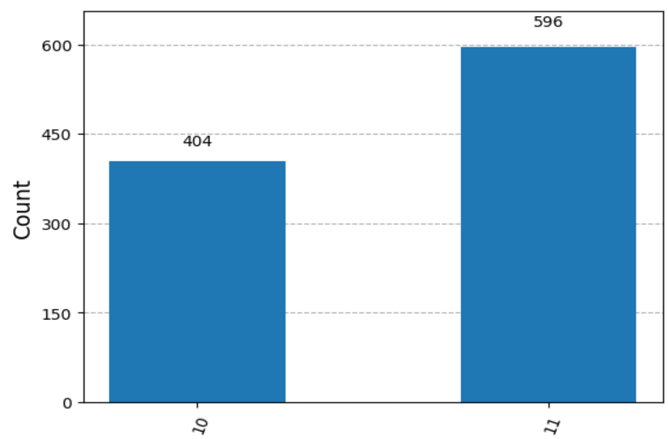
$$U_{Bell} \cdot \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} A+D \\ B+C \\ A-D \\ B-C \end{bmatrix}$$



The trial wavefunction after applying the U_{Bell} unitary gate:

$$U_{Bell} \cdot |\phi(\vec{\theta})\rangle = U_{Bell} \cdot \begin{bmatrix} 0 \\ -\sin\left(\frac{\theta}{2}\right) \\ \cos\left(\frac{\theta}{2}\right) \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ \cos\left(\frac{\theta}{2}\right) - \sin\left(\frac{\theta}{2}\right) \\ 0 \\ -\cos\left(\frac{\theta}{2}\right) - \sin\left(\frac{\theta}{2}\right) \end{bmatrix} \begin{matrix} |00\rangle & \\ |01\rangle & \approx 0.39\% \\ |10\rangle & \\ |11\rangle & \approx 0.61\% \end{matrix}$$

Using $\theta \approx -3.37$ we have:



We can see the counts of $|11\rangle$ is dominant, which means the state is $|\Psi^-\rangle$. Therefore, the sign between $|01\rangle$ and $|10\rangle$ is negative.

$$0.99|01\rangle - 0.13|10\rangle = |\phi(\vec{\theta})\rangle \tag{2}$$

Reference.

Now we plug in the θ to equation (1) to compare with equation (2), we have:

$$-\sin\left(\frac{-3.37}{2}\right)|01\rangle + \cos\left(\frac{-3.37}{2}\right)|10\rangle = |\phi(\vec{\theta})\rangle$$
$$0.993|01\rangle - 0.11|10\rangle = |\phi(\vec{\theta})\rangle$$

Mathematically we can use the Hamiltonian and the trial wavefunction, we can get our cost function (energy) as:

$$E = \langle\phi(\vec{\theta})|H|\phi(\vec{\theta})\rangle$$

$$\begin{bmatrix}0 & -\sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) & 0\end{bmatrix}\cdot\begin{bmatrix}g_0+g_1+g_2+g_3 & 0 & 0 & g_5-g_4\\ 0 & g_0+g_1-g_2-g_3 & g_5+g_4 & 0\\ 0 & g_5+g_4 & g_0-g_1+g_2-g_3 & 0\\ g_5-g_4 & 0 & 0 & g_0-g_1-g_2+g_3\end{bmatrix}\cdot\begin{bmatrix}0\\ -\sin(\frac{\theta}{2})\\ \cos(\frac{\theta}{2})\\ 0\end{bmatrix}$$

Plug in $g_0 = -0.4804, g_1 = 0.3435, g_2 = -0.4347, g_3 = 0.5716, g_4 = 0.091, g_5 = 0.091$ we have:

$$\begin{bmatrix}0 & -\sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) & 0\end{bmatrix}\cdot\begin{bmatrix}0 & 0 & 0 & 0\\ 0 & -0.2738 & 0.182 & 0\\ 0 & 0.182 & -1.8302 & 0\\ 0 & 0 & 0 & 0.1824\end{bmatrix}\cdot\begin{bmatrix}0\\ -\sin(\frac{\theta}{2})\\ \cos(\frac{\theta}{2})\\ 0\end{bmatrix}$$

$$\begin{bmatrix}0 & \frac{910\cdot\cos\left(\frac{\theta}{2}\right)+1369\cdot\sin\left(\frac{\theta}{2}\right)}{5000} & \frac{-9151\cdot\cos\left(\frac{\theta}{2}\right)-910\cdot\sin\left(\frac{\theta}{2}\right)}{5000} & 0\end{bmatrix}\cdot\begin{bmatrix}0\\ -\sin(\frac{\theta}{2})\\ \cos(\frac{\theta}{2})\\ 0\end{bmatrix} = \frac{-3891\cdot\cos(\theta) - 910\cdot\sin(\theta) - 5260}{5000}$$

The minimum energy can be found using classical optimization techniques.

$$E_{min} = \langle\phi_{min}(\vec{\theta}) \mid H \mid \phi_{min}(\vec{\theta})\rangle$$