Ansatz

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Reference from Scalable Quantum Simulation of Molecular Energies

Contents

We start with defining the Hamiltonian of the molecular Hydrogen.

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

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.

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

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

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

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

1 Decomposing the UCCSD ansatz

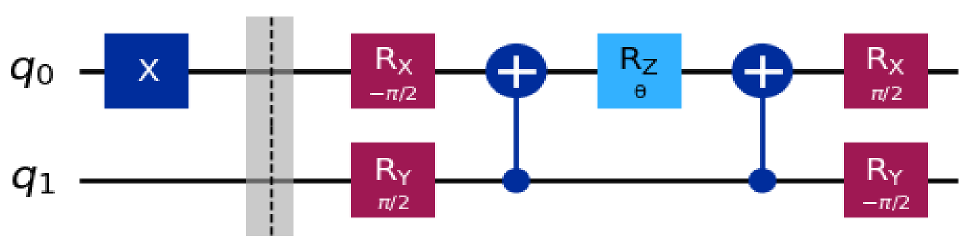
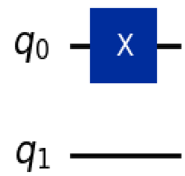


Figure 1: The UCCSD ansatz for the Hydrogen molecule.

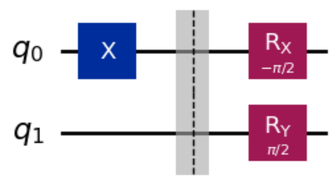
Reference state $|10\rangle$



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

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

Apply parameterized ansatz



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

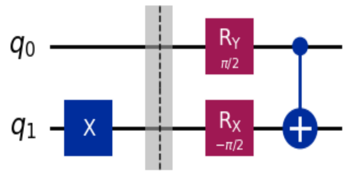
$$R_x(\frac{-\pi}{2}) = e^{-iX(\frac{-\pi}{4})} = \begin{bmatrix}\cos(\frac{-\pi}{4}) & -i\sin(\frac{-\pi}{4})\\ -i\sin(\frac{-\pi}{4}) & \cos(-\frac{\pi}{4})\end{bmatrix} = \begin{bmatrix}\frac{\sqrt{2}}{2} & \frac{i\sqrt{2}}{2}\\ \frac{i\sqrt{2}}{2} & \frac{\sqrt{2}}{2}\end{bmatrix}$$

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

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

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

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:

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

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

The second CNOT (entanglement)

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

The final rotation gates:

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

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

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

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

Reverse to match the qiskit ordering:

$$\begin{bmatrix} 0 \\ \cos(\frac{\theta}{2}) \\ -\sin(\frac{\theta}{2}) \\ 0 \end{bmatrix} = |\phi(\vec{\theta})\rangle = \cos\left(\frac{\theta}{2}\right)|01\rangle - \sin\left(\frac{\theta}{2}\right)|10\rangle \tag{2}$$

Use $\theta = -3.37$:

$$\begin{bmatrix} 0 \\ \cos(\frac{-3.37}{2}) \\ -\sin(\frac{-3.37}{2}) \\ 0 \end{bmatrix} \approx \begin{bmatrix} 0 \\ -0.1139 \\ 0.9935 \\ 0 \end{bmatrix}$$

***Note: This does not match the calculation, I had to switch place between the $|01\rangle$ and $|10\rangle$ to match the qiskit ordering**

2 Unitary Couple Cluster Single Double (UCCSD)

2.1 Coupled Cluster Theory

Couple Cluster theory was introduced for calculation nuclear binding energies. It is the gold standard for the balance between accucarcy and effiency.
Key concepts:

- First quantization: individual particles are described by wavefucntion $\psi(x)$ that satisfies the Schrodinger equation.
- Second quantization: instead of describing each particle separately, we define creation and annihilation operators that act on quantum states of an entire system.

The fundamental operators:

- Creation operator: $a_i^\dagger$ creates a particle in state i.
- Annihilation operator: a_i removes a particle from state i.

Fermionic Second Quantization: We described electron using second quantization.

$$|\Psi\rangle = a_1^\dagger a_3^\dagger |0\rangle$$

Which means we have occupied states 1 and 3 in the vaccum sate $|0\rangle$.

2.2 Unitary Coupled Cluster

The UCC ansatz $|\phi(\vec{\theta}\rangle)$ is constructed from the reference state (Hatree-Fock state $|\varphi\rangle$)

$$|\phi(\vec{\theta}\rangle) = e^{T(\vec{\theta}) - T(\vec{\theta})^\dagger} |\varphi\rangle \tag{3}$$

Where $T(\vec{\theta})$ is the anti-Hermitian cluster operator.

3 Pauli Measurement

The expectation value (Pauli Measurement):

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:

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

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

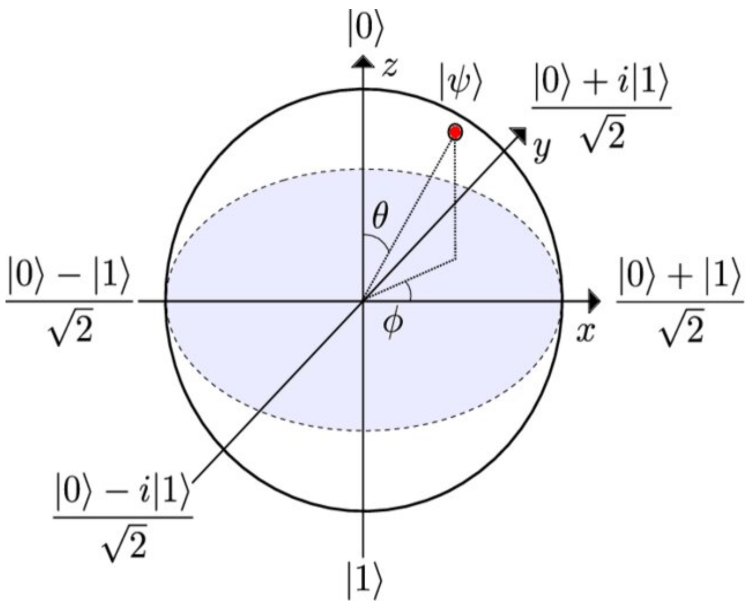


Figure 2: Reference

Let say we have a 1-qubit state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. This state is a superposition of $|0\rangle$ and $|1\rangle$. This is also called the Z basis (computational basis).

Measurement in the X basis - Diagonal basis/ Hadamard basis: superposition collapses the quantum state of the qubit $|\psi\rangle$ to either $|+\rangle$ or $|-\rangle$.

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$
$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$
$$|0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$$
$$|1\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)$$

$$
\begin{aligned}
H|\psi\rangle &= H(\alpha|0\rangle + \beta|1\rangle) && (4)\\
&= \alpha H|0\rangle + \beta H|1\rangle && (5)\\
&= \alpha \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} && (6)\\
&= \alpha \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} + \beta \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} && (7)\\
&= \alpha|+\rangle + \beta|-\rangle \quad \text{X basis} && (8)
\end{aligned}
$$

Measurement in the Y basis (Imaginary basis):

$$
\begin{aligned}
(S^\dagger \cdot H)|\psi\rangle &= (S^\dagger \cdot H)(\alpha|0\rangle + \beta|1\rangle)\\
&= \alpha(S^\dagger \cdot H)|0\rangle + \beta(S^\dagger \cdot H)|1\rangle\\
&= \alpha \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix}\\
&= \alpha \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} \end{bmatrix} + \beta \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{bmatrix}\\
&= \alpha \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle) + \beta \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle) \quad \text{Y basis}
\end{aligned}
$$

Pauli Measurement	**Unitary Transformation**
$Z \otimes 1$	$1 \otimes 1$
$X \otimes 1$	$H \otimes 1$
$Y \otimes 1$	$HS^\dagger \otimes 1$
$1 \otimes Z$	SWAP
$1 \otimes X$	$(H \otimes 1)$SWAP
$1 \otimes Y$	$(HS^\dagger \otimes 1)$SWAP
$Z \otimes Z$	CNOT_{10}
$X \otimes Z$	$\text{CNOT}_{10}(H \otimes 1)$
$Y \otimes Z$	$\text{CNOT}_{10}(HS^\dagger \otimes 1)$
$Z \otimes X$	$\text{CNOT}_{10}(1 \otimes H)$
$X \otimes X$	$\text{CNOT}_{10}(H \otimes H)$
$Y \otimes X$	$\text{CNOT}_{10}(HS^\dagger \otimes H)$
$Z \otimes Y$	$\text{CNOT}_{10}(1 \otimes HS^\dagger)$
$X \otimes Y$	$\text{CNOT}_{10}(H \otimes HS^\dagger)$
$Y \otimes Y$	$\text{CNOT}_{10}(HS^\dagger \otimes HS^\dagger)$

$$
\langle H\rangle = g_0\mathbb{I} + g_1\langle Z_0\rangle + g_2\langle Z_1\rangle + g_3\langle Z_0Z_1\rangle + g_4\langle Y_0Y_1\rangle + g_5\langle X_0X_1\rangle
$$

$$
\langle P\rangle = \sum_{\text{bitstring}} (-1)^{\text{parity}} \left(\frac{\text{count}}{\text{shots}}\right)
$$

Where:

- parity = bitstring.count('1') mod 2
- count = number of times the bitstring was measured
- shots = total number of measurements

3.1 Theoretical Analysis (XX)

- For the XX operator

$$XX = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

The expectation value of an observable O is given by:

$$\langle O \rangle = \sum_i \lambda_i p_i$$

Where p_i is the probability of measuring the state in the i^{th} eigenstate. λ_i is the expectation value correspoding to eigenstate.

From equation (4) we can see that $H|0\rangle = |+\rangle, H|1\rangle = |-\rangle$. The corresponding eigenvalues for the operator X are

$$\langle +|X|+\rangle = 1 \text{ and } \langle -|X|-\rangle = -1$$

For the 2 qubit states, we have:

$$(H \otimes H)|00\rangle = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} = |++\rangle = \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle)$$

$$(H \otimes H)|01\rangle = |+-\rangle = \frac{1}{2}(|00\rangle - |01\rangle + |10\rangle - |11\rangle)$$

$$(H \otimes H)|10\rangle = |-+\rangle = \frac{1}{2}(|00\rangle + |01\rangle - |10\rangle - |11\rangle)$$

$$(H \otimes H)|11\rangle = |--\rangle$$

Apply the operator XX on each state:

$$\begin{aligned}
XX|++\rangle &= \frac{1}{2}(XX|00\rangle + XX|01\rangle + XX|10\rangle + XX|11\rangle) \\
&= \frac{1}{2}(|11\rangle + |10\rangle + |01\rangle + |00\rangle) = |++\rangle \\
&\Rightarrow \langle ++|XX|++\rangle = \langle ++|++\rangle = 1 \\
XX|+-\rangle &= \frac{1}{2}(XX|00\rangle - XX|01\rangle + XX|10\rangle - XX|11\rangle) \\
&= \frac{1}{2}(|11\rangle - |10\rangle + |01\rangle - |00\rangle) = \frac{1}{2}\begin{bmatrix} -1 \\ 1 \\ -1 \\ 1 \end{bmatrix} \\
&\Rightarrow \langle +-|XX|+-\rangle = \begin{bmatrix} \frac{1}{2} & \frac{-1}{2} & \frac{1}{2} & \frac{-1}{2} \end{bmatrix} \cdot \begin{bmatrix} \frac{-1}{2} \\ \frac{1}{2} \\ \frac{-1}{2} \\ \frac{1}{2} \end{bmatrix} = -1
\end{aligned}$$

and so we can get the remaining expectation values $\langle -+|XX|-+\rangle = -1, \langle --|XX|--\rangle = 1$

Measurement	XX basis equivalent	XX Expectation Value
$\|00\rangle$	$\|++\rangle$	1
$\|01\rangle$	$\|+-\rangle$	-1
$\|10\rangle$	$\|-+\rangle$	-1
$\|11\rangle$	$\|--\rangle$	1

3.2 Experimental Analysis (XX)

From our circuit that produce the wavefunction $|\phi(\vec{\theta})\rangle$ (see Figure 1). We just need to apply two Hadamard gates to the qubits and measure the expectation value of the XX operator.

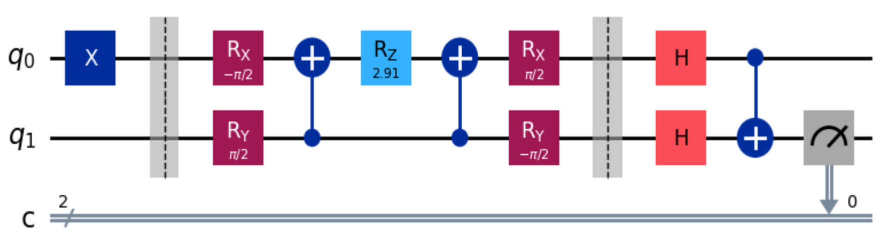


Figure 3: Circuit for the XX operator

Give the trial wavefunction $|\phi(\vec{\theta})\rangle = \cos\left(\frac{\theta}{2}\right)|01\rangle - \sin\left(\frac{\theta}{2}\right)|10\rangle$. Applying the Hadamard gates given:

$$
\begin{aligned}
&(H \otimes H)|\phi(\vec{\theta})\rangle \\
&= (H \otimes H)(\cos\left(\frac{\theta}{2}\right)|01\rangle - \sin\left(\frac{\theta}{2}\right)|10\rangle) \\
&= \cos\left(\frac{\theta}{2}\right)(H|0\rangle \otimes H|1\rangle) - \sin\left(\frac{\theta}{2}\right)(H|1\rangle \otimes H|0\rangle) \\
&= \cos\left(\frac{\theta}{2}\right)\left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)\right] - \sin\left(\frac{\theta}{2}\right)\left[\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right] \\
&= \cos\left(\frac{\theta}{2}\right)\left[\frac{1}{2}(|00\rangle - |01\rangle + |10\rangle - |11\rangle)\right] - \sin\left(\frac{\theta}{2}\right)\left[\frac{1}{2}(|00\rangle + |01\rangle - |10\rangle - |11\rangle)\right] \\
&= \frac{1}{2}\left\{\left[\cos\left(\frac{\theta}{2}\right) - \sin\left(\frac{\theta}{2}\right)\right]|00\rangle - \left[\cos\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)\right]|01\rangle + \left[\cos\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)\right]|10\rangle + \left[\sin\left(\frac{\theta}{2}\right) - \cos\left(\frac{\theta}{2}\right)\right]|11\rangle\right\}
\end{aligned}
$$

Then we apply the CNOT_{01} gate to the state:

$$
\begin{aligned}
&\text{CNOT}_{01}\left\{\cos\left(\frac{\theta}{2}\right)\left[\frac{1}{2}(|00\rangle - |01\rangle + |10\rangle - |11\rangle)\right] - \sin\left(\frac{\theta}{2}\right)\left[\frac{1}{2}(|00\rangle + |01\rangle - |10\rangle - |11\rangle)\right]\right\} \\
&= \cos\left(\frac{\theta}{2}\right)\left[\frac{1}{2}\text{CNOT}_{01}(|00\rangle - |01\rangle + |10\rangle - |11\rangle)\right] - \sin\left(\frac{\theta}{2}\right)\left[\frac{1}{2}\text{CNOT}_{01}(|00\rangle + |01\rangle - |10\rangle - |11\rangle)\right] \\
&= \cos\left(\frac{\theta}{2}\right)\left[\frac{1}{2}(|00\rangle - |01\rangle + |11\rangle - |10\rangle)\right] - \sin\left(\frac{\theta}{2}\right)\left[\frac{1}{2}(|00\rangle + |01\rangle - |11\rangle - |10\rangle)\right] \\
&= \frac{1}{2}\left\{\left[\cos\left(\frac{\theta}{2}\right) - \sin\left(\frac{\theta}{2}\right)\right]|00\rangle - \left[\cos\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)\right]|01\rangle + \left[\sin\left(\frac{\theta}{2}\right) - \cos\left(\frac{\theta}{2}\right)\right]|10\rangle + \left[\sin\left(\frac{\theta}{2}\right) + \cos\left(\frac{\theta}{2}\right)\right]|11\rangle\right\}
\end{aligned}
$$

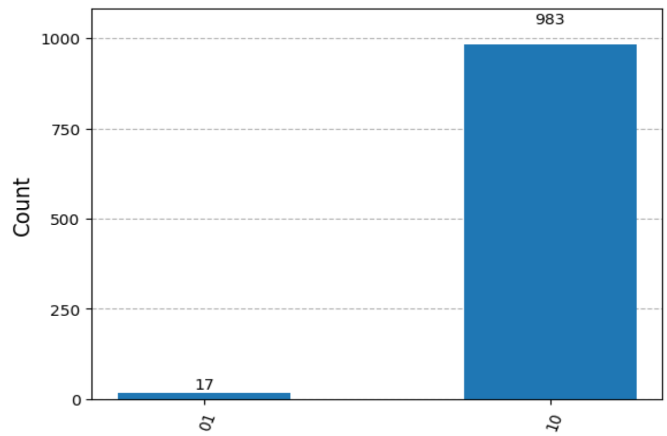
After applying CNOT_{01} gate.

$$
\underbrace{|00\rangle}_{even} \rightarrow |0\textcolor{red}{0}\rangle\,;\ \underbrace{|01\rangle}_{odd} \rightarrow |0\textcolor{blue}{1}\rangle\,;\ \underbrace{|10\rangle}_{odd} \rightarrow |1\textcolor{blue}{1}\rangle\,;\ \underbrace{|11\rangle}_{even} \rightarrow |1\textcolor{red}{0}\rangle
$$

We can see that after applying the CNOT_{01} gate, the second qubit is flipped (the colored). Now measuring just the second qubit give us the parity of the state. If the parity is even we will see 0 and if the parity is odd we will see 1. A CNOT gate is used to compute the parity of two qubits and store it in one qubit without fully collapsing the state.

4 Bell Measurement (Work In Progress)

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 $|10\rangle$.

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

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.

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

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

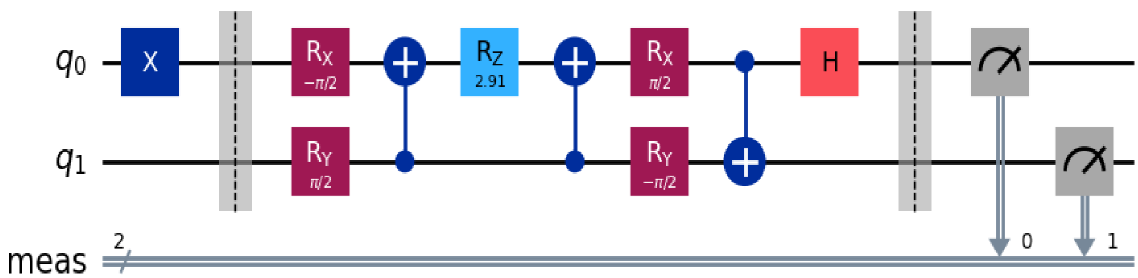
$$\begin{aligned}U|\Phi^+\rangle &= |00\rangle \\ U|\Phi^-\rangle &= |01\rangle \\ U|\Psi^+\rangle &= |10\rangle \\ U|\Psi^-\rangle &= |11\rangle\end{aligned}$$

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

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

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

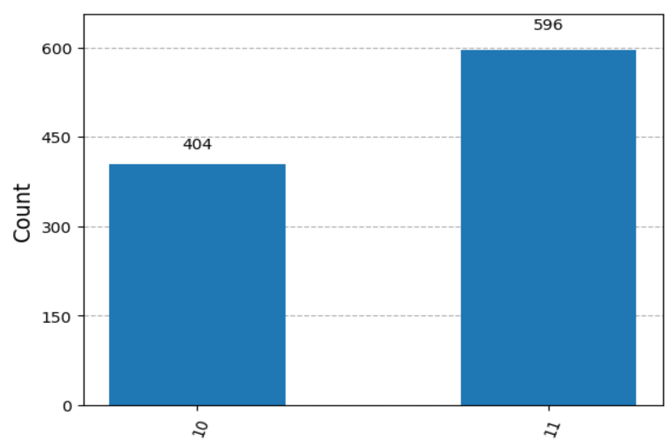
$$U_{Bell} \cdot \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} A+D \\ A-D \\ B+C \\ B-C \end{bmatrix}$$



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

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

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.

$$0.13|01\rangle - 0.99|10\rangle = |\phi(\vec{\theta})\rangle \tag{9}$$

Reference.

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

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

There is a mistake for my bell measurement, I will correct it later.

5 Cost Function

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

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

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

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:

$$\begin{bmatrix}0 & \cos(\frac{\theta}{2}) & -\sin(\frac{\theta}{2}) & 0\end{bmatrix} \cdot \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -0.2738 & 0.182 & 0 \\ 0 & 0.182 & -1.8302 & 0 \\ 0 & 0 & 0 & 0.1824 \end{bmatrix} \cdot \begin{bmatrix} 0 \\ \cos(\frac{\theta}{2}) \\ -\sin(\frac{\theta}{2}) \\ 0 \end{bmatrix} \approx -1.851 \quad (\text{with } \theta = -3.37)$$

The minimum energy can be found using classical optimization techniques.

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

6 Experiment

6.1 Mapping

From equation (2), we have a trial wavefunction of:

$$|\phi(\vec{\theta})\rangle = 0\,|00\rangle + \cos\left(\frac{\theta}{2}\right)|01\rangle - \sin\left(\frac{\theta}{2}\right)|10\rangle + 0\,|11\rangle \tag{10}$$

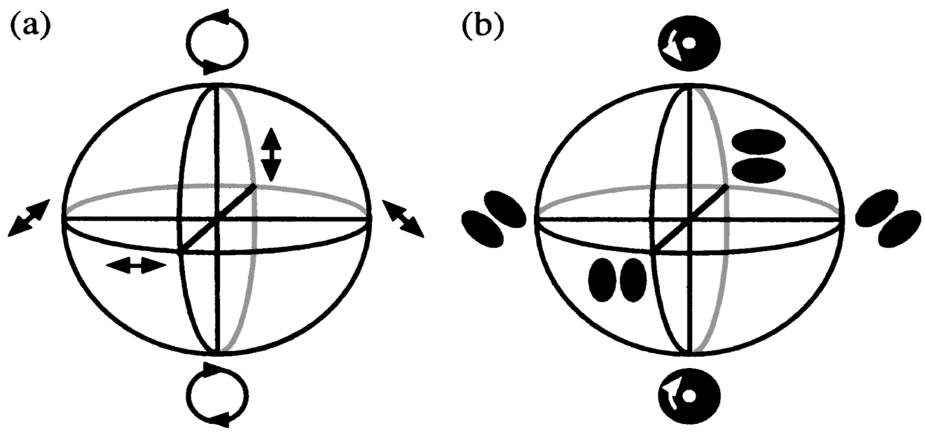


Figure 4: Poincare

For this experiment, we will use "01"/"10" Spatial Mode as our first qubit and Polarization as our second qubit.

$$|0\rangle = \text{Spatial Mode 10 and Horizontal Polarization or } |0\rangle_s, |0\rangle_p$$

$$|1\rangle = \text{Spatial Mode 01 and Vertical Polarization or } |1\rangle_s, |1\rangle_p$$

$$\frac{|0\rangle - i|1\rangle}{\sqrt{2}} = \text{South Pole of the Poincare Sphere or Left-circular Polarization} \frac{|L\rangle_s}{\sqrt{2}}, \frac{|L\rangle_p}{\sqrt{2}}$$

$$\frac{|0\rangle + i|1\rangle}{\sqrt{2}} = \text{North Pole of the Poincare Sphere or Right-circular Polarization} \frac{|R\rangle_s}{\sqrt{2}}, \frac{|R\rangle_p}{\sqrt{2}}$$

$$|+\rangle = \text{Diagonal Polarization} \frac{|D\rangle_s}{\sqrt{2}}, \frac{|D\rangle_p}{\sqrt{2}}$$

$$|-\rangle = \text{Anti-diagonal Polarization} \frac{|A\rangle_s}{\sqrt{2}}, \frac{|A\rangle_p}{\sqrt{2}}$$

Therefore our initial state is $|0\rangle_p \otimes |0\rangle_s \equiv |0_p 0_s\rangle$

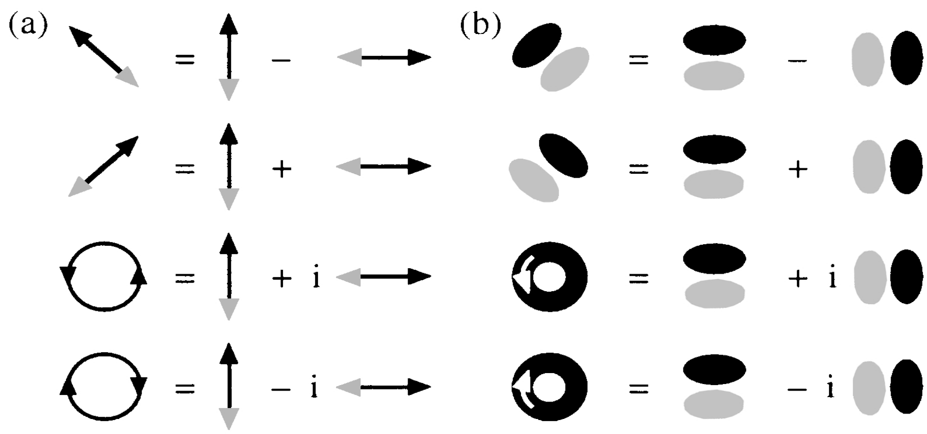


Figure 5: Geometric Phase Shift

7 Optical Circuit

7.1 Optical Components

Reference

Quarter-wave plate (QWP):

$$e^{\frac{-i\pi}{4}}\begin{bmatrix}\cos^2(\theta)+i\sin^2(\theta) & (1-i)\sin(\theta)\cos(\theta)\\(1-i)\sin(\theta)\cos(\theta) & \sin^2(\theta)+i\cos^2(\theta)\end{bmatrix}$$

Quarter-wave plate with fast axis vertical (QWPv):

$$e^{\frac{i\pi}{4}}\begin{bmatrix}1 & 0\\0 & -i\end{bmatrix}$$

Quarter-wave plate with fast axis horizontal (QWPh):

$$e^{\frac{-i\pi}{4}}\begin{bmatrix}1 & 0\\0 & i\end{bmatrix}$$

Half-wave plate (HWP):

$$\begin{bmatrix}\cos(2\phi) & \sin(2\phi)\\\sin(2\phi) & -\cos(2\phi)\end{bmatrix}$$

Dove Prism (DP) using Rotation matrix:

$$\begin{bmatrix}\cos(\omega) & -\sin(\omega)\\\sin(\omega) & \cos(\omega)\end{bmatrix}$$

7.2 Realization of the Circuit

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

$$R_y(\frac{\pi}{2}) = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

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

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$S^\dagger = \begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix}$$

$R_x(\frac{\pi}{2})$ realization in the optical circuit for Polarization:

$$\text{QWP}(\frac{\pi}{4}) = \begin{bmatrix} \cos^2(\frac{\pi}{4}) + i\sin^2(\frac{\pi}{4}) & (1-i)\sin(\frac{\pi}{4})\cos(\frac{\pi}{4}) \\ (1-i)\sin(\frac{\pi}{4})\cos(\frac{\pi}{4}) & \sin^2(\frac{\pi}{4}) + i\cos^2(\frac{\pi}{4}) \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{2} + i\frac{1}{2} & (1-i)\frac{1}{2} \\ (1-i)\frac{1}{2} & \frac{1}{2} + i\frac{1}{2} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1+i & (1-i) \\ (1-i) & 1+i \end{bmatrix} = \frac{1+i}{2} \begin{bmatrix} 1 & \frac{1-i}{1+i} \\ \frac{1-i}{1+i} & 1 \end{bmatrix}$$

$$= \frac{1+i}{2} \begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix}$$

$R_y(\frac{\pi}{2})$ realization in the optical circuit for Spatial Mode:

$$\text{DP}(\frac{\pi}{4}) = \begin{bmatrix} \cos(\frac{\pi}{4}) & -\sin(\frac{\pi}{4}) \\ \sin(\frac{\pi}{4}) & \cos(\frac{\pi}{4}) \end{bmatrix}$$

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

$R_z(\theta)$ realization in the optical circuit for Polarization:

$$\text{QWPh} \cdot \text{QWP}(\frac{-\pi}{4}) \cdot \text{HWP}(\frac{\pi}{2} - \frac{\phi}{4}) \cdot \text{QWP}(\frac{-\pi}{4}) \cdot \text{QWPh} = \begin{bmatrix} -ie^{-\frac{i\phi}{2}} & 0 \\ 0 & -ie^{\frac{i\phi}{2}} \end{bmatrix}$$

Hadamard gate (H) realization in the optical circuit for Polarization:

$$\text{HWP}(\frac{\pi}{8}) = \begin{bmatrix} \cos(\frac{\pi}{8}) & \sin(\frac{\pi}{8}) \\ \sin(\frac{\pi}{8}) & -\cos(\frac{\pi}{8}) \end{bmatrix}$$

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

Mach-Zehnder Interferometer (MZI) realization in the optical circuit for Spatial Mode: