In [1]:

```
from qiskit import QuantumCircuit, ClassicalRegister, QuantumRegister, Aer
from qiskit import execute
from qiskit.tools.visualization import plot_histogram
import numpy as np
import matplotlib.pyplot as plt
from qiskit.ignis.mitigation.measurement import (complete_meas_cal,CompleteMeasFitter)
```

2-site DMFT Hamiltonian calculation for the 4-qubit DMFT state

$$\hat{H} = \frac{U}{4}\hat{\sigma}_1^z\hat{\sigma}_3^z + \left(\frac{\mu}{2} - \frac{U}{4}\right)(\hat{\sigma}_1^z + \hat{\sigma}_3^z) + \frac{V}{2}(\hat{\sigma}_1^x\hat{\sigma}_2^x + \hat{\sigma}_1^y\hat{\sigma}_2^y + \hat{\sigma}_3^x\hat{\sigma}_4^x + \cdots$$

In [2]:

```
def result_calc(qc):
    simulator = Aer.get_backend('qasm_simulator')
    result = execute(qc, backend=simulator, shots=1024).result()
    my_his = plot_histogram(result.get_counts(qc))
    return my_his
```

In [3]:

```
def two_site_ham(term):
    # Create a Quantum Register and classical registers with 2 qubits and 2 classical
    qr = QuantumRegister(4)
    cr = ClassicalRegister(4)
    qc = QuantumCircuit(qr, cr)

    # Need to add coefficients terms
    # V = 1.23
    # U = 0.3

    # QC for the 4 qubit DMFT calculation based on the PT approach:
    # Whilst minimising the need for rotation gates
    qc.ry(1.60127,2)
    qc.ry(1.5708,0)
    qc.cx(0,1)
    qc.cx(1,2)
    qc.cx(2,3)
    qc.ry(-np.pi,1)
    qc.ry(np.pi,3)
    qc.barrier()

    if term == 'gs':
        # This is the wavefunction of the system after DMFT
        qc.measure([i for i in range(4)],[i for i in range(4)])
        qc.barrier()

    elif term == 1:
        # First term describing the Hamiltonian
        # sigma_{1}^{z} sigma_{3}^{z}
        qc.measure(0,0)
        qc.measure(2,2)
        qc.barrier()

        qc.measure(1,1)
        qc.measure(3,3)
        qc.barrier()

    elif term == 2:
        # Second term describing the Hamiltonian
        # sigma_{1}^{z}
        qc.measure(0,0)
        qc.barrier()
        qc.measure(1,1)
        qc.measure(2,2)
        qc.measure(3,3)
        qc.barrier()

    elif term == 3:
        # Third term describing the Hamiltonian
        # sigma_{3}^{z}
        qc.measure(2,2)

        qc.barrier()
        qc.measure(0,0)
        qc.measure(1,1)
        qc.measure(3,3)
        qc.barrier()

    elif term == 4:
```

```
        # Fourth term describing the Hamiltonian
        # Applying a hadmard gate to measure along the x-basis
        # sigma_{1}^{x} sigma_{2}^{x}
        qc.h(qr[0])
        qc.h(qr[1])
        qc.measure(0,0)
        qc.measure(1,1)
        qc.barrier()

        qc.measure(2,2)
        qc.measure(3,3)

    elif term == 5:
        # fith term describing the Hamiltonian:
        # Applying a hadmard gate to change the basis to x-basis,
        # on the 2nd qubit and then,
        # applying a complex conjugate S gate to measure along the y-basis
        # sigma_{1}^{y} sigma_{2}^{y}
        qc.sdg(qr[0])
        qc.sdg(qr[1])

        qc.h(qr[0])
        qc.h(qr[1])

        qc.measure(0,0)
        qc.measure(1,1)
        qc.barrier()


        qc.measure(2,2)
        qc.measure(3,3)

    elif term == 6:
        # sixth term describing the Hamiltonian
        # Applying a hadmard gate to measure along the x-basis
        # sigma_{3}^{x} sigma_{4}^{x}
        qc.h(qr[2])
        qc.h(qr[3])
        qc.measure(2,2)
        qc.measure(3,3)
        qc.barrier()

        qc.measure(0,0)
        qc.measure(1,1)
    else:
        # seventh term describing the Hamiltonian:
        # Applying a hadmard gate to change the basis to x-basis,
        # on the 2nd qubit and then,
        # applying a complex conjugate S gate to measure along the y-basis
        # sigma_{3}^{y} sigma_{4}^{y}
        qc.sdg(qr[2])
        qc.sdg(qr[3])

        qc.h(qr[2])
        qc.h(qr[3])

        qc.measure(2,2)
        qc.measure(3,3)
        qc.barrier()

        qc.measure(0,0)
```

```
        qc.measure(1,1)

    print(qc)
    simulator = Aer.get_backend('qasm_simulator')
    result = execute(qc, backend=simulator, shots=1024).result()
    my_his = plot_histogram(result.get_counts(qc))

    return my_his
```

Ground state wave function

The two_site_ham(gs) measurement is the groundstate of the system given by:

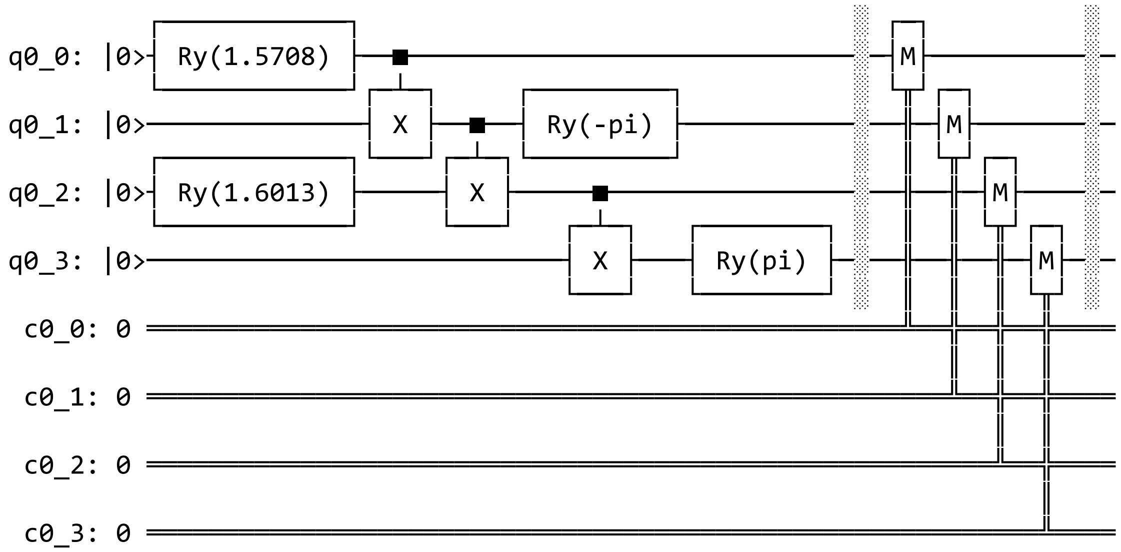
$$\left|\psi_{gs}\right\rangle \propto a\left|0101\right\rangle + b\left|0110\right\rangle + c\left|1001\right\rangle + d\left|1010\right\rangle.$$

From Mathematica:

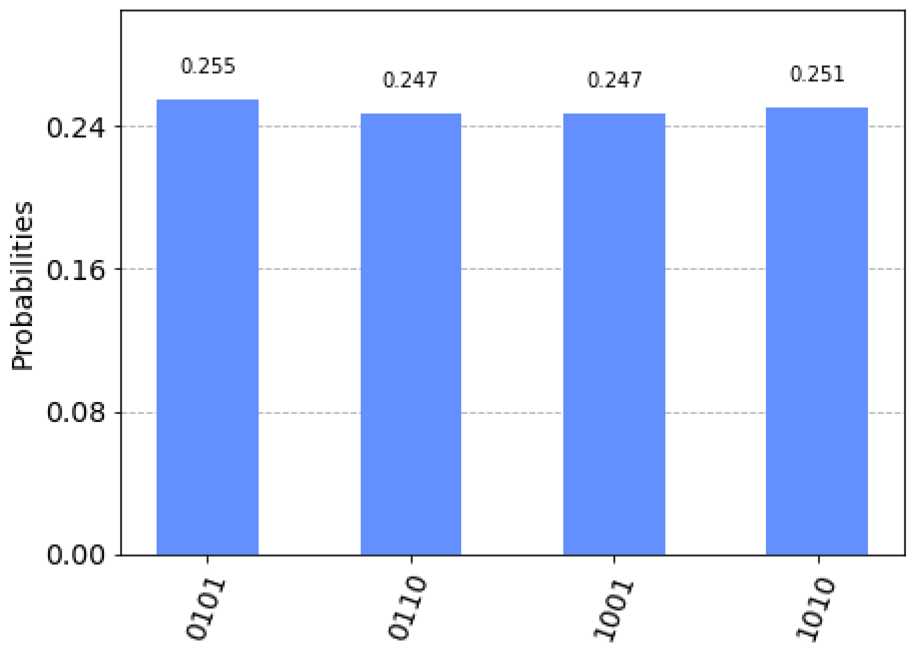
$$\left|\psi_{gs}\right\rangle = -a\left|0101\right\rangle + b\left|0110\right\rangle + c\left|1001\right\rangle - d\left|1010\right\rangle.$$
$$\left\langle\psi_{gs}\right| = -a^{\dagger}\left\langle 1010\right| + b^{\dagger}\left\langle 0110\right| + c^{\dagger}\left\langle 1001\right| - d^{\dagger}\left\langle 0101\right|.$$

In [4]:

```
1 two_site_ham('gs')
```



Out[4]:



Measurement of the first term:

$$H_1 = \hat{\sigma}_1^z \hat{\sigma}_3^z.$$

$$H_1 \left|\psi_{gs}\right\rangle = \hat{\sigma}_1^z \hat{\sigma}_3^z(-a\,|0101\rangle + b\,|0110\rangle + c\,|1001\rangle - d\,|1010\rangle)$$

$$H_1 \left|\psi_{gs}\right\rangle = -a\,|0101\rangle - b\,|0110\rangle - c\,|1001\rangle - d\,|1010\rangle$$

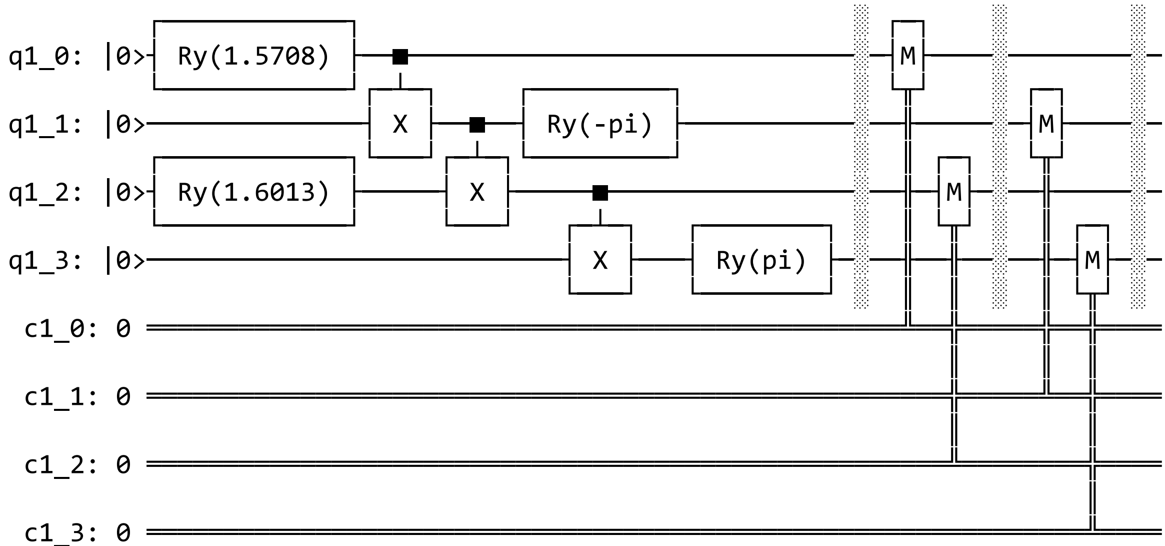
$$\left\langle\psi_{gs}\right| H_1 \left|\psi_{gs}\right\rangle = (-a^\dagger\,\langle 1010| + b^\dagger\,\langle 0110| + c^\dagger\,\langle 1001| - d^\dagger\,\langle 0101|)(-a\,|0101\rangle - b\,|0110\rangle - c\,|1001\rangle - d$$

$$\langle H_1\rangle = |a|^2_{|0101\rangle} - |b|^2_{|0110\rangle} - |c|^2_{|1001\rangle} + |d|^2_{|1010\rangle}$$

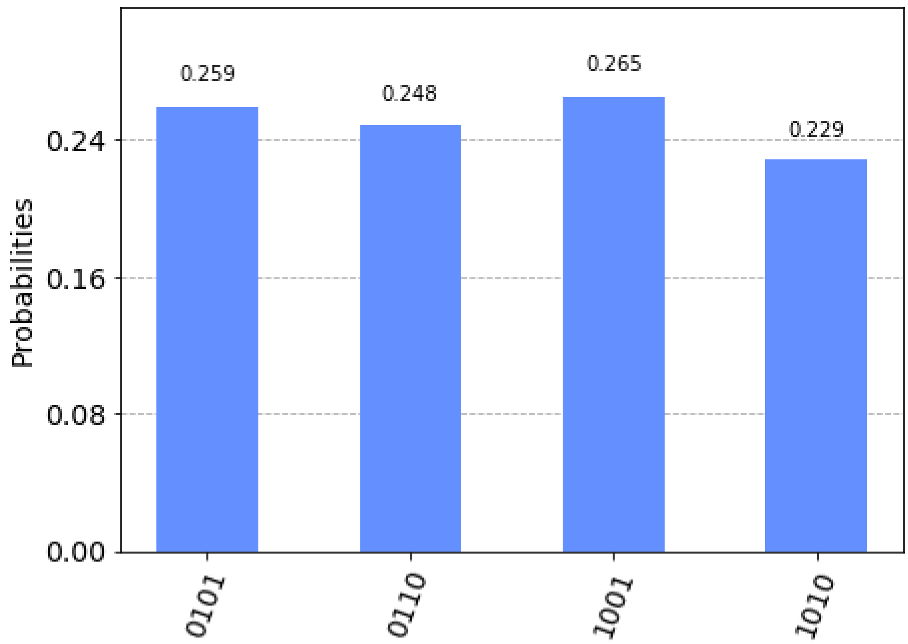
$$\langle H_1\rangle = 0.259 - 0.248 - 0.265 + 0.229 = -0.025$$

In [5]:

```
1 two_site_ham(1)
```



Out[5]:



Measurement of the second term:

$$H_2 = \hat{\sigma}_1^z.$$

$$H_2 \left|\psi_{gs}\right\rangle = \hat{\sigma}_1^z(-a\,|0101\rangle + b\,|0110\rangle + c\,|1001\rangle - d\,|1010\rangle)$$

$$H_2 \left|\psi_{gs}\right\rangle = -a\,|0101\rangle + b\,|0110\rangle - c\,|1001\rangle + d\,|1010\rangle$$

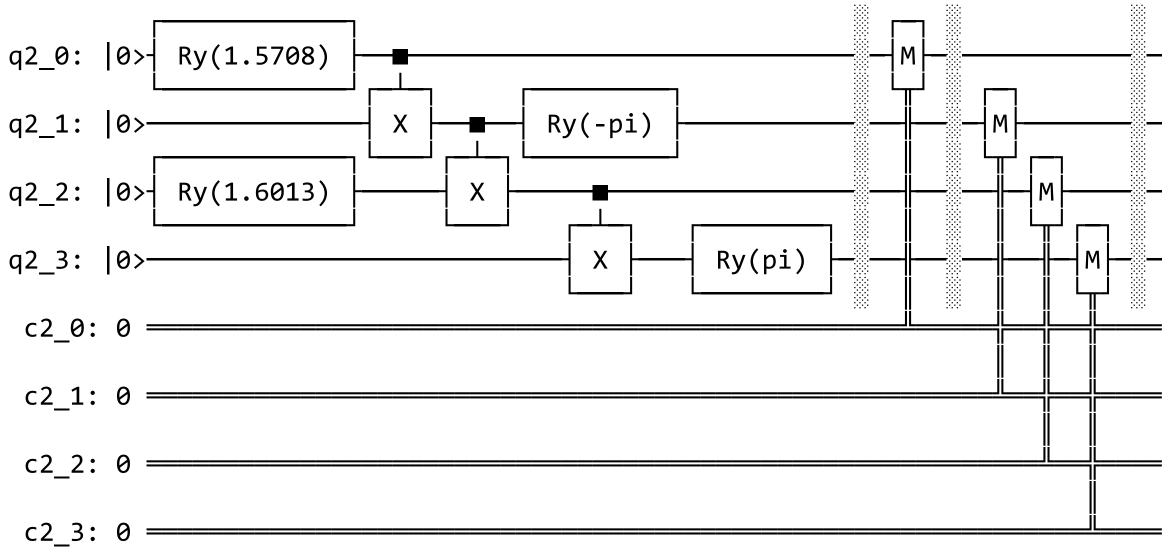
$$\left\langle\psi_{gs}\right| H_2 \left|\psi_{gs}\right\rangle = (-a^\dagger\,\langle 1010| + b^\dagger\,\langle 0110| + c^\dagger\,\langle 1001| - d^\dagger\,\langle 0101|)(-a\,|0101\rangle + b\,|0110\rangle - c\,|1001\rangle + d$$

$$\langle H_2\rangle = |a|^2_{|0101\rangle} + |b|^2_{|0110\rangle} - |c|^2_{|1001\rangle} - |d|^2_{|1010\rangle}$$

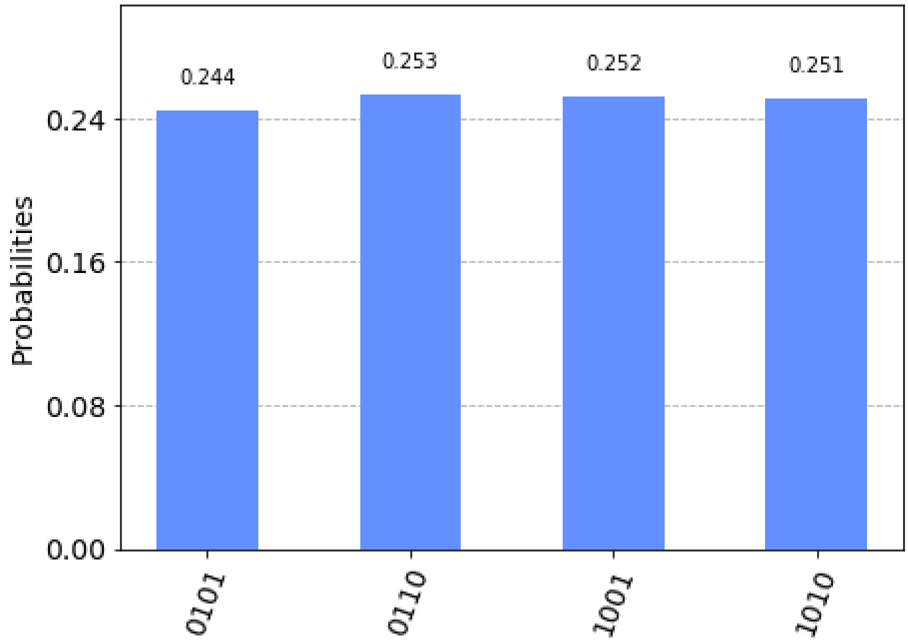
$$\langle H_2\rangle = 0.244 + 0.253 - 0.252 - 0.251 = -0.006$$

In [6]:

```
1  two_site_ham(2)
```



Out[6]:



Measurement of the third term:

$$H_3 = \hat{\sigma}^z_3.$$

$$H_3 \left|\psi_{gs}\right\rangle = \hat{\sigma}^z_3(-a\,|0101\rangle + b\,|0110\rangle + c\,|1001\rangle - d\,|1010\rangle)$$

$$H_3 \left|\psi_{gs}\right\rangle = -a\,|0101\rangle - b\,|0110\rangle + c\,|1001\rangle + d\,|1010\rangle$$

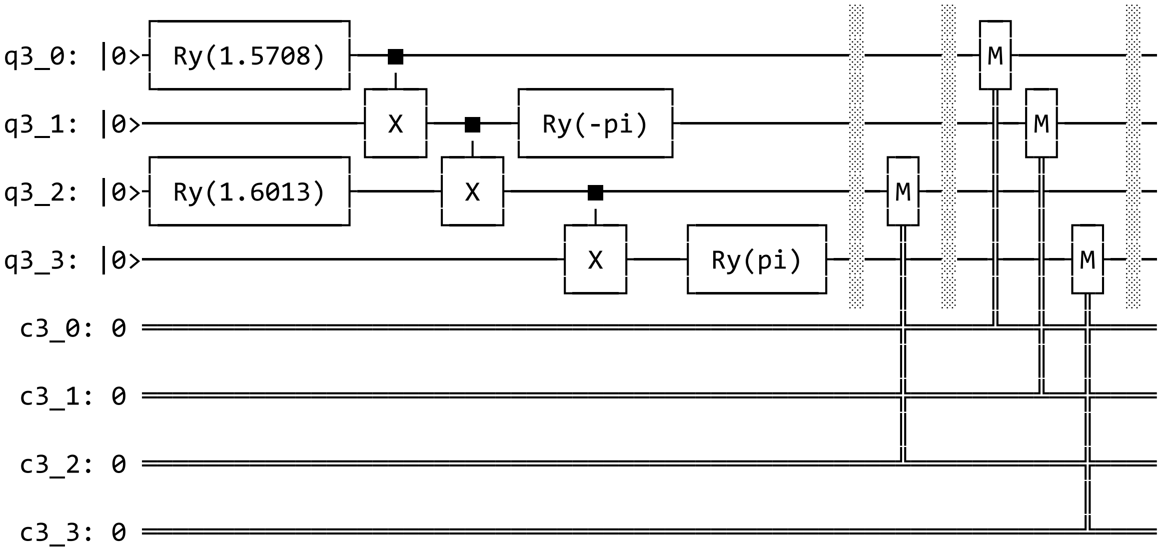
$$\left\langle\psi_{gs}\right| H_3 \left|\psi_{gs}\right\rangle = (-a^\dagger\,\langle 1010| + b^\dagger\,\langle 0110| + c^\dagger\,\langle 1001| - d^\dagger\,\langle 0101|)(-a\,|0101\rangle - b\,|0110\rangle + c\,|1001\rangle + d$$

$$\langle H_3\rangle = |a|^2_{|0101\rangle} - |b|^2_{|0110\rangle} + |c|^2_{|1001\rangle} - |d|^2_{|1010\rangle}$$

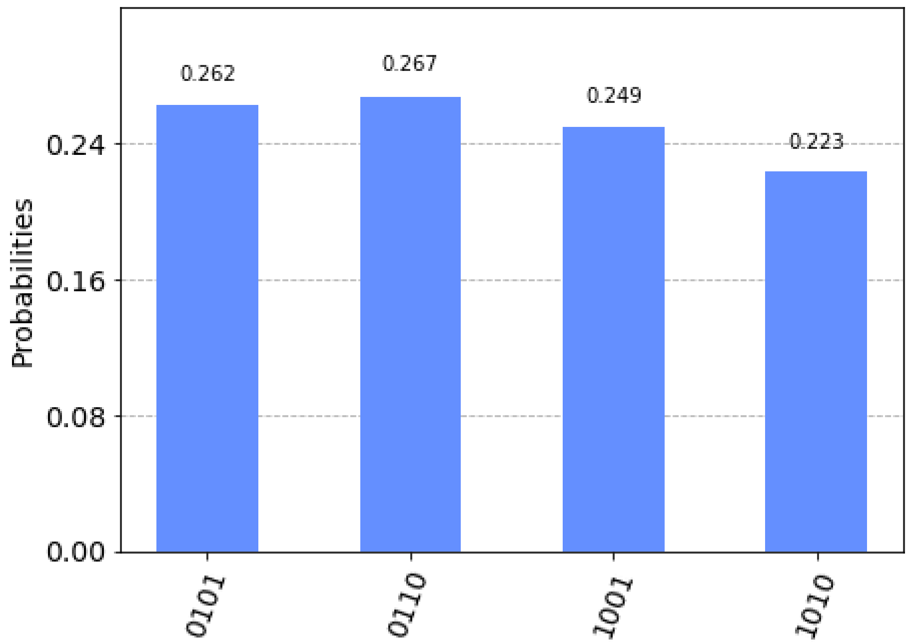
$$\langle H_3\rangle = 0.262 - 0.267 + 0.249 - 0.223 = 0.021$$

In [7]:

```
two_site_ham(3)
```



Out[7]:



Measurement of the fourth term: $H_4 = \hat{\sigma}_1^x \hat{\sigma}_2^x.$

$$H_4 \left|\psi_{gs}\right\rangle = \hat{\sigma}_1^x \hat{\sigma}_2^x(-a\,|0101\rangle + b\,|0110\rangle + c\,|1001\rangle - d\,|1010\rangle)$$

$$H_4 \left|\psi_{gs}\right\rangle = -a\,|1001\rangle + b\,|1010\rangle + c\,|0101\rangle - d\,|0110\rangle$$

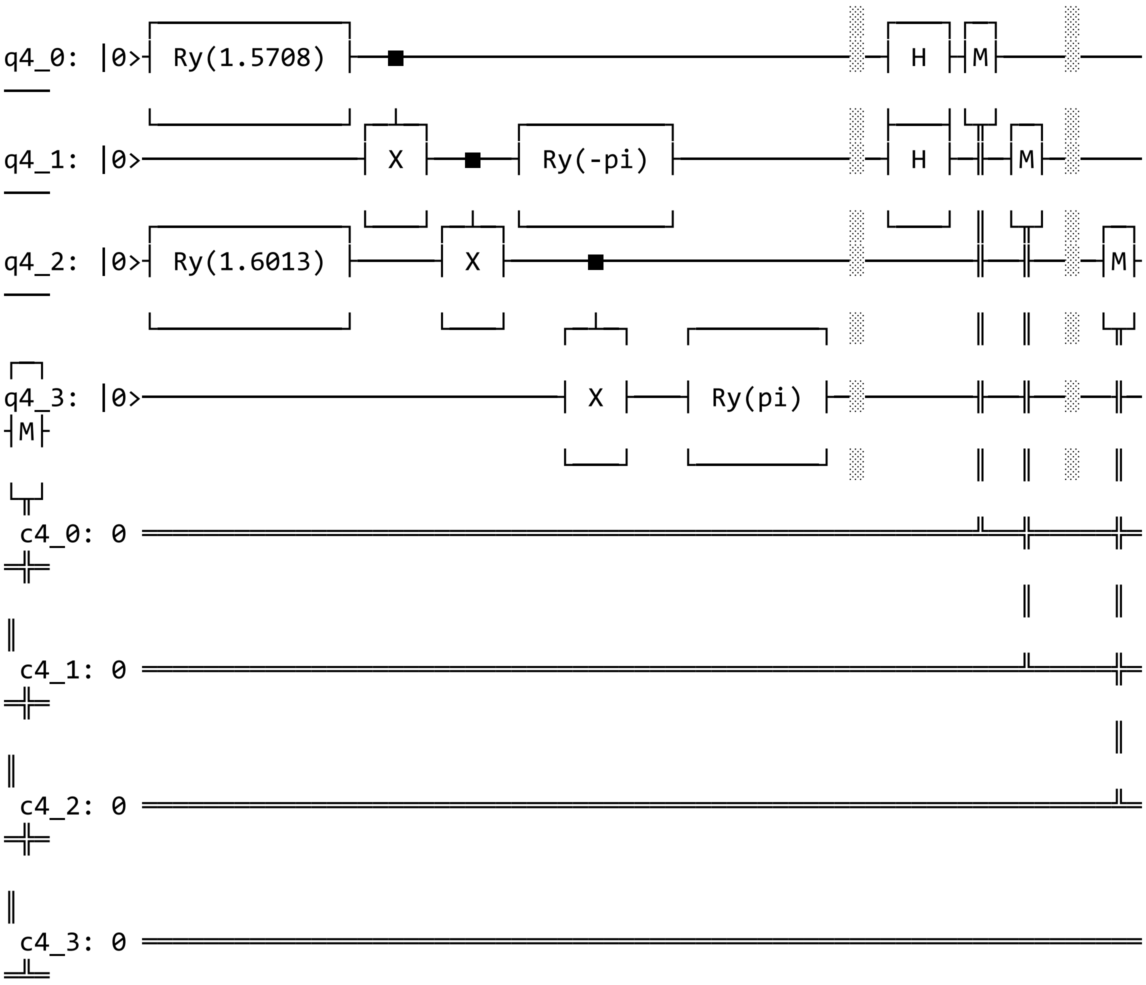
$$\left\langle\psi_{gs}\right| H_4 \left|\psi_{gs}\right\rangle = (-a^\dagger\,\langle 1010| + b^\dagger\,\langle 0110| + c^\dagger\,\langle 1001| - d^\dagger\,\langle 0101|)(-a\,|1001\rangle + b\,|1010\rangle + c\,|0101\rangle - d$$

$$\langle H_4\rangle = -(ac^\dagger)_{|1001\rangle} - (bd^\dagger)_{|1010\rangle} - (ca^\dagger)_{|0101\rangle} - (db^\dagger)_{|0110\rangle}$$

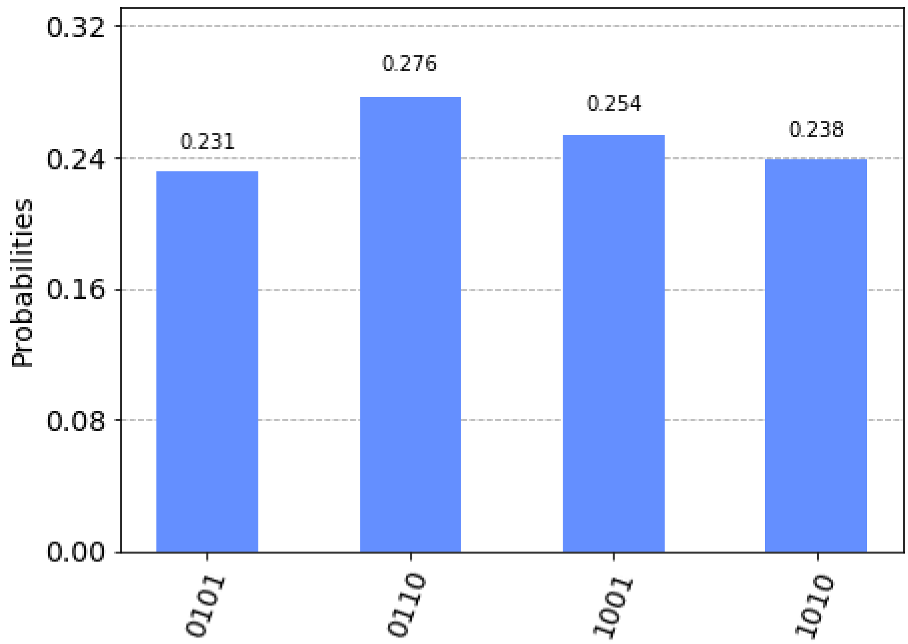
$$\langle H_4 \rangle = -0.254 - 0.238 - 0.231 - 0.276 = -1$$

In [8]:

```
two_site_ham(4)
```



Out[8]:



Measurement of the fith term:

$$H_5 = \hat{\sigma}^y_1 \hat{\sigma}^y_2.$$

$$H_5 \left|\psi_{gs}\right\rangle = \hat{\sigma}^y_1 \hat{\sigma}^y_2 (-a\left|0101\right\rangle + b\left|0110\right\rangle + c\left|1001\right\rangle - d\left|1010\right\rangle)$$

$$H_5 \left|\psi_{gs}\right\rangle = i^2 a\left|1001\right\rangle - i^2 b\left|1010\right\rangle - i^2 c\left|0101\right\rangle + i^2 d\left|0110\right\rangle$$

$$\left\langle\psi_{gs}\right| H_5 \left|\psi_{gs}\right\rangle = (-a^\dagger \left\langle 1010\right| + b^\dagger \left\langle 0110\right| + c^\dagger \left\langle 1001\right| - d^\dagger \left\langle 0101\right|)(-a\left|1001\right\rangle + b\left|1010\right\rangle + c\left|0101\right\rangle - d$$

$$\langle H_5\rangle = -(ac^\dagger)_{\left|1001\right\rangle} - (bd^\dagger)_{\left|1010\right\rangle} - (ca^\dagger)_{\left|0101\right\rangle} - (db^\dagger)_{\left|0110\right\rangle}$$

$$\langle H_5\rangle = -0.252 - 0.257 - 0.238 - 0.253 = -1$$

In [9]:

```
1 two_site_ham(5)
```

```
         ┌────────────┐                                  ░ ┌─────┐┌───┐┌─┐
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q5_0: |0>┤ Ry(1.5708) ├─■────────────────────────────────░─┤ Sdg ├┤ H ├┤M├───
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         └────────────┘┌─┴─┐     ┌─────────┐             ░ ├─────┤├───┤└╥┘┌─┐
░ »
q5_1: |0>──────────────┤ X ├──■──┤ Ry(-pi) ├─────────────░─┤ Sdg ├┤ H ├─╫─┤M├─
░─»
         ┌────────────┐└───┘┌─┴─┐└─────────┘             ░ └─────┘└───┘ ║ └╥┘
░ »
q5_2: |0>┤ Ry(1.6013) ├─────┤ X ├───■────────────────────░──────────────╫──╫─
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         └────────────┘     └───┘ ┌─┴─┐  ┌────────┐      ░               ║  ║
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q5_3: |0>─────────────────────────┤ X ├──┤ Ry(pi) ├──────░──────────────╫──╫─
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                                  └───┘  └────────┘      ░               ║  ║
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 c5_1: 0 ══════════════════════════════════════════════════════════════════╩═
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 c5_2: 0 ════════════════════════════════════════════════════════════════════
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 c5_3: 0 ════════════════════════════════════════════════════════════════════
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«      └╥┘┌─┐
«q5_3: ─╫─┤M├
«       ║ └╥┘
«c5_0: ═╬══╬═
«       ║  ║
«c5_1: ═╬══╬═
«       ║  ║
«c5_2: ═╩══╬═
«          ║
«c5_3: ════╩═
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```
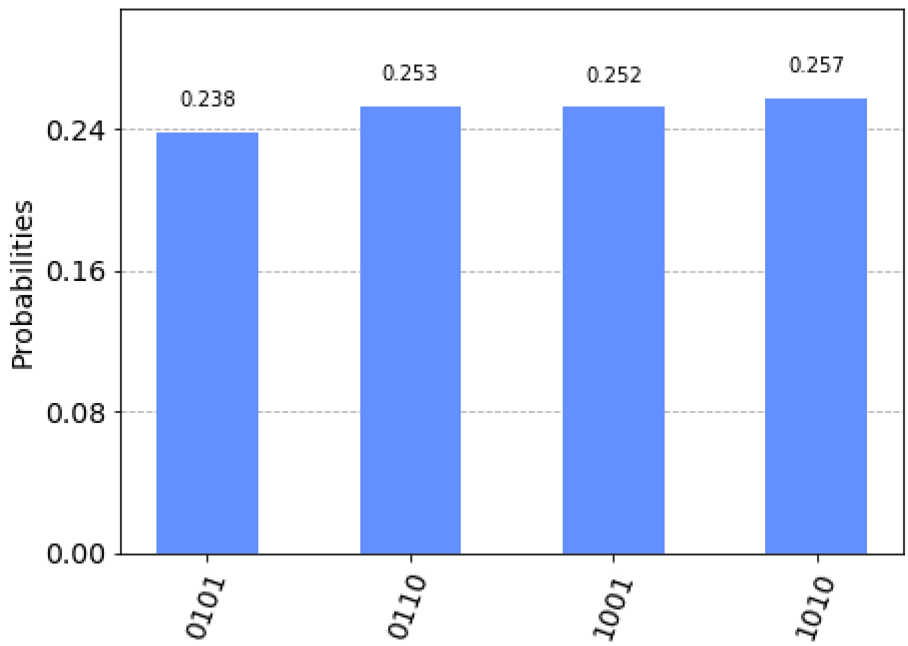

Out[9]:



Measurement of the fith term:

$$H_6 = \hat{\sigma}_3^x \hat{\sigma}_4^x .$$

$$H_6 \left|\psi_{gs}\right\rangle = \hat{\sigma}_3^x \hat{\sigma}_4^x (-a\left|0101\right\rangle + b\left|0110\right\rangle + c\left|1001\right\rangle - d\left|1010\right\rangle)$$

$$H_6 \left|\psi_{gs}\right\rangle = -a\left|0110\right\rangle + b\left|0101\right\rangle + c\left|1010\right\rangle - d\left|1001\right\rangle$$

$$\left\langle\psi_{gs}\right| H_6 \left|\psi_{gs}\right\rangle = (-a^\dagger \left\langle 1010\right| + b^\dagger \left\langle 0110\right| + c^\dagger \left\langle 1001\right| - d^\dagger \left\langle 0101\right|)(-a\left|0110\right\rangle + b\left|0101\right\rangle + c\left|1010\right\rangle - d$$

$$\langle H_6\rangle = -(ab^\dagger)_{|0110\rangle} - (ba^\dagger)_{|0101\rangle} - (cd^\dagger)_{|1010\rangle} - (dc^\dagger)_{|1001\rangle}$$

$$\langle H_6\rangle = -0.260 - 0.260 - 0.231 - 0.249 = -1$$

In [10]:

```
1 two_site_ham(6)
```

```
         ┌────────────┐                                                  ░                ░ ┌─┐
q6_0: |0>┤ Ry(1.5708) ├──■───────────────────────────────────────────────░────────────────░─┤M├───
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         └────────────┘┌─┴─┐     ┌─────────┐                             ░                ░ └╥┘┌─
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q6_1: |0>──────────────┤ X ├──■──┤ Ry(-pi) ├─────────────────────────────░────────────────░──╫─┤M
├
         ┌────────────┐└───┘┌─┴─┐└─────────┘                             ░ ┌───┐┌─┐       ░  ║ └╥
┘
q6_2: |0>┤ Ry(1.6013) ├─────┤ X ├─────■──────────────────────────────────░─┤ H ├┤M├───────░──╫──╫
─
         └────────────┘     └───┘   ┌─┴─┐     ┌────────┐                 ░ ├───┤└╥┘┌─┐    ░  ║  ║
q6_3: |0>───────────────────────────┤ X ├─────┤ Ry(pi) ├─────────────────░─┤ H ├─╫─┤M├────░──╫──╫
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                                    └───┘     └────────┘                 ░ └───┘ ║ └╥┘    ░  ║  ║
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```
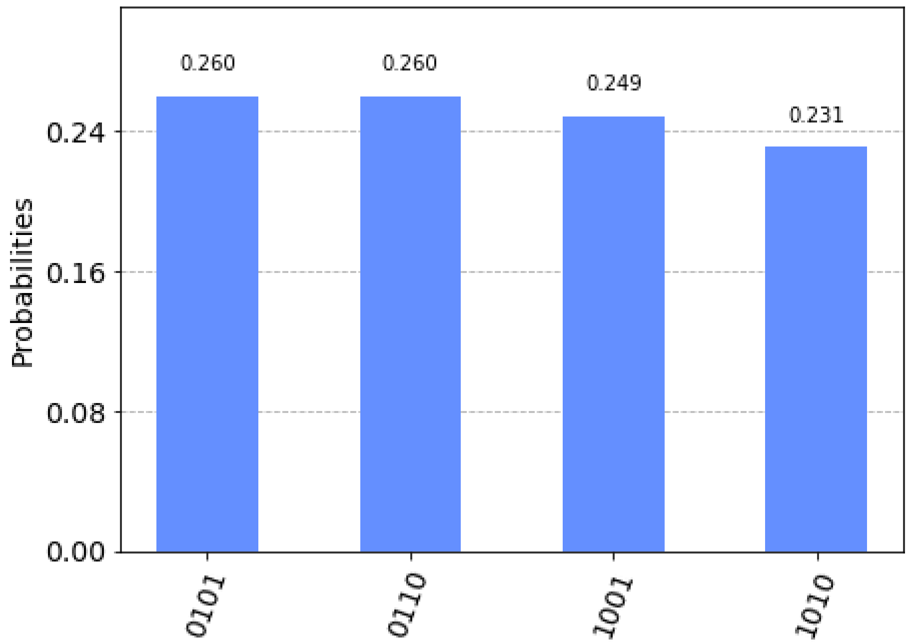

Out[10]:



Measurement of the fith term:

$$H_7 = \hat{\sigma}_3^y \hat{\sigma}_4^y.$$

$$H_7 \left|\psi_{gs}\right\rangle = \hat{\sigma}_3^y \hat{\sigma}_4^y(-a\left|0101\right\rangle + b\left|0110\right\rangle + c\left|1001\right\rangle - d\left|1010\right\rangle)$$

$$H_7 \left|\psi_{gs}\right\rangle = i^2 a\left|0110\right\rangle - i^2 b\left|0101\right\rangle - i^2 c\left|1010\right\rangle + i^2\left|1001\right\rangle$$
$$\left\langle\psi_{gs}\right| H_7 \left|\psi_{gs}\right\rangle = (-a^\dagger\left\langle 1010\right| + b^\dagger\left\langle 0110\right| + c^\dagger\left\langle 1001\right| - d^\dagger\left\langle 0101\right|)(-a\left|0110\right\rangle + b\left|0101\right\rangle + c\left|1010\right\rangle - d$$

$$\langle H_7\rangle = -(ab^\dagger)_{|0110\rangle} - (ba^\dagger)_{|0101\rangle} - (cd^\dagger)_{|1010\rangle} - (dc^\dagger)_{|1001\rangle}$$

$$\langle H_7\rangle = 0.260 - 0.267 - 0.228 - 0.246 = -1$$

In [11]:

```
1 two_site_ham(7)
```

```
         ┌────────────┐                                          ░                         
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q7_0: |0>┤ Ry(1.5708) ├──■───────────────────────────────────────░─────────────────────────
░─»
         └────────────┘┌─┴─┐     ┌─────────┐                     ░                         
░ »
q7_1: |0>──────────────┤ X ├──■──┤ Ry(-pi) ├─────────────────────░─────────────────────────
░─»
         ┌────────────┐└───┘┌─┴─┐└─────────┘                     ░ ┌─────┐┌───┐┌─┐        
░ »
q7_2: |0>┤ Ry(1.6013) ├─────┤ X ├───────■────────────────────────░─┤ Sdg ├┤ H ├┤M├────────
░─»
         └────────────┘     └───┘     ┌─┴─┐   ┌─────────┐        ░ ├─────┤├───┤└╥┘┌─┐     
░ »
q7_3: |0>─────────────────────────────┤ X ├───┤ Ry(pi)  ├────────░─┤ Sdg ├┤ H ├─╫─┤M├─────
░─»
                                      └───┘   └─────────┘        ░ └─────┘└───┘ ║ └╥┘     
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«      ┌─┐   
«q7_0: ┤M├───
«      └╥┘┌─┐
«q7_1: ─╫─┤M├
«       ║ └╥┘
«q7_2: ─╫──╫─
«       ║  ║ 
«q7_3: ─╫──╫─
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«c7_0: ═╩══╬═
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«c7_1: ════╩═
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«            
«c7_3: ══════
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```
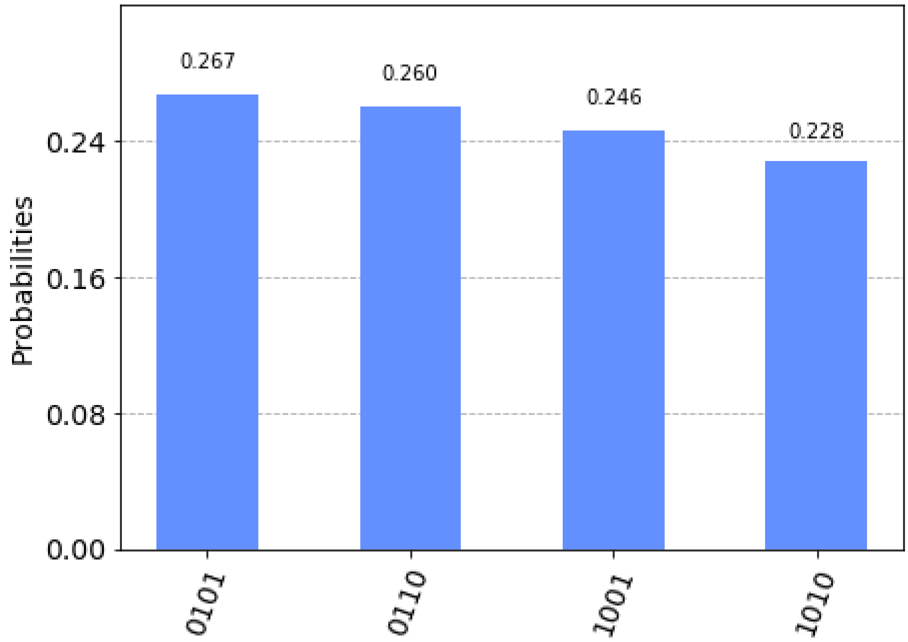

Out[11]:



$$\hat{H} = \frac{U}{4}\hat{\sigma}_1^z\hat{\sigma}_3^z + \left(\frac{\mu}{2} - \frac{U}{4}\right)(\hat{\sigma}_1^z + \hat{\sigma}_3^z)$$

$$+ \frac{V}{2}(\hat{\sigma}_1^x\hat{\sigma}_2^x + \hat{\sigma}_1^y\hat{\sigma}_2^y + \hat{\sigma}_3^x\hat{\sigma}_4^x + \hat{\sigma}_3^y\hat{\sigma}_4^y)$$

$$U = 0.3$$
$$V = 1.23$$
$$\mu = 0.15$$

The result for $\hat{H}$ using Qiskit:
$\langle \hat{H} \rangle = -0.025\frac{0.3}{4} + (\frac{0.15}{2} - \frac{0.3}{4})(-0.006 + 0.021) + \frac{1.23}{2}(-4) = -0.001875 - 2.46 = -2.461875$

The mathematica calculated value for the Hamiltonian descibing the 2-site DMFT system:

$$\langle \hat{H} \rangle = -2.53614$$

The difference between the measurements of the Hamiltonian using Qiskit and Mathematica differ due to the random nature of quantum mechanics. The results differ by 0.074.

In [ ]:

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