In [1]:

```
################################  All necessary imports  ##########################
import numpy as np
from scipy.optimize import minimize
import matplotlib.pyplot as plt
from qiskit import *
%matplotlib inline
plt.style.use('ggplot')
```

Find the lowest eigen value of the matrix below using VQE

Contents:

1. Exact solution using Numpy linalg module
2. Pauli gate decomposition and its verification
3. Expeectation value calculation on quantum computer
4. Measurement and basis transformation
5. Variational Ansatz: 2 trial wave functions
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7. VQE with scipy optimizer using Ansatz-1
8. VQE with scipy optimizer using Ansatz-2

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

We can evaluate the lowest eigen values by using Numpy library

1. Exact solution with Numpy linalg module

In [2]:

```
M = np.array([[1,0,0,0],
              [0,0,-1,0],
              [0,-1,0,0],
              [0,0,0,1]])

eig_vals,eig_vecs = np.linalg.eig(M)


print('Our given matrix is:\n\n',M)
print('\nEigen values are:',eig_vals)
print('\nLowest eigen value is:',round(eig_vals.min()))
```

```
Our given matrix is:

 [[ 1  0  0  0]
 [ 0  0 -1  0]
 [ 0 -1  0  0]
 [ 0  0  0  1]]

Eigen values are: [ 1. -1.  1.  1.]

Lowest eigen value is: -1.0
```

2. Solving this using VQE requires Pauli gate decomposition

Decomposition of M matrix into a sum of 2-qubit operators,

$$H = aX_1 \otimes X_2 + bY_1 \otimes Y_2 + cZ_1 \otimes Z_2 + dI_1 \otimes I_2$$

where the subscripts $1, 2$ denote the first and second qubit on which the operator acts on, and $\otimes$ indicates the tensor product, and a, b, c, d are the coefficients. Pauli matrices X, Y, Z are,

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Here XX,YY,ZZ and II are,

$$XX = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \qquad YY = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}, \qquad ZZ = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \qquad II =$$

Respective coefficients can be found by solving linear equation analytically,

$$a = -0.5, b = -0.5, c = 0.5, d = 0.5$$

M in 2 qubit pauli operator decomposed format is

$$M = \frac{1}{2}(-X_1 \otimes X_2 - Y_1 \otimes Y_2 + Z_1 \otimes Z_2 + I_1 \otimes I_2),$$

Verification of pauli decomposition

In [3]:

```
############   checking the result of Pauli decomposition   #################

X = np.array([[0,1],[1,0]])       # pauli's sigma-x matrix
Y = np.array([[0, -1j],[1j, 0]])  # pauli's sigma-y matrix
Z = np.array([[1,0],[0,-1]])      # pauli's sigma-z matrix
I = np.array([[1,0],[0,1]])       # 2X2 Identity matrix



XX = np.kron(X,X)
YY = np.kron(Y,Y)
ZZ = np.kron(Z,Z)
II = np.kron(I,I)

a,b,c,d = -0.5,-0.5,0.5,0.5
M1 = (a*XX) + (b*YY) + (c*ZZ) + (d*II)
print('M1 matrix is\n\n',M1.astype(int),'\n\nPauli decomposition verified:',np.arra
```

```
M1 matrix is

 [[ 1  0  0  0]
 [ 0  0 -1  0]
 [ 0 -1  0  0]
 [ 0  0  0  1]]

Pauli decomposition verified: True
```

3. Expectation value calculation on Quantum computer

General 2 qubit state can be represented as,

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

Expectation value of the above operator M on $\langle\psi\rangle$,

$$E = \langle\psi| M |\psi\rangle$$

Now if we want to measure expectation value of any operator (say, $Z_1 \otimes Z_2$) for the above state on computational basis, it follows

$$\begin{aligned}\langle\psi| Z_1 \otimes Z_2 |\psi\rangle = \alpha_{00}^2 - \alpha_{01}^2 - \alpha_{10}^2 + \alpha_{11}^2 &= (\alpha_{00}^2 + \alpha_{11}^2) - (\alpha_{01}^2 + \alpha_{10}^2) \\ &= (\text{prob}(00) + \text{prob}(11))\text{ - }(\text{prob}(01) + \text{prob}(10)) \\ &= \frac{(\text{count}(00)\text{+count}(11))\text{-}(\text{count}(01)\text{+count}(10))}{\text{shots}}\end{aligned}$$

Hence, we'll also measure other 2 qubit operators $X_1 \otimes X_2$ and $Y_1 \otimes Y_2$ in the computational basis.

4. Measurement and Basis Transformation

We have to measure every observables in their respective basis.

1. The first term in the hamiltonian $X_1 \otimes X_2$ is in the hadamard basis. Since

$$X\left|+\right\rangle = \left|+\right\rangle \qquad X\left|-\right\rangle = -\left|-\right\rangle$$

where

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

So we need to apply some basis transformation such that $\left|+\right\rangle$ goes to $\left|0\right\rangle$ and $\left|-\right\rangle$ goes to $\left|1\right\rangle$. Such a gate is hadamard H gate.

$$H\left|+\right\rangle = \left|0\right\rangle \qquad H\left|-\right\rangle = \left|1\right\rangle$$

So, we will apply hadamard gate on both qubits before measurement. We could have used $R_y(-\pi/2)$ or U_3 on both qubits.

so,

$$X_1 \otimes X_2 = (H_1 \otimes H_2)^\dagger Z_1 \otimes Z_2 \, (H_1 \otimes H_2)\,,$$

2. The 2nd term $Y_1 \otimes Y_2$ is also not in the Z basis. Y has two eigen vectors,

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

In this case our transformation will be $HS^\dagger$, which will be applied to every qubit before measurement as,

$$HS^\dagger\left|+i\right\rangle = \left|0\right\rangle \qquad HS^\dagger\left|-i\right\rangle = \left|1\right\rangle$$

We could have used $R_x(\pi/2)$ or $U_3(\pi/2, 0, \pi/2)$ gate on each qubits. So,

$$Y_1 \otimes Y_2 = \left(H_1S_1^\dagger \otimes H_2S_2^\dagger\right)^\dagger Z_1 \otimes Z_2 \left(H_1S_1^\dagger \otimes H_2S_2^\dagger\right),$$

where,

$$S^\dagger = \begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix} \qquad H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

3. $Z_1 \otimes Z_2$ is already in Z basis, so we dont need to do any basis transformation.

4. The 4th term $I_1 \otimes I_2$ is just a constant. No measurement is required.

These identities allow us to write our original matrix M as the sum of operators

$$M = -\frac{1}{2}(H_1 \otimes H_2)^\dagger \, (Z_1 \otimes Z_2)\,(H_1 \otimes H_2) - \frac{1}{2}\left(H_1S_1^\dagger \otimes H_2S_2^\dagger\right)^\dagger (Z_1 \otimes Z_2)\left(H_1S_1^\dagger \otimes H_2S_2^\dagger\right) +$$

The expectation value of the above matrix on the state $\left|\psi\right\rangle$ is given as

$$\left\langle\psi\right| M \left|\psi\right\rangle = -\frac{1}{2}\left\langle\phi_1\right|(Z_1 \otimes Z_2)\left|\phi_1\right\rangle - \frac{1}{2}\left\langle\phi_2\right|(Z_1 \otimes Z_2)\left|\phi_2\right\rangle + \frac{1}{2}\left\langle\psi\right|(Z_1 \otimes Z_2)\left|\psi\right\rangle + \frac{1}{2}$$

where new states $\left|\phi_1\right\rangle$ and $\left|\phi_2\right\rangle$ are

$$\left|\phi_1\right\rangle = (H_1 \otimes H_2)\left|\psi\right\rangle,$$
$$\left|\phi_2\right\rangle = \left(H_1S_1^\dagger \otimes H_2S_2^\dagger\right)\left|\psi\right\rangle$$

In [4]:

```
## All the necessary functions for the algorithm are written here ##

def XX(theta):
    """
    Gives expectation value of XX
    sub-hamiltonian from measurement
    on parametric state.
    :param theta: angle in radian
    :return: expectation value of XX
    """
    circuit = ansatz(theta)
    q = circuit.qregs[0]
    c = circuit.cregs[0]
    ###########  Transformation on XX ###########

    circuit.h(q[0])              #circuit.ry(-np.pi/2, q[0])
    circuit.h(q[1])              #circuit.ry(-np.pi/2, q[1])

    ############  XX measurement  ##############
    circuit.measure(q,c)
    exp_XX = measurement(circuit)
    return exp_XX

def YY(theta):
    """
    Gives expectation value of YY
    sub-hamiltonian from measurement
    on parametric state.
    :param theta: angle in radian
    :return: expectation value of YY
    """
    circuit = ansatz(theta)
    q = circuit.qregs[0]
    c = circuit.cregs[0]
    ########### Transformation on YY #########

    circuit.sdg(q[0])           #circuit.rx(np.pi/2, q[0])
    circuit.h(q[0])             #circuit.rx(np.pi/2, q[1])
    circuit.sdg(q[1])
    circuit.h(q[1])

    ############ YY Measurement ###########
    circuit.measure(q,c)
    exp_YY = measurement(circuit)
    return exp_YY

def ZZ(theta):
    """
    Gives expectation value of ZZ
    sub-hamiltonian from measurement
    on parametric state.
    :param theta: angle in radian
    :return: expectation value of ZZ
    """
    circuit = ansatz(theta)
    q = circuit.qregs[0]
    c = circuit.cregs[0]

    ###########  ZZ measurement ###############
```

```
    circuit.measure(q,c)
    exp_ZZ = measurement(circuit)
    return exp_ZZ

def vqe(theta):    #------------------- creates ansatz measures and performs additi
    """
    Contains the complete Hamiltonian
    :param theta: angle is radian
    :return: expectation value of whole hamiltonian
    """                                                                  # H = aXX +
    E = (-0.5*XX(theta)) + (-0.5*YY(theta)) + (0.5*ZZ(theta)) + 0.5    #Hamiltonian
    return E

def key_check(my_dict: dict, my_key: str):
    """
    If key is missing returns 0
    otherwise the corresponding value.
    :param my_dict: the dictionary
    :param my_key: key (string)
    :return: 0 or value corresponding to key
    """
    response = 0
    if my_key in my_dict:
        response = my_dict[my_key]
    return response


def measurement(circuit):  # ------------------ Takes a quantum circuit and perform
    """
    Takes the quantum circuit as
    input to perform measurement
    :param circuit: quantumm circuit
    :return: expectation value
    """
    shots =1024
    backend = BasicAer.get_backend('qasm_simulator')
    job = execute(circuit, backend, shots=shots)
    result = job.result()
    counts = result.get_counts()

    n00 = key_check(counts,'00')
    n01 = key_check(counts,'01')
    n10 = key_check(counts,'10')
    n11 = key_check(counts,'11')
    expectation_value = ((n00+n11)-(n01+n10))/shots
    return expectation_value
```

5. Variational Ansatz : Trial wave function

According to the theory of Variational methods for Quantum mechanics, to measure the expectation value of M we need a trial wave function or ansatz $|\psi(\theta)\rangle$.

$$E(\theta) = \langle\psi(\theta)|\, M \,|\psi(\theta)\rangle$$

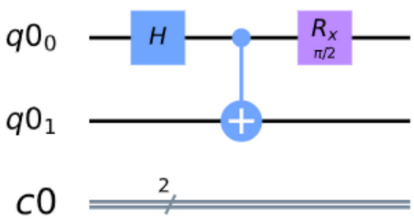
Here we have discussed the solution with two ansatz.

Ansatz 1: Given in the question of Task 4 with 1 parametric $R_x(\theta)$ gate

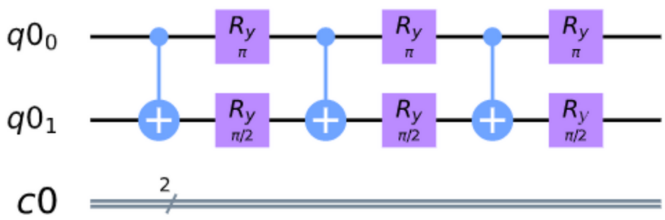
$$|\psi(\theta)\rangle_1 = (R_x(\theta) \otimes I)CX(H \otimes I)\,|00\rangle\,.$$

Ansatz 2: Circuit with 6 parametric $R_y(\theta)$ gates

$$|\psi(\theta)\rangle_2 = CX(R_y(\theta_0) \otimes R_y(\theta_1))CX(R_y(\theta_0) \otimes R_y(\theta_1))CX(R_y(\theta_0) \otimes R_y(\theta_1))\,|00\rangle\,.$$



Ansatz 1



Ansatz 2

Attention! Mechanism of $ansatz(\theta)$ function $|\psi(\theta)\rangle$

A single function is presented below for both ansatz. The working mechanism is little different. The $theta - \theta$ in function $ansatz(theta)$ is a list or array with one or two elements. When $theta - \theta$ with one-parameter(list or array with one element) is passed into $ansatz(theta)$, it automatically starts using Ansatz-1, as there is only one parametric angle is Ansatz-1. Similarly if we pass $theta - \theta$ list or array with 2 parameters (list or array with 2 elements), the $ansatz(theta)$ function will use Ansatz-2.

In [5]:

```
def ansatz(theta):
    """
    Creates ANSATZ with an
    angle taking as parameter &
    returns a quantum circuit.
    :param theta: angle in radian
    :return: quantum circuit
    """
    q = QuantumRegister(2)
    c = ClassicalRegister(2)
    circuit = QuantumCircuit(q,c)
    if len(theta) ==1:    #--------------- Ansatz 1
        circuit.h(q[0])
        circuit.cx(q[0],q[1])
        circuit.rx(theta[0],q[0])
        return circuit
    elif len(theta)==2:   #--------------- Ansatz 2
        for i in range(3):  #----------------circuit depth
            circuit.cx(q[0],q[1])
            circuit.ry(theta[0],q[0])
            circuit.ry(theta[1],q[1])
        return circuit
```

As Ansatz-1 contains one parametric angle, it is easier to search over all spaces from 0 to 2π , but for Ansatz-2 there are 6 parametric gates (taking depth of the circut into account), which is little difficult for searching. Hence, searching is performed with Ansatz-1. Later on there are solutions using Scipy optimizers with Ansatz-1 and Ansatz-2 both.

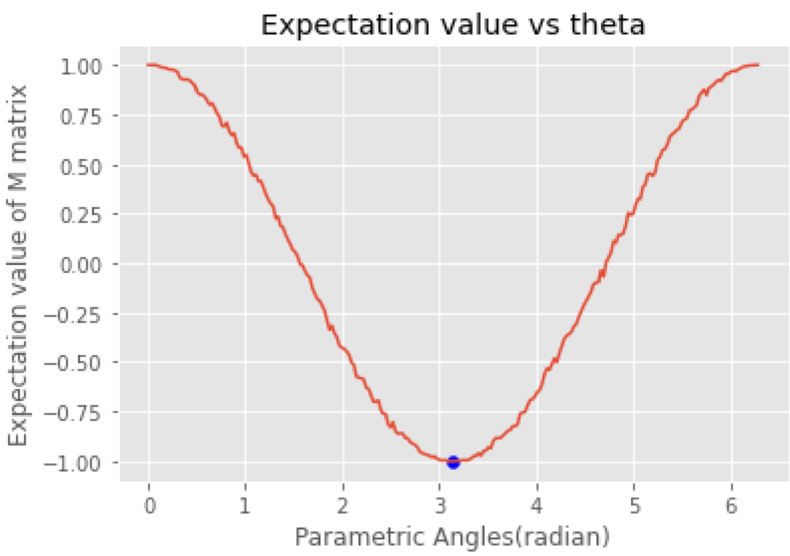
6. θ exploration of $R_x(\theta)$ with Ansatz 1

Ansatz 1 uses one parametric gate $R_x(\theta)$. Here N equispaced angles are introduced between 0 to 2π and for each angle (theta) expectation value is calculated using for loop. No optimizer is used here.

In [6]:

```
#################   Exploration   ###############
N =  250
all_angles = np.linspace(0,2*np.pi,N)
angles = []        #---------------------------------- list for storing Parametric a
energies = []      #---------------------------------- list for storing eigen values
print("Search in progress.... Please wait!")

for theta in all_angles.reshape(N,1):
    E = vqe(theta)
    angles.append(theta)
    energies.append(E)
    #print('Parametric angle is {} and energy eigen value is {} \n'.format(round(fl


print('\n \n \nMinimum energy eigen value is:',min(energies))
print('Angle corresponds to this energy is {} radian\n'.format(round(all_angles[np.

plt.plot(angles,energies)
plt.scatter(all_angles[np.argmin(energies)],min(energies),color='blue')
plt.title('Expectation value vs theta', color='k')
plt.xlabel('Parametric Angles(radian)')
plt.ylabel('Expectation value of M matrix')
plt.show()
```

```
Search in progress.... Please wait!



Minimum energy eigen value is: -1.0
Angle corresponds to this energy is 3.12898 radian
```



In VQE state preparation and measurement is carried by Quantum module (QPU)

and optimization of the angle of the parametric gates are done by classical optimizers (CPU).

7. Finding solution of VQE with Ansatz 1 using Scipy optimizer

One parametric angle is passed within the $theta$.Function $ansatz(theta)$ will use Ansatz-1

In [7]:

```
###########  VQE by Scipy Optimizers with Ansatz 1 ##############

theta = [2] #------------- One parameter in the list


result = minimize(vqe, theta, method="Powell")  # Powell, COBYLA, Nelder-Mead and o
print(result.message)
print('\nLowest eigen value of M using VQE with ansatz_1 is {}'.format(result.fun))
print('Parametric angle is {} radian.'.format(round(float(result.x),5)))
print('Success Status:',result.success)
```

```
Optimization terminated successfully.

Lowest eigen value of M using VQE with ansatz_1 is -1.0
Parametric angle is 3.13097 radian.
Success Status: True
```

8. Finding solution of VQE with Ansatz 2 using Scipy optimizer

Two parametric angles are passed within the $theta$. Function $ansatz(theta)$ will use Ansatz-2. These 2 angles will be used in 6 parametric gates as the depth is 3.

In [8]:

```
###########  VQE by Scipy Optimizers with Ansatz 2  ##############

theta = [2,2]  #---------------------- 2 parameters in the list


result = minimize(vqe, theta, method="Powell")  # Powell, Nelder-Mead, COBYLA  and
print(result.message)
print('\nLowest eigen value of M using VQE with ansatz_2 is {}'.format(result.fun))
print('Success Status:',result.success)
```

```
Optimization terminated successfully.

Lowest eigen value of M using VQE with ansatz_2 is -1.0
Success Status: True
```

In [ ]:

```

```