QOSF Mentorship Assessment Task

Applicant: Utkarsh, *Center for Computational Natural Sciences and Bioinformatics, IIIT Hyderabad*

Question:

Find the lowest eigenvalue of the following matrix:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

using VQE-like circuits, created by yourself from scratch.

Solution:

My solution involves usage of Qiskit platform and is based on a very generalizable approach, i.e., not restrictive to the current Hamiltonian itself and can be outlined as follows:

1. Hamiltonian in Pauli Basis
2. Calculations of Expectation Value
3. Designing Ansatze
4. Running Simulations
5. Running Noisy Simulations
6. Extension to Excited Energy States
7. Interpreting the Results

Necessary Imports

In [1]:
```
import numpy as np
import scipy as sp
import itertools
import functools as ft
%matplotlib notebook
import matplotlib.pyplot as plt
from mpl_toolkits import mplot3d
import re
```

In [2]:
```
#!pip install qiskit
from qiskit import *
from qiskit.providers.aer.noise import NoiseModel
from qiskit.providers.aer.noise import QuantumError, ReadoutError
from qiskit.providers.aer.noise import phase_amplitude_damping_error
from qiskit.providers.aer.noise import depolarizing_error
from qiskit.providers.aer.noise import thermal_relaxation_error
from qiskit.ignis.mitigation.measurement import complete_meas_cal, CompleteMeasFitter
```

Hamiltonian in Pauli Basis

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The normalized Pauli matrices $\{\sigma_0, \sigma_x, \sigma_y, \sigma_z\}/\sqrt{2}$ form an orthogonal basis of $\mathcal{M}_2$, this vector space can be endowed with a scalar product called the Hilbert-Schmidt inner product: $\langle A, B\rangle = Tr(A^\dagger B)$. Since the Pauli matrices anticommute, their product is traceless, and since they are Hermitian this implies that they are orthogonal with respect to that scalar product. Hence this property can be used for decomposing a Hamiltonian as:

$$H = \sum_{i_1,\ldots,i_n=\{0,x,y,z\}} h_{i_1,\ldots,i_n} \cdot \frac{1}{2^n} \sigma_{i_1} \otimes \ldots \otimes \sigma_{i_n}$$

$$h_{i_1,\ldots,i_n} = \frac{1}{2^n} \mathrm{Tr}\big((\sigma_{i_1} \otimes \ldots \otimes \sigma_{i_n})^\dagger \cdot H\big) = \frac{1}{2^n} \mathrm{Tr}\big((\sigma_{i_1} \otimes \ldots \otimes \sigma_{i_n}) \cdot H\big)$$

Decomposing Hamiltonian into Pauli Terms

In [3]:
```
def decompose_ham_to_pauli(H):
    """Decomposes a Hermitian matrix into a linear combination of Pauli operators.

    Args:
        H (array[complex]): a Hermitian matrix of dimension 2**n x 2**n.

    Returns:
        tuple[list[float], list[string], list [ndarray]]: a list of coefficients,
        a list of corresponding string representation of tensor products of Pauli
        observables that decompose the Hamiltonian, and
        a list of their matrix representation as numpy arrays
```

```
    """

    n = int(np.log2(len(H)))
    N = 2 ** n

    # Sanity Checks
    if H.shape != (N, N):
        raise ValueError(
            "The Hamiltonian should have shape (2**n, 2**n), for any qubit number n>=1"
        )

    if not np.allclose(H, H.conj().T):
        raise ValueError("The Hamiltonian is not Hermitian")

    sI = np.eye(2, 2, dtype=complex)
    sX = np.array([[0, 1], [1, 0]], dtype=complex)
    sZ = np.array([[1, 0], [0,-1]], dtype=complex)
    sY = complex(0,-1)*np.matmul(sZ,sX)
    paulis = [sI, sX, sY, sZ]
    paulis_label = ['I', 'X', 'Y', 'Z']
    obs = []
    coeffs = []
    matrix = []

    for term in itertools.product(paulis, repeat=n):
        matrices = [pauli for pauli in term]
        coeff = np.trace(ft.reduce(np.kron, matrices) @ H) / N
        coeff = np.real_if_close(coeff).item()

        # Hilbert-Schmidt-Product
        if not np.allclose(coeff, 0):
            coeffs.append(coeff)
            obs.append(''.join([paulis_label[[i for i, x in enumerate(paulis)
            if np.all(x == t)][0]]+str(idx) for idx, t in enumerate(reversed(term))]))
            matrix.append(ft.reduce(np.kron, matrices))

    return obs, coeffs , matrix
```

Composing Hamiltonian into Pauli Terms

In [4]:

```
def compose_ham_from_pauli(terms, coeffs):
    """Composes a Hermitian matrix from a linear combination of Pauli operators.

    Args:
        tuple[list[float], list[string]]: a list of coefficients,
        a list of corresponding string representation of tensor products of
        Pauli observables that decompose the Hamiltonian.

    Returns:
        H (array[complex]): a Hermitian matrix of dimension 2**n x 2**n.
    """

    pauli_qbs = [re.findall(r'[A-Za-z]|-?\d+\.\d+|\d+', x) for x in terms]
    qubits = max([max(list(map(int, x[1:][::2]))) for x in pauli_qbs])

    N = int(2**np.ceil(np.log2(qubits+1)))

    sI = np.eye(2, 2, dtype=complex)
    sX = np.array([[0, 1], [1, 0]], dtype=complex)
    sZ = np.array([[1, 0], [0,-1]], dtype=complex)
    sY = complex(0,-1)*np.matmul(sZ,sX)
    paulis = [sI, sX, sY, sZ]
    paulis_label = ['I', 'X', 'Y', 'Z']
    paulis_term = {'I':sI, 'X':sX, 'Y':sY, 'Z':sZ}
    hamil = np.zeros((2**N, 2**N), dtype=complex)

    for coeff, pauli_qb in zip(coeffs, pauli_qbs):
      term_str = ['I'] * N
      for term, index in zip(pauli_qb[0:][::2], pauli_qb[1:][::2]):
        term_str[int(index)] = term
      matrices = [paulis_term[pauli] for pauli in term_str]
      term_matrix = np.asarray(ft.reduce(np.kron, matrices[::-1]))
      hamil += coeff*term_matrix

    # Sanity Check
    if not np.allclose(hamil, hamil.conj().T):
        raise ValueError("The Hamiltonian formed is not Hermitian")

    return hamil
```

Test Hamiltonian

$$H_0 = \begin{bmatrix} 0.7056 & 0 & 0. & 0. \\ 0. & -1.1246 & 0.182 & 0. \\ 0. & 0.182 & 0.4318 & 0. \\ 0. & 0 & 0. & 0.888 \end{bmatrix}$$

In [5]:

```
H0 = np.array([
                [ 0.7056    ,  0.         , -0.        ,  0.        ],
                [ 0.        ,  -1.1246    , 0.182     ,  0.        ],
                [-0.        , 0.182       ,  0.4318   , -0.        ],
                [ 0.        ,  0.         , -0.       ,  0.888     ]
```

```
                ])
H0
```

Out[5]:
```
array([[ 0.7056,  0.    , -0.    ,  0.    ],
       [ 0.    , -1.1246,  0.182 ,  0.    ],
       [-0.    ,  0.182 ,  0.4318, -0.    ],
       [ 0.    ,  0.    , -0.    ,  0.888 ]])
```

In [6]:
```
a, b , c = decompose_ham_to_pauli(H0)
a, b
```

Out[6]:
```
(['I0I1', 'Z0I1', 'X0X1', 'Y0Y1', 'I0Z1', 'Z0Z1'],
 [0.2252, 0.3435, 0.091, 0.091, -0.43470000000000003, 0.5716])
```

$$H_0 = 0.2252 \times I_0I_1 + 0.3435 \times Z_0 - 0.4347 \times Z_1 + 0.91 \times X_0X_1 + 0.91 \times Y_0Y_1 + 0.5716 \times Z_0Z_1$$

In [7]:
```
compose_ham_from_pauli(a, b)
```

Out[7]:
```
array([[ 0.7056+0.j,  0.    +0.j,  0.    +0.j,  0.    +0.j],
       [ 0.    +0.j, -1.1246+0.j,  0.182 +0.j,  0.    +0.j],
       [ 0.    +0.j,  0.182 +0.j,  0.4318+0.j,  0.    +0.j],
       [ 0.    +0.j,  0.    +0.j,  0.    +0.j,  0.888 +0.j]])
```

In [8]:
```
assert(np.isclose(compose_ham_from_pauli(a, b).real, H0).all())
```

Given Hamiltonian

$$H_1 = \begin{bmatrix} 1. & 0 & 0. & 0. \\ 0. & 0 & -1 & 0. \\ 0. & -1 & 0 & 0. \\ 0. & 0 & 0. & 1. \end{bmatrix}$$

In [9]:
```
H1 = np.array([[1, 0, 0, 0],
               [0, 0, -1, 0],
               [0, -1, 0, 0],
               [0, 0, 0, 1]])
H1
```

Out[9]:
```
array([[ 1,  0,  0,  0],
       [ 0,  0, -1,  0],
       [ 0, -1,  0,  0],
       [ 0,  0,  0,  1]])
```

In [10]:
```
a, b, c = decompose_ham_to_pauli(H1)
a, b
```

Out[10]:
```
(['I0I1', 'X0X1', 'Y0Y1', 'Z0Z1'], [0.5, -0.5, -0.5, 0.5])
```

$$H_1 = 0.5 \times (I_0I_1 - X_0X_1 - Y_0Y_1 + Z_0Z_1)$$

In [11]:
```
compose_ham_from_pauli(a, b)
```

Out[11]:
```
array([[ 1.+0.j,  0.+0.j,  0.+0.j,  0.+0.j],
       [ 0.+0.j,  0.+0.j, -1.+0.j,  0.+0.j],
       [ 0.+0.j, -1.+0.j,  0.+0.j,  0.+0.j],
       [ 0.+0.j,  0.+0.j,  0.+0.j,  1.+0.j]])
```

In [12]:
```
assert(np.isclose(compose_ham_from_pauli(a, b).real, H1).all())
```

Calculating the Expectation values

For an n-qubit quantum state, measuring one qubit corresponds to projecting the quantum state onto one of two half-spaces determined by the unique eigenvalues of our measurement operator.

By convention, performing a computational basis measurement is equivalent to measuring in measuring `Pauli Z`, which gives us two eigenvectors $|0\rangle$ and $|1\rangle$, with corresponding eigenvalues ± 1. Therefore, doing a computation measurement of a qubit and obtaining 0 means the state of our qubit is in the $+1$ eigenstate of the Z operator. In general, we can then use the definition of the tensor product to perform multi-qubit measurements as will be explained below.

For some qubit $|\psi\rangle$ we have $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, we can calculate expectation value of a single-qubit operator $M = \sum_m m|m\rangle\langle m|$, as $\langle M\rangle = \langle\psi|\sum_m m|m\rangle\langle m|\psi\rangle = \sum_m m\langle\psi|m^\dagger m|\psi\rangle = \sum_m m\, p(m) = (+1)p(0) + (-1)p(1) = p(0) - p(1)$. Similarly, for a two-qubit operator M we will get $\langle M\rangle = p(00) + p(11) - p(01) - p(10)$.

Change of Basis

Therefore, to measure a qubit, we can use any 2×2 operator that is a unitary transformation of Z. That is, we could also use a measurement operator $M = U^\dagger ZU$, where U is an unitary operator and M gives two unique outcomes of a measurement in its ± 1 eigenvectors. Thereofre, to measure in a basis other than the computational (or Z), we need to find the corresponding unitary equivalence. Similar to the one-qubit case, all two-qubit Pauli-measurements can be written as $(U_1^\dagger \otimes U_2^\dagger)[Z \otimes Z](U_1 \otimes U_2)$ for 2×2 unitary matrices U_1 and U_2.

For X, and Y basis measurements, these unitary equivalence are given below:

$$X = (H)^\dagger ZH$$

$$Y = (HS^\dagger)^\dagger Z (HS^\dagger)$$

This feature can be exploited to create circuits for both X basis and Y basis measurements from the standard Z basis. It is done by applying the corresponding unitary operation to the prepared quantum state and then performing a measurement in Z basis.

For example: In order to do a Y basis measurement, first apply $HS^\dagger$ to the quantum state and then do a normal Z basis measurement.

Similar to the one-qubit case, all multi-qubit Pauli-measurements can be written as a generalization of above.

For example: For two-qubit X basis measurement, $X \otimes X = (H \otimes H)[Z \otimes Z](H \otimes H)$.

Constructing Measurement Circuits

In [13]:
```
def measure_circuit(basis, num_qubits):
    """
    Generate measurement circuit according to the Pauli observable
    string provided.

    Args:
    basis (str): String representation of tensor products of Pauli
    observables
    num_qubits (int): Number of qubits in the circuit

    Returns:
    measure_qc (QuantumCircuit): Measurement Circuit for the
    corresponding basis.

    """

    basis_qb = re.findall(r'[A-Za-z]|-?\d+\.\d+|\d+', basis)
    basis = basis_qb[0:][::2]
    qubit = list(map(int, basis_qb[1:][::2]))

    measure_qc = QuantumCircuit(num_qubits, num_qubits)
    for base, qb in zip(basis, qubit):
      if base == 'I' or base == 'Z':
        pass
      elif base == 'X':
        measure_qc.h(qb)
      elif base == 'Y':
        measure_qc.sdg(qb)
        measure_qc.h(qb)
      else:
        raise ValueError("Wrong Basis provided")

    for qb in range(num_qubits):
        measure_qc.measure(qb, qb)

    return measure_qc
```

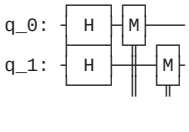
In [14]:
```
def calculate_expecation_val(circuit, basis, shots=2048, backend='qasm_simulator'):
    """
    Calculate expectation value for the measurement of a circuit in a
    given basis.

    Args:
    circuit (QuantumCircuit): Circuit using which expectation value
    will be calculated for a given basis.
    basis (str): String representation of tensor products of Pauli
    observables.
    shots (int): Number of times measurements needed to be done for calculating
    probability.
    backend (str): Backend for running the circuit.

    Returns:
    exp (float): Expectation value for the measurement of a circuit
    in a given basis.

    """
    exp_circuit = circuit + measure_circuit(basis, circuit.num_qubits)

    result = execute(exp_circuit, backend=Aer.get_backend(backend),
                     shots=shots).result()

    exp = 0.0
    for key, counts in result.get_counts().items():
        exp += (-1)**(int(key[0])+int(key[1])) * counts

    return exp/shots
```

Examples

Measurements in XX, YY, ZZ basis

In [15]:
```
measure_circuit('X0X1', 2).draw()
```

Out[15]:



```
c: 2/═══════╩═╩═
            0 1
```

In [16]:
```
measure_circuit('Y0Y1', 2).draw()
```

Out[16]:
```
q_0: ┤ SDG ├┤ H ├┤ M ├──────
q_1: ┤ SDG ├┤ H ├──┤ M ├───
c: 2/═══════════════╩═╩═══
                    0 1
```

In [17]:
```
measure_circuit('Z0Z1', 2).draw()
```

Out[17]:
```
q_0: ┤ M ├──────
q_1: ──┤ M ├───
c: 2/═══╩═╩═══
        0 1
```

Measurements in XY, YZ, ZX basis (To show flexibility of the function)

In [18]:
```
measure_circuit('X0Y1', 2).draw()
```

Out[18]:
```
q_0: ┤ H ├──────┤ M ├──────
q_1: ┤ SDG ├┤ H ├──┤ M ├───
c: 2/═══════════════╩═╩═══
                    0 1
```

In [19]:
```
measure_circuit('Y0Z1', 2).draw()
```

Out[19]:
```
q_0: ┤ SDG ├┤ H ├┤ M ├──────
q_1: ──┤ M ├──────┤ M ├───
c: 2/═══╩═══════════╩═══
        1           0
```

In [20]:
```
measure_circuit('Z0X1', 2).draw()
```

Out[20]:
```
q_0: ──────┤ M ├──────
q_1: ┤ H ├──┤ M ├───
c: 2/═══════╩═╩═══
            0 1
```

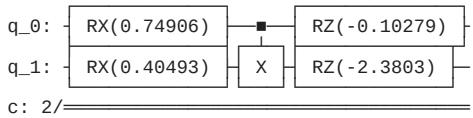
Determining the Ansatz

Designing Ansatze

Ansatze are simply a parameterized quantum circuits (PQC), which play an essential role in the performance of many variational hybrid quantum-classical (HQC) algorithms. Major challenge while designing an asatz is to choose an effective template circuit that well represents the solution space while maintaining a low circuit depth and number of parameters. Here, we make a choice of two ansatze, one randomly and another inspired from the given hint.

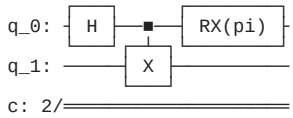
Ansatz 1 (Random Choice)

In [21]:
```
def ansatz1(params, num_qubits):
    """
    Generate an templated ansatz with given parameters

    Args:
    params (array[float]): Parameters to initialize the parameterized unitary.
    num_qubits (int): Number of qubits in the circuit.

    Returns:
    ansatz (QuantumCircuit): Generated ansatz circuit

    """

    ansatz = QuantumCircuit(num_qubits, num_qubits)
    params = params.reshape(2,2)

    for idx in range(num_qubits):
      ansatz.rx(params[0][idx], idx)

    ansatz.cnot(0, 1)

    for idx in range(num_qubits):
      ansatz.rz(params[1][idx], idx)

    return ansatz

ansatz1(np.random.uniform(-np.pi, np.pi, (2,2)), 2).draw()
```

Out[21]:


Ansatz 2 (From Hint)

In [22]:
```python
def ansatz2(params, num_qubits):
    """
    Generate an templated ansatz with given parameters

    Args:
    params (array[float]): Parameters to initialize the parameterized unitary.
    num_qubits (int): Number of qubits in the circuit.

    Returns:
    ansatz (QuantumCircuit): Generated ansatz circuit

    """
    params = np.array(params).reshape(1)
    ansatz = QuantumCircuit(num_qubits, num_qubits)
    ansatz.h(0)
    ansatz.cx(0, 1)
    ansatz.rx(params[0], 0)

    return ansatz

ansatz2([np.pi], 2).draw()
```

Out[22]:


Checking Expressibility of Ansatze

We quantify expressibility of ansatze using the Hilbert-Schmidt norm of A defined as:

$$A = \int_{Haar} |\psi\rangle\langle\psi| d\psi - \int_{\theta} |\psi_\theta\rangle\langle\psi_\theta| d\theta$$

This quantity needs to be taken with a pinch of salt as it is an oversimplification of the A which actually has to be calculated with the definition of an ϵ-approximate state t-design [1].

Here, the first term, i.e. a Haar integral, is the integral over a group of unitaries distributed randomly according to the Haar measure. Whereas, the second term, is taken over all states over the measure induced by uniformly sampling the parameters θ of the PQC.

In [23]:
```python
def random_unitary(N):
    """
        Return a Haar distributed random unitary from U(N)
    """

    Z = np.random.randn(N, N) + 1.0j * np.random.randn(N, N)
    [Q, R] = sp.linalg.qr(Z)
    D = np.diag(np.diagonal(R) / np.abs(np.diagonal(R)))
    return np.dot(Q, D)

def haar_integral(num_qubits, samples):
    """
        Return calculation of Haar Integral for a specified number of samples.
    """

    N = 2**num_qubits
    randunit_density = np.zeros((N, N), dtype=complex)


    zero_state = np.zeros(N, dtype=complex)
    zero_state[0] = 1

    for _ in range(samples):
      A = np.matmul(zero_state, random_unitary(N)).reshape(-1,1)
      randunit_density += np.kron(A, A.conj().T)

    randunit_density/=samples

    return randunit_density

def pqc_integral(num_qubits, ansatze, size, samples):
    """
        Return calculation of Integral for a PQC over the uniformly sampled
        the parameters θ for the specified number of samples.
    """

    N = num_qubits
    randunit_density = np.zeros((2**N, 2**N), dtype=complex)

    for _ in range(samples):
      params = np.random.uniform(-np.pi, np.pi, size)
```

```
        ansatz = ansatze(params, N)
        result = execute(ansatz,
                         backend=Aer.get_backend('statevector_simulator')).result()
        U = result.get_statevector(ansatz, decimals=5).reshape(-1,1)
        randunit_density += np.kron(U, U.conj().T)

    return randunit_density/samples
```

Sanity Check (Comparing Two Haar Integrals)

In [24]:
```
np.linalg.norm(haar_integral(2, 2048) - haar_integral(2, 2048))
```

Out[24]: 0.025708942385801254

Ansatz 1 (Random Choice)

In [25]:
```
np.linalg.norm(haar_integral(2, 2048) - pqc_integral(2, ansatz1, (2,2), 2048))
```

Out[25]: 0.02432573321735785

Ansatz 2 (From Hint)

In [26]:
```
np.linalg.norm(haar_integral(2, 2048) - pqc_integral(2, ansatz2, 1, 2048))
```

Out[26]: 0.49896675806724666

Ansatz 3 (Empty Circuit)

In [27]:
```
def ansatz3(params, num_qubits):
    """
    Generate an templated ansatz with no parameters

    Args:
    params (array[float]): Parameters to initialize the parameterized unitary.
    num_qubits (int): Number of qubits in the circuit.

    Returns:
    ansatz (QuantumCircuit): Generated ansatz circuit

    """

    ansatz = QuantumCircuit(num_qubits, num_qubits)
    return ansatz

np.linalg.norm(haar_integral(2, 2048) - pqc_integral(2, ansatz3, 0, 2048))
```

Out[27]: 0.8589639169688795

Clearly, expressibility are in the order: Ansatz 3 < Ansatz 2 < Ansatz 1, i.e. the power to probe Hilbert space is much more for our randomly chosen ansatz, which is guessable.

Checking Entangling Capability of Ansatze

We quantify entanlging capability [1] of ansatze by calculating the average Meyer-Wallach entanglement, Q, of the states generated by it:

$$Q = \frac{2}{|S|} \sum_{\theta_i \in S} \left(1 - \frac{1}{n} \sum_{k=1}^{n} Tr(\rho_k^2(\theta_i)) \right)$$

Here, ρ_k is the density operator for the k^{th} qubit after tracing out the rest, and S is the set of sampled parameters. The quantity within the first summation can also be called as the average subsystem linear entropy for the system, and to calculate it we make use of qiskit's `partial_trace`.

In [28]:
```
def meyer_wallach(circuit, num_qubits, size, sample=1024):
    """
        Returns the meyer-wallach entanglement measure for the given circuit.
    """

    res = np.zeros(sample, dtype=complex)
    N = num_qubits

    for i in range(sample):
        params = np.random.uniform(-np.pi, np.pi, size)
        ansatz = circuit(params, N)
        result = execute(ansatz,
                         backend=Aer.get_backend('statevector_simulator')).result()
        U = result.get_statevector(ansatz, decimals=5)
        entropy = 0
        qb = list(range(N))

        for j in range(N):
            dens = quantum_info.partial_trace(U, qb[:j]+qb[j+1:]).data
            trace = np.trace(dens**2)
            entropy += trace

        entropy /= N
        res[i] = 1 - entropy

    return 2*np.sum(res).real/sample
```

Sanity Check (Empty circuit aka Ansatz 3)

In [29]:
```
meyer_wallach(ansatz3, 2, 0)
```

Out[29]:
```
0.0
```

Ansatz 1 (Random Choice)

In [30]:
```
meyer_wallach(ansatz1, 2, (2,2))
```

Out[30]:
```
0.6190388917964508
```

Ansatz 2 (From Hint)

In [31]:
```
meyer_wallach(ansatz2, 2, 1)
```

Out[31]:
```
1.0
```

Clearly, the entangling capability are in the order: Ansatz 3 < Ansatz 1 < Ansatz 2. Therefore, we can guess limited expressibility of Ansatz 2 is compensated by its higher entangling capability.

Running Simulations

Variational Quantum Eigensolver (VQE) is based on *Rayleigh-Ritz variational principle*. To perform VQE, the first step is to enocde the problem into a Hermitian matrix M, whose expectation value w.r.t a trial wave function $|\psi(\theta)\rangle$ which is yielded by an ansatz $U(\theta)$, i.e., nothing but a unitary paramterized by $\{\vec{\theta}\}$.

Here, we optimize these parameters $\{\vec{\theta}\}$ using `scipy.optimize` library based on a cost function $C(\theta)$, which is nothing but the calculated expectation value of Hamiltonian, H_1 for $|\psi(\theta)\rangle$:

$$C(\theta) = \langle\psi(\theta)|H_1|\psi(\theta)\rangle$$

In [32]:
```
def vqe(params, meas_basis, coeffs, circuit, num_qubits, shots=2048):
    """
        Return the calculated energy scalar for a given asnatz and
        decomposed Hamiltoian.

        Args:
        params (matrix(np.array)): Parameters for initializing the ansatz.
        meas_basis (list[str]): String representation of measurement basis, i.e.
        the decomposed pauli term with their corresponding qubits.
        coeffs (vector(np.array)): Coefficients for the decomposed Pauli Term
        circuit (QuantumCircuit): Template for Ansatz circuit
        num_qubits (int): Number of qubits in the given asatze.
        shots (int): Number of shots to get the probability distribution.

        Return:
        energy (float): Expectation value of the Hamiltonian whose
        decomposition was provided.
    """

    N = num_qubits
    circuit = circuit(params, num_qubits)
    energy = 0

    for basis, coeff in zip(meas_basis, coeffs):
      if basis.count('I') != N:
        energy += coeff*calculate_expecation_val(circuit, basis, shots)

    energy += 0.5

    return energy
```

Ansatz 1 (Random Choice)

In [33]:
```
a, b, c = decompose_ham_to_pauli(H1)

params = np.random.uniform(-np.pi, np.pi, (2,2))
func = ft.partial(vqe, meas_basis=a, coeffs=b, circuit=ansatz1,
                  num_qubits=2, shots=2048)
```

In [34]:
```
res = sp.optimize.minimize(func, params, method='Powell')
res
```

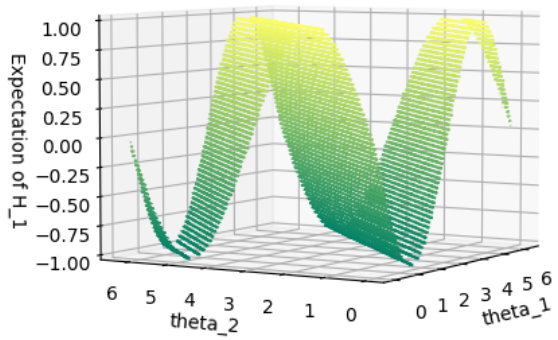
Out[34]:
```
   direc: array([[1., 0., 0., 0.],
       [0., 1., 0., 0.],
       [0., 0., 1., 0.],
       [0., 0., 0., 1.]])
     fun: array(-1.)
 message: 'Optimization terminated successfully.'
    nfev: 190
     nit: 3
  status: 0
 success: True
       x: array([ 4.7130171 , -3.15044759, -1.59558296, -0.02529809])
```

In [35]:
```
assert(float(res.fun) == min(np.linalg.eig(H1)[0])) #Sanity Check
```

Visualizing the Result

After looking at multiple results' `res.x`, we realize that first and second parameters always have the values $\pm n\pi/2$ and $\pm\pi$ respectively. So, while keeping them fixed, we do a parameters search-scan in the range $\theta_{3,4} \in [0, 2\pi]$ and visualize how they affect our expectation value.

In [36]:
```
def energy_expectation(x, y):
  """ Returns meshgrid values for plotting """
  energy = np.zeros(x.shape)
  for idx, thetas in enumerate(x):
    for ind, theta1 in enumerate(thetas):
      params = np.array([np.pi/2, np.pi, theta1, y[idx][ind]])
      energy[idx][ind] = func(params)
  return energy

theta1 = np.linspace(0.0, 2*np.pi, 200)
theta2 = np.linspace(0.0, 2*np.pi, 200)

X, Y = np.meshgrid(theta1, theta2)
Z = energy_expectation(X, Y)

fig = plt.figure()
ax = plt.axes(projection='3d')
ax.contour3D(X, Y, Z, 50, cmap='summer')
ax.set_xlabel('theta_1')
ax.set_ylabel('theta_2')
ax.set_zlabel('Expectation of H_1');
plt.show()
```



Ansatz 2 (From Hint)

In [37]:
```
a, b, c = decompose_ham_to_pauli(H1)
params = np.random.uniform(-np.pi, np.pi, 1)
func = ft.partial(vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                  num_qubits=2, shots=2048)
```

In [38]:
```
res = sp.optimize.minimize(func, params, method='Powell')
res
```

Out[38]:
```
   direc: array([[1.]])
     fun: array(-1.)
 message: 'Optimization terminated successfully.'
    nfev: 26
     nit: 2
  status: 0
 success: True
       x: array([3.13590442])
```

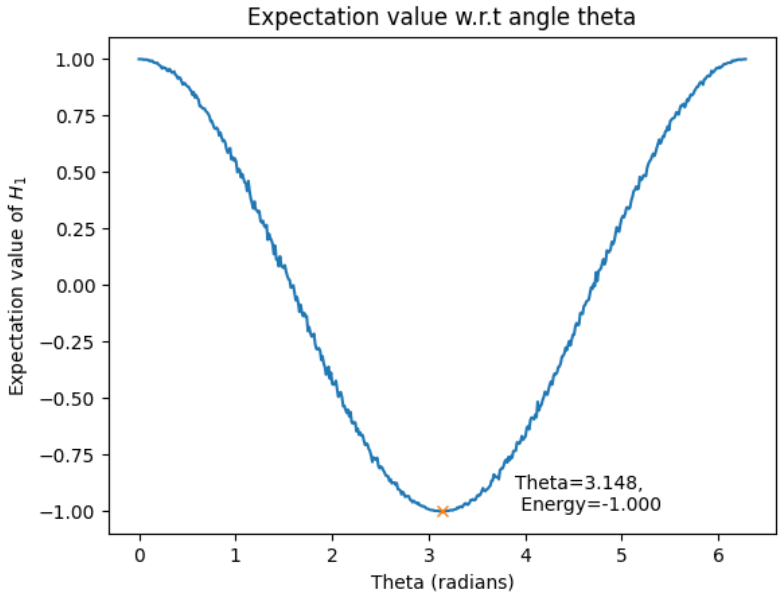
In [39]:
```
assert(float(res.fun) == min(np.linalg.eig(H1)[0])) #Sanity Check
```

Visualizing the Result

We scan over the paramter $\theta \in [0, 2\pi]$, to visualize the change in expectation value for the ansatz2, which is inspired from the hint given.

In [40]:
```
thetas = np.linspace(0.0, 2*np.pi, 500)
energy = np.zeros(len(thetas))

for idx, theta in enumerate(thetas):
    energy[idx] = func([theta])

fig = plt.figure()
plt.plot(thetas, energy)
plt.title('Expectation value w.r.t angle theta')
plt.ylabel('Expectation value of $H_1$')
```

```
plt.xlabel('Theta (radians)')
indices = [idx for idx, x in enumerate(energy) if x <= -1.0]
xmin = thetas[indices[len(indices)//2]]
ymin = energy.min()
text= "Theta={:.3f}, \n Energy={:.3f}".format(xmin, ymin)
plt.plot(xmin,ymin,'x')
plt.annotate(text, xy=(xmin+0.75, ymin))
fig.show()
```

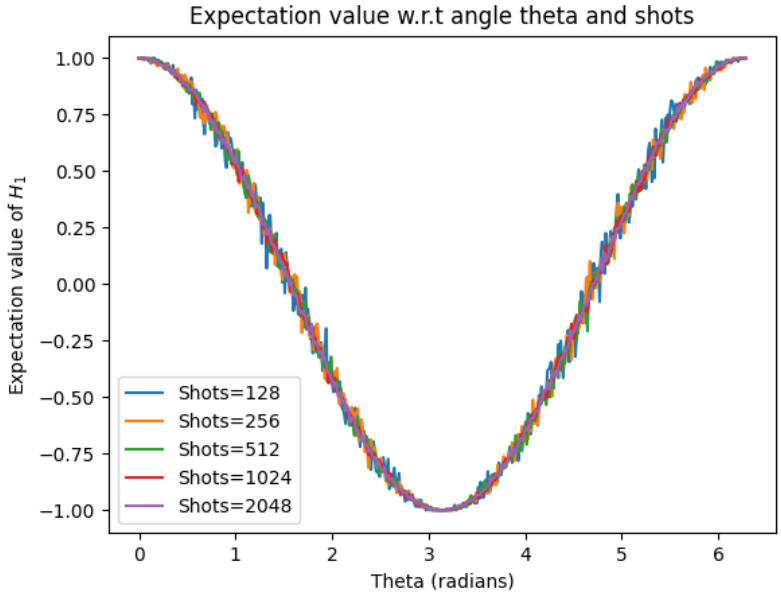


Number of Measurements (or Shots)

In order to obtain results from a quantum computer, one needs to perform sampling. This allows us to obtain the probability distribution, and hence know the most probable results from the measurement. Here, we see the change of expectation value of H_1 with the number of shots, i.e., number of measurements for ansatz 2.

In [41]:
```
thetas = np.linspace(0.0, 2*np.pi, 500)
shots = [128, 256, 512, 1024, 2048]
shot_energy = np.zeros((len(shots), len(thetas)))

for ind, shot in enumerate(shots):
    for idx, theta in enumerate(thetas):
        func = ft.partial(vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                          num_qubits=2, shots=shot)
        shot_energy[ind][idx] = func([theta])
```

In [45]:
```
plt.figure()
for ind, shot in enumerate(shots):
    plt.plot(thetas, shot_energy[ind], label='Shots=' + str(shot))

plt.title('Expectation value w.r.t angle theta and shots')
plt.ylabel('Expectation value of $H_1$')
plt.xlabel('Theta (radians)')
plt.legend()
plt.show()
```



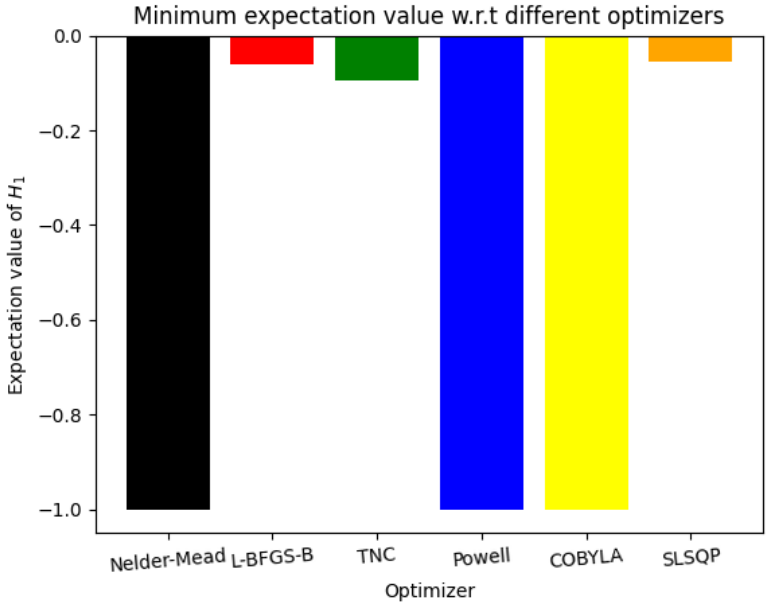
Performance of Classical Optimizers

Successful application of hybrid-quantum classical algorithms, with the classical step involving an optimizer, on current hardware, requires the classical optimizer to be noise-aware. In order to study this, we study the change of expectation value of H_1 with different classical optimizers for ansatz 2, first in absence of noise, then later in the presence of noise.

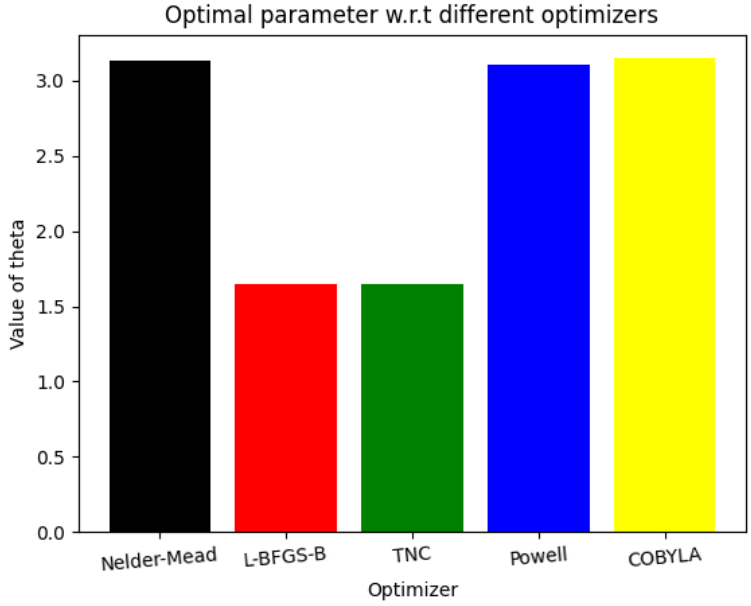
In [43]:
```
a, b, c = decompose_ham_to_pauli(H1)
params = np.random.uniform(-np.pi, np.pi, 1)
func = ft.partial(vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                  num_qubits=2, shots=2048)
```

In [44]:
```
optimizers = ['Nelder-Mead', 'L-BFGS-B', 'TNC', 'Powell', 'COBYLA', 'SLSQP']
opt_val = []
opt_param = []
opt_feval = []
opt_iter = []
init_params = params

for opt in optimizers:

    params = init_params
    res = sp.optimize.minimize(func, params, method=opt)

    opt_val.append(float(res.fun))
    opt_param.append(float(res.x))
    opt_feval.append(int(res.nfev))
    try:
        opt_iter.append(int(res.nit))
    except:
        opt_iter.append(1)
```

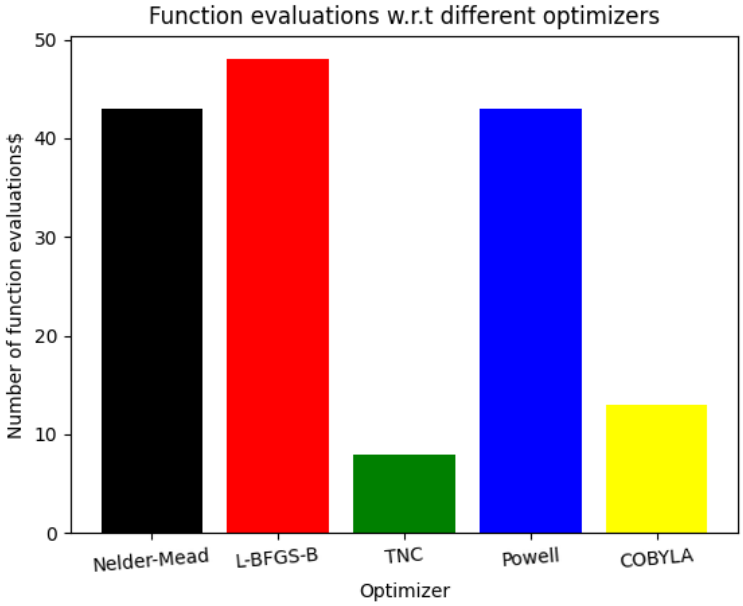
In [46]:
```
fig = plt.figure()
plt.bar(optimizers, opt_val, color=['black', 'red', 'green', 'blue', 'yellow', 'orange'])
plt.title('Minimum expectation value w.r.t different optimizers')
plt.ylabel('Expectation value of $H_1$')
plt.xlabel('Optimizer')
plt.xticks(rotation=5)
fig.show()
```



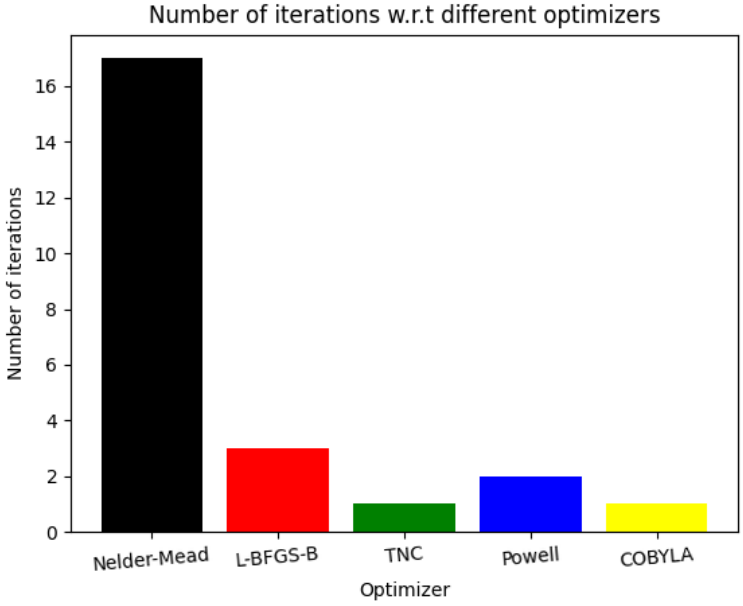
In [47]:
```
fig = plt.figure()
plt.bar(optimizers[:-1], opt_param[:-1], color=['black', 'red', 'green', 'blue', 'yellow'])
plt.title('Optimal parameter w.r.t different optimizers')
plt.ylabel('Value of theta')
plt.xlabel('Optimizer')
plt.xticks(rotation=5)
fig.show()
```



In [48]:
```
fig = plt.figure()
plt.bar(optimizers[:-1], opt_feval[:-1], color=['black', 'red', 'green', 'blue', 'yellow'])
plt.title('Function evaluations w.r.t different optimizers')
plt.ylabel('Number of function evaluations$')
plt.xlabel('Optimizer')
plt.xticks(rotation=5)
fig.show()
```



In [49]:
```
fig = plt.figure()
plt.bar(optimizers[:-1], opt_iter[:-1], color=['black', 'red', 'green', 'blue', 'yellow'])
plt.title('Number of iterations w.r.t different optimizers')
plt.ylabel('Number of iterations')
plt.xlabel('Optimizer')
plt.xticks(rotation=5)
fig.show()
```



Noisy Simulation

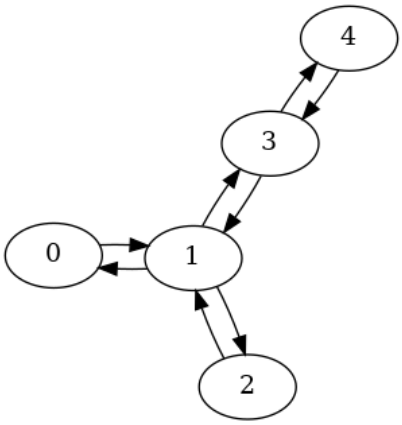
Computational power of NISQ processors suffers a lot from the limited capabilities of their physical qubits. This is essentially due to present of decoherence, limited connectivity, and absence of error-correction. Hence, it is essential to see how our ansatz would perform on a real device. Here, we replicate the noise model from a real device, and then test the perfrormance of our VQE module.

In [54]:
```
# Noise Model Preparation
provider = IBMQ.load_account()
noisy_backend = provider.get_backend('ibmq_vigo')
coupling_map = noisy_backend.configuration().coupling_map
noise_model = providers.aer.noise.NoiseModel.from_backend(noisy_backend)
basis_gates = noise_model.basis_gates
```

Qubit coupling map of this real device is the following:

In [53]:
```
qiskit.transpiler.CouplingMap(noisy_backend.configuration().coupling_map).draw()
```

Out[53]:



In [57]:
```
noise_model
```

Out[57]:
```
NoiseModel:
  Basis gates: ['cx', 'id', 'u2', 'u3']
  Instructions with noise: ['id', 'measure', 'cx', 'u2', 'u3']
  Qubits with noise: [0, 1, 2, 3, 4]
  Specific qubit errors: [('id', [0]), ('id', [1]), ('id', [2]), ('id', [3]), ('id', [4]), ('u2', [0]), ('u2', [1]), ('u
2', [2]), ('u2', [3]), ('u2', [4]), ('u3', [0]), ('u3', [1]), ('u3', [2]), ('u3', [3]), ('u3', [4]), ('cx', [0, 1]), ('c
x', [1, 0]), ('cx', [1, 2]), ('cx', [1, 3]), ('cx', [2, 1]), ('cx', [3, 1]), ('cx', [3, 4]), ('cx', [4, 3]), ('measure',
[0]), ('measure', [1]), ('measure', [2]), ('measure', [3]), ('measure', [4])]
```

In [50]:
```
def calculate_noisy_expecation_val(circuit, basis, mitigated=False, shots=2048, backend='qasm_simulator'):
    """
    Calculate expectation value for the measurement of a circuit in a
    given basis in presence of noise.

    Args:
    circuit (QuantumCircuit): Circuit using which expectation value
    will be calculated for a given basis.
    basis (str): String representation of tensor products of Pauli
    observables.
    mitigated (bool): Whether mitigation has to be performed or not.
    shots (int): Number of times measurements needed to be done for calculating
    probability.
    backend (str): Backend for running the circuit.

    Returns:
    exp (float): Expectation value for the measurement of a circuit
    in a given basis.

    """
    exp_circuit = circuit + measure_circuit(basis, circuit.num_qubits)

    result = execute(exp_circuit, backend=Aer.get_backend(backend),
                     shots=shots, coupling_map=coupling_map,
                     basis_gates=basis_gates,
                     noise_model=noise_model).result()

    if mitigated:
        meas_calibs, state_labels = complete_meas_cal(qr=exp_circuit.qregs[0], cr=exp_circuit.cregs[0])
        cal_results = qiskit.execute(meas_calibs, backend=Aer.get_backend(backend),
                                     coupling_map=coupling_map, basis_gates=basis_gates,
                                     shots=shots, noise_model=noise_model).result()
        meas_fitter = CompleteMeasFitter(cal_results, state_labels)
        meas_filter = meas_fitter.filter
        result = meas_filter.apply(result)

    exp = 0.0
    for key, counts in result.get_counts().items():
        exp += (-1)**(int(key[0])+int(key[1])) * counts

    return exp/shots


def noisy_vqe(params, meas_basis, coeffs, circuit, num_qubits, mitigated=False, shots=2048):
    """
        Return the calculated energy scalar for a given asnatz and
        decomposed Hamiltoian in presence of noise.

        Args:
        params (matrix(np.array)): Parameters for initializing the ansatz.
        meas_basis (list[str]): String representation of measurement basis, i.e.
        the decomposed pauli term with their corresponding qubits.
        coeffs (vector(np.array)): Coefficients for the decomposed Pauli Term
        circuit (QuantumCircuit): Template for Ansatz circuit
        num_qubits (int): Number of qubits in the given asatze.
        mitigated (bool): Whether mitigation has to be performed or not.
        shots (int): Number of shots to get the probability distribution.

        Return:
        energy (float): Expectation value of the Hamiltonian whose
        decomposition was provided.
    """

    N = num_qubits
    circuit = circuit(params, num_qubits)
```

```
    energy = 0

    for basis, coeff in zip(meas_basis, coeffs):
      if basis.count('I') != N:
        energy += coeff*calculate_noisy_expecation_val(circuit, basis, mitigated, shots)

    energy += 0.5

    return energy
```

```
/home/whatsis/.local/lib/python3.8/site-packages/qiskit/providers/ibmq/ibmqfactory.py:192: UserWarning: Timestamps in IB
MQ backend properties, jobs, and job results are all now in local time instead of UTC.
  warnings.warn('Timestamps in IBMQ backend properties, jobs, and job results '
```

Ansatz 1 (Random Choice)

In [43]:
```
a, b, c = decompose_ham_to_pauli(H1)

params = np.random.uniform(-np.pi, np.pi, (2,2))
func = ft.partial(noisy_vqe, meas_basis=a, coeffs=b, circuit=ansatz1,
                  num_qubits=2, mitigated=False, shots=8192)
```

In [44]:
```
res = sp.optimize.minimize(func, params, method='Powell')
res
```

Out[44]:
```
  direc: array([[1., 0., 0., 0.],
       [0., 1., 0., 0.],
       [0., 0., 1., 0.],
       [0., 0., 0., 1.]])
    fun: array(-0.87451172)
message: 'Optimization terminated successfully.'
   nfev: 266
    nit: 3
 status: 0
success: True
      x: array([1.64212384, 3.14620703, 2.15383843, 0.53103981])
```

In [45]:
```
a, b, c = decompose_ham_to_pauli(H1)

params = np.random.uniform(-np.pi, np.pi, (2,2))
func = ft.partial(noisy_vqe, meas_basis=a, coeffs=b, circuit=ansatz1,
                  num_qubits=2, mitigated=True, shots=8192)
```

In [46]:
```
res = sp.optimize.minimize(func, params, method='Powell')
res
```

Out[46]:
```
  direc: array([[1., 0., 0., 0.],
       [0., 1., 0., 0.],
       [0., 0., 1., 0.],
       [0., 0., 0., 1.]])
    fun: -0.9619728377818637
message: 'Optimization terminated successfully.'
   nfev: 257
    nit: 3
 status: 0
success: True
      x: array([ 1.58409174, -3.11397559, -0.50929574, -1.96419365])
```

Ansatz 2 (From Hint)

In [47]:
```
a, b, c = decompose_ham_to_pauli(H1)
params = np.random.uniform(-np.pi, np.pi, 1)
func = ft.partial(noisy_vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                  num_qubits=2, mitigated=False, shots=8192)
```

In [48]:
```
res = sp.optimize.minimize(func, params, method='Powell')
res
```

Out[48]:
```
  direc: array([[-0.1127984]])
    fun: array(-0.88122559)
message: 'Optimization terminated successfully.'
   nfev: 88
    nit: 5
 status: 0
success: True
      x: array([3.17376448])
```

In [49]:
```
a, b, c = decompose_ham_to_pauli(H1)
params = np.random.uniform(-np.pi, np.pi, 1)
func = ft.partial(noisy_vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                  num_qubits=2, mitigated=True, shots=8192)
```

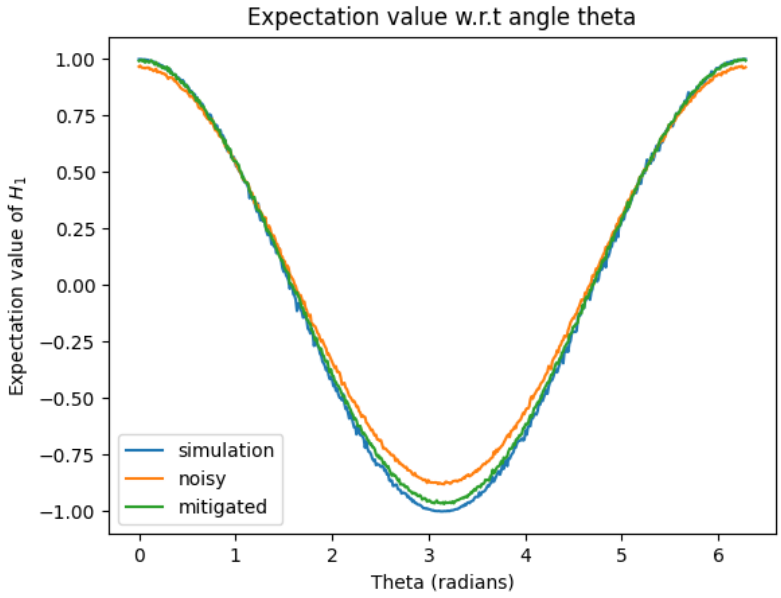
In [50]:
```
res = sp.optimize.minimize(func, params, method='Powell')
res
```

Out[50]:
```
  direc: array([[3.01441921e-09]])
    fun: -0.9702586386528804
message: 'Optimization terminated successfully.'
   nfev: 120
    nit: 5
 status: 0
success: True
      x: array([-3.12601157])
```

Visualizing the Result (Noisy v/s Mitigated v/s Ideal)

In [55]:
```
thetas = np.linspace(0.0, 2*np.pi, 500)
energy1 = np.zeros(len(thetas))
energy2 = np.zeros(len(thetas))
func1 = ft.partial(noisy_vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                   num_qubits=2, mitigated=False, shots=8192)
func2 = ft.partial(noisy_vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                   num_qubits=2, mitigated=True, shots=8192)

for idx, theta in enumerate(thetas):
    energy1[idx] = func1([theta])
    energy2[idx] = func2([theta])
```

In [54]:
```
plt.plot(thetas, energy, label='simulation')
plt.plot(thetas, energy1, label='noisy')
plt.plot(thetas, energy2, label='mitigated')
plt.title('Expectation value w.r.t angle theta')
plt.ylabel('Expectation value of $H_1$')
plt.xlabel('Theta (radians)')
plt.legend()
plt.show()
```

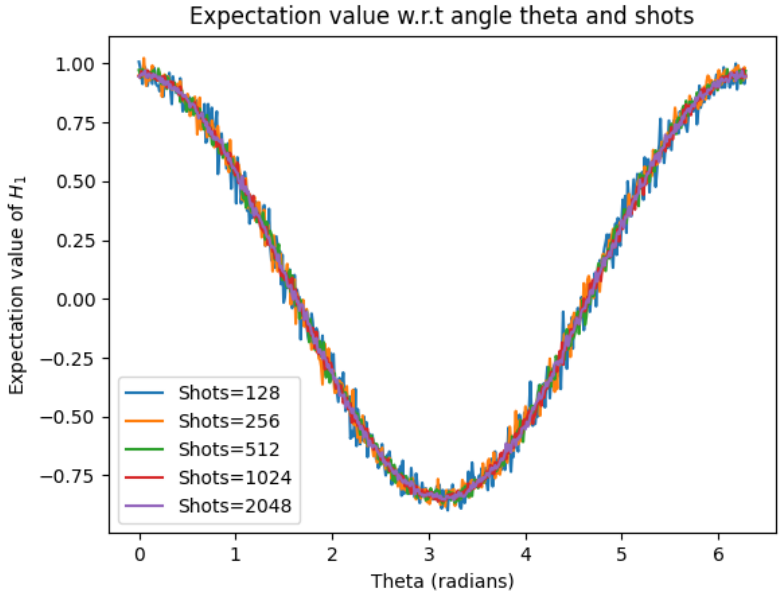


Number of Measurements (or Shots)

Let's see the change of expectation value of H_1 with the number of shots for ansatz 2.

In [129…
```
thetas = np.linspace(0.0, 2*np.pi, 500)
shots = [128, 256, 512, 1024, 2048]
noisy_shot_energy = np.zeros((len(shots), len(thetas)))

for ind, shot in enumerate(shots):
    for idx, theta in enumerate(thetas):
        func = ft.partial(noisy_vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                          num_qubits=2, shots=shot)
        noisy_shot_energy[ind][idx] = func([theta])
```

In [131…
```
plt.figure()
for ind, shot in enumerate(shots):
    plt.plot(thetas, noisy_shot_energy[ind], label='Shots=' + str(shot))

plt.title('Expectation value w.r.t angle theta and shots')
plt.ylabel('Expectation value of $H_1$')
plt.xlabel('Theta (radians)')
plt.legend()
plt.show()
```



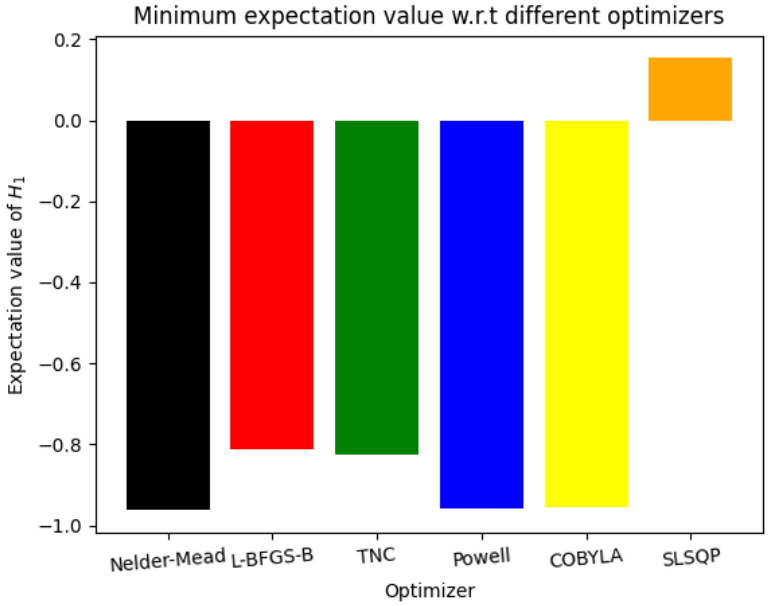
Peformance of Classical Optimizers

Let's see the change of expectation value of H_1 with different classical optimizers for ansatz 2.

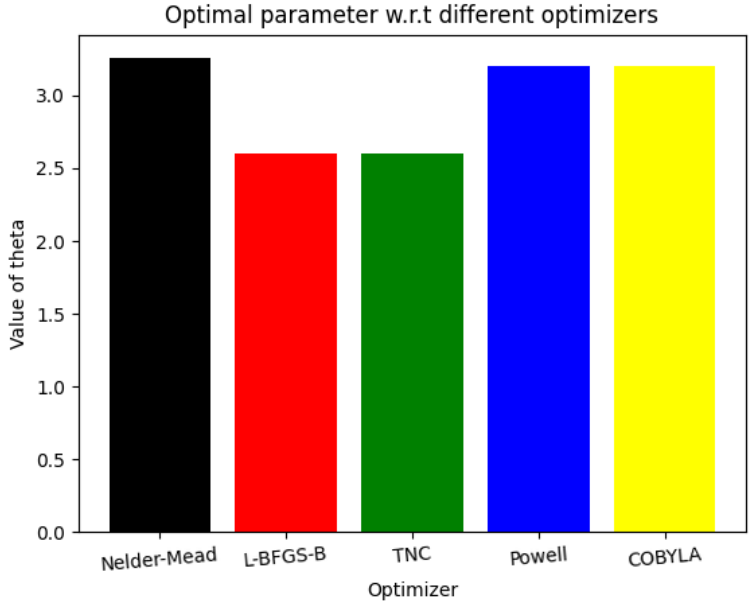
In [123…
```
a, b, c = decompose_ham_to_pauli(H1)
params = np.random.uniform(-np.pi, np.pi, 1)
func = ft.partial(noisy_vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                  num_qubits=2, mitigated=True, shots=8192)
```

In [124…
```
optimizers = ['Nelder-Mead', 'L-BFGS-B', 'TNC', 'Powell', 'COBYLA', 'SLSQP']
opt_val = []
opt_param = []
opt_feval = []
opt_iter = []

init_params = params

for opt in optimizers:

    params = init_params
    res = sp.optimize.minimize(func, params, method=opt)

    opt_val.append(float(res.fun))
    opt_param.append(float(res.x))
    opt_feval.append(int(res.nfev))
    try:
        opt_iter.append(int(res.nit))
    except:
        opt_iter.append(1)
```

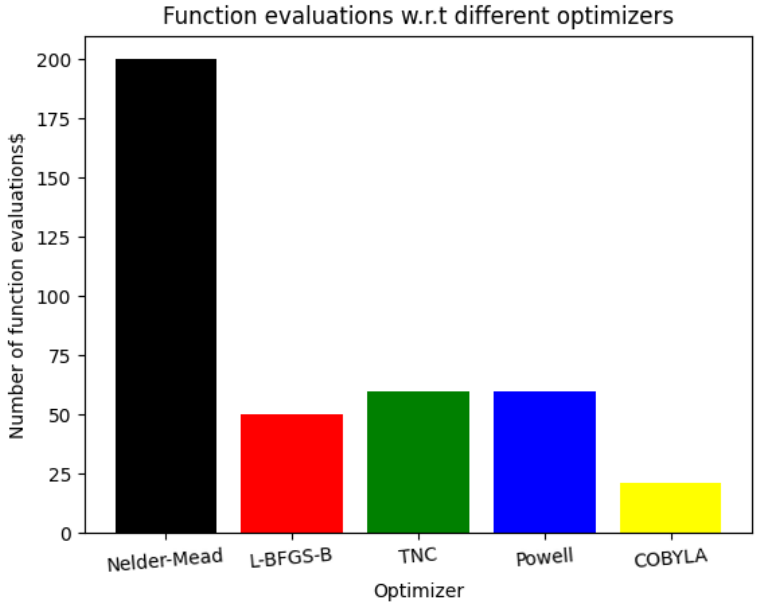
In [125…
```
fig = plt.figure()
plt.bar(optimizers, opt_val, color=['black', 'red', 'green', 'blue', 'yellow', 'orange'])
plt.title('Minimum expectation value w.r.t different optimizers')
plt.ylabel('Expectation value of $H_1$')
plt.xlabel('Optimizer')
plt.xticks(rotation=5)
fig.show()
```



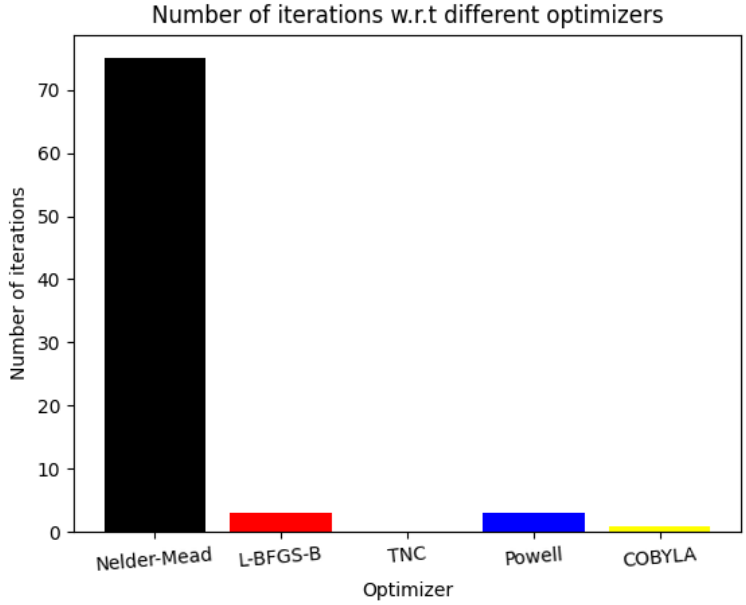
In [126…
```
fig = plt.figure()
plt.bar(optimizers[:-1], opt_param[:-1], color=['black', 'red', 'green', 'blue', 'yellow'])
plt.title('Optimal parameter w.r.t different optimizers')
plt.ylabel('Value of theta')
plt.xlabel('Optimizer')
plt.xticks(rotation=5)
fig.show()
```



In [127…
```
fig = plt.figure()
plt.bar(optimizers[:-1], opt_feval[:-1], color=['black', 'red', 'green', 'blue', 'yellow'])
plt.title('Function evaluations w.r.t different optimizers')
plt.ylabel('Number of function evaluations')
plt.xlabel('Optimizer')
plt.xticks(rotation=5)
fig.show()
```



In [128…]:
```
fig = plt.figure()
plt.bar(optimizers[:-1], opt_iter[:-1], color=['black', 'red', 'green', 'blue', 'yellow'])
plt.title('Number of iterations w.r.t different optimizers')
plt.ylabel('Number of iterations')
plt.xlabel('Optimizer')
plt.xticks(rotation=5)
fig.show()
```



Comparing the performance of VQE in presence of errors due to Readout, Thermal Relaxation, Amplitude-Phase damping and Depolarization

Readout

Describes classical readout errors

In [33]:
```
# Measurement miss-assignement probabilities
p0given1 = 0.1
p1given0 = 0.05
noise_readout = ReadoutError([[1 - p1given0, p1given0], [p0given1, 1 - p0given1]])
noise_readout
```

Out[33]:
```
ReadoutError([[0.95 0.05]
 [0.1  0.9 ]])
```

Thermal Relaxation

Single qubit thermal relaxation error is characterized by relaxation time constants T_1, T_2, and the gate time t.

In [34]:
```
num_qubits = 2

T1s = np.random.normal(50e3, 10e3, num_qubits) # Sampled from normal distribution
T2s = np.random.normal(80e3, 20e3, num_qubits)  # Sampled from normal distribution
T2s = np.array([min(T2s[j], 2 * T1s[j]) for j in range(num_qubits)]) # Ensuring T2s < 2*T1s
```

```
# Instruction times (in nanoseconds)
time_u1 = 0   # virtual gate
time_u2 = 50  # (single X90 pulse)
time_u3 = 100 # (two X90 pulses)
time_cx = 300
time_measure = 1000 # 1 microsecond

# Add depolarizing error to all single qubit u1, u2, u3, cx, measure gates
errors_thermal_u1  = [thermal_relaxation_error(t1, t2, time_u1)
              for t1, t2 in zip(T1s, T2s)]
errors_thermal_u2  = [thermal_relaxation_error(t1, t2, time_u2)
              for t1, t2 in zip(T1s, T2s)]
errors_thermal_u3  = [thermal_relaxation_error(t1, t2, time_u3)
              for t1, t2 in zip(T1s, T2s)]
errors_thermal_cx = [[thermal_relaxation_error(t1a, t2a, time_cx).expand(
             thermal_relaxation_error(t1b, t2b, time_cx))
              for t1a, t2a in zip(T1s, T2s)]
               for t1b, t2b in zip(T1s, T2s)]
errors_thermal_measure = [thermal_relaxation_error(t1, t2, time_measure)
                  for t1, t2 in zip(T1s, T2s)]

# Add errors to noise model
noise_thermal = NoiseModel()
for j in range(num_qubits):
    noise_thermal.add_quantum_error(errors_thermal_u1[j], "u1", [j])
    noise_thermal.add_quantum_error(errors_thermal_u2[j], "u2", [j])
    noise_thermal.add_quantum_error(errors_thermal_u3[j], "u3", [j])
    for k in range(num_qubits):
        noise_thermal.add_quantum_error(errors_thermal_cx[j][k], "cx", [j, k])
    noise_thermal.add_quantum_error(errors_thermal_measure[j], "measure", [j])

noise_thermal
```

Out[34]:
```
NoiseModel:
  Basis gates: ['cx', 'id', 'u2', 'u3']
  Instructions with noise: ['u2', 'u3', 'cx', 'measure']
  Qubits with noise: [0, 1]
  Specific qubit errors: [('u2', [0]), ('u2', [1]), ('u3', [0]), ('u3', [1]), ('cx', [0, 0]), ('cx', [0, 1]), ('cx', [1,
0]), ('cx', [1, 1]), ('measure', [0]), ('measure', [1])]
```

Amplitude-Phase Damping

Single-qubit generalized combined phase and amplitude damping error is given by an amplitude damping parameter λ, and a phase damping parameter γ.

In [35]:
```
lamb = 0.05
gamma = 0.1

errors_phase_amplitude_1 =  phase_amplitude_damping_error(lamb, gamma)
errors_phase_amplitude_2 =  phase_amplitude_damping_error(lamb, gamma).expand(phase_amplitude_damping_error(lamb, gamma))

# Add errors to noise model
noise_phase_amplitude = NoiseModel()
noise_phase_amplitude.add_all_qubit_quantum_error(errors_phase_amplitude_1, ['u1', 'u2', 'u3', 'measure'])
noise_phase_amplitude.add_all_qubit_quantum_error(errors_phase_amplitude_2, ['cx'])
noise_phase_amplitude
```

Out[35]:
```
NoiseModel:
  Basis gates: ['cx', 'id', 'u1', 'u2', 'u3']
  Instructions with noise: ['u2', 'u3', 'u1', 'cx', 'measure']
  All-qubits errors: ['u1', 'u2', 'u3', 'measure', 'cx']
```

Depolarization

N-qubit depolarizing error is given by a depolarization probability p.

In [36]:
```
# Add depolarizing error to all single qubit u1, u2, u3, cx, measure gates
error_depol_1 = depolarizing_error(0.05, 1)
error_depol_2 = depolarizing_error(0.1, 2)
error_depol_3 = depolarizing_error(0.1, 1)

# Add errors to noise model
noise_depol = NoiseModel()
noise_depol.add_all_qubit_quantum_error(error_depol_1, ['u1', 'u2', 'u3'])
noise_depol.add_all_qubit_quantum_error(error_depol_2, ['cx'])
noise_depol.add_all_qubit_quantum_error(error_depol_3, ['measure'])
noise_depol
```

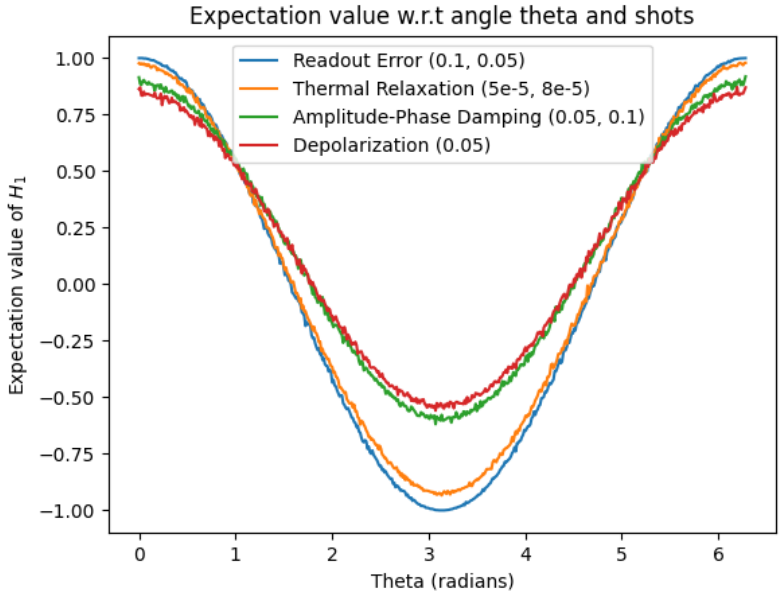
Out[36]:
```
NoiseModel:
  Basis gates: ['cx', 'id', 'u1', 'u2', 'u3']
  Instructions with noise: ['u2', 'u3', 'u1', 'cx', 'measure']
  All-qubits errors: ['u1', 'u2', 'u3', 'cx', 'measure']
```

In [37]:
```
def calculate_restricted_noisy_expecation_val(circuit, basis, noise_model, shots=2048, backend='qasm_simulator'):
    """
    Calculate expectation value for the measurement of a circuit in a
    given basis in presence of a particular kind of noise.

    Args:
    circuit (QuantumCircuit): Circuit using which expectation value
    will be calculated for a given basis.
    basis (str): String representation of tensor products of Pauli
    observables.
    noise_model (NoiseModel): Noise Model for execution
    shots (int): Number of times measurements needed to be done for calculating
    probability.
    backend (str): Backend for running the circuit.
```

```
    Returns:
    exp (float): Expectation value for the measurement of a circuit
    in a given basis.

    """
    exp_circuit = circuit + measure_circuit(basis, circuit.num_qubits)

    result = execute(exp_circuit, backend=Aer.get_backend(backend),
                     shots=shots, noise_model=noise_model).result()

    exp = 0.0
    for key, counts in result.get_counts().items():
        exp += (-1)**(int(key[0])+int(key[1])) * counts

    return exp/shots


def restricted_noisy_vqe(params, meas_basis, coeffs, circuit, num_qubits, noise_model, shots=2048):
    """
        Return the calculated energy scalar for a given asnatz and
        decomposed Hamiltoian in presence of a particular kind of noise.

        Args:
        params (matrix(np.array)): Parameters for initializing the ansatz.
        meas_basis (list[str]): String representation of measurement basis, i.e.
        the decomposed pauli term with their corresponding qubits.
        coeffs (vector(np.array)): Coefficients for the decomposed Pauli Term
        circuit (QuantumCircuit): Template for Ansatz circuit
        num_qubits (int): Number of qubits in the given asatze.
        noise_model (NoiseModel): Noise Model for execution
        shots (int): Number of shots to get the probability distribution.

        Return:
        energy (float): Expectation value of the Hamiltonian whose
        decomposition was provided.
    """

    N = num_qubits
    circuit = circuit(params, num_qubits)
    energy = 0

    for basis, coeff in zip(meas_basis, coeffs):
      if basis.count('I') != N:
        energy += coeff*calculate_restricted_noisy_expecation_val(circuit, basis, noise_model, shots)

    energy += 0.5

    return energy
```

In [38]:
```
noise_models = [noise_readout, noise_thermal, noise_phase_amplitude, noise_depol]

thetas = np.linspace(0.0, 2*np.pi, 500)
noisy_energy = np.zeros((len(noise_models), len(thetas)))

for ind, model in enumerate(noise_models):
    func3 = ft.partial(restricted_noisy_vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                   num_qubits=2, noise_model=model, shots=4096)
    for idx, theta in enumerate(thetas):
        noisy_energy[ind][idx] = func3([theta])
```

In [39]:
```
noise_models_name = ['Readout Error (0.1, 0.05)', 'Thermal Relaxation (5e-5, 8e-5)',
                     'Amplitude-Phase Damping (0.05, 0.1)', 'Depolarization (0.05)']

plt.figure()
for ind, model in enumerate(noise_models):
    plt.plot(thetas, noisy_energy[ind], label=noise_models_name[ind])

plt.title('Expectation value w.r.t angle theta and shots')
plt.ylabel('Expectation value of $H_1$')
plt.xlabel('Theta (radians)')
plt.legend()
plt.show()
```



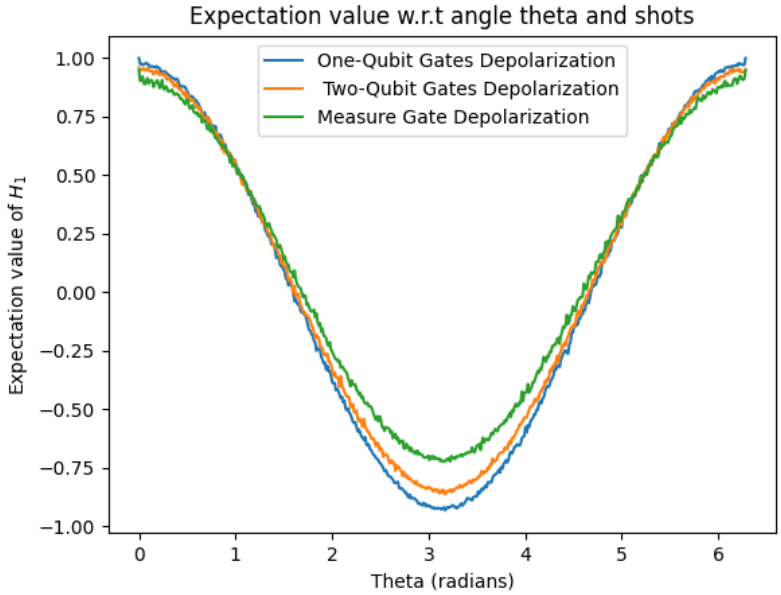
We see from the above plot that the presence of noise due to depolarization has affected our VQE results the most. This can be explained via its definiton that it is the uniform contraction of the Bloch sphere, parameterized by p. So, we now do a quick comparision between the effects of depolarization on single qubit gates v/s two-qubit gates v/s measure gates.

In [43]:
```
# Add depolarizing error to all single qubit u1, u2, u3, cx, measure gates
error_depol_1 = depolarizing_error(0.05, 1)
error_depol_2 = depolarizing_error(0.1, 2)
error_depol_3 = depolarizing_error(0.1, 1)

# Add errors to noise model
noise_depol_single = NoiseModel()
noise_depol_two = NoiseModel()
noise_depol_measure = NoiseModel()
noise_depol_single.add_all_qubit_quantum_error(error_depol_1, ['u1', 'u2', 'u3'])
noise_depol_two.add_all_qubit_quantum_error(error_depol_2, ['cx'])
noise_depol_measure.add_all_qubit_quantum_error(error_depol_3, ['measure'])
noise_depol_single, noise_depol_two, noise_depol_measure
```

Out[43]:
```
(NoiseModel:
   Basis gates: ['cx', 'id', 'u1', 'u2', 'u3']
   Instructions with noise: ['u2', 'u3', 'u1']
   All-qubits errors: ['u1', 'u2', 'u3'],
 NoiseModel:
   Basis gates: ['cx', 'id', 'u3']
   Instructions with noise: ['cx']
   All-qubits errors: ['cx'],
 NoiseModel:
   Basis gates: ['cx', 'id', 'u3']
   Instructions with noise: ['measure']
   All-qubits errors: ['measure'])
```

In [44]:
```
depol_noise_models = [noise_depol_single, noise_depol_two, noise_depol_measue]

thetas = np.linspace(0.0, 2*np.pi, 500)
depol_noisy_energy = np.zeros((len(depol_noise_models), len(thetas)))

for ind, model in enumerate(depol_noise_models):
    func3 = ft.partial(restricted_noisy_vqe, meas_basis=a, coeffs=b, circuit=ansatz2,
                       num_qubits=2, noise_model=model, shots=4096)
    for idx, theta in enumerate(thetas):
        depol_noisy_energy[ind][idx] = func3([theta])
```

In [45]:
```
depol_noise_models_name = ['One-Qubit Gates Depolarization', ' Two-Qubit Gates Depolarization',
                           'Measure Gate Depolarization']

plt.figure()
for ind, model in enumerate(depol_noise_models):
    plt.plot(thetas, depol_noisy_energy[ind], label=depol_noise_models_name[ind])

plt.title('Expectation value w.r.t angle theta and shots')
plt.ylabel('Expectation value of $H_1$')
plt.xlabel('Theta (radians)')
plt.legend()
plt.show()
```



Excited States of the Hamiltonian

One of the way to find the k^{th} exicted states of a Hamiltonian would be to update the Hamiltonain H to H_k as follows:

$$H_k = H + \sum_{i=0}^{k-1} \beta_i |i\rangle\langle i|$$

For example: To find the first excited state, we find $H_1 = H + \beta_0 |g\rangle\langle g|$, where g is the ground state of the Hamiltonian. This works because of spectral decomposition.

This can be used to update our cost function, C_k, as follows:

$$C(\theta_k) = \langle\psi(\theta_k)|H|\psi(\theta_k)\rangle + \sum_{i=0}^{k-1} \beta_i |\langle\psi(\theta_k)|\psi(\theta_i)\rangle|^2$$

We'd already calculated the first term in VQE, but to calculate the next summation term, we refer to [2]. It suggests us to rewrite the overlap term $|\langle\psi(\theta_k)|\psi(\theta_i)\rangle|^2$ as $|\langle 00|U(\theta_k)^\dagger U(\theta_i)|00\rangle|^2$. Therefore, we can prepare the state $U(\theta_k)^\dagger U(\theta_i)|00\rangle$ using the trial state preparation circuit for current state and i^{th} previously-computed state.

This technique is known as ***Variational Quantum Deflation*** and requires the same number of qubits as ***Variational Quantum Eigensolver*** and around twice the circuit depth.

In [185…

```
def vqd_cost(thetak, thetai, func, circuit, num_qubits, beta, shots=2048):
    """  Returns cost for VQD """

    energy = func(thetak)

    for idx, theta in enumerate(thetai):
        ansatz = circuit(theta, num_qubits) + circuit(thetak, num_qubits).inverse()
        ansatz.measure_all()
        backend = Aer.get_backend('qasm_simulator')
        result = execute(ansatz, backend, shots=shots).result()
        energy += beta[idx]*result.get_counts().get('00 00', 0)/shots

    return energy

def vqd(hamiltonian, circuit, num_qubits, params_shape, beta):
    """
        Runs Variational Quantum Deflation algorithm on a given Hamiltonian
        to give its excited eigenvalues.

        Args:
        hamiltonian (matrix(ndarray)): Hamiltonian for
        circuit (Quantum Circuit): ansatz template
        num_qubits (int): number of qubits to make an ansatz
        params_shape (tuple): shape tuple for parameters in ansatz
        beta (int): beta coefficent for VQD

        Returns:
        energy (vector(ndarray)): Calculated eigen energies for the Hamiltonian.
    """

    a, b, c = decompose_ham_to_pauli(hamiltonian)
    initial_params  = np.random.uniform(-np.pi, np.pi, params_shape)
    func  = ft.partial(vqe, meas_basis=a, coeffs=b, circuit=circuit,
                       num_qubits=num_qubits, shots=2048)
    res1 = sp.optimize.minimize(func, initial_params, method='Powell')
    energies = [float(res1.fun)]
    thetas = [np.reshape(res1.x, params_shape)]
```

```
    if len(beta) != np.shape(hamiltonian)[0]-1:
        raise ValueError('Length mismatch! Provide sufficient amount of beta_{i}')

    for eigst in range(np.shape(hamiltonian)[0]-1):
        cost = ft.partial(vqd_cost, thetai=thetas, func=func, circuit=circuit,
                  num_qubits=num_qubits, beta=beta, shots=2048)
        res2 = sp.optimize.minimize(cost, initial_params, method='Powell')
        if res2.success:
            thetas.append(np.reshape(res2.x, params_shape))
            energies.append(float(res2.fun))
        else:
            raise ValueError('Minimization was not successful.')

    return energies
```

Ansatz 1

In [194…
```
excited_energies = vqd(H1, ansatz1, 2, (2,2), [3.5, 1e-1, 1e-3])
excited_energies
```

Out[194…
```
[-1.0, 0.9921875, 0.994189453125, 1.0003808593749999]
```

In [195…
```
assert(np.allclose(np.asarray(excited_energies),  np.sort(np.linalg.eig(H1)[0]), atol=1e-2))
```

Ansatz 2

In [196…
```
excited_energies = vqd(H1, ansatz2, 2, 1, [2.7, 1e-2, 1e-3])
excited_energies
```

Out[196…
```
[-1.0, 0.99365234375, 1.0012158203125, 1.0074306640625]
```

In [197…
```
assert(np.allclose(np.asarray(excited_energies),  np.sort(np.linalg.eig(H1)[0]), atol=1e-2))
```

Interpreting the Results

1. Both of our ansatz produced accurate results despite of ansatz 2 being more expressible than ansatz 1. One reason for this can be that the the ansatz 2 expressibility was covered the interested solution subspace. Another reason could be due to its more entangling capability.
2. Convergence of VQE depends upon both the type of optimizer (gradient-based or point-search) and the choice of ansatz. In general more the number of parameters, and the depth of ansatz, more difficult will be the convergence.
3. Number of shots did matter for non-optimal values of theta in ansatz 2. However, at optimal values of theta, less shots also gave good results. For noisy simulations, higher number of shots were required to get agreeable results.
4. COBYLA and Powell performed far better than others in both noisy and ideal conditions. Next one in line was Nelder-Mead. Gradient-based optimizers gave much poor results. In future, it would nice to see results from specialized optimizers such as rotosolve and rotoselect, and also optimizers that calculate gradients via parameter-shift rule.
5. Ansatz 2 performed better than ansatz 1 under Noisy simulation. However, mitigation improved the result for both of them.
6. Out of all the all the noise models tested, we saw VQE still gave the (deviated) minima at the optimal value of theta, and performed worst for errors due to damping and depolarization.
7. Even with depolarization, presence of errors in measurement gates gave much poor result than two-qubit gates which in turn gave worse results than single-qubit gates.
8. VQD was able to perform better as we adjusted the values of β_i based on the difference between the eigen-energies. In general, values of these β_i should be larger than the largest difference between the consecutive eigen-energies.

In [ ]:
```
```