

QOSF Mentorship Assessment Task

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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 outlined as follows:

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

Necessary Imports

```
In [241... import numpy as np
import scipy as sp
import itertools
import functools as ft
import matplotlib.pyplot as plt
from mpl_toolkits import mplot3d
%matplotlib notebook
import re
```

```
In [184... #!pip install qiskit
from qiskit import *
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: $\langle A, B \rangle = \text{Tr}(A^\dagger B)$. 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:

$$H = \sum_{i_1, \dots, i_n = \{0, x, y, z\}} h_{i_1, \dots, i_n} \cdot \frac{1}{2^n} \sigma_{i_1} \otimes \dots \otimes \sigma_{i_n}$$
$$h_{i_1, \dots, i_n} = \frac{1}{2^n} \text{Tr}((\sigma_{i_1} \otimes \dots \otimes \sigma_{i_n})^\dagger \cdot H) = \frac{1}{2^n} \text{Tr}((\sigma_{i_1} \otimes \dots \otimes \sigma_{i_n}) \cdot H)$$

Decomposing Hamiltonian into Pauli Terms

```
In [5]: 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 [6]: 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 [7]: 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[7]: array([[ 0.7056, 0., -0., 0. ],
               [ 0., -1.1246, 0.182, 0. ],
               [ -0., 0.182, 0.4318, -0. ],
               [ 0., 0., -0., 0.888 ]])

```

```

In [8]: a, b, c = decompose_ham_to_pauli(H0)
a, b

```

```

Out[8]: (['I0I1', 'Z0I1', 'X0X1', 'Y0Y1', 'I0Z1', 'Z0Z1'],
        [0.2252, 0.3435, 0.091, 0.091, -0.43470000000000003, 0.5716])

```

$$H_0 = 0.2252 \times I_0 I_1 + 0.3435 \times Z_0 - 0.4347 \times Z_1 + 0.91 \times X_0 X_1 + 0.91 \times Y_0 Y_1 + 0.5716 \times Z_0 Z_1$$

```

In [9]: compose_ham_from_pauli(a, b)

```

```

Out[9]: 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 [10]: 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 [11]: H1 = np.array([[1, 0, 0, 0],
                        [0, 0, -1, 0],
                        [0, -1, 0, 0],
                        [0, 0, 0, 1]])
H1

```

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

```
In [12]: a, b, c = decompose_ham_to_pauli(H1)
a, b
```

```
Out[12]: (['I0I1', 'X0X1', 'Y0Y1', 'Z0Z1'], [0.5, -0.5, -0.5, 0.5])
```

$$H_1 = 0.5 \times (I_0 I_1 - X_0 X_1 - Y_0 Y_1 + Z_0 Z_1)$$

```
In [13]: compose_ham_from_pauli(a, b)
```

```
Out[13]: 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 [14]: 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 $\text{Pauli } Z$, 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 $M = U^\dagger Z U$, where U is a unitary operator and M gives two unique outcomes of a measurement in its ± 1 eigenvectors. Therefore, 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:

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

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

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 [205...

```
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 [206...

```
def calculate_expectation_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
```

Determining the Ansatz

Designing Ansatzes

Ansatzes 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 ansatz 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 ansätze, one randomly and another inspired from the given hint.

Ansatz 1 (Random Choice)

```
In [18]: 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[18]:
```

```

graph LR
    q0[q_0] -- RX(0.88304) --> X
    q1[q_1] -- RX(-1.352) --> X
    X --> RZ1[RZ(0.26428)]
    RZ1 --> RZ2[RZ(3.0658)]
    style X fill:#fff,stroke:#000,stroke-width:1px
    style RZ1 fill:#fff,stroke:#000,stroke-width:1px
    style RZ2 fill:#fff,stroke:#000,stroke-width:1px

```

c: 2/

Ansatz 2 (From Hint)

```
In [19]: 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

        """

        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[19]:

```
graph LR
    q0[q_0] --> H[H]
    H --> CNOT1[CNOT]
    q1[q_1] --> CNOT1
    CNOT1 --> CNOT2[CNOT]
    q0 --> CNOT2
    CNOT2 --> RX[RX(pi)]
    RX --> c[c: 2/3]
```

Checking Expressibility of Ansätze

We quantify expressibility of ansatz 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 [27]: 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, ansatz, size, samples):
    """
    Return calculation of Integral for a PQC over the uniformly sampled
    the parameters  $\theta$  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 = ansatz(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 [28]: np.linalg.norm(haar_integral(2, 2048) - haar_integral(2, 2048))
```

```
Out[28]: 0.024868548351111183
```

Ansatz 1 (Random Choice)

```
In [29]: np.linalg.norm(haar_integral(2, 2048) - pqc_integral(2, ansatz1, (2,2), 2048))
```

```
Out[29]: 0.02801342169578825
```

Ansatz 2 (From Hint)

```
In [30]: np.linalg.norm(haar_integral(2, 2048) - pqc_integral(2, ansatz2, 1, 2048))
```

```
Out[30]: 0.5020624523202759
```

Ansatz 3 (Empty Circuit)

```
In [31]: 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[31]: 0.8735321855793371
```

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 Ansatz

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

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

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 [32]: 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 [33]: meyer_wallach(ansatz3, 2, 0)
```

```
Out[33]: 0.0
```

Ansatz 1 (Random Choice)

```
In [34]: meyer_wallach(ansatz1, 2, (2,2))
```

```
Out[34]: 0.6275200677278762
```

Ansatz 2 (From Hint)

```
In [35]: meyer_wallach(ansatz2, 2, 1)
```

```
Out[35]: 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 encode 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 parameterized 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 [204... def vqe(params, meas_basis, coeffs, circuit, num_qubits, shots=2048):
    """
    Return the calculated energy scalar for a given ansatz and
    decomposed Hamiltonian.

    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 ansatz.
    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_expectation_val(circuit, basis, shots)

    energy += 0.5

    return energy
```

Ansatz 1 (Random Choice)

```
In [207... 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 [208]: res = sp.optimize.minimize(func, params, method='Powell')
res
```

```
Out[208]: 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: 200
nit: 3
status: 0
success: True
x: array([-1.57091826,  3.16113411,  3.51294118, -1.21586596])
```

```
In [67]: assert(float(res.fun) == min(np.linalg.eig(H1)[0])) #Sanity Check
```

Visualizing the Result

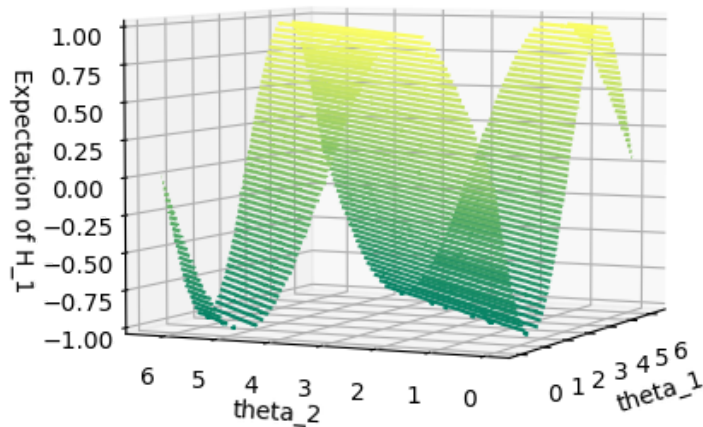
After looking at multiple results' `res.x`, we realize that first and second parameters always have the values $\pm\pi/2$ and $\pm\pi$ respectively. So, while keeping them fixed, we do a parameters search-scan in the range $\theta_{3,4} \in [0, 2\pi]$ and visualize how they affect our expectation value.

```
In [68]: 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, 100)
theta2 = np.linspace(0.0, 2*np.pi, 100)

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 [69]: 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 [70]: res = sp.optimize.minimize(func, params, method='Powell')
         res
```

```
Out[70]: direc: array([[ -7.27080612e-05]])
         fun: array(-1.)
         message: 'Optimization terminated successfully.'
         nfev: 52
         nit: 2
         status: 0
         success: True
         x: array([-3.12289634])
```

```
In [71]: assert(float(res.fun) == min(np.linalg.eig(H1)[0])) #Sanity Check
```

Visualizing the Result

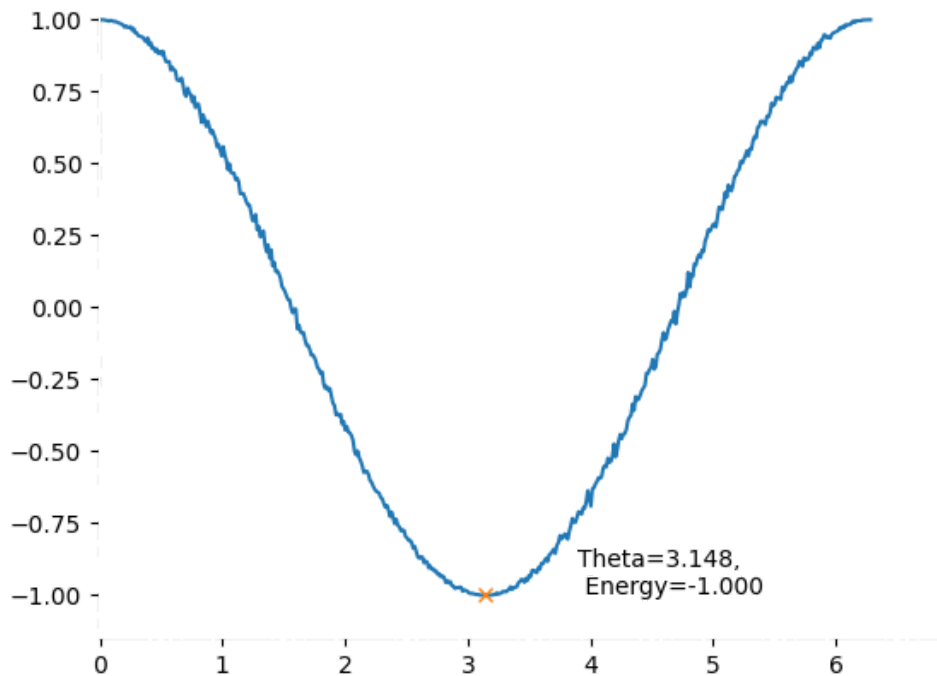
We scan over the parameter $\theta \in [0, 2\pi]$, to visualize the change in expectation value for the ansatz2, which is inspired from the hint given.

```
In [73]: 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()
```



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 performance of our VQE module.

```
In [226... # 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

def calculate_noisy_expectation_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.
    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 ansatz and
    decomposed Hamiltonian 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 ansatz.
    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_expectation_val(circuit, basis, mitigated, shots)

    energy += 0.5

    return energy

```

Ansatz 1 (Random Choice)

```

In [234...] 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 [235...] res = sp.optimize.minimize(func, params, method='Powell')
res

```

```

Out[235...] direc: array([[1., 0., 0., 0.],
        [0., 1., 0., 0.],
        [0., 0., 1., 0.],
        [0., 0., 0., 1.]])
fun: array(-0.86547852)
message: 'Optimization terminated successfully.'
nfev: 190
nit: 3
status: 0
success: True
x: array([ 1.51991209,  3.18646575, -2.04197874,  2.67050187])

```

```

In [232...] 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 [233...] res = sp.optimize.minimize(func, params, method='Powell')

```

res

```
Out[233...   direc: array([[1., 0., 0., 0.],
                [0., 1., 0., 0.],
                [0., 0., 1., 0.],
                [0., 0., 0., 1.]])
   fun: -0.96031367246352
   message: 'Optimization terminated successfully.'
   nfev: 220
   nit: 3
   status: 0
   success: True
   x: array([1.58069027, 3.23188154, 2.69054865, 1.0999503 ])
```

Ansatz 2 (From Hint)

```
In [236... 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 [237... res = sp.optimize.minimize(func, params, method='Powell')
   res
```

```
Out[237...   direc: array([[1.]])
   fun: array(-0.87097168)
   message: 'Optimization terminated successfully.'
   nfev: 73
   nit: 4
   status: 0
   success: True
   x: array([-3.19115317])
```

```
In [238... 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 [239... res = sp.optimize.minimize(func, params, method='Powell')
   res
```

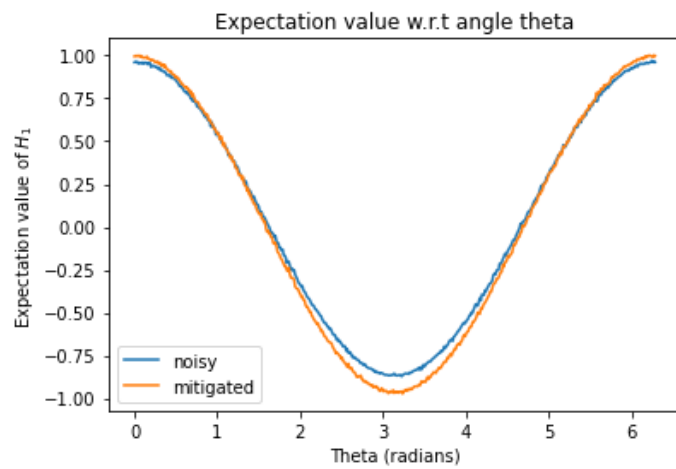
```
Out[239...   direc: array([[ -0.02716262]])
   fun: -0.9725933344219455
   message: 'Optimization terminated successfully.'
   nfev: 118
   nit: 4
   status: 0
   success: True
   x: array([3.13032988])
```

```
In [240... 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])

   fig = plt.figure()
   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()
```

<ipython-input-240-ab06563cfc35>:20: UserWarning: Matplotlib is currently using module://ipykernel.pylab.backend_inline, which is a non-GUI backend, so cannot show the figure.
fig.show()



Excited States of the Hamiltonian

One of the way to find the k^{th} excited states of a Hamiltonian would be to update the Hamiltonian 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 coefficient 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. Ansatz 2 performed better than ansatz 1 under Noisy simulation. However, mitigation improved the result for both of them.
4. 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 [ ]:

```