Variational Principle and Static Perturbation Theory

Arjun Kudinoor

Quantum Mechanics 2 - PHYS 6037, Spring 2022

Abstract

In this class, we have largely been able to solve for the energies and eigenstates of Hamiltonians exactly. However, this is not always possible. We turn to approximation methods like the Variational Principle, Perturbation Theory, and the WKB Method to help us find approximate eigenstates and energies to complicated Hamiltonians. In this lecture, we will study the Variational Principle and Time Independent Perturbation Theory. We will also work through a couple of examples, and implement the Variational Principle on physical quantum systems using a quantum computer.

Contents

1 Variational Principle

1.1 Theory

Suppose we have a Hamiltonian H with energies E_n and corresponding eigenstates $|u_n\rangle$ are unknown. Assume $E_0 < E_1 < ...$, i.e. the energies are ascending. We know that the eigenstates must form an orthonormal basis, i.e.

$$\langle u_n|u_m\rangle = \delta_{nm} \text{ and } \mathbb{1} = \sum_n |u_n\rangle\langle u_n|$$

Goal: To find the ground state energy of the Hamiltonian H.

Method: We begin by guessing a potential ground state $|\psi(\lambda)\rangle$, often referred to as an ansatz. Then, we examine what the energy of this ansatz wavefunction is in this Hamiltonian.

$$E_\psi(\lambda) = \frac{\langle\psi(\lambda)|H|\psi(\lambda)\rangle}{\langle\psi(\lambda)|\psi(\lambda)\rangle}$$

Let us examine this $E_\psi(\lambda)$ more closely. Note that

$$\begin{aligned}
\langle\psi|H|\psi\rangle &= \langle\psi|\mathbb{1}H\mathbb{1}|\psi\rangle \\
&= \sum_{n,m}\langle\psi|u_n\rangle\langle u_n|H|u_m\rangle\langle u_m|\psi\rangle = \sum_{n,m} E_m\langle\psi|u_n\rangle\langle u_n|u_m\rangle\langle u_m|\psi\rangle \\
&= \sum_{n,m} E_m\langle\psi|u_n\rangle\delta_{nm}\langle u_m|\psi\rangle = \sum_n E_n|\langle\psi|u_n\rangle|^2 \\
&\geq E_0\sum_n |\langle\psi|u_n\rangle|^2 = E_0|\langle\psi|\psi\rangle|
\end{aligned}$$

Thus,

$$E_\psi(\lambda) = \frac{\langle\psi(\lambda)|H|\psi(\lambda)\rangle}{\langle\psi(\lambda)|\psi(\lambda)\rangle} \geq E_0$$

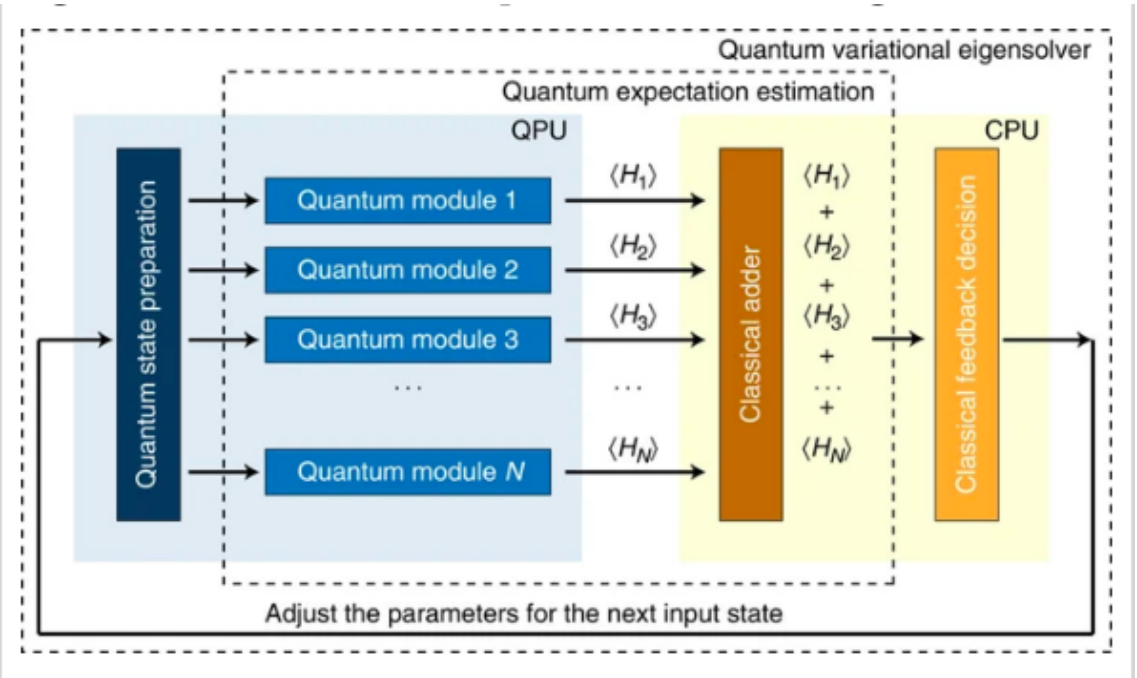
So, for any guess function (ansatz) ψ, we cannot find an energy lower than the ground state energy. Our goal is to find a good approximation for the ground state energy - we do this by minimizing $E_\psi(\lambda)$ with respect to lambda. So, we set

$$\boxed{\frac{\partial E_\psi(\lambda)}{\partial\lambda} = 0}$$

1.2 Quantum Computing Experiment

We can test the physical implementation of the variational principle on quantum states using modern-day quantum computers. A quantum computer is a system that performs operations on quantum bits of information (qubits). These operations are conducted by a series of quantum logic gates, measurements, and possibly classical computations as well.

We can test the experimental validity of the variational principle using a quantum algorithm called the "Variational Quantum Eigensolver" (VQE). This algorithm has 4 parts: state preparation, quantum gate operations, energy measurement, and classical optimization.
In a VQE experiment, we are given a Hamiltonian H, whose ground state energy is unknown. We prepare a guess function (an ansatz) and encode it onto a collection of qubits. Once this state is prepared, we feed these qubits into a set of quantum modules that perform a series of quantum gate operations on these qubits - these gate operations are determined by the Hamiltonian H. Then, we measure the energies of each qubit and add them to get the total state energy. Finally, we optimize this energy by classically varying the variational parameters of our initial quantum state. We repeat this process with our new parameters until a minimum energy is found.



1.2.1 A Simple Example

Suppose we want to find the ground state energy of the Hamiltonian $H = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. It is easy to see that the ground state vector is $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and corresponds to a ground state energy of -1. We denote the vectors

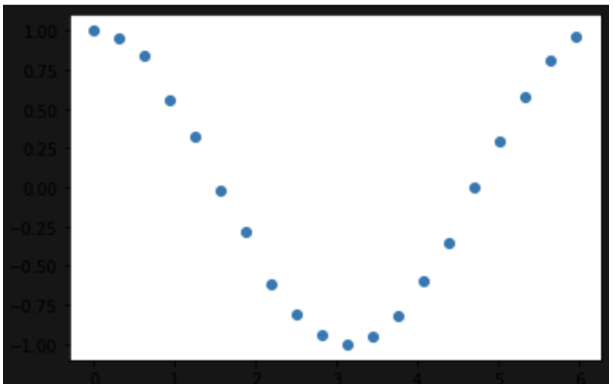
$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

If we wanted to find the ground state and ground state energy of the Hamiltonian using the variational principle, we would first guess some initial wavevector. We could just guess the wavevector $|1\rangle$, but this would be a very uninteresting exercise because it is already the ground state. Instead, let us guess an initial wavevector $U(\theta)|0\rangle$, where θ is our variational parameter and $U(\theta)$ is the rotation matrix

$$U(\theta) = \begin{pmatrix} cos(\theta/2) & -sin(\theta/2) \\ sin(\theta/2) & cos(\theta/2) \end{pmatrix}$$

Then, if we run this state through our variational quantum eigensolver, we get a plot of energies as a function of angle θ. This particular example was run on IBM's Qiskit cloud quantum computing platform (code in the Appendix 3). We should expect the minimum measured energy to be -1 with angle $\theta = \pi$ since $U(\pi)|0\rangle = |1\rangle$, the theoretical ground state.
We find that the minimum energy is -1 and it occurs at $\theta = \pi$, just as we expected. This demonstrates that the variational principle theory we built physically works in nature!

```
(3.141592653589793, -1.0)
```



2 Time Independent Perturbation Theory

The Varational Principle is a good method to approximate the ground state energies of a Hamiltonian. However, it does not give us a prescription for finding good approximations to the eigenstates of an arbitrary Hamiltonian. The Time Independent Perturbation Theory method helps us do just that.

2.1 Nondegenerate Perturbation Theory

Suppose we have a Hamiltonian H_0 whose eigenstates $|n^{(0)}\rangle$ and corresponding energies $E_n^{(0)}$ are known to us. The superscript (0) indicates that these are the eigenstates and energies of the Hamiltonian H_0. Examples of Hamiltonians whose states and energies we know are the infinite square well, simple harmonic oscillator, hydrogen atom, etc.

Now, suppose we have a Hamiltonian $H = H_0 + \lambda H'$ that is a perturbation of our original Hamiltonian by another Hamiltonian H' and some real parameter λ. We do not know the eigenstates or energies of H'.

Goal: We want to find the eigenstates $|n\rangle$ and energies E_n of this total Hamiltonian H. More specifically, we want to find states $|n\rangle$ and energies E_n such that the Schrodinger equation is satisfied:

$$H|n\rangle = E_n|n\rangle$$

Method: We want to leverage the information we already know from the unperturbed Hamiltonian states $|n^{(0)}\rangle$ and energies $E_n^{(0)}$ to construct the new eigenstates and energies for the perturbed Hamiltonian. So, we expand the eignestates $|n\rangle$ and energies E_n in a polynomial over our variational parameter λ.

$$|n\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + ...$$
$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...$$

We then substitute these expansions into the Schrodinger equation, equate terms, and solve for the energy and eigenstate corrections. Before we do that, let's examine the states $|n^{(i)}\rangle$ to understand their orthonormality properties.

2.1.1 Orthonormality of States

Even in perturbation theory, we want our states $|n\rangle$ to be orthonormal, i.e.

$$\langle n|m\rangle = \delta_{nm}$$

If we work to first order in λ, we may write $|n\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle$. The inner product $\langle n|n\rangle$ yields

$$\begin{aligned}
1 = \langle n|n\rangle &= (\langle n^{(0)}| + \lambda\rangle n^{(1)}|)(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle) \\
&= \langle n^{(0)}|n^{(0)}\rangle + \lambda\langle n^{(0)}|n^{(1)}\rangle + \lambda\langle n^{1}|n^{(0)}\rangle + \lambda^2\langle n^{(1)}|n^{(1)}\rangle \\
&= 1 + \lambda(\langle n^{(0)}|n^{(1)}\rangle + \langle n^{(1)}|n^{(0)}\rangle) \text{ (only keeping terms upto first order in } \lambda) \\
&= 1 + 2\lambda\langle n^{(0)}|n^{(1)}\rangle
\end{aligned}$$

So, we can see that $\langle n^{(0)}|n^{(1)}\rangle = 0$. If we worked to higher orders in λ, we would similarly find that

$$\boxed{\langle n^{(i)}|n^{(j)}\rangle = \delta_{ij}}$$

Thus, all our expansion eigenstates are orthonormal.

2.1.2 1st Order Corrections

Now that we know all our expansion states are orthonormal, we can turn back to the Schrodinger equation, and solve for the energy and eigenstate corrections. We begin with the Schrodinger equation $H|n\rangle = E_n|n\rangle$ and expand it in terms of our eigenstate and energy expansions.

$$(H_0+\lambda H')(|n^{(0)}\rangle+\lambda|n^{(1)}\rangle+\lambda^2|n^{(2)}\rangle+...) = (E_n^{(0)}+\lambda E_n^{(1)}+\lambda^2 E_n^{(2)}+...)(|n^{(0)}\rangle+\lambda|n^{(1)}\rangle+\lambda^2|n^{(2)}\rangle+...)$$

If we expand both sides of this equation, they yield polynomials in *lambda* on the left and right hand sides. Linear algebra tells us that we have to then equate the coefficients of each λ^i term. If we do this, we get the following:

$$\begin{aligned}
&\lambda^0 : H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle \text{ (as expected)} \\
&\lambda^1 : H_0|n^{(1)}\rangle + H'|n^{(0)}\rangle = E_n^{(0)}|n^{(1)}\rangle + E_n^{(1)}|n^{(0)}\rangle \ (\star) \\
&\lambda^2 : H_0|n^{(2)}\rangle + H'|n^{(1)}\rangle = E_n^{(0)}|n^{(2)}\rangle + E_n^{(1)}|n^{(1)}\rangle + E_n^{(2)}|n^{(0)}\rangle \ (\dagger) \\
&\text{and so on ...}
\end{aligned}$$

To find the first oder energy corrections $E_n^{(1)}$, we inner product equation $(\star)$ with $\langle n^{(0)}|$.

$$\langle n^{(0)}|H_0|n^{(1)}\rangle + \langle n^{(0)}|H'|n^{(0)}\rangle = E_n^{(0)}\langle n^{(0)}|n^{(1)}\rangle + E_n^{(1)}\langle n^{(0)}|n^{(0)}\rangle$$

Our discussion of orthonormality of expansion states told us that $\langle n^{(0)}|n^{(1)}\rangle = 0$. Thus,

$$\boxed{E_n^{(1)} = \langle n^{(0)}|H'|n^{(0)}\rangle}$$

To find the first order eigenstate corrections $|n^{(1)}\rangle$, we examine how the perturbation term H' in our Hamiltonian acts on each unperturbed basis state $|n^{(0)}\rangle$.

$$\begin{aligned} H'|n^{(0)}\rangle = \mathbb{1}H'|n^{(0)}\rangle &= \sum_m |m^{(0)}\rangle\langle m^{(0)}|H'|n^{(0)}\rangle \\ &= \sum_{m\neq n} |m^{(0)}\rangle\langle m^{(0)}|H'|n^{(0)}\rangle + |n^{(0)}\rangle\langle n^{(0)}|H'|n^{(0)}\rangle \\ &= \sum_{m\neq n} |m^{(0)}\rangle\langle m^{(0)}|H'|n^{(0)}\rangle + E_n^{(1)}|n^{(0)}\rangle \end{aligned}$$

If we compare this equation with equation ($\star$) from above (the λ^1 equation), we deduce

$$(E_n^{(0)} - H_0)|n^{(1)}\rangle = \sum_{m\neq n} |m^{(0)}\rangle\langle m^{(0)}|H'|n^{(0)}\rangle$$

Inner-producting this with $\langle m^{(0)}$, a fixed bra vector with $m \neq n$ yields

$$(E_n^{(0)} - E_m^{(0)})\langle m^{(0)}|n^{(1)}\rangle = \langle m^{(0)}|H'|n^{(0)}\rangle \implies \langle m^{(0)}|n^{(1)}\rangle = \frac{\langle m^{(0)}|H'|n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}$$

Since $|n^{(1)}\rangle = \sum_{m\neq n} |m^{(0)}\rangle\langle m^{(0)}|n^{(1)}\rangle$,

$$\boxed{|n^{(1)}\rangle = \sum_{m\neq n} \frac{\langle m^{(0)}|H'|n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}|m^{(0)}\rangle}$$

Notice that this expression for $|n^{(1)}\rangle$ is well-defined because we are working in the nondegenerate case, i.e. $E_n^{(0)} \neq E_m^{(0)}$ for $m \neq n$. We will treat the degenerate case differently later.

2.1.3 2nd Order Corrections

Let us find the 2nd order corrections $E_n^{(2)}$ to the energies of our nondegenerate system. To do so, we examine the λ^2 equation (†) from above. Similar to the 1st order correction case, we inner product equation (†) with $\langle n^{(0)}|$. Simplifying terms, we get

$$E_n^{(2)} = \langle n^{(0)}|H'|n^{(1)}\rangle$$

Substituing the expression for $|n^{(1)}\rangle$ above, we simplify and find

$$\boxed{E_n^{(2)} = \sum_{m\neq n} \frac{|\langle m^{(0)}|H'|n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}}}$$

2.1.4 Example: Harmonic Oscillator in an Electric Field

Suppose we have a Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - qEx$. Find the energies of this Hamiltonian up to 2nd order in our perturbative expansion.

We may write this Hamiltonian as $H = H_0 + \lambda H'$ with $H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$, $H' = -qEx$, and $\lambda = 1$. We know the energies of H_0, the simple harmonic oscillator.

$$E_n^{(0)} = \hbar\omega(n + \frac{1}{2})$$

To make our lives easier, we express H' using the lowering and raising operators.

$$H' = -qEx = -qE\sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$$

To find the 1st order corrections to the energies, we use the expression $E_n^{(1)} = \langle n^{(0)}|H'|n^{(0)}\rangle$.

$$E_n^{(1)} = -qE\sqrt{\frac{\hbar}{2m\omega}}\langle n^{(0)}|(a + a^\dagger)|n^{(0)}\rangle = 0$$

To find the 2nd order corrections to the energies, we write

$$\begin{aligned} E_n^{(2)} &= \sum_{m\neq n} \frac{|\langle m^{(0)}|H'|n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}} = E_n^{(2)} \\ &= \frac{q^2E^2\hbar}{2m\omega}\sum_{m\neq n}\frac{|\langle m^{(0)}|(a + a^\dagger)|n^{(0)}\rangle|^2}{\hbar\omega(n-m)} \\ &= \frac{q^2E^2}{2m\omega^2}\left(\frac{|\sqrt{n}|^2}{n-(n-1)} + \frac{|\sqrt{n+1}|^2}{n-(n+1)}\right) \\ &= -\frac{q^2E^2}{2m\omega^2} \end{aligned}$$

So, up to 2nd order, $E_n = \hbar\omega(n + \frac{1}{2}) - \frac{q^2E^2}{2m\omega^2}$. If you were to solve this Hamiltonian exactly, by completing the square, you would find that these are the exact values of the energy for H! This is a rare case where perturbation theory gives us the exact values of energies for the Hamiltonian - however, this is not generally the case.

2.2 Degenerate Perturbation Theory

Suppose that the total Hamiltonian $H = H_0 + \lambda H'$ has energy E_n with N degenerate states $n_i^{(0)}$, $i = 1, ..., N$. Here, we have fixed n - so only for the nth energy state is there an N-fold degeneracy.

Goal: We want to find the 1st order corrections $E_n^{(1)}$ for the state $|n\rangle$.

Method: We expand our eigenstate $|n\rangle$ in powers of λ, similar to our nondegenerate case analysis. However, we replace the 0-th order term $|n^{(0)}\rangle$ with a linear combination $\sum_j c_j|n_j^{(0)}\rangle$ of the degenerate states. We do this because we are unsure of what combination of these states yields the "correct" 0-th order contribution to $|n\rangle$. So,

$$|n\rangle = \sum_j c_j|n_j^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + ...$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...$$

We work with the Schrodinger equation $H|n\rangle = E_n$. Then, the λ^1 equation $(\star)$ becomes

$$H_0|n^{(1)}\rangle + \sum_j c_j H'|n_j^{(0)}\rangle = E_n^{(0)}|n^{(1)}\rangle + E_n^{(1)} \sum_j c_j |n_j^{(0)}\rangle$$

We inner product this equation with $\langle n_i^{(0)}|$ to yield

$$\sum_j \langle n_i^{(0)}|H'|n_j^{(0)}\rangle c_j = E_n^{(1)} \sum_j c_j \langle n_i^{(0)}|n_j^{(0)}\rangle = E_n^{(1)} \sum_j c_j \delta_{ij} = E_n^{(1)} c_i$$

The terms $\langle n_i^{(0)}|H'|n_j^{(0)}\rangle = H'_{ij}$ are the matrix elements of H' in the $\{|n_i^{(0)}\rangle\}$ basis of degenerate 0-th order states. So,

$$\boxed{\sum_j H'_{ij} c_j = E_n^{(1)} c_i}$$

This is precisely an eigenvalue equation. The first order corrections $E_n^{(1)}$ are the eigenvalues of H' in the degenerate state basis and the corresponding vectors c_i characterize the "correct" linear combination $\sum_j c_j |n_i^{(0)}\rangle$ in the 0-th order term of the eigenstate $|n\rangle$.

Finding eigenvalues and eigenvectors of a matrix are equivalent to diagonlizing it - so, when we carry about this procedure for finding the 1st order corrections to the energies of degenerate states, we diagonalize the perturbation Hamiltonian H'.

3 Appendix - Code

The code below is the code for executing Example 1.2.1 on IBM's Qiskit cloud quantum computing platform.

```
# Preamble
import numpy as np
import math as m
import matplotlib.pyplot as plt
from qiskit import QuantumCircuit, QuantumRegister, ClassicalRegister, execute,
    BasicAer, IBMQ
from qiskit.visualization import plot_histogram, plot_bloch_multivector

import qiskit
print(qiskit.__qiskit_version__)


# Defining our ansatz
def ansatz(param, qc):
    # We apply some unitary gate onto our general state to create our ansatz.
    # Sets theta = param, and the next two (phi, lambda) to 0. Last argument is the
    qubit number
    # Since our example just has one qubit, let's just set that to 0
    qc.u(param, 0, 0, 0)
    return

```

```
20
21 # Calculating the energy of our ansatz
22 def expectation(param, shots_number = 1024):
23     # We run the quantum circuit. Then, using the resulting measurement, we
       calculate the expectation value
24     # This function is hard-coded for our Hamiltonian
25     # We assume we are in the z-basis. Then, we need only find the amplitudes of
       being in |0> and |1>.
26     # <H> = (Counts(0) - Counts(1)) / Normalization
27
28     # Creating the circuit
29     q = QuantumRegister(1)
30     c = ClassicalRegister(1)
31     qc = QuantumCircuit(q, c)
32
33     # Next, apply our ansatz onto the state
34     ansatz(param, qc) # Applying the ansatz preparation on a given |0>
35
36     # make a measurement in the Z basis
37     qc.measure(0,0) # measures onto the classical registry
38
39     backend = BasicAer.get_backend('qasm_simulator')
40     counts = execute(qc, backend, shots=shots_number).result().get_counts() #
       executs the job
41
42     # Go through the results and return the relative counts of being in either the 0
        or 1 state
43     # I use if/else statements to avoid key errors if we are 100% in one state.
44     if ('0' in counts.keys()):
45         freq_0 = counts['0'] / shots_number
46     else:
47         freq_0 = 0
48
49     if ('1' in counts.keys()):
50         freq_1 = counts['1'] / shots_number
51     else:00
52         freq_1 = 0
53
54     # From the results above, return an expectation value.
55     exp = (1* freq_0) + (-1*freq_1) # This can be seen from <psi | H | psi>
56     return exp
57
58
59 # Iterating through theta and finding the minimum energy
60 def brute_force(step_size, min_theta, max_theta):
61     # This is an extremely naive optimization method, but I am using it return a
       graph
62     # We will pick a step size, start at min_theta, and work all the way to the
       max_theta.
63     # This really only works because our ansatz is a one-parameter wave function
64
65     # Create our array of thetas and the corresponding np.array for expectations.
66     thetas = np.arange(min_theta, max_theta, step_size)
67     expectations = np.zeros(np.size(thetas)) # creating a zero array of equal length
68
69     # Iterate through the thetas to find the expectation value.
70     i = 0
71     while i < np.size(thetas):
```

```
        expectations[i] = expectation(thetas[i])
        i += 1

    # Plot the results and find the minimum value and minimum index.
    plt.scatter(thetas, expectations)
    min_value = np.amin(expectations)
    min_index = np.where(expectations == min_value)[0][0]
    # returns the index of the first instance of the minimum value
    opt_theta = thetas[min_index]

    print("The minimum expectation value is " + str(min_value) + ", which occurs at position "
          + str(min_index) + " and corresponds to theta = " + str(opt_theta))
    # return the theta corresponding to the minimum value, and also the minimum value.
    return opt_theta, min_value


# Now, we run it!
brute_force(m.pi/10, 0.0, 2*m.pi)
```

References

[1] Eugene Commins. *Quantum Mechanics: An Experimentalist's Approach*. Cambridge University Press, 2014. ISBN: 9781107063990.

[2] John Townsend. *A Modern Approach to Quantum Mechanics*. University Science Books, 2000. ISBN: 9781891389788.

[3] A. Peruzzo, J. McClean, and P.A. Shadbolt. "A variational eigenvalue solver on a photonic quantum processor". In: *Nature Communications* 5 (2014). DOI: https://doi.org/10.1038/ncomms5213.

[4] *Perturbation theory*. URL: https://en.wikipedia.org/wiki/Perturbation_theory.