

Quantum Chemistry Challenge:



Project Name: QSpark Dinamics

Team Name: QSpark

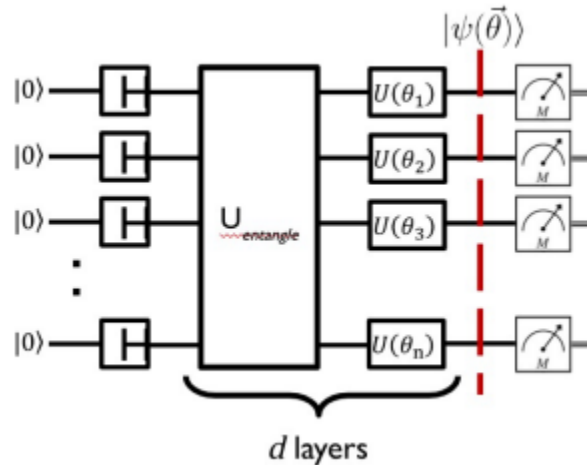
In this hackathon we will face a molecule a bit larger than normal BeH₂

Your goal will be, with the help of a quantum computational algorithm, to obtain a result as close as possible to the real ground state energy value.

The Variational Quantum Eigensolver (VQE) was originally developed by Peruzzo and its theoretical framework was extended and formalized by McClean . The VQE is among the most promising examples of NISQ algorithms. In its most general description, it aims to compute an upper bound for the ground-state energy of a Hamiltonian, which is generally the first step in computing the energetic properties of molecules and materials. The study of electronic structures is a critical application for quantum chemistry

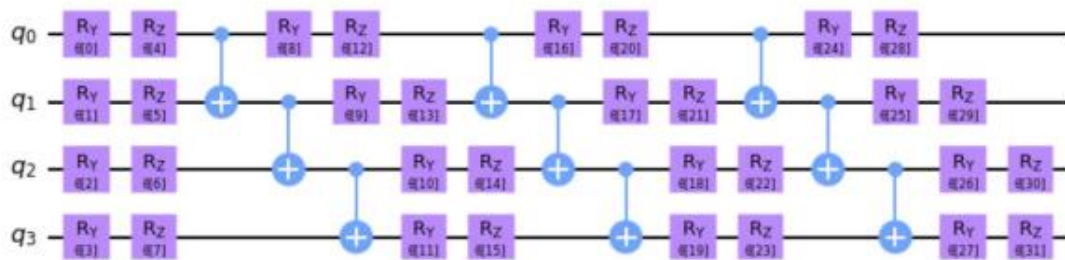
1.Near-Term Vs. Long-term Quantum Algorithms: A near-term quantum algorithm is implemented on Noisy Intermediate-Scale Quantum (NISQ) devices that are available now or in the next few years. Near-term quantum algorithms are often hybrid algorithms, which leverage both classical and quantum devices. On the other hand, long-term quantum algorithms are algorithms that we cannot implement with today's quantum devices, but we know we could once we get fault tolerant devices. This includes Grover's algorithm, Shor's algorithm, and others.

2. Tunable Gates & Tunable Circuits: Variational algorithms are ones with a circuit that can be varied and rerun to produce better results each time. This is called a tunable circuit and comes in many forms. Each form or template is called an ansatz. Designing a good ansatz is the key to working with hybrid algorithms.



The gate operations used in creating a tunable circuit can include:

1. Rx - This gate rotates θ radians around the x axis.
2. Ry - This gate rotates θ radians around the y axis.
3. Rz - This gate rotates θ radians around the z axis.
4. CNOT - This gate is used to entangle qubits



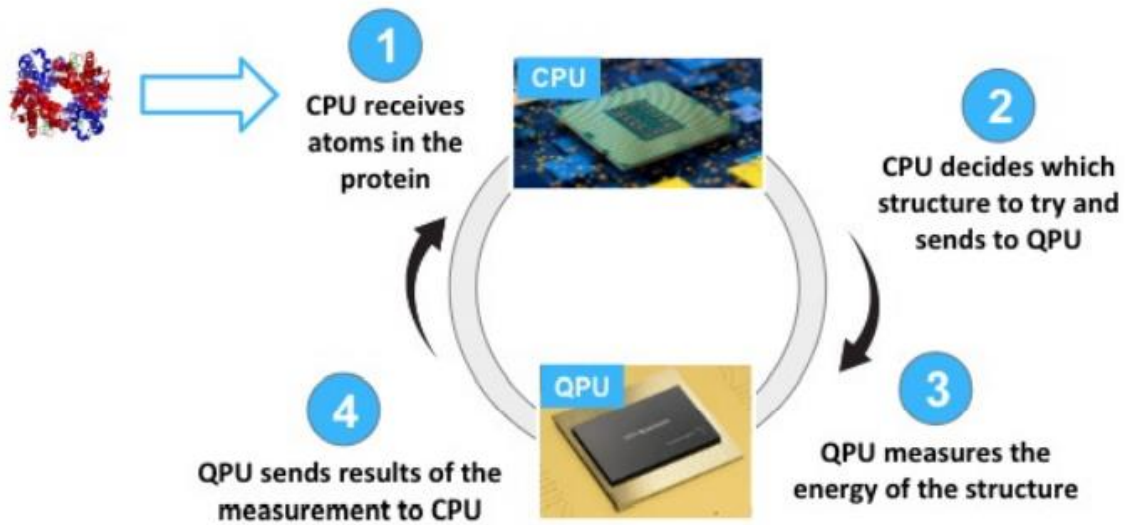
Constrained Optimization Problems: These are problems where we need to find an optimal combination of elements within certain parameters. VQE can be utilized to find these optimal combinations. Classic examples include:

- a. The knapsack problem.
- b. Chemistry - in protein folding & drug discovery via molecular combination.
- c. Finance - in portfolio optimization and risk management.

d. Transport - in route optimizations such as the traveling salesman problem.

e. Molecular simulation - discovering optimizations in carbon capture, battery design, & alternative renewable resources.

4. Steps in VQE:



Quantum computational algorithm:

```
In [1]: # Non-qiskit imports
import math
import numpy as np
import matplotlib.pyplot as plt
import warnings
warnings.filterwarnings("ignore")

# General Qiskit and VQE imports
from qiskit import Aer, IBMQ
from qiskit import QuantumCircuit
from qiskit.visualization import visualize_transition
from qiskit.algorithms import VQE
from qiskit.circuit.library import EfficientSU2
from qiskit.algorithms.optimizers import SPSA, COBYLA
from qiskit.algorithms import NumPyMinimumEigensolver
from qiskit.utils import QuantumInstance
from qiskit_optimization.algorithms import MinimumEigenOptimizer
from qiskit_optimization.converters import QuadraticProgramToQubo

# Knapsack and Electronic Structure Problem imports
from qiskit_optimization.applications import Knapsack
from qiskit_nature.algorithms import (GroundStateEigensolver,
                                     NumPyMinimumEigensolverFactory)
from qiskit_nature.drivers import Molecule
from qiskit_nature.drivers.second_quantization import (
    ElectronicStructureMoleculeDriver, ElectronicStructureDriverType)
from qiskit_nature.problems.second_quantization import ElectronicStructureProblem
from qiskit_nature.converters.second_quantization import QubitConverter
from qiskit_nature.mappers.second_quantization import ParityMapper
from qiskit_nature.second_q.mappers import JordanWignerMapper
from qiskit.opflow import TwoQubitReduction

print("Libraries imported successfully!")

Libraries imported successfully!
```

Finding the Structure of a Molecule

In this section, we will use VQE to determine the structure of the hydrogen molecule *BeH2*.

Setting Up the Problem

The problem of finding the electronic structure of *BeH2* with a distance of 2.4566439619345806 Angstroms between the atoms.

```

dist = 2.4566439619345806
molecule = Molecule(

    geometry=[
        ["Be", [0.0, 0.0, 0.0]],
        ["H", [0.0, 0.0, -dist]],
        ["H", [0.0, 0.0, dist]],
    ],

    multiplicity=1, charge=0)

driver = ElectronicStructureMoleculeDriver(
    molecule=molecule,
    basis="sto3g",
    driver_type=ElectronicStructureDriverType.PYSCF)

problem = ElectronicStructureProblem(driver)

second_q_ops = problem.second_q_ops() # Get 2nd Quant OP
num_spin_orbitals = problem.num_spin_orbitals

num_particles = problem.num_particles
print(num_spin_orbitals)

print(num_particles)
mapper = ParityMapper() # Set Mapper

hamiltonian = second_q_ops['ElectronicEnergy'] # second_q_ops[0] # Set Hamiltonian
#fermionic_op = problem.hamiltonian.second_q_op()
# Do two qubit reduction
#
converter = QubitConverter(JordanWignerMapper(), z2symmetry_reduction="auto", two_qubit_reduction=True)

qubit_op = converter.convert(hamiltonian, sector_locator=problem.symmetry_sector_locator)
#converter = QubitConverter(mapper, two_qubit_reduction=True)
reducer = TwoQubitReduction(num_particles)

qubit_op = reducer.convert(qubit_op)

```

With this algorithm we determine the structure of the hydrogen molecule BeH_2 .

14 Number of qubit first Hamiltonian

Then we need to reduce the number of qubits

```

converter = QubitConverter(JordanWignerMapper(), z2symmetry_reduction="auto", two_qubit_reduction=True)

qubit_op = converter.convert(hamiltonian, sector_locator=problem.symmetry_sector_locator)
#converter = QubitConverter(mapper, two_qubit_reduction=True)
reducer = TwoQubitReduction(num_particles)

qubit_op = reducer.convert(qubit_op)

```

This is the new Hamiltonian with 7 qubits

```

-11.093231605554427 * IIIIIIIII
- 2.2342764803467845 * ZZZIZIIZZ
- 0.030876146934990606 * ZZZIZIIZX
- 0.030876146934990606 * IIIIIIIIX
- 0.025339430508280948 * IZZIIIZXI
- 0.025339430508280948 * ZIIIZIZXZ
- 0.02590563633267814 * IIIIIIIIZ
+ 0.0006538430653180042 * ZIIIZIZYY

```

+ 0.0006538430653180042 * ZIIIZIZXX
- 0.05148801520855965 * ZIIIZIZII
- 0.019318265789275747 * ZZZIZIXZI
+ 0.019318265789275747 * IZZIIIXZI
- 0.09749119599845107 * IIIIIIZI
- 0.30273691642572265 * IIZIIIIII
- 0.30273691642572215 * IZIIIIIIII
- 0.18663477321114838 * IIIIIIZII
- 2.234276480346781 * ZZZZZZIII
- 0.030876146934990658 * ZZZZZXIII
- 0.030876146934990658 * IIIIIXIII
- 0.025339430508281087 * ZZZXIIIIII
- 0.025339430508281087 * IIXZZIII
- 0.025905636332678308 * IIIIIZIII
+ 0.0006538430653179987 * IIIYZYIII
+ 0.0006538430653180004 * IIXZXIII
- 0.05148801520855987 * IIIIZIIII
+ 0.019318265789275705 * YZZZYIIII
+ 0.019318265789275712 * XZZZXIIII
- 0.09749119599845088 * IIZIIIIII
- 0.18663477321114796 * ZIIIIIIII
- 0.1009807490521759 * ZZZIZIIZI
- 0.03899192293517185 * IZZIIIZXX
- 0.03899192293517185 * IZZIIIZYY
- 0.0767589087014456 * IZZIIIZZZ
- 0.03902371098891915 * IIIIIIXIZ
+ 0.03902371098891915 * ZIIIZIXIZ
- 0.08559398342317932 * ZZZIZIIIZ
- 0.2806905855808315 * ZZIIZIIZZ
- 0.2806905855808316 * ZIZIZIIZZ
- 0.11868762887323264 * ZZZIZIZZZ
+ 2.4136596381977108e-05 * IZZIIIZXZ
+ 2.413659638197705e-05 * ZIIIZIZXI
- 0.0019352036246316534 * IZZIIIZZX
- 0.001935203624631653 * ZIIIZIZIX
- 0.0035036756262935434 * IIIIIIXIX
+ 0.002264319839091843 * ZIIIZIXIX
- 0.0012393557872017005 * ZIIIZIYIY
+ 0.0012393557872017005 * ZZZIZIYZY
- 0.002264319839091843 * ZZZIZIXZX
+ 0.0035036756262935434 * IZZIIIXZX
- 5.277374917102631e-05 * ZZZIZIIIX
- 5.277374917102631e-05 * IIIIIIZX
- 0.007488850784653309 * ZZIIZIIZX
- 0.007488850784653309 * IIZIIIIIX
- 0.007488850784653311 * ZIZIZIIZX
- 0.007488850784653318 * IZIIIIIIIX
- 0.00417965060217814 * ZZZIZIZZX
- 0.00417965060217814 * IIIIIIZIX
- 0.0006329701208549004 * ZZZIZIIXI
- 0.0006329701208549004 * IIIIIIXZ
+ 0.0011785344662138127 * IIIIIIXXI
+ 0.002326988206739397 * IIIIIYYI
- 0.001148453740525584 * ZIIIZIYYI

+ 0.001148453740525584 * ZZZIZIYYZ
- 0.002326988206739397 * IZZIIIIYYZ
- 0.0011785344662138127 * IZZIIIXXZ
- 0.006268862976815363 * IZIIIIIZXI
- 0.006268862976815363 * ZIZIZIZXZ
- 0.006268862976815364 * IIZIIIIIZXI
- 0.006268862976815364 * ZZIIIZIZXZ
- 0.004279015499804545 * IZZIIIIIXI
- 0.004279015499804545 * ZIIIZIIXZ
+ 0.5684960111762645 * IIZIZIZIZ
+ 0.0487826880494432 * IIZIZIZIX
+ 0.0487826880494432 * ZZZZZZIIIX
+ 0.04204809284915808 * ZIIZZZZXI
+ 0.04204809284915808 * IZZZIZXZX
+ 0.04878268804944321 * ZZZIZXIZZ
+ 0.04878268804944321 * IIZIXIZZ
+ 0.006538334032144781 * ZZZIZXIZX
+ 0.006538334032144781 * IIZIXIZX
+ 0.006538334032144781 * IIIIIXIIX
+ 0.006538334032144781 * ZZZZZXIIX
+ 0.005668859159946176 * IZZIIXZXI
+ 0.005668859159946176 * ZIIZZXZXI
+ 0.005668859159946176 * ZIIIZXZXZ
+ 0.005668859159946176 * IZZZIXZXZ
+ 0.0009207193056845817 * IZZIXZZZI
+ 0.0009207193056845817 * ZIIZXIZZI
+ 0.0009207193056845817 * IIIIXZIIZ
+ 0.0009207193056845817 * ZZZZXIIIZ
+ 0.0017301765665305607 * IIIIXZXII
+ 0.0017301765665305607 * ZZZZXIXII
- 0.0017301765665305607 * ZZZIYZYZZ
- 0.0017301765665305607 * IIZYIYZZ
+ 0.04204809284915808 * ZZZXIZIZZ
+ 0.04204809284915808 * IIXZIIIZ
+ 0.005668859159946176 * ZZZXIZIZX
+ 0.005668859159946176 * IIXZIIIZX
+ 0.005668859159946176 * IIXZZIIX
+ 0.005668859159946176 * ZZXIIIIIX
+ 0.004916093794680817 * IZZXZZZXI
+ 0.004916093794680817 * ZIIXIIZXI
+ 0.004916093794680817 * ZIIXIZZXZ
+ 0.004916093794680817 * IZZXZIZXZ
+ 0.003913769747552855 * IZXZZZZII
+ 0.003913769747552855 * ZIXIIIZII
+ 0.003913769747552855 * ZIXZIZZZZ
+ 0.003913769747552855 * IZXIZIZZZ
+ 0.003913769747552856 * IXXZZZZII
+ 0.003913769747552856 * ZXIIIIIZII
+ 0.003913769747552856 * ZXIZIZZZZ
+ 0.003913769747552856 * IXXIZIZZZ
+ 0.001730176566530561 * XIIZZZZZI
+ 0.001730176566530561 * XZZIIIZZI
+ 0.001730176566530561 * XZZZZZIIZ
+ 0.001730176566530561 * XIIIIIIIZ

+ 0.003253180587401158 * XZZZZZXII
+ 0.003253180587401158 * XIIIIIXII
- 0.003253180587401158 * YIIZIZYZZ
- 0.003253180587401158 * YZZIZIYZZ
- 0.10751908308432068 * ZZZIZZIZZ
- 0.0016321780112546938 * ZZZIZZIZX
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- 0.0013707570742804364 * IZZIIZZXI
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- 0.0014965621494616886 * IIIIYYIIZ
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- 0.0027479322766393185 * IIIIYYXII
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- 0.0016575830309382988 * YZZYIIIIIZ
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- 0.0030776852368264896 * YZZYIIXII
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- 0.0014493467185287619 * ZIIIIIIIX
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+ 0.15178604822659766 * IIZIIIIIZ
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+ 0.06957087339139933 * IIIIIIZIZ
- 0.014007198555236706 * IIIIIIIYY
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- 0.0014965621494616886 * ZIIIZZZIY
- 0.0014965621494616886 * IZZZYIZIY
- 0.0014965621494616886 * IIIIXZIIIX
- 0.0014965621494616886 * ZZZZXIIIX
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- 0.0015085764894376178 * IIZYIXZY
+ 0.0015085764894376178 * ZZZIYZYZX
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- 0.002747932276639318 * XIIIIIIIX
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+ 0.0027303038836493793 * YIIZIZYZX
+ 0.0027303038836493793 * YZZIZIYZX
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- 0.004579116052267363 * ZIIIZZZXX
+ 0.031683519845633654 * ZIIIXYZIY
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+ 0.031683519845633654 * IIIIXXIIX
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+ 0.004888253998068427 * ZZZIXYXZY
+ 0.004888253998068427 * ZZZIYXYZX

- 0.004888253998068427 * ZZZIXYYZX
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- 0.004579116052267363 * IIIYZYIIZ
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+ 0.025279463797686242 * ZIIYIYZYY
+ 0.025279463797686242 * ZIIXIXZXX
+ 0.025279463797686242 * ZIIYIYZXX
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- 0.013023640233644792 * ZIXZIZZZY
+ 0.013023640233644792 * ZIXZIXZZX
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+ 0.013023640233644797 * ZXIZIXZZX
+ 0.013023640233644797 * ZYIZIYZZX
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+ 0.004888253998068428 * XZZZIZIZY
- 0.004888253998068428 * XZZZZXIIX
- 0.004888253998068428 * YZZZZYIIX
+ 0.014395444810409776 * YIIZIXXZY
- 0.014395444810409776 * XIIZIYXZY
- 0.014395444810409776 * YIIZIXYZX
+ 0.014395444810409776 * XIIZIYYZX
+ 0.07675793468144508 * IIIIZIIIZ
+ 0.012547997076855817 * ZIIIIIZYY
+ 0.012547997076855817 * ZIIIIIZXX
- 0.02655519563209253 * ZIIXYIZIY
+ 0.02655519563209253 * ZIIYXIZIY
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- 0.02655519563209253 * IIIYYIIIX
+ 0.01650892119410557 * ZZZXYIXZY
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- 0.01650892119410557 * ZZZXYIYZX
+ 0.01650892119410557 * ZZZYXIYZX
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- 0.02370453745554476 * YZZZYIZYY
- 0.02370453745554476 * XZZZXIZYY
- 0.02370453745554476 * YZZZYIZXX
- 0.02370453745554476 * XZZZXIZXX
+ 0.07791027959537972 * IIIZIIIIIZ
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+ 0.010849983760835005 * ZXIXZIZZX
+ 0.010849983760835005 * ZYIYZIZZX
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- 0.02929100398176276 * XZZYZIZIY
+ 0.02929100398176276 * XZZXIIIIIX

+ 0.02929100398176276 * YZZYIIIIIX
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+ 0.004420566043489543 * XIIYZIXZY
+ 0.004420566043489543 * YIIXZIIYZX
- 0.004420566043489543 * XIIYZIIYZX
+ 0.08396631820180912 * ZIIIIIIIZ
- 0.00685853524506079 * IIIIZIZYY
- 0.00685853524506079 * IIIIZIZXX
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+ 0.1282034845597751 * ZZIIZIZII
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- 0.01660899095903293 * IZZIIIXII
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- 0.04341371115795717 * IZIIIIIXZI
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- 0.043413711157957176 * IIZIIIXZI
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- 0.0140071985552367 * IIIIIYY
- 0.0140071985552367 * IIIIIXX
- 0.012782082787657177 * ZZIZXYX
+ 0.005586466526218001 * ZZIZYXY
+ 0.007195616261439185 * ZZIIYXY
+ 0.007195616261439185 * ZZIZYYX
+ 0.005586466526218001 * ZZIIYYX
+ 0.012782082787657177 * ZZIIXXX
- 0.04042319649030313 * IZIZZYY
- 0.04042319649030313 * IZIZZXX
- 0.04042319649030315 * ZIIZZYY
- 0.04042319649030315 * ZIIZZXX
- 0.011279101288550333 * IIZIYY
- 0.011279101288550333 * IIZIXX
- 0.04605567576578045 * ZZZIZYY
- 0.04605567576578045 * ZZZIZXX
- 0.030186957696171954 * IIIYZIY
- 0.0014965621494616881 * ZZZYZIY
- 0.030186957696171954 * IIIXIIX
+ 0.0063968304875060425 * ZZIYXZY
- 0.0015085764894376171 * IIZYXZY
- 0.0063968304875060425 * ZZIYYZX
+ 0.0015085764894376171 * IIZYYZX
+ 0.005949873126547797 * IIXZIIZ
- 0.026479777419378587 * IIXIZYY
+ 0.0012003136216923547 * ZZXZZYY
- 0.026479777419378587 * IIXIZXX
+ 0.0012003136216923547 * ZZXZZXX
- 0.009062512367771062 * IYZIZZY
- 0.003961127865873723 * ZYIZZZY
- 0.009062512367771062 * IXZIZZX
- 0.003961127865873723 * ZXIZZZX
- 0.009062512367771072 * YIZIZZY
- 0.003961127865873723 * YZIZZZY
- 0.009062512367771072 * XIZIZZX
- 0.003961127865873723 * XZIZZZX
- 0.002747932276639317 * ZZZIZIY
+ 0.002747932276639317 * IIZZIY
- 0.0027303038836493775 * IIZIXZY
+ 0.0027303038836493784 * ZZIZXZY
+ 0.0027303038836493775 * IIZIYZX
- 0.0027303038836493784 * ZZIZYZX
- 0.03168351984563364 * IIIXZIY
+ 0.03168351984563364 * IIIYIIX
+ 0.004888253998068425 * ZZIXXZY
- 0.004888253998068425 * ZZIXYZX
- 0.004579116052267361 * IIZZIIZ
+ 0.02527946379768623 * IIZIZYY
+ 0.02527946379768623 * IIZIZXX
- 0.013023640233644787 * IXZIZZY
+ 0.013023640233644787 * IYZIZZX
- 0.013023640233644792 * XIZIZZY
+ 0.013023640233644792 * YIZIZZX
+ 0.07675793468144505 * IIZZIIZ

+ 0.012547997076855812 * IIIIZYY
+ 0.012547997076855812 * IIIIZXX
- 0.02655519563209252 * IIXYZIY
+ 0.02655519563209252 * IIXXZIY
- 0.02655519563209252 * IIXXIIX
- 0.02655519563209252 * IYYIIX
+ 0.016508921194105564 * ZZXYXZY
- 0.016508921194105564 * ZZYXXZY
- 0.016508921194105564 * ZZXYYZX
+ 0.016508921194105564 * ZZYXYZX
+ 0.0054240411392868755 * ZZZYIIZ
+ 0.02370453745554475 * ZZZYZZY
- 0.02370453745554475 * ZZZXZYY
+ 0.02370453745554475 * ZZZYZXX
- 0.02370453745554475 * ZZZXZXX
+ 0.07791027959537969 * IIZIIIZ
+ 0.00863919256866846 * IIZZZYY
+ 0.00863919256866846 * IIZZZXX
+ 0.010849983760835001 * IYXZZZY
- 0.010849983760835001 * IXYZZZY
+ 0.010849983760835001 * IXXZZZX
+ 0.010849983760835001 * IYYZZZX
+ 0.010849983760835001 * YIXZZZY
- 0.010849983760835001 * XIYZZZY
+ 0.010849983760835001 * XIXZZZX
+ 0.010849983760835001 * YIYZZZX
- 0.02929100398176275 * ZZXZZIY
- 0.02929100398176275 * ZZYZZIY
- 0.02929100398176275 * ZZYIIIX
+ 0.004420566043489541 * IIXZXZY
+ 0.004420566043489541 * IIZZXZY
- 0.004420566043489541 * IIXZYZX
- 0.004420566043489541 * IIZZYZX
+ 0.0506642647630694 * IIZZZI
+ 0.12820348455977504 * IZIZZII
+ 0.12820348455977504 * ZIIZZII
+ 0.016608990959032923 * ZZIZXII
- 0.016608990959032923 * ZZIIXII
+ 0.043413711157957155 * ZIIZXZI
- 0.043413711157957155 * ZIIIXZI
+ 0.04341371115795716 * IZIZXZI
- 0.04341371115795716 * IZIIXZI
+ 0.07811826948230013 * ZZZIZII
+ 0.04150963090510393 * IIZIXZI
- 0.04150963090510393 * IIZZXZI
+ 0.02683861560588802 * IIIYZYI
- 0.0002834199737954983 * ZZZYZYI
+ 0.02683861560588802 * IIXIXI
- 0.0002834199737954983 * ZZZXIXI
- 0.012198446929796415 * IIXIZII
- 0.0003495501470594015 * ZZXZZII
+ 0.024373942631345853 * ZZXIXZI
- 0.0006694051758010979 * IIXZXZI
- 0.024373942631345853 * ZZXZXZI

+ 0.0006694051758010979 * IIXIXZI
- 0.0004790485647244852 * ZZZIZYI
+ 0.00047904856472448585 * IIIZZYI
- 0.03253879382348664 * ZZZZIXI
- 0.00047904856472448585 * IIIIIXI
+ 0.02655519563209252 * IIXZYZI
- 0.02655519563209252 * IIIYIXI
+ 0.012547997076855817 * IYIZII
- 0.023704537455544756 * ZZYIXZI
+ 0.023704537455544756 * ZZYXZI
+ 0.03357735811188127 * IIXYZYI
- 0.03357735811188127 * IIXYZYI
+ 0.03357735811188127 * IIXXIXI
+ 0.03357735811188127 * IYYIXI
+ 0.0017682056417195001 * IYZYZZI
+ 0.0017682056417195001 * IXZXZZI
+ 0.0017682056417195001 * IXZXIZI
+ 0.0017682056417195001 * IYZYIZI
+ 0.0017682056417195004 * YIZYZZI
+ 0.0017682056417195004 * XIZXZZI
+ 0.0017682056417195004 * XIZXIZI
+ 0.0017682056417195004 * YIZYIZI
+ 0.01941490171160182 * ZZZYZII
- 0.01941490171160182 * ZZZXZII
- 0.04905541480408368 * IIZYXZI
+ 0.04905541480408368 * IIZXXZI
+ 0.08424162287495071 * IIZZZII
- 0.008019115593261543 * ZZZZXZI
+ 0.008019115593261543 * ZZZIXZI
+ 0.024628106552294464 * ZZXZZYI
+ 0.024628106552294464 * ZZYZZYI
- 0.024628106552294464 * ZZXIIXI
+ 0.024628106552294464 * ZZYIIXI
- 0.0027892656656257515 * ZYIZZZI
+ 0.0027892656656257515 * ZXIZZZI
+ 0.0027892656656257515 * ZXIIIZI
- 0.0027892656656257515 * ZYIIIZI
- 0.002789265665625753 * YZIZZZI
+ 0.002789265665625753 * XZIZZZI
+ 0.002789265665625753 * XZIIIZI
- 0.002789265665625753 * YZIIIZI
+ 0.13386560804014777 * IZIIIZI
+ 0.1338656080401478 * ZIIIIIZI
+ 0.05377187022075583 * IIIIZZI
+ 0.09176316458872351 * ZZZZIZI
- 0.027633420950824456 * ZZIXYYI
- 0.0016575830309382982 * IIZXYYI
- 0.027633420950824456 * ZZIXXXI
- 0.0016575830309382982 * IIZXXXI
- 0.007619463200286027 * IIXZIZI
- 0.001019729368382432 * ZZXIIZI
- 0.007443448010270441 * IYZZIIYI
- 0.0034065357505645593 * ZYIIIIYI
- 0.007443448010270441 * IXZZIXI

- 0.0034065357505645593 * ZXIIIXI
- 0.007443448010270441 * YIZZIIYI
- 0.00340653575056456 * YZIIIIYI
- 0.007443448010270441 * XIZZIXI
- 0.00340653575056456 * XZIIIXI
+ 0.01191881732380557 * IIZZYYI
- 0.003077685236826488 * ZZIIYYI
+ 0.01191881732380557 * IIZZXXI
- 0.003077685236826488 * ZZIIXXI
+ 0.029291003981762754 * ZZIYYYYI
+ 0.029291003981762754 * ZZIYXXI
+ 0.00863919256866846 * IIZIZI
- 0.010849983760835 * IXZZIYI
+ 0.010849983760835 * IYZZIXI
- 0.010849983760835001 * XIZZIIYI
+ 0.010849983760835001 * YIZZIXI
+ 0.08424162287495068 * IIZIZI
- 0.024628106552294464 * ZZXXYYI
- 0.024628106552294464 * ZZZYYYI
- 0.024628106552294464 * ZZZXXXI
- 0.024628106552294464 * ZZZYXXI
+ 0.00801911559326154 * ZZZXIZI
- 0.00801911559326154 * ZZZYIZI
+ 0.0848934910661167 * IIZIIZI
+ 0.009135938253688584 * IYXIIYI
- 0.009135938253688584 * IXYIIYI
+ 0.009135938253688584 * IXXIIXI
+ 0.009135938253688584 * IYYIIXI
+ 0.009135938253688585 * YIXIIYI
- 0.009135938253688585 * XIYIIYI
+ 0.009135938253688585 * XIXIIXI
+ 0.009135938253688585 * YIYIIXI
+ 0.02824079809276439 * IIXIYYI
- 0.02824079809276439 * IYIYYI
+ 0.02824079809276439 * IIXIXXI
- 0.02824079809276439 * IYIXXI
+ 0.3892355930337426 * ZZIIIII
+ 0.1708833603026625 * IZIIIZI
+ 0.2881794363654847 * ZIZZIII
+ 0.0466920594671185 * IZXZIII
- 0.006268862976815361 * ZIXIIII
- 0.04042319649030313 * IZYZIII
+ 0.12820348455977504 * IZIZIII
+ 0.0027892656656257515 * ZYZXYII
- 0.0027892656656257515 * ZXZYYII
+ 0.0027892656656257515 * ZXZXXII
+ 0.0027892656656257515 * ZYZYXII
- 0.043413711157957155 * ZIZXIII
+ 0.043413711157957155 * ZIZYIII
+ 0.13386560804014774 * IZZIIII
+ 0.012124689610585573 * YYIIIII
+ 0.012124689610585573 * XXIIIII
+ 0.004560303161411231 * IYIIYII
+ 0.004560303161411231 * IXIIYII

```

+ 0.004560303161411231 * IXIIXII
- 0.004560303161411231 * IYIIXII
+ 0.1708833603026625 * ZIIIZII
+ 0.2881794363654848 * IZZZIII
+ 0.046692059467118505 * ZIXZIII
- 0.006268862976815361 * IZXIIII
- 0.04042319649030314 * ZIYZIII
+ 0.12820348455977504 * ZIIZIII
+ 0.002789265665625753 * YZZXYII
- 0.002789265665625753 * XZZYYII
+ 0.002789265665625753 * XZZXXII
+ 0.002789265665625753 * YZZYXII
- 0.04341371115795717 * IZZXIII
+ 0.04341371115795717 * IZZYIII
+ 0.13386560804014777 * ZIZIIII
+ 0.004560303161411232 * YIIIIYII
+ 0.004560303161411232 * XIIIIYII
+ 0.004560303161411232 * XIIIXII
- 0.004560303161411232 * YIIIXII
+ 0.12339015617916253 * ZZZZZII
+ 0.008059865508038841 * IIXZZII
- 0.001201330262978055 * ZZXIZII
- 0.006858535245060787 * IIZZZII
+ 0.08201266831352023 * IIZIZII
- 0.038991922935171834 * ZZYIIII
+ 0.07869411232607722 * ZZZIIII
+ 0.04252738661521268 * IIXIIII
- 0.04252738661521268 * IIIYIII
+ 0.08564675717235033 * ZZIZIII
- 0.0006329701208549001 * ZZXZIII
+ 0.014640168676091601 * IIXIIII
+ 0.0011785344662138123 * IIXXIII
- 0.0023269882067393963 * IIYXIII
- 0.0011484537405255836 * IIYYIII
- 0.021126152789621946 * ZZYYIII
+ 0.0032594783194786047 * ZZYXIII
- 0.018799164582882548 * ZZXXIII
- 0.0140071985552367 * IIYIIII
+ 0.005586466526218001 * ZZXYIII
+ 0.0506642647630694 * IIZZIII
+ 0.016608990959032923 * ZZIYIII
- 0.016608990959032923 * ZZIXIII

```

Next, we will set up VQE. Specifically, we will create:

- The tunable circuit using `EfficientSU2` with the correct number of qubits and 1 repetition.
- A classical optimizer that uses the `COBYLA` algorithm provided by Qiskit.
- The VQE solver combining all of these components.


```

tunable_circuit = EfficientSU2(num_qubits = qubit_op.num_qubits, reps=1)# COMPLETE THIS LINE

optimizer = COBYLA(maxiter=500)

method = VQE(ansatz = tunable_circuit, optimizer = optimizer, quantum_instance = Aer.get_backend('qasm_simulator'))
#method = VQE(ansatz = tunable_circuit, optimizer = optimizer, quantum_instance = provider.get_backend('ibm_nairobi'))

```

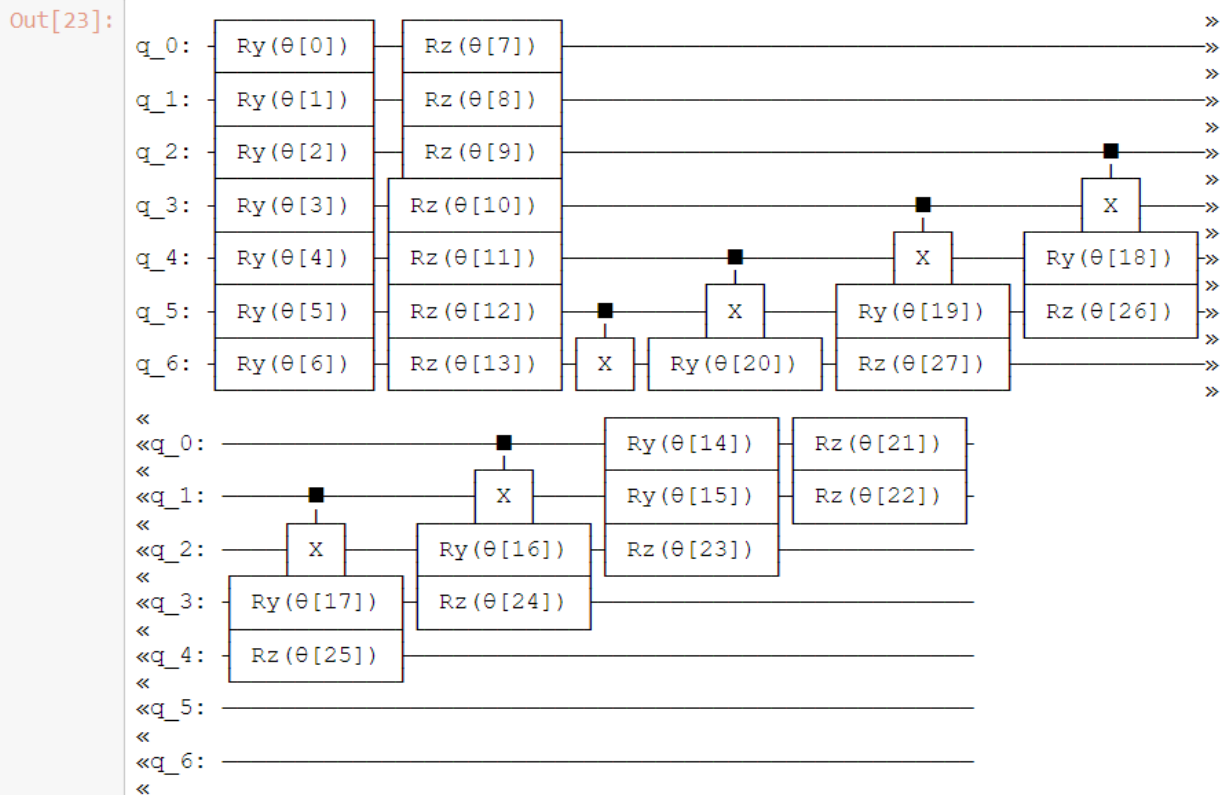
Visualize the Circuit

Before solving the problem, let's visualize the tunable circuit we will be using.

```

In [23]: #var_form.decompose().draw()# COMPLETE THIS LINE
tunable_circuit.decompose().draw()# COMPLETE THIS LINE

```



Using VQE to Solve the Problem

Finally, it's time to find the energy of this structure and print the results.

```
calc = GroundStateEigensolver(converter, method)
result = calc.solve(problem)

print("Total energy = ", result.total_energies)
```

Total energy = [-14.06252947]

Verify the Solution

it's difficult for us to determine if this solution is correct just by looking at it. So, let's use an exact solver that is guaranteed to give us the correct answer.

```
method = NumPyMinimumEigensolver()

calc = GroundStateEigensolver(converter, method)
exact_result = calc.solve(problem)
print("Total energy = ", exact_result.total_energies)
```

Total energy = [-15.3561025]

Run the code below to exactly calculate the error in VQE's answer.

```
print("Error % = ", (exact_result.total_energies - result.total_energies)/(exact_result.total_energies)*100)
```

Error % = [8.42]