VQE3

September 6, 2024

0.0.1 Constructing the Molecule

[16]:
```
from qiskit_nature.units import DistanceUnit
from qiskit_nature.second_q.drivers import PySCFDriver

driver = PySCFDriver(
    atom="He 0 0 0; H+ 0 0 0.772",
    basis="sto-3g",
    charge=1,
    spin=0,

)

problem = driver.run()
print(problem)
```

```
<qiskit_nature.second_q.problems.electronic_structure_problem.ElectronicStructur
eProblem object at 0x71cef0589d00>
```

0.0.2 Converting to fermionic operator

[17]:
```
fermionic_op = problem.hamiltonian.second_q_op()
#print(fermionic_op)
```

0.0.3 Jordan-Wigner Mapping

[18]:
```
from qiskit_nature.second_q.mappers import JordanWignerMapper

mapper = JordanWignerMapper()
qubit_jw_op = mapper.map(fermionic_op)
#print(qubit_jw_op)
```

0.0.4 Constructing the Optimization Log

[19]:
```
class OptimizerLog:
    """Log to store optimizer's intermediate results"""
    def __init__(self):
        self.evaluations = []
```

```
        self.parameters = []
        self.costs = []
    def update(self, evaluation, parameter, cost, _stepsize):
        self.evaluations.append(evaluation)
        self.parameters.append(parameter)
        self.costs.append(cost)
```

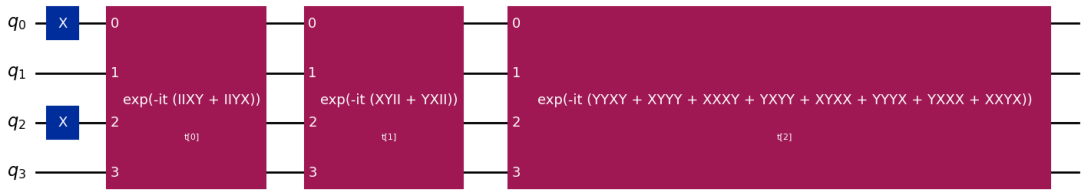
0.0.5 Chosing the Optimization Method and Variational Form

[20]:
```
from qiskit_algorithms import VQE
from qiskit_algorithms.optimizers import SLSQP,SPSA,COBYLA, L_BFGS_B
from qiskit.primitives import Estimator
from qiskit_nature.second_q.circuit.library import HartreeFock, UCCSD
import numpy as np
#this is the optimization method
log = OptimizerLog()
# Sequential Least Squares Programming

Optimizer = SLSQP()

# Using Unitary Coupled Cluster as Variational Form and HatreeFock for intial␣
 ↪states

# The Variation Form does affect the number parameters(theta) which also impact␣
 ↪the number
# of iteration and expectation value (ground-state energy)

ansatz = UCCSD(
    problem.num_spatial_orbitals,
    problem.num_particles,
    mapper,
    initial_state=HartreeFock(
        problem.num_spatial_orbitals,
        problem.num_particles,
        mapper,
    ),
)

vqe_solver = VQE(Estimator(), ansatz, optimizer=Optimizer,callback=log.update)

#Set the initial parameters(theta) as random - this will
# also affect the convergence of the plot and number of iteration.

#maybe we can a away to appoximate the intial points

vqe_solver.initial_point = np.random.random(ansatz.num_parameters)
```

```
ansatz.decompose().draw('mpl')
```

```
/tmp/ipykernel_156137/2768004495.py:25: DeprecationWarning: The class
``qiskit.primitives.estimator.Estimator`` is deprecated as of qiskit 1.2. It
will be removed no earlier than 3 months after the release date. All
implementations of the `BaseEstimatorV1` interface have been deprecated in favor
of their V2 counterparts. The V2 alternative for the `Estimator` class is
`StatevectorEstimator`.
  vqe_solver = VQE(Estimator(), ansatz, optimizer=Optimizer,callback=log.update)
```

[20]:



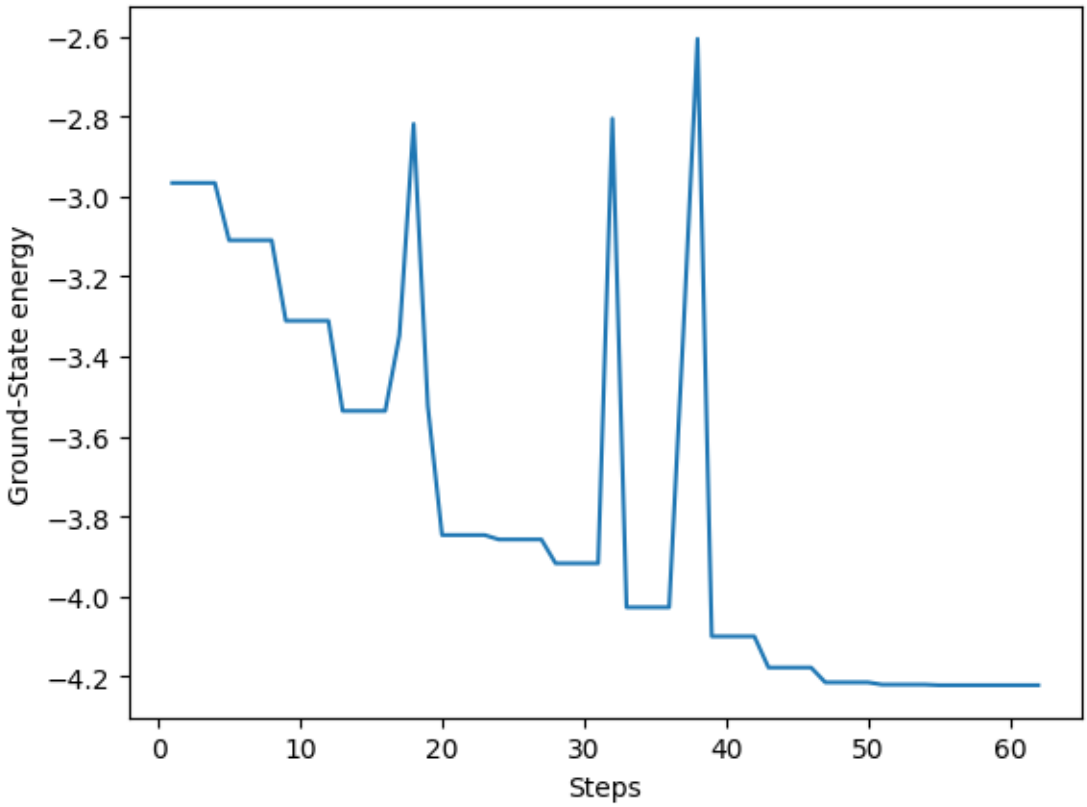
0.0.6 Solving the Ground-state energy

[21]:
```
from qiskit_nature.second_q.algorithms import GroundStateEigensolver
#from qiskit_aer import AerSimulator, Aer
calc = GroundStateEigensolver(mapper, vqe_solver)
res = calc.solve(problem)
print(res)
```

```
=== GROUND STATE ENERGY ===

* Electronic ground state energy (Hartree): -4.221949415588
  - computed part:      -4.221949415588
~ Nuclear repulsion energy (Hartree): 1.370925416891
> Total ground state energy (Hartree): -2.851023998697

=== MEASURED OBSERVABLES ===

  0:  # Particles: 2.000 S: 0.000 S^2: 0.000 M: 0.000

=== DIPOLE MOMENTS ===

~ Nuclear dipole moment (a.u.): [0.0  0.0  1.45886857]

  0:
  * Electronic dipole moment (a.u.): [0.0  0.0  0.386347815215]
    - computed part:      [0.0  0.0  0.386347815215]
  > Dipole moment (a.u.): [0.0  0.0  1.072520754785]  Total: 1.072520754785
                 (debye): [0.0  0.0  2.726075586203]  Total: 2.726075586203
```

0.0.7 Ploting the Optimization value over iteration

[22]:
```
import matplotlib.pyplot as plt

figfig = plt.figure()
plt.plot(log.evaluations, log.costs)
plt.xlabel('Steps')
plt.ylabel('Ground-State energy')
plt.show()
```



0.0.8 Ploting the Paramaters(theta) over iteration

[23]:
```
# Extract parameters
data = log.parameters
iterations = range(len(data))
param1 = [row[0] for row in data]
param2 = [row[1] for row in data]
param3 = [row[2] for row in data]

# Plotting the parameters
plt.figure(figsize=(10, 6))
```

```
plt.plot(iterations, param1, label='Parameter 1')
plt.plot(iterations, param2, label='Parameter 2')
plt.plot(iterations, param3, label='Parameter 3')

plt.xlabel('Iteration')
plt.ylabel('Parameter Value')
plt.title('Parameters Over Iterations')
plt.legend()
plt.grid(True)
plt.show()
```