VQE3.3

September 9, 2024

0.0.1 Constructing the Molecule

[120]:
```
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 0x79e09ec680e0>
```

0.0.2 Converting to fermionic operator

[121]:
```
fermionic_op = problem.hamiltonian.second_q_op()
#print(fermionic_op)
```

0.0.3 Jordan-Wigner Mapping

[122]:
```
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

[123]:
```
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

[124]:
```
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()

Optimizer = SLSQP()
# Sequential Least Squares Programming
Optimizer2 = SPSA()
#Simultanious Pertubation Stochastic Approximation
'''
The main feature of SPSA is the stochastic gradient approximation,
which requires only two measurements of the objective function, regardless of␣
 ↪the dimension of the optimization problem.
'''
Optimizer3 = COBYLA()

Optimizer4 = L_BFGS_B()

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

```
/tmp/ipykernel_7640/3046545942.py:37: 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)
```

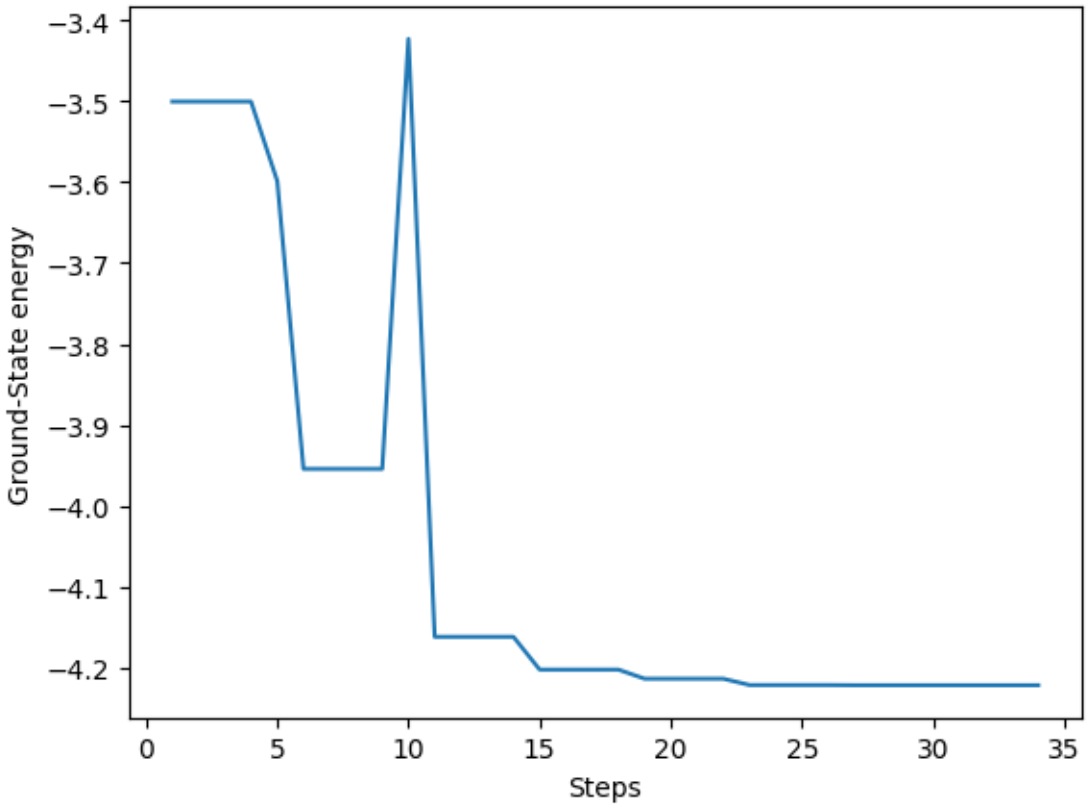
0.0.6 Solving the Ground-state energy

[125]:
```
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): -4.221949436267
  - computed part:      -4.221949436267
~ Nuclear repulsion energy (Hartree): 1.370925416891
> Total ground state energy (Hartree): -2.851024019376

=== 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  0.386320566725]
    - computed part:      [0.0  0.0  0.386320566725]
  > Dipole moment (a.u.): [0.0  0.0  1.072548003275]  Total: 1.072548003275
                 (debye): [0.0  0.0  2.726144844949]  Total: 2.726144844949
```

0.0.7 Ploting the Optimization value over iteration

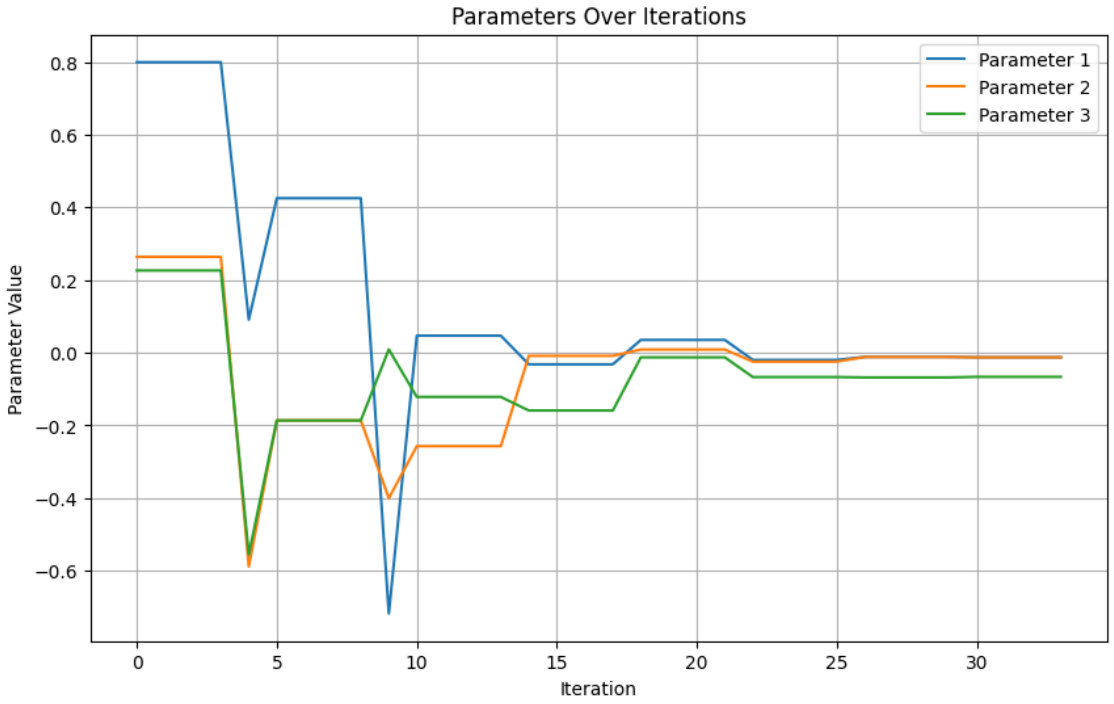
[126]:
```
import matplotlib.pyplot as plt

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

[127]:
```
# 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()
```



0.0.9 A Different Variational Method.

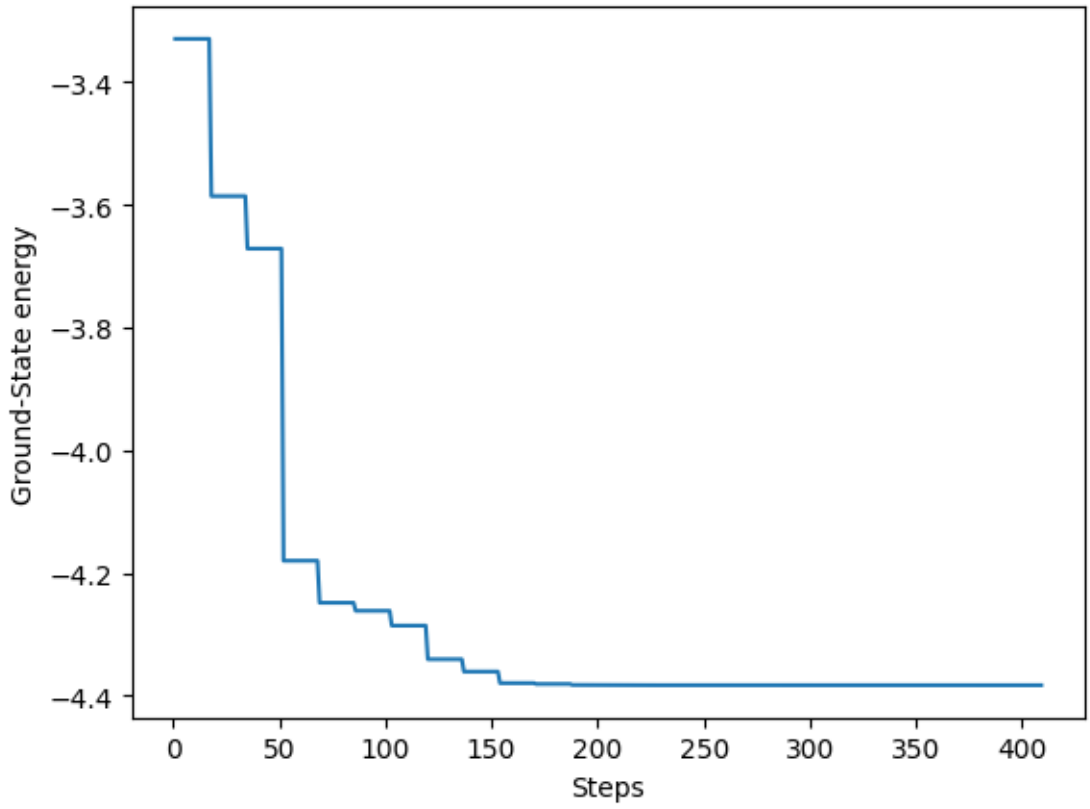
[128]:
```
log2 = OptimizerLog()
```

[129]:
```
from qiskit import QuantumCircuit
from qiskit.circuit.library import TwoLocal
import numpy as np
# Initial States base on HatreeFock approximation
reference_circuit = QuantumCircuit(4)
reference_circuit.x(0)
reference_circuit.x(2)
ansatz2 = TwoLocal(
```

```
    4,
    rotation_blocks=["rz", "ry"],
    entanglement_blocks="cx",
    entanglement="linear",
    reps=1,
)
ansatz2 = reference_circuit.compose(ansatz2)
vqe_solver2 = VQE(Estimator(), ansatz2, optimizer=Optimizer,callback=log2.
 ↪update)
vqe_solver2.initial_point= np.random.random(ansatz2.num_parameters)

from qiskit_nature.second_q.algorithms import GroundStateEigensolver
#from qiskit_aer import AerSimulator, Aer
calc2 = GroundStateEigensolver(mapper, vqe_solver2)
res2 = calc2.solve(problem)
print(res2)
```

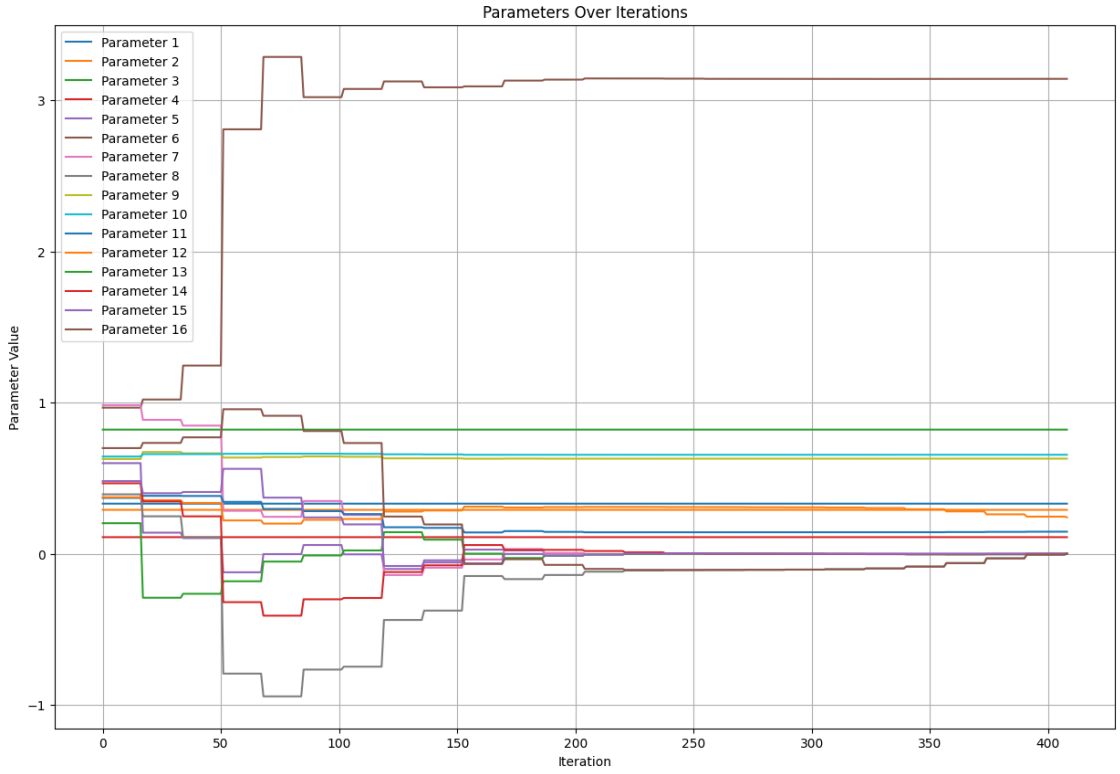
```
/tmp/ipykernel_7640/2111297350.py:16: DeprecationWarning: The class
``qiskit.primitives.estimator.Estimator`` is deprecated as of qiskit 1.2. It
will be removed no earlier than 3 months after the release date. All
implementations of the `BaseEstimatorV1` interface have been deprecated in favor
of their V2 counterparts. The V2 alternative for the `Estimator` class is
`StatevectorEstimator`.
  vqe_solver2 = VQE(Estimator(), ansatz2,
optimizer=Optimizer,callback=log2.update)
=== GROUND STATE ENERGY ===

* Electronic ground state energy (Hartree): -4.383100342663
  - computed part:      -4.383100342663
~ Nuclear repulsion energy (Hartree): 1.370925416891
> Total ground state energy (Hartree): -3.012174925772

=== MEASURED OBSERVABLES ===

  0:  # Particles: 3.000 S: 0.500 S^2: 0.750 M: -0.500

=== DIPOLE MOMENTS ===

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

  0:
  * Electronic dipole moment (a.u.): [0.0  0.0  1.743455202196]
    - computed part:      [0.0  0.0  1.743455202196]
  > Dipole moment (a.u.): [0.0  0.0  -0.284586632196]  Total: 0.284586632196
                 (debye): [0.0  0.0  -0.723346999792]  Total: 0.723346999792
```

[130]:
```
import matplotlib.pyplot as plt

figfig = plt.figure()
plt.plot(log2.evaluations, log2.costs)
plt.xlabel('Steps')
plt.ylabel('Ground-State energy')
plt.show()
```



[134]:
```
# Extract parameters
data2 = log2.parameters
iterations = range(len(data2))

# Extract all 16 parameters
parameters = [[row[i] for row in data2] for i in range(16)]

# Plotting the parameters
plt.figure(figsize=(15, 10))

# Plot each parameter
for i in range(16):
    plt.plot(iterations, parameters[i], label=f'Parameter {i+1}')
```

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



[ ]: