QHack2023 – Simulations of BeH_2

The Entangled Cats

Chemistry Challenge

Objective: Obtaining a value for the ground state energy of BeH_2 as close as possible to the real value

Define the Molecule:

```
driver_ana = PySCFDriver(
    atom="H 0 0 0; Be 0 0 1.334; H 0 0 2.668",
    basis="sto3g",
    charge=0,
    spin=0,
    unit=DistanceUnit.ANGSTROM,
)
```

Theoretical Result:

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

* Electronic ground state energy (Hartree): -18.966849762441
  - computed part:      -18.966849762441
~ Nuclear repulsion energy (Hartree): 3.37181881021
> Total ground state energy (Hartree): -15.595030952231
```

Active Space

Using the freeze core approximation and removing inactive orbitals we can reduce the problem to 8 qubits

```
problem = ElectronicStructureProblem(
    driver,
    [FreezeCoreTransformer(freeze_core=True, remove_orbitals=[2,3])])
```

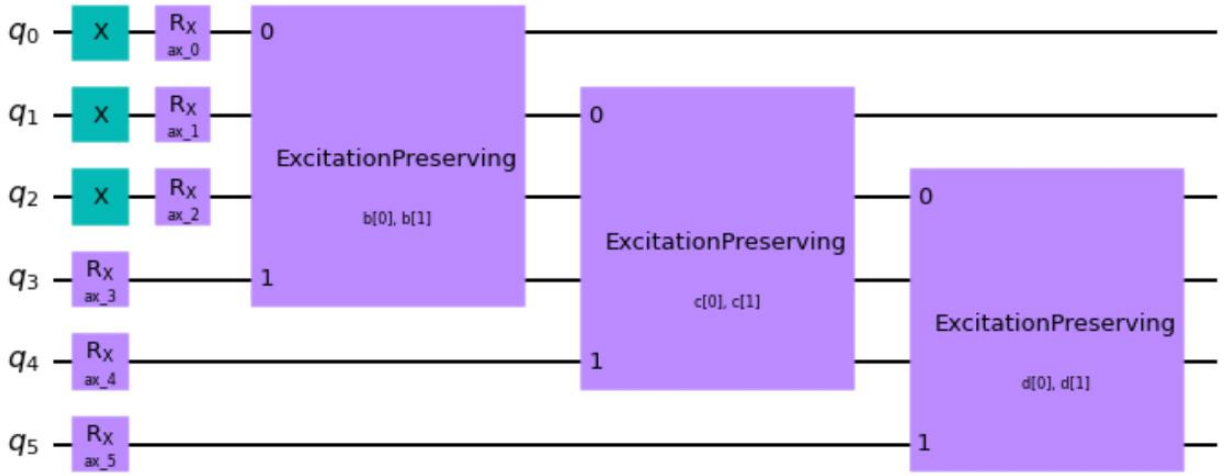
Using the parity mapper we can remove 2 extra qubits: we have a 6 qubit problem that can be run on IBM systems available with the power ups

```
mapper = ParityMapper()#JordanWignerMapper()
converter = QubitConverter(mapper, two_qubit_reduction=True)
```

Ansatz Selection

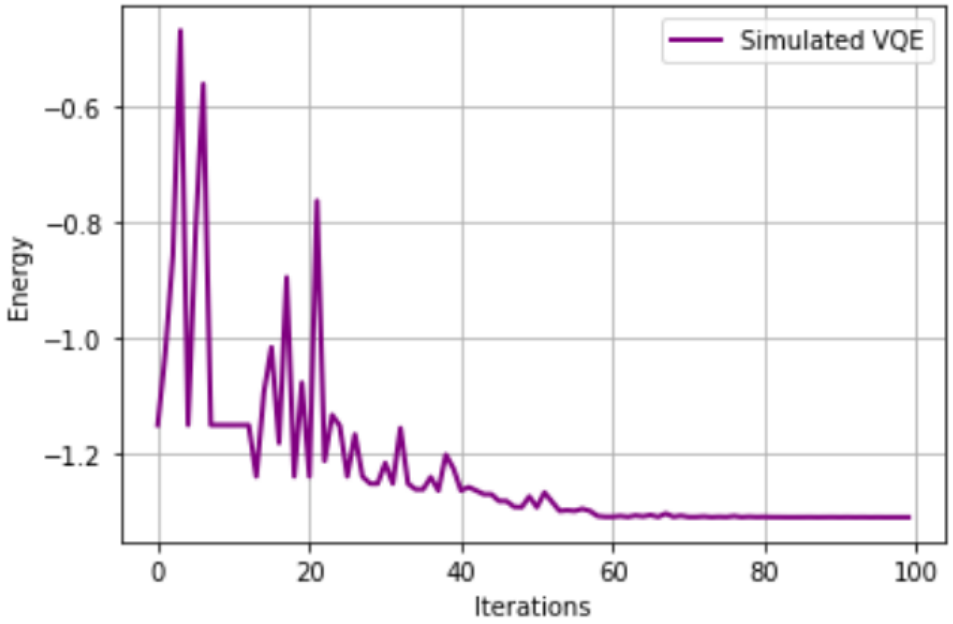
Initial Ansatz: UCCSD, however this has 212 CNOT gates – too much, there will be too much noise running it in an actual Quantum Computer

Simplified Ansatz: Start with Hartree Fock, apply RX gates and 3 single excitations



Ansatz Selection

With this simplified Ansatz in an Ideal Simulation we get:



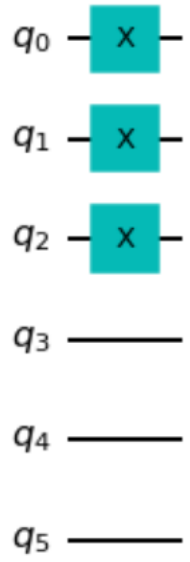

```
=== GROUND STATE ENERGY ===

* Electronic ground state energy (Hartree): -18.931641207513
  - computed part:      -1.312125344753
  - FreezeCoreTransformer extracted energy part: -17.619515862759
~ Nuclear repulsion energy (Hartree): 3.37181881021
> Total ground state energy (Hartree): -15.559822397303
```

Relative Error: 0.23 %

Ansatz Selection

The same result can be achieved by just using the Hartree Fock state




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

* Electronic ground state energy (Hartree): -18.94205799966
  - computed part:      -1.313985122467
  - FreezeCoreTransformer extracted energy part: -17.628072877192
~ Nuclear repulsion energy (Hartree): 3.381959618662
> Total ground state energy (Hartree): -15.560098380998

=== MEASURED OBSERVABLES ===


=== DIPOLE MOMENTS ===

~ Nuclear dipole moment (a.u.): [15.08001447  0.0  0.0]
```

Relative Error: 0.23 %

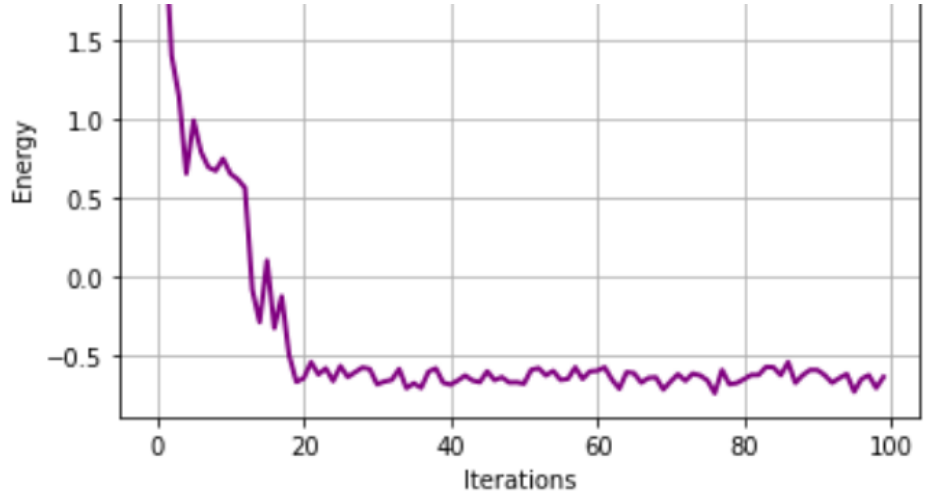
Advantage: It is much Faster, no CNOT

Running on Quantum Computers

Running in an actual 7 Qubit Quantum Computer (ibm_nairobi) the VQE with the simplified Ansatz

Zero Noise Extrapolation

Dynamical Decoupling




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

* Electronic ground state energy (Hartree): -18.365263480836
  - computed part:      -0.745747618077
  - FreezeCoreTransformer extracted energy part: -17.619515862759
~ Nuclear repulsion energy (Hartree): 3.37181881021
> Total ground state energy (Hartree): -14.993444670626
```

Relative Error: 3.85 %

Running on Quantum Computers

Running in an actual 7 Qubit Quantum Computer (ibm_nairobi) just the Hartree Fock state preparation

Probabilistic Error Cancelation

Dynamical Decoupling

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

* Electronic ground state energy (Hartree): -19.062418158777
  - computed part:      -1.442902296017
  - FreezeCoreTransformer extracted energy part: -17.619515862759
~ Nuclear repulsion energy (Hartree): 3.37181881021
> Total ground state energy (Hartree): -15.690599348567
```

Relative Error: 0.61 %

Entanglement Forging

If we did not have access to power ups the problem would solvable on a 5 qubit system by using Entanglement Forging

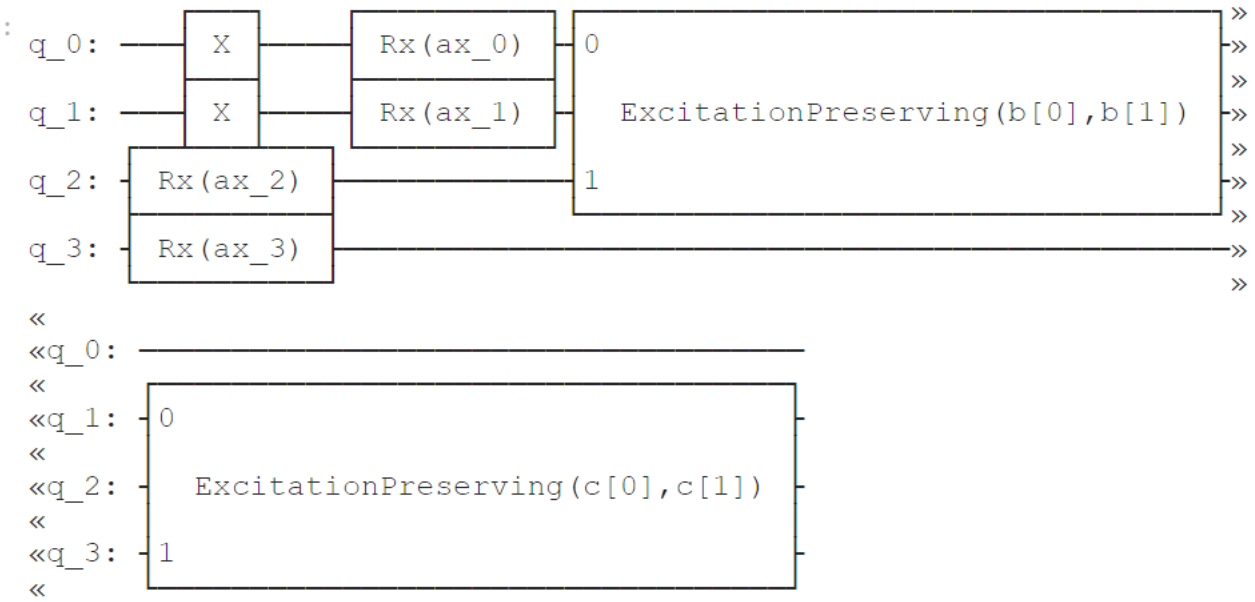
It allows us to simulate 2n qubit systems using only n qubits

4 qubit ansatz with bit strings (1,1,1,1) and (0,0,0,0) representing fully occupied and unoccupied states

Ansatz inspired on simplified ansatz, 2 PauliX followed by RX gates and 2 single excitations

Entanglement Forging

Ansatz:



Promising Results:

- Ideal simulation: - 15.56 Ha, error: 0.23 %
- Noisy simulation: -15.05 Ha, error: 3.51%

Conclusions

Successfully run VQE on a Quantum computer to obtain the energy of the ground state of BeH_2

With simplified Ansatz: Energy : **-14.99 Ha**, relative error **3.85%**

Just Hartree Fock Energy: **-15.69 Ha**, relative error **0.61%**

Successfully explored advanced simulation techniques like Entanglement Forging