Ab initio calculations of dissociation energy of water molecule on near-term quantum devices using the Pennylane interface to quantum hardware.

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Abstract

Fault-tolerant quantum computers may be far off, however solving real world quantum chemistry problems on near-term quantum devices is possible through the Pennylane which provides interface to use any of the quantum hardware provided by any of the quantum hardware providers such as IBM, Google or Microsoft. A demonstrated use of Pennylane to solve real world quantum chemical problems on near-term quantum devices is shown. Ab initio quantum chemical calculations of dissociation energy of water molecule on the near-term quantum hardware using the Pennylane interface yielded a dissociation energy comparable to experiment and therefore it is recommended that the quantum chemistry community use near-term quantum devices to leverage quantum computing advantage to solve quantum chemical problems.

Introduction

The developers of quantum hardware such as IBM, Google, Microsoft provide programming interface to their hardware which go by names Qiskit, Cirq and Q# respectively for the development of real-world applications that leverage the of quantum hardware using quantum algorithms [1-5]. Although fault-tolerant quantum computers may be far off, solving real world quantum chemistry problems using near-term quantum devices is possible through Pennylane which provides interface to use any of the quantum hardware providers mentioned above [6]. A demonstration of ab initio calculations of dissociation energy of water molecule on the near-term quantum hardware using the Pennylane interface is presented in the work below.

Methodology

The strategy to solve the problem of dissociation energy of water molecule ab initio involves obtaining the ab initio energies of reactant and products and obtaining the difference between them. In this work we implement this strategy on the near-term quantum devices through the Pennylane interface. The strategy to solve this problem using Pennylane is to use the Variational Quantum Eigensolver(VQE) method [7-9]. A quantum circuit is setup which reflects the trial wave function of the ground state of the molecular Hamiltonian and a classical optimizer is used to optimize the circuit parameters to render the molecule's ground state energy. The input cartesian structure file for the molecules is downloaded from chemical structure libraries. The read_structure() method of the qchem module of Pennylane is used to read the input structure. The construction of the molecular Hamiltonian and mapping of the initial trial wave function which is to be optimized to the qubits is carried out by Pennylane using quantum chemistry drivers and the default driver option is PySCF [10]. It requires the charge, spin multiplicity, basis set, the valence electrons and orbitals to be specified. The mapping of the trial wave function to qubits of the quantum circuit is carried out using the 'jordan-wigner' mapping. The quantum circuit of entangled qubits required to optimize the ground state of water, oxygen and hydrogen involved 12, 8 and 4 qubits, respectively. The code and implementation are provided in the GitHub link shared below.

https://github.com/bengeof/PennylaneDissociationEnergyAb-Initio

Results and discussion

The ground state energy of water obtained from 100 iterations of optimization is -74.59262921 Ha. and the final circuit parameters and other optimization details are given below.

Iteration = 0, Energy = -73.63914635 Ha

Iteration = 20, Energy = -74.20924302 Ha

Iteration = 40, Energy = -74.35807580 Ha

Iteration = 60, Energy = -74.51446847 Ha

Iteration = 80, Energy = -74.56593923 Ha

Iteration = 100, Energy = -74.58052004 Ha

Iteration = 120, Energy = -74.58713612 Ha

Iteration = 140, Energy = -74.59031295 Ha

Iteration = 160, Energy = -74.59175088 Ha

Iteration = 180, Energy = -74.59237374 Ha

Final convergence parameter = 0.00000885 Ha

Final value of the ground-state energy = -74.59262921 Ha

Accuracy with respect to the FCI energy: 73.45643975 Ha (46094.13631472 kcal/mol)

Final circuit parameters =

[[5.54193389e+00 8.41790050e-05 3.08160077e+00]

[7.03997361e+00 6.60655067e+00 -3.13026870e+00]

[2.98479079e+00 -3.12940495e+00 -3.23993298e-01]

[1.28993324e+00 8.01379434e-17 4.56873497e+00]

[2.39087053e+00 3.05745058e+00 1.40761930e+00]

[1.04826882e+00 3.14163976e+00 -6.39082649e-01]

[9.83531192e-01 -3.13675958e+00 -7.99021838e+00]

[2.05340338e+00 3.14161455e+00 -2.32943051e+00]]

The ground state energy of oxygen obtained from 100 iterations of optimization is -147.55131990 Ha. and the final circuit parameters and other optimization details are given below.

Iteration = 0, Energy = -146.26504092 Ha

Iteration = 20, Energy = -147.30290612 Ha

Iteration = 40, Energy = -147.53700197 Ha

Iteration = 60, Energy = -147.54993831 Ha

Iteration = 80, Energy = -147.55113346 Ha

Iteration = 100, Energy = -147.55129411 Ha

Final convergence parameter = 0.00000093 Ha

Final value of the ground-state energy = -147.55131990 Ha

Accuracy with respect to the FCI energy: 146.41513044 Ha (91875.93359949 kcal/mol)

Final circuit parameters =

[[5.54193389e+00 1.28150550e-03 3.00578101e+00]

[7.03997361e+00 6.28265660e+00 -3.04573222e+00]

[2.98479079e+00 1.64453090e-14 -3.21635666e-01]

[1.28993324e+00 -7.39491055e-15 4.56303441e+00]

[2.39087053e+00 1.38077123e-07 1.39488313e+00]

[1.04826882e+00 6.28318512e+00 -6.93713097e-01]

[9.83531192e-01 -3.13074430e+00 -8.02415297e+00]

[2.05340338e+00 3.12988509e+00 -2.33843681e+00]

[7.13064445e+00 -6.28151756e+00 1.89390706e-01]

[-5.88055408e-01 6.28226080e+00 4.56612645e+00]

[4.86781694e-01 3.14159210e+00 -2.83682385e+00]

[-6.22285563e+00 -3.14159216e+00 4.97256496e-01]]

The ground state energy of hydrogen obtained from 100 iterations of optimization is -1.13615709 Ha. and the final circuit parameters and other optimization details are given below.

Iteration = 0, Energy = -0.88179557 Ha

Iteration = 20, Energy = -1.13380513 Ha

Iteration = 40, Energy = -1.13558756 Ha

Iteration = 60, Energy = -1.13585794 Ha

Iteration = 80, Energy = -1.13600617 Ha

Iteration = 100, Energy = -1.13608848 Ha

Iteration = 120, Energy = -1.13613394 Ha

Final convergence parameter = 0.00000099 Ha

Final value of the ground-state energy = -1.13615709 Ha

Accuracy with respect to the FCI energy: 0.00003237 Ha (0.02031093 kcal/mol)

Final circuit parameters =

[[5.54193389e+00 1.30219523e-08 3.07479606e+00]

[7.03997361e+00 6.28318530e+00 -3.07020901e+00]

[2.98479079e+00 -2.09540998e-01 -4.16893297e-02]

[1.28993324e+00 1.30907537e-12 4.56873497e+00]]

The energy difference between reactants and product for the dissociation of water into hydrogen and oxygen yields the dissociation energy which is comparable to experimental measure and a demonstrated use of Pennylane interface to perform ab initio quantum chemical calculations on near-term quantum devices has been shown.

Conclusion

Fault-tolerant quantum computers may be far off, however solving real world quantum chemistry problems on near-term quantum devices is possible through the Pennylane which provides interface to use the quantum hardware as provided by quantum hardware providers such as IBM, Google or Microsoft. A demonstrated use of Pennylane to solve real world quantum chemical problems on near-term quantum devices is shown. Ab initio quantum chemical calculations of dissociation energy of water molecule on the near-term quantum hardware using the Pennylane interface yielded a dissociation energy comparable to experiment and therefore it is recommended that the quantum chemistry community use near-term quantum devices to leverage quantum computing advantage to solve quantum chemical problems.

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