The Variational Quantum Eigensolver (VQE) for Estimating the Ground State of the H_2 Molecule

Q-TrashPandas

Zhi Han, Xinbo Li, Jonas Jäger, Nabil Zerradi

Every member independently implemented the full workshop materials, and contributed to a column of the poster according to the author order

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Introduction

Motivation

- Every known chemical interaction is an electron-electron interaction
- However, simulating large many body interactions is computationally difficult
- Jordan Wigner transformation: fermion operators (electrons) → quantum logic gates
- Enabling quantum computers to efficiently simulate **all** of chemistry
- VQE algorithm: quantum logic gates → ground state

Problem Statement

- Calculate ground state energy of H_2

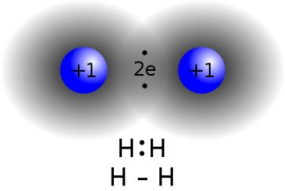
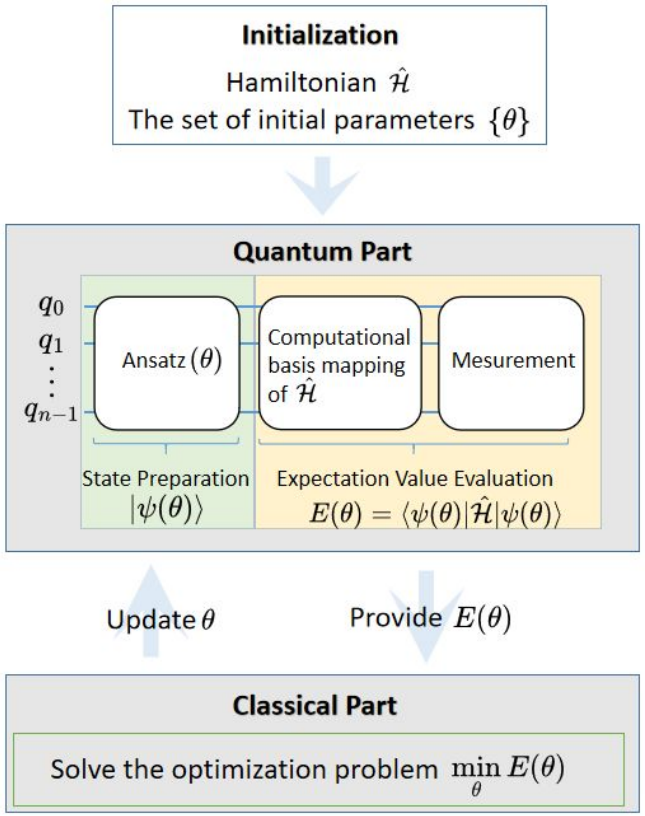


Figure credit: Wikipedia: Covalent Bond

Methodology

VQE: A hybrid quantum-classical algorithm

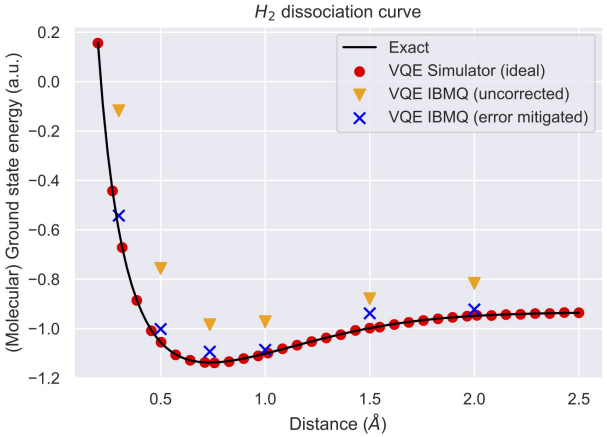


- Second quantization and Jordan-Wigner mapping
- Ansatz has
  - only one parameter
  - |0101> and |1010> basis states

Results & Benchmarking

Experiments

- VQE for H_2 with different bond distances
- QASM Simulator (ideal simulation)
- Real 5-qubit IBM Quantum Computer (`ibmq-lima`)



Main results

1. **Simulated VQE** matches **exact** solutions ●
2. (Uncorrected) **IBMQ overestimates** ▼
3. **Error mitigation improves IBMQ** results by mitigating the overestimation **x**

Experimental details

- 8192 Shots per expectation estimation
- Qiskit Runtime minimal error mitigation: *Twirled Readout Error eXtinction* (resilience level 1)

Conclusion

- Our implementation is successful
- The simulated VQE applied to the H_2 molecule converges to the exact solution
- Error mitigation is an effective approach to obtaining better result in the NISQ era

Future Work

Possible improvement can be achieved if

- molecular symmetries are exploited (indicating other mapping like the parity mapping)
- more advanced classical optimizers are used
- simultaneous estimation circuit is implemented to reduce runtime

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