Exploring the Potential Energy Surface of various Molecules with a Problem-Inspired Ansatz

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Team: Qanything

Project Aim

Image Source: https://en.wikipedia.org/wiki/Potential_energy_surface#/media/File:Potential_Energy_Surface_for_Water.png

- H_2: Hydrogen molecule
- He_2: Helium Dimer
- LiH: Lithium Hydride

Aim: Explore Potential Energy Surface (PES) of H_2, He_2, and LiH, using Variational Quantum Eigensolver (VQE) with a Problem-Inspired Ansatz.

Motivation: PES enables us to study molecular properties, such as the equilibrium molecular bond lengths.

Objectives:

- We shall use PennyLane to build our problem-inspired ansatz and perform VQE optimization.
- We shall implement the IBMQ noise models and Mitig zero noise extrapolation and study how NISQ devices can affect the PES.
- We use QAMUY to cross check our results.

Molecular Hamiltonian and the Problem-Inspired Ansatz

$$\hat{H} = \sum_i c_i \sigma_i + \sum_{ij} c_{ij} \sigma_i \sigma_j + \sum_{ijk} c_{ijk} \sigma_i \sigma_j \sigma_k + \dots$$

- Molecular Hamiltonian is an energy operator consisting of all electrons and the nucleus of the molecule
- It can be decomposed as a linear combination of Pauli strings
- VQE can be used to find the minimum energy of the molecular Hamiltonian

Our Problem-Inspired Ansatz

$$|\psi_{PI}\rangle = \prod_\alpha U_\alpha(\theta_\alpha) |1_1 \dots 1_n 0_{n-1} \dots 0_m\rangle$$

n: Number of electrons
m: Number of molecular orbitals

Disentangled UCC

$$U_\alpha(\theta_\alpha) \in \{U_{i,k}(\theta_{i,k}), U_{ij,kl}(\theta_{ij,kl})\}$$

Singles Doubles

θ: Parameters to Optimise

- We used the Disentangled UCC, a problem-inspired ansatz
- It consists of singles and doubles excitation operators applied to the Hartree-Fock state.
- As an example, shown below is the Disentangled UCC ansatz for H_2, requiring 4 qubits

Measurement
$\langle\psi_{PI}| \hat{H} |\psi_{PI}\rangle$

Hartree-Fock state

PennyLane Quantum Circuit for H_2

```
0:─┌|1⟩──────────────────────────────────────────┌DoubleExcitation(0)─┌SingleExcitation(0)─┌SingleExcitation(0)─┤
1:─├|1⟩─┌SingleExcitation(0)─┌SingleExcitation(0)─├DoubleExcitation(0)─│────────────────────│────────────────────┤
2:─├|0⟩─│────────────────────└SingleExcitation(0)─├DoubleExcitation(0)─│────────────────────└SingleExcitation(0)─┤
3:─└|0⟩─└SingleExcitation(0)─────────────────────└DoubleExcitation(0)─└SingleExcitation(0)─────────────────────┤
```

Performing VQE Energy Optimisation using PennyLane

VQE optimization of Hydrogen Molecule H_2

H_2: Hydrogen molecule

Bond length:
$r = 1.4$ Bohr

- Parameters are Optimized using Gradient Descent with Default Settings

No. of Electrons: 2
No. of Qubits: 4
No. of Pauli Strings (to measure): 15
No. of Single Excitations Rotations Gate : 4
No. of Double Excitations Rotations Gate : 1
Total No. of Excitations Parameter: 5

```
0:─┌|1⟩──────────────────────────────────────────┌DoubleExcitation(0)─┌SingleExcitation(0)─┌SingleExcitation(0)─┤
1:─├|1⟩─┌SingleExcitation(0)─┌SingleExcitation(0)─├DoubleExcitation(0)─│────────────────────│────────────────────┤
2:─├|0⟩─│────────────────────└SingleExcitation(0)─├DoubleExcitation(0)─│────────────────────└SingleExcitation(0)─┤
3:─└|0⟩─└SingleExcitation(0)──────────────────────└DoubleExcitation(0)─└SingleExcitation(0)──────────────────────┤
```

Benchmarking Using PennyLane Built-in Classical Optimizers

VQE optimization of Hydrogen Molecule H_2

H_2: Hydrogen molecule

Bond length:
$r = 1.4$ Bohr

We tested the various optimizers available in PennyLane applied to H_2 using our Disentangled UCC ansatz and ranked them according to their accuracy.

Optimiser Ranking:
1. RMSProp
2. Adam
3. Nesterov
4. Momentum
5. QNG
6. Adagrad
7. Gradient Descent

Implementing VQE on H_2 and Tetra Hydrogen H_4 with QAMUY

VQE optimization of H_2 in QAMUY
(BFGS Only)

VQE Optimisation of Tetra Hydrogen H_4 Various
in QAMUY (Various Optimisers)

QAMUY
with their
UCCSD
Ansatz

The optimizers from QAMUY were able to
provide accurate results with quick convergence

Image Source H_4: Henry Rzepa, https://www.ch.imperial.ac.uk/rzepa/blog/?p=17483

Potential Energy Surface for H_2 using Exact Quantum Simulator

Bond lengths:
$r = 1.0$ to 4.0 Bohr

Potential Energy Surface for H_2 using various IBMQ Device Noise Models

Open Providers

Best performing

Worst performing

Exclusive providers

Best performing

Worst performing

<u>Legend</u>

GREY Dots: Our Optimised Problem Inspired Ansatz

+ : Problem Inspired Ansatz w/ Mitiq Zero Noise Extrapolation

CYAN Dots: Hartree-Fock (HF) State Only

X : HF w/ Mitiq Zero Noise Extrapolation

Bond lengths:
$r = 1.0$ to 4.0 Bohr

- Note: From the plots, our implementation of Mitig as an error mitigation technique did not appear to help with improving the accuracy of our results. (???)

Actual Quantum Circuit Implemented:

```
0: ──╭|1⟩──╭DoubleExcitation(0)──┤
1: ──├|1⟩──├DoubleExcitation(0)──┤
2: ──├|0⟩──├DoubleExcitation(0)──┤
3: ──╰|0⟩──╰DoubleExcitation(0)──┤
```

- Turns out for H_2, the only gate that contributes to PES is Double Excitations.
- We remove all Singles Excitations from quantum circuit to reduce circuit noise.
- All Noise model obtained from IBMQ Device backends
- Number of Shots Per Pauli String Expectation: $20{,}000$

Potential Energy Surface for H_2 using various IBMQ Device Noise Models

Open Providers

Best performing

Worst performing

Exclusive Providers

Best performing

Worst performing

ibmq_manila Error Map

ibmq_santiago Error Map

ibm_hanoi Error Map

ibmq_guadalupe Error Map

Simulated IBM Quantum Devices Noise Map

Potential Energy Surface for H_2 using various IBMQ Device Noise Models

Other Open Providers

Potential Energy Surface for H_2 using various IBMQ Device Noise Models

Other Exclusive Providers

ibmq_toronto Error Map

ibmq_brooklyn Error Map

ibmq_jakarta Error Map

ibm_perth Error Map

ibmq_casablanca Error Map

Potential Energy Surface for H_2 using various IBMQ Device Noise Models

Other Exclusive Providers

ibm_lagos Error Map

ibm_auckland Error Map

ibm_cairo Error Map

ibmq_montreal Error Map

ibmq_mumbai Error Map

Potential Energy Surface for He_2 using Exact Quantum simulator

Zoomed In

Distance:
$r = 5.4$ to 6.8 Bohr

No. of Electrons: 4
No. of Qubits: 8
No. of Pauli Strings (to measure): 185
No. of Single Excitations Rotation Gate: 16
No. of Double Excitations Rotations Gate: 36
Total No. of Excitations Rotation Parameter: 52
Hartree-Fock State: |1 1 1 1 0 0 0 0>

Energy Optimisation of He_2@ 6Bohr

Note: Optimizers provided by PennyLane were unsuccessful in converging to the reference energy <u>exactly</u> in a limited number of steps (30 Iterations Max)

Potential Energy Surface for He_2 with QAMUY

He_2 Morse Curve (6-31G)

QAMUY with their UCCSD Ansatz

$\Delta E \approx 10^{-6}$ Hartree

Total Runtime: ~5 min

Distance:
$\mathrm{r} = 5.4$ to 6.8 Bohr

There should be no Helium Bond as the energy depth is too shallow to support it

Potential Energy Surface for LiH using Exact Quantum simulator

Max Optimiser Iterations: 20
Total Runtime: ~5 Hours

Total Runtime: ~2 Hours

No. of Electrons: 4
No. of Qubits: 12
No. of Pauli Strings (to measure): 631
No. of Single Excitations Rotations Gate : 32
No. of Double Excitations Rotations Gate: 168
Total No. of Excitations Rotation Parameter: 200
Hartree-Fock State: |1 1 1 1 0 0 0 0 0 0 0 0>

Bond lengths:
$r = 2.1$ to 3.9 Bohr

Contributing Members

Team Members (NUS, CQT):

- Chee Chong Hian (Main Lead, Coder, Curator)
- Benjamin Tan (Proofreading, Curator)
- Gan Beng Yee & Supanut Thanasilp (Tried in Running Our Quantum Circuit on Real IBM Devices, but it didn’t work due to Technical Issues)
- Adrain Mak (Basic Proofreading, ASTAR)