Variational Quantum Eigensolver

Review of NISQ-Era Algorithms

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Outline

- NISQ-Era – Quantum Devices and Algorithms
- Variational Quantum Eigensolver
- Running VQE: Hartree-Fock
- Simulating H_2
- Simulating H_2O
- Conclusion

NISQ-Era of Quantum Devices

- NISQ or Noisy Intermediate-Scale Quantum[1] is characterized by:
  - Devices with 50 to few hundreds of qubits
  - "Noisy" $\implies$ Perturbations due to device environment leads to inability to perfectly control qubits
  - Moreso a step towards practical fault-tolerant quantum computation, where proof-of-concepts arise.
- Question:
  - What are the capabilities and practical use-cases of NISQ-Era quantum devices?
  - Do they show quantum advantage?

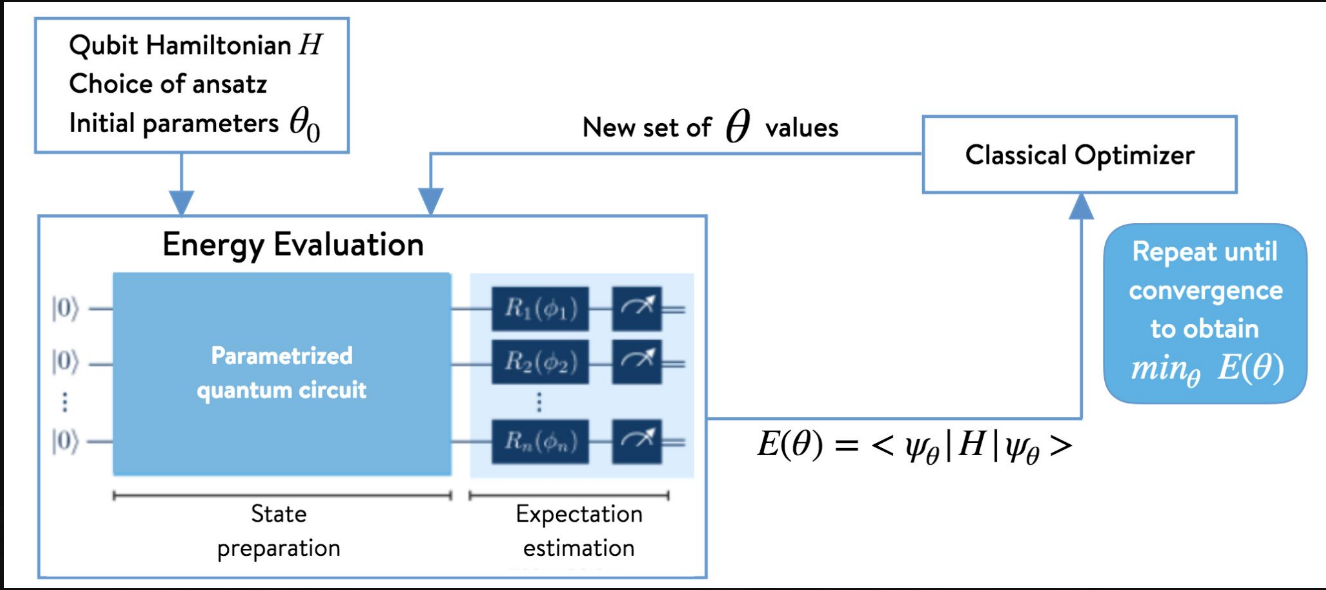
[1] https://arxiv.org/pdf/1801.00862.pdf

NISQ-Era Algorithms and Further Considerations

- Variational Quantum Algorithms (VQA)
  - Applicable to quantum chemistry (quantum simulations, in general) and optimization problems
- Adiabatic Quantum Computing:
  - Similar applications as VQA but a completely different approach to quantum computing $\Longrightarrow$ Quantum Annealing
- Resource Estimation:
  - How many qubits do we need?
  - How many (non-Clifford) gates do we need?

Variational Quantum Eigensolver

- **Goal:** Find ground state energy of given Hamiltonian H
- Hybrid quantum-classical algorithm
- Applicable to quantum chemistry problems



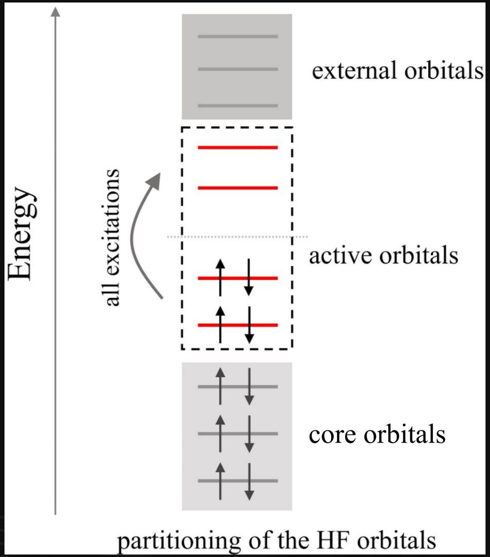
Source: 1QBit

Running VQE: Estimating Resources

- # of shots (IBM default = 1024)

- # of non-Clifford gates
  - Clifford gates = I, X, Y, Z, CNOT
  - non-Clifford = Controlled phase[2]

- # of qubits required to represent Hamiltonian of the molecule
  - Max simulatable: ~20



Source: Pennylane

[1]https://arxiv.org/pdf/2111.09967.pdf
[2]Stancil, Principles of Superconducting Quantum Computers

Running VQE: Hartree-Fock[1]

In our simulations, we varied

- Molecules: H_2, H_2O
  - # of qubits to represent Hamiltonian
- # of shots
- # of gates

[1]https://arxiv.org/pdf/2111.09967.pdf

Running VQE: Parameterized Circuit Construction

- Goal: Construct quantum variational circuits “to prepare fermionic states of interest”[1]
  - Consequence: Short-depth circuits
- Primary way this is achieved: **Givens Rotations**

$$G(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta/2) & -\sin(\theta/2) & \\ & \sin(\theta/2) & \cos(\theta/2) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Single Excitation

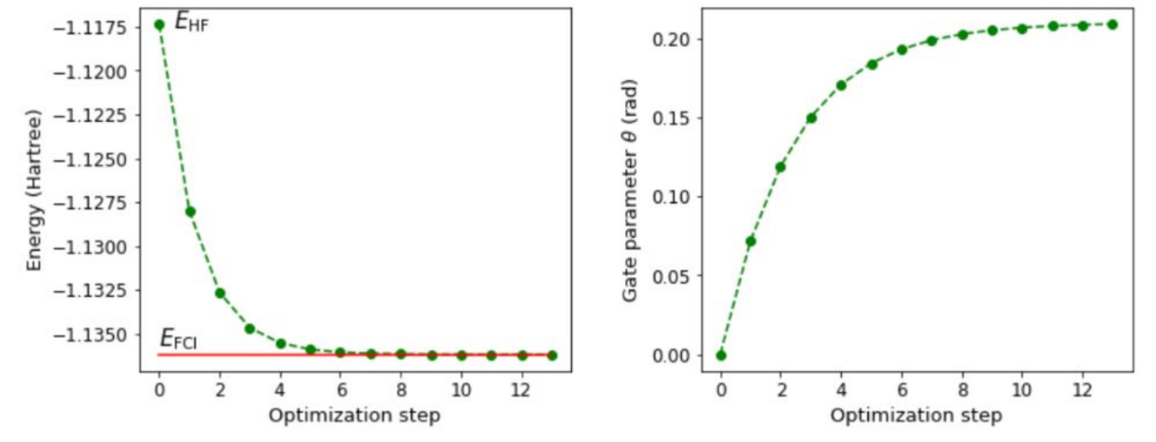
$$G^{(2)}(\theta)\,|\,0011\rangle = \cos(\theta/2)\,|\,0011\rangle + \sin(\theta/2)\,|\,1100\rangle$$

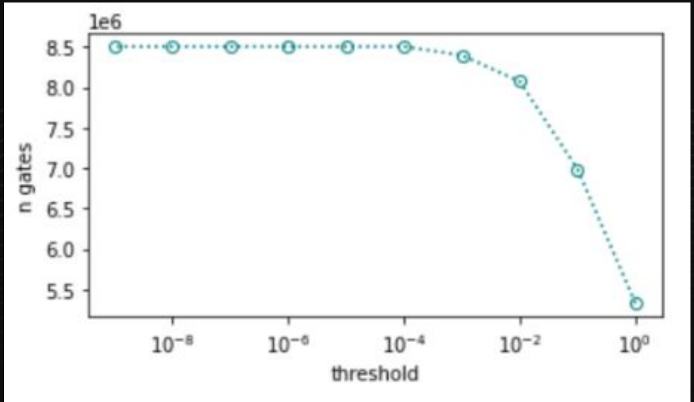
$$G^{2}(\theta)\,|\,1100\rangle = \cos(\theta/2)\,|\,1100\rangle - \sin(\theta/2)\,|\,0011\rangle$$

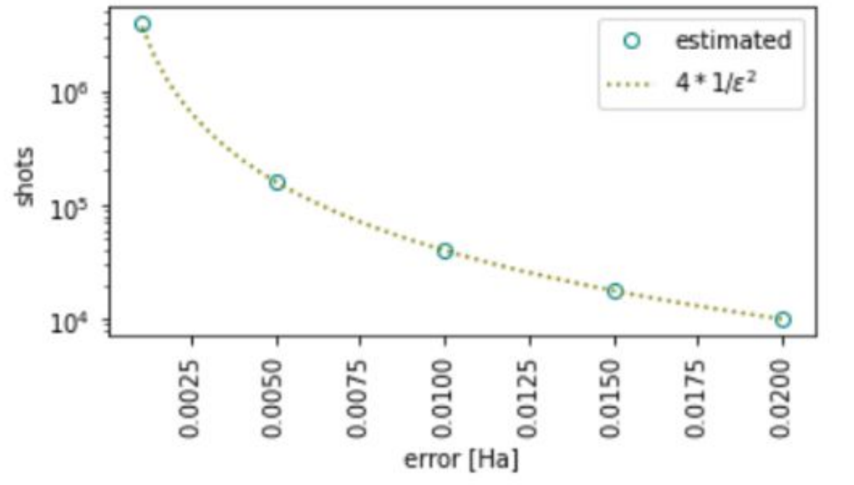
Double Excitation

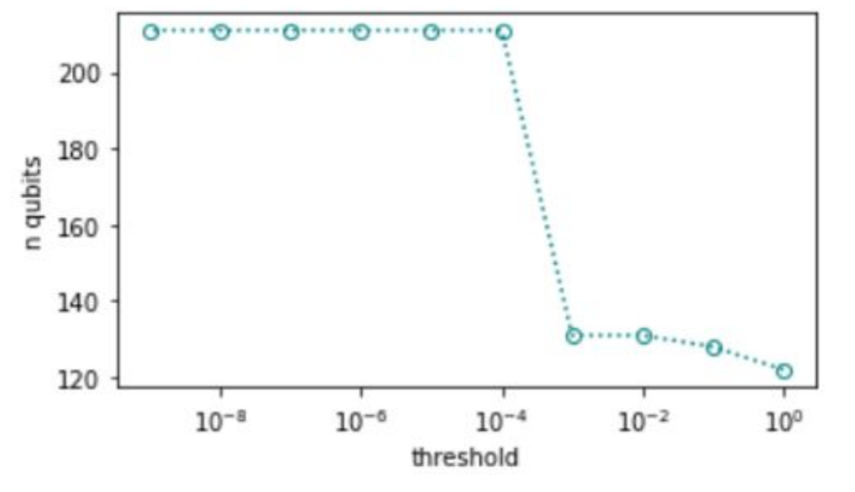
[1]https://arxiv.org/pdf/2111.09967.pdf

H_2 Resource Estimation (Pennylane)

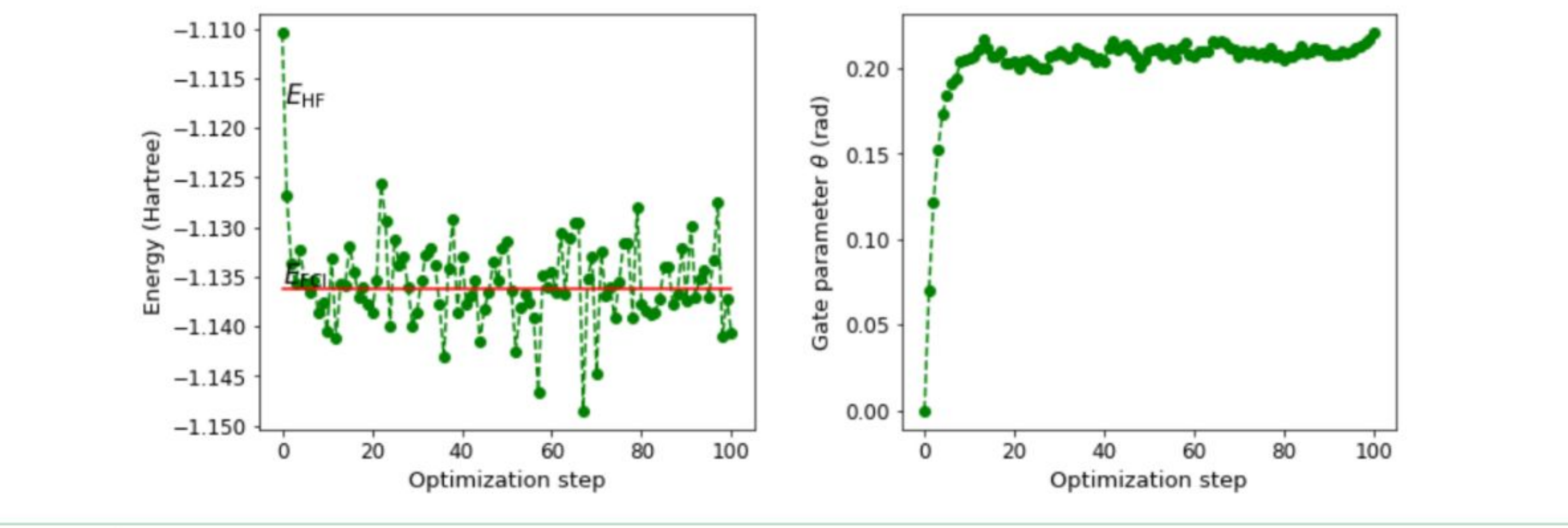





estimated
$4 * 1/\varepsilon^2$
shots
10^6
10^5
10^4
0.0025
0.0050
0.0075
0.0100
0.0125
0.0150
0.0175
0.0200
error [Ha]


n qubits
200
180
160
140
120
10^{-8}
10^{-6}
10^{-4}
10^{-2}
10^{0}
threshold

Simulating H_2 (IBM Device)



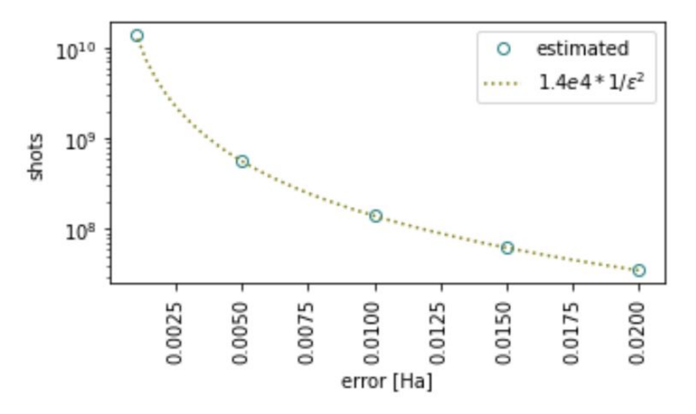
Simulating H_2O

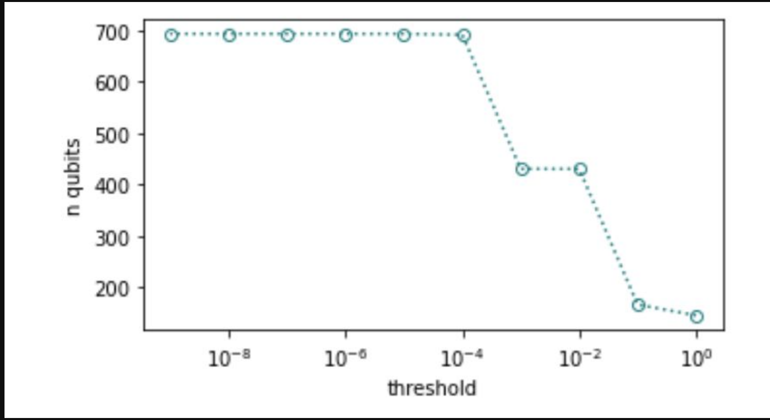
Using precomputed simulation from Pennylane Database:

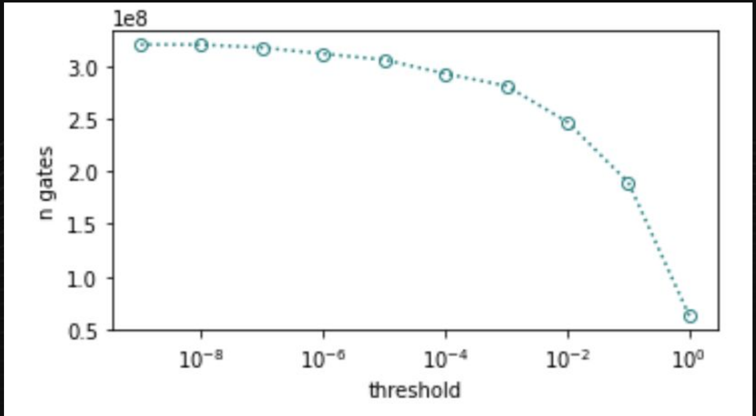
```
In [24]:
H2Odatasets = qml.data.load("qchem", molname="H2O", basis="STO-3G", bondlength=1.98)
print('fci_energy',H2Odatasets[0].fci_energy)
print('vqe_energy',H2Odatasets[0].vqe_energy)
```

```
fci_energy -74.76404151230251
vqe_energy -74.7570250805498
```

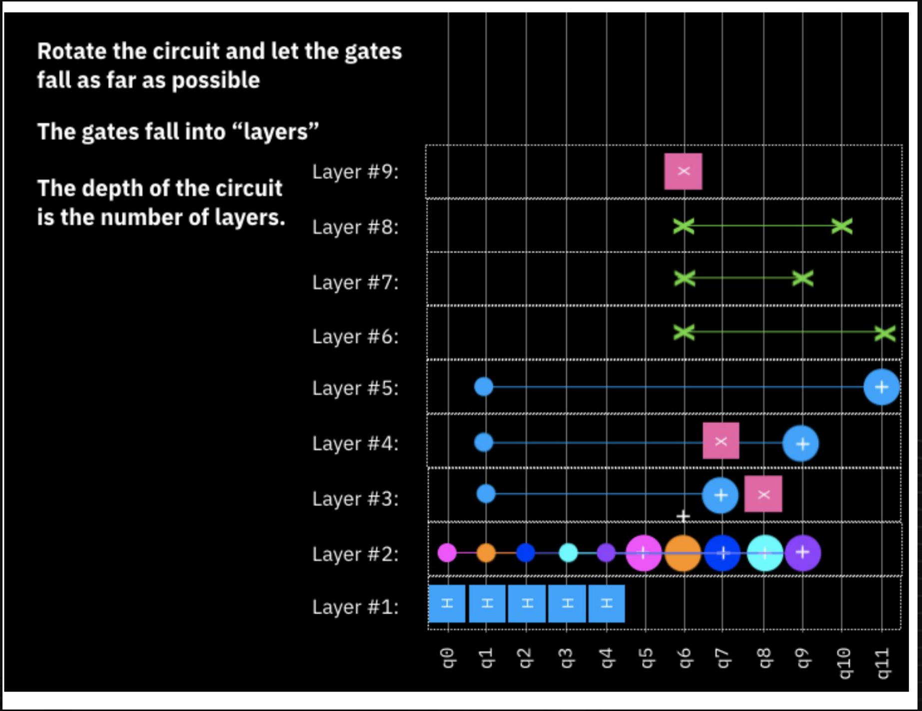
Resource Estimation for H2O (Pennylane)







SRI(QED-C) Circuit Width vs Depth For VQE IBM QASM Simulator



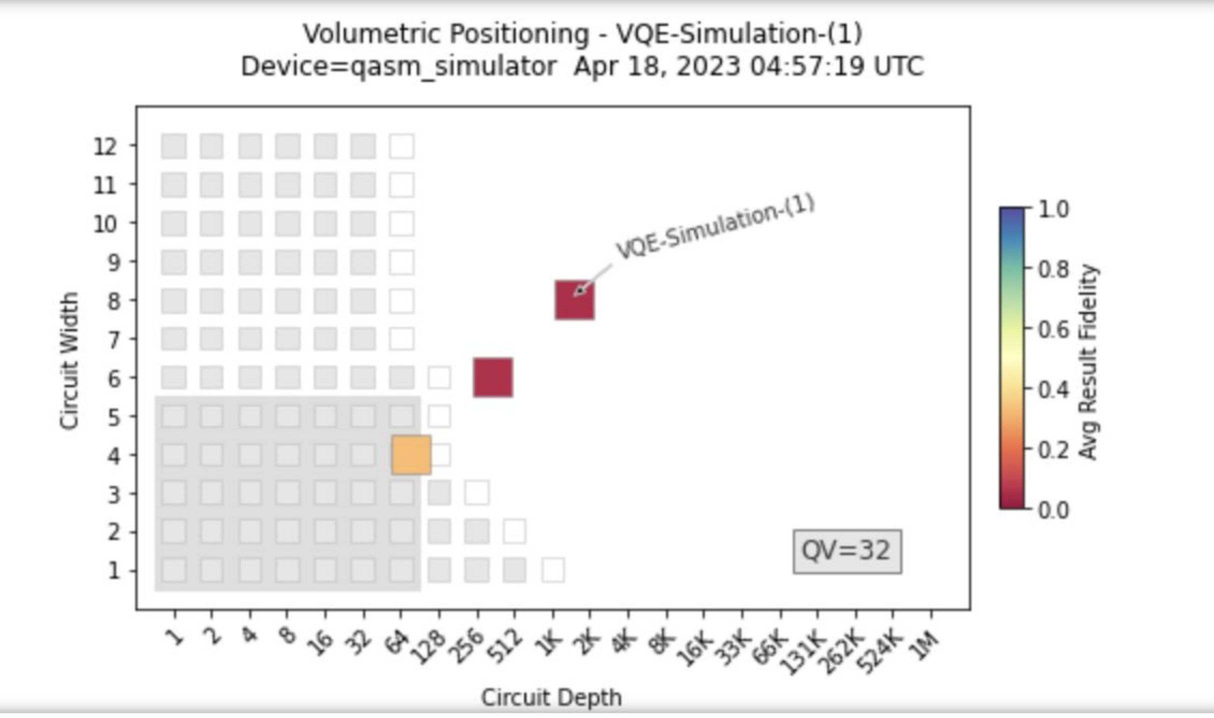
Source: IBM

Circuit Width:

- Number of Qubits

Circuit Depth:

- Number of layers of circuit



Source: Lubinski, Johri, et al. 2021

Future Plans

- Run VQE on different hardwares, such as IonQ’s ion trap and Xanadu’s photonic quantum computers

- Test how different types of errors (e.g. bit flip, Pauli-X, depolarizing) affect the convergence rate or lack of convergence

Challenges

- # of simulatable qubits is very low ~20
- Running simulation on actual device takes a very long time
  - Erroneous $\implies$ Does not converge

References

https://pennylane.ai/qml/demos/tutorial_quantum_chemistry.html
https://pennylane.ai/qml/demos/tutorial_adaptive_circuits.html#romero2017
https://pennylane.ai/qml/demos/tutorial_vqe.html
https://discuss.pennylane.ai/t/co2-active-electrons-orbitals/1589
https://pennylane.ai/qml/demos/tutorial_noisy_circuits.html
https://pennylane.ai/qml/demos/tutorial_quantum_chemistry.html
https://arxiv.org/pdf/2111.09967.pdf
https://arxiv.org/pdf/2110.03137.pdf