Quantum Simulation of Hamiltonian Using Variational Approach Involving Linear Combination of Unitary Operators

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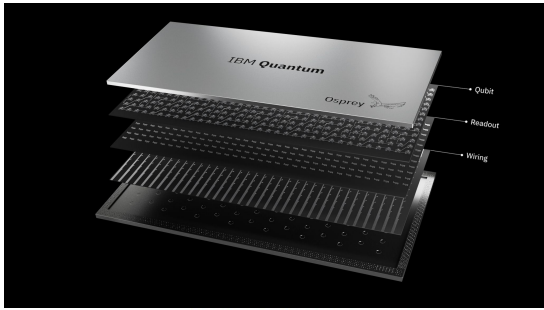
Outline

- Introduction
- Motivation
- Solving nuclear physics problems
- Algorithms
- Modified algorithm
- Conclusion

Introduction

- Why Quantum simulations?
  - Certain problems can be solved in polynomial time on the quantum computer, which cannot be solved in polynomial time on a classical computer.
  - Classical simulations face difficulty in simulating any quantum system due to exponential growth in resource requirements.
- Similar complexities occur in nuclear many-body problems.
- We are trying to solve the smaller problem on the quantum computer of the present NISQ era.
- Also, trying to give proof of concept that problems can be solved on the quantum computer once they are a practical reality in the near future.

P.C.: IBM Quantum



Motivation for current work..

- In the last decade, quantum computers have been used to simulate various molecules, and a wide variety of chemistry problems are being simulated.
- In recent years researchers have drawn their attention to nuclear physics problems which can be solved on a quantum computer.

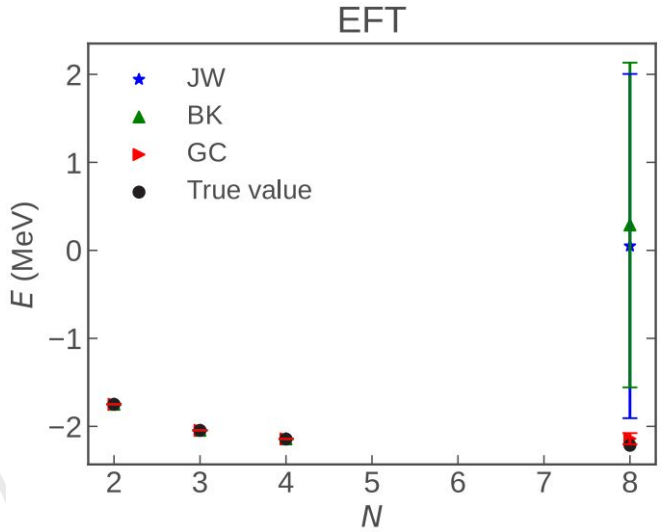


Fig. 1: Deuteron binding energy as function of number of basis states.

E. Dumitrescu et al. PRL **120** (2018) 210501.

PS and PA, PRC ***104 (***2021) *235501*.

A. Roggero et al. PRC **100** (2019) 034610.

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- In Childs *et al. QIC* ***12*** *(2012), 901-924* , a new approach for simulating Hamiltonian dynamics based on implementing linear combinations of unitary (LCU) operations is proposed.
- LCU method is used in PS and PA, PRC ***105*** (2022) *064318*, to calculate the expectation value of operators.
- In TB and SK, JCP **154** (2021) 194107 , proposed a technique to simulate molecular resonances.
- In A. Roggero et al. PRC **102** (2020) 064624, used LCU for creation of excited states.
- Motivated by these, we are trying to modify the variational algorithm and implement it for complex energy calculations.

Encodings and quantum algorithms

- We transform the nuclear problem in such a way that it can be solved on a quantum computer.

$$H = \sum_{ij} h_{ij} a_i^\dagger a_j \quad \text{Where,} \quad h_{ij} = < i \left| \hat{T} + \hat{V} \right| j >$$

- We map many-body basis states and operators to qubit basis states and operations respectively.
- This mapping is done via various encodings, among which we will primarily use **Jordan-Wigner transformation** (JWT) and **Gray code encoding** (GC).

$$a_j^\dagger = \frac{1}{2}(X_j - iY) \otimes \prod_{k<j} Z_k, \qquad a_j = \frac{1}{2}(X_j + iY) \otimes \prod_{k<j} Z_k.$$

- After mapping, the second quantized hamiltonian transforms to Pauli strings which can be applied to quantum circuits.
- We have various algorithms like VQE, Quantum phase estimation (QPE) and LCU etc., which can be used to simulate the problem.

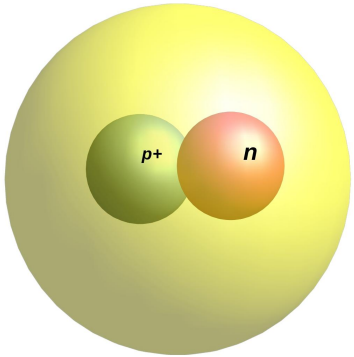
BE of Deuteron

- For simplicity, we choose the problem of deuteron BE calculation.
- Hamiltonian for N=2 , N=3 and N= 4 are:

$$H_2 = 5.9067091 I_0 - 6.34329 Z_0 - 4.28661 X_0$$

$$H_3 = 7.765855 I_0 I_1 - 7.984145 Z_0 - 1.859145 I_0 Z_1 + 1.640855 Z_0 Z_1 - 2.143305 (X_0 I_1 + X_0 Z_1) - 3.91312 (I_0 X_1 - Z_0 X_1)$$

$$H_4 = 14.328 I - 7.814 X_0 - 3.913 X_1 + 3.913 Z_0 X_1 - 1.422 Z_0 - 8.422 Z_1 + 3.527 X_0 Z_1 - 4.922 Z_0 Z_1$$



- O. D. Matteo et al. PRA **103** (2021), 042405.
- PS and PA, PRC ***104 (***2021) *235501*.

Variational Quantum Eigensolver (VQE)

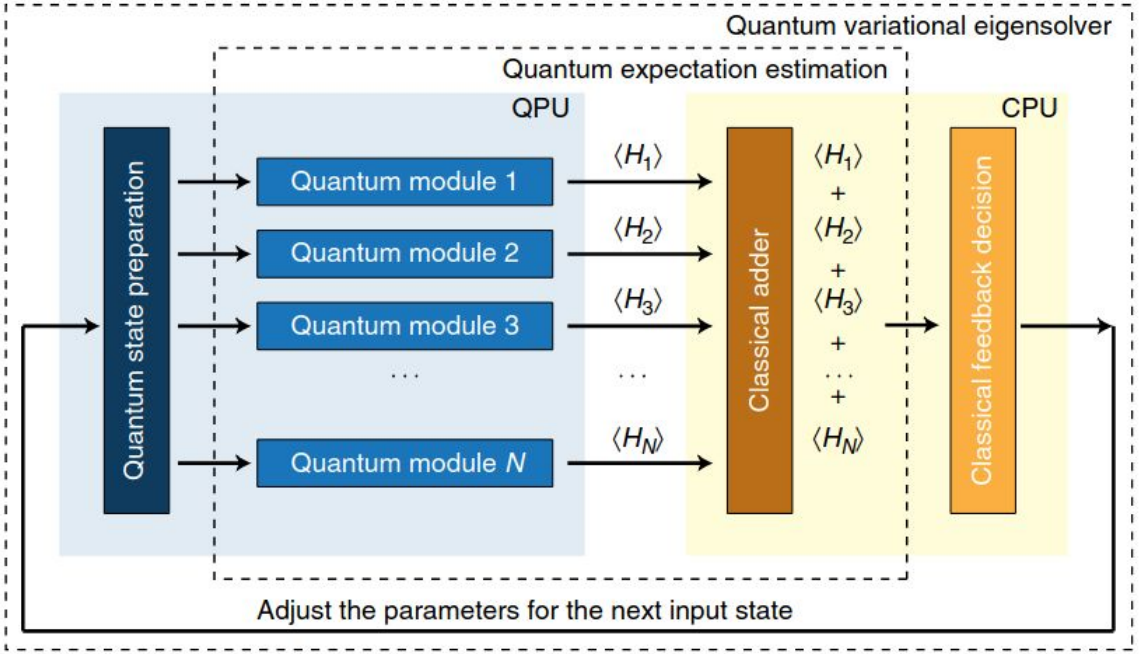


Fig. 2: Architecture of the variational-quantum eigensolver.

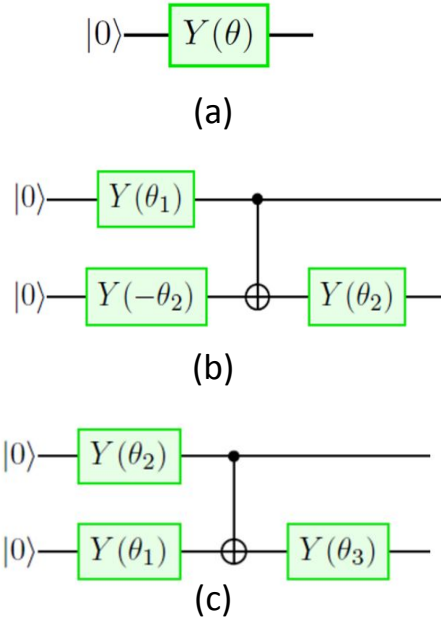


Fig. 3: Parameterized ansatz for N=2, 3 and 4 for GC encoding.

- A. Peruzzo and J. McClean et al. *Nature Communications* **5**, 4213 (2014)
- PS and PA, PRC ***104*** **(**2021) *235501*

Results for binding energy through VQE

Basis size (N)	True Value	VQE (Results)
2	-1.74916	-1.7335918 ± 0.107
3	-2.04567	-1.9751983 ± 0.150
4	-2.145	-1.8317920 ± 0.451

Table 1: Energy calculated with QASM simulator for EFT potential

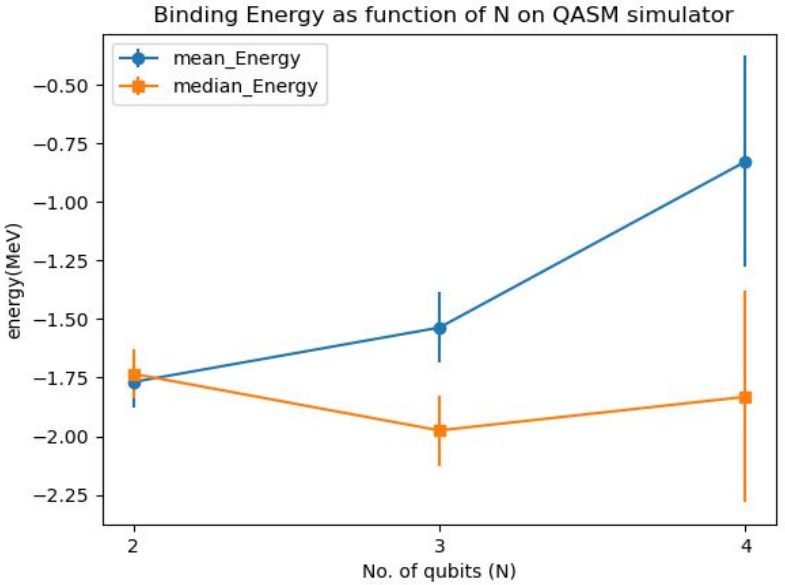


Fig. 4: Energy as a function of number of states for EFT potential for GC encoding

Expectation value through LCU

- The method for calculating expectation value based on LCU is discussed in PS and PA, PRC **105** (2022) 064318 and A. Roggero et al. PRC 102 (2020) 064624.

$$\mathcal{O} = \sum_{i=0}^{k-1} \beta_i U_i$$

$$V_P \left|0\right\rangle^{\otimes n_a} = \frac{1}{\sqrt{\Lambda}} \sum_i \sqrt{\beta_i} \left|i\right\rangle,$$

Where, $\Lambda = \sum_i \beta_i$ and $W = V_P^\dagger V_S V_P$

$$W \left|0\right\rangle^{\otimes n_a} \left|\psi\right\rangle = \frac{1}{\Lambda} \left|0\right\rangle^{\otimes n_a} \mathcal{O} \left|\psi\right\rangle + \left|\Psi^\perp\right\rangle.$$

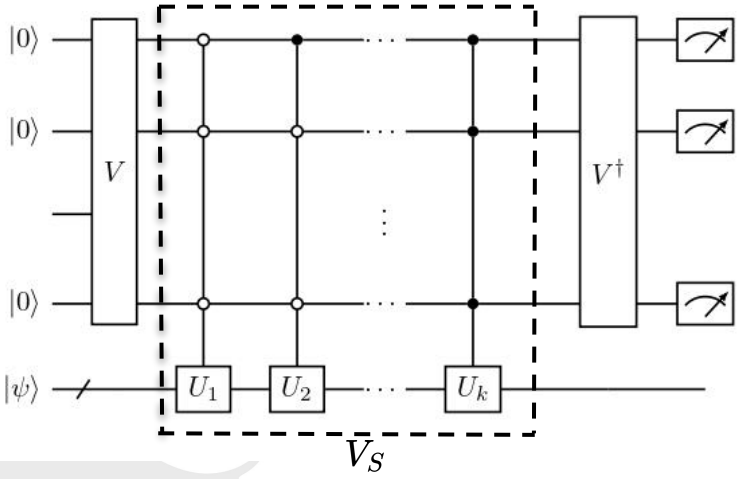


Fig. 5: General circuit for LCU

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- Once we get the $\mathcal{O}|\psi\rangle$ we can calculate expectation value of operator by taking its overlap with $|\psi\rangle$

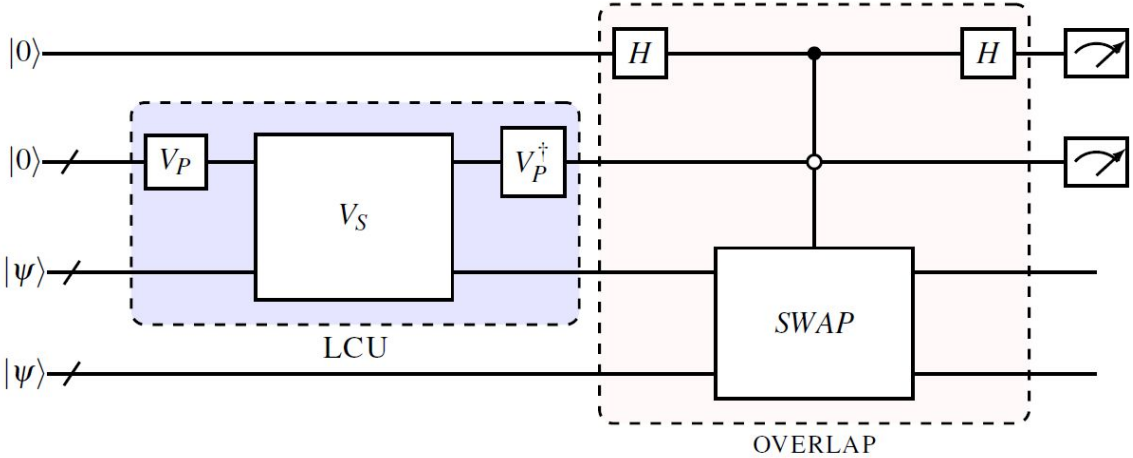

Fig. 6: Expectation Value Calculator

- J.C. Garcia-Escartin et al. PRA **87** (2013), 052330.
- PS and PA, PRC **105** (2022), 064318

Modified algorithm

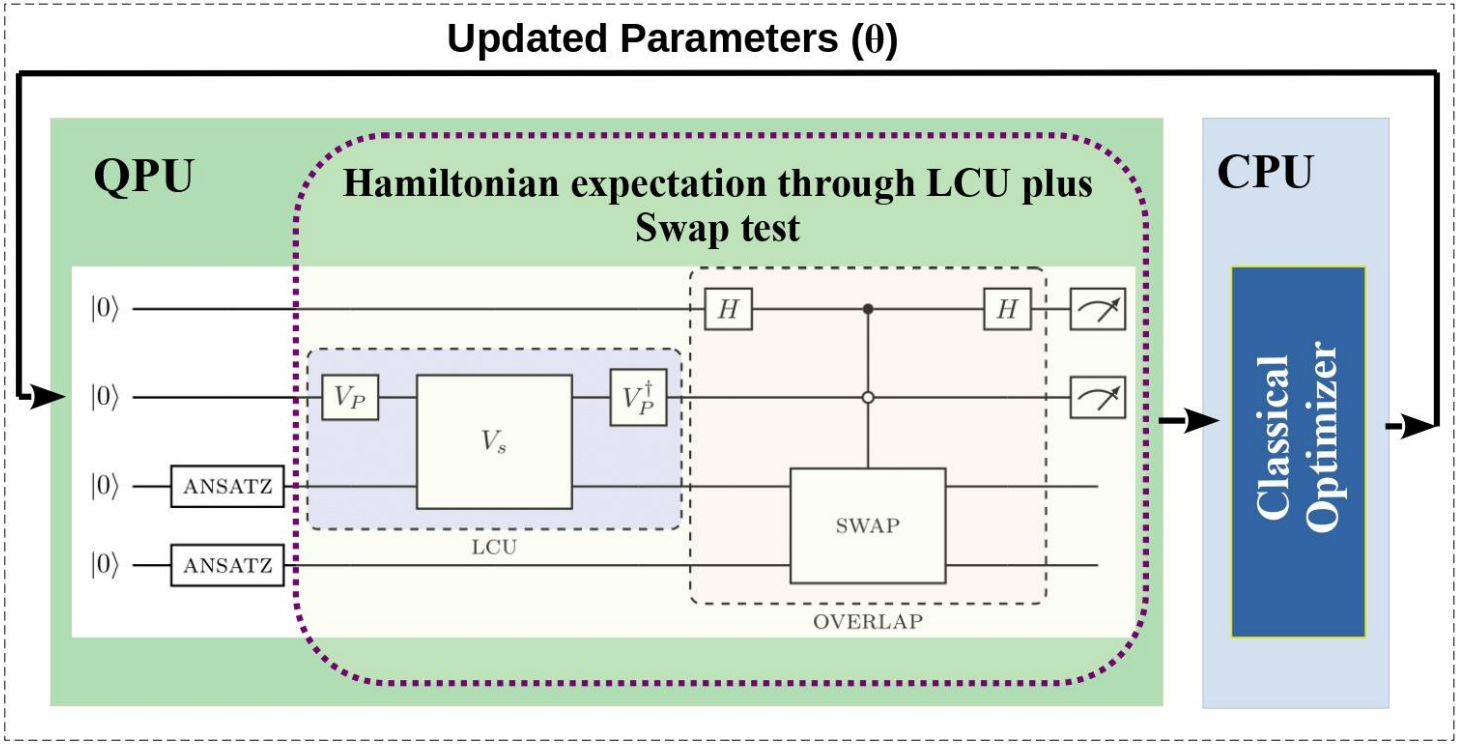

Fig. 7: Modified variational algorithm for expectation value calculation

Results and discussion

- We have applied this algorithm for binding energy of deuteron under EFT potential, and Hamiltonian is encoded via Gray Code encoding.
- Classical optimizer used for our calculation is SPSA optimizer.
- Executed the algorithm for 100000 shots and 100 independent runs.
- For error bar we used MAD.

Basis size (N)	True Value	Modified variational algorithm
2	-1.74916	-1.7459993 ± 0.025
3	-2.04567	-2.0464696 ± 0.044
4	-2.145	-2.0992413 ± 0.078

Table 2: Energy calculated with QASM simulator for EFT potential through modified algorithm

Results

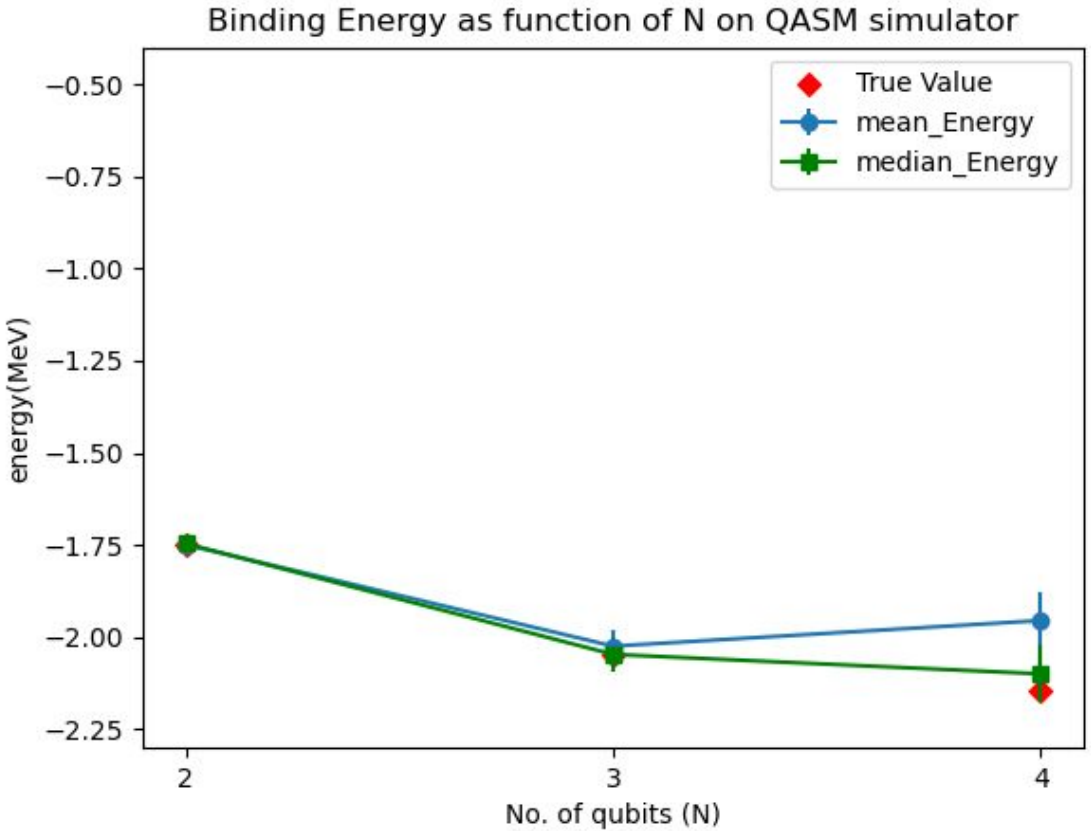

Fig. 8: Energy as function of number of states for EFT potential for GC encoding using modified variational algorithm using LCU.

Conclusions

- We modified the variational algorithm such that it can be applied to system having non hermitian Hamiltonian.
- We calculated the BE of deuteron with our method and results are in agreement with the published VQE results.
- Even though this method is more prone to error due to larger gate depth, this method can be applied to the non-hermitian matrix, which occurs in the case of resonances.
- This shows a validity of method and further it can be extended for the Hamiltonian having complex energies.

Thank you