QAGC SUBMISSION

Daichi Suzuki(team: 81ueman)

Motivation

- VQE is hard to optimize due to
  - *T1,T2 noise*
  - *Depolarizing noise*
  - *Measurement noise*
  - *Statistical error of observables*

- Are there any way to avoid it?

Overview of the method

The idea In short:

Quantum Selected Configuration Interaction
with the sampled basis from the HF wavefunction

1. HF on a Quantum Computer?
2. Quantum Selected Configuration Interaction?

Hartree-Fock ansatz

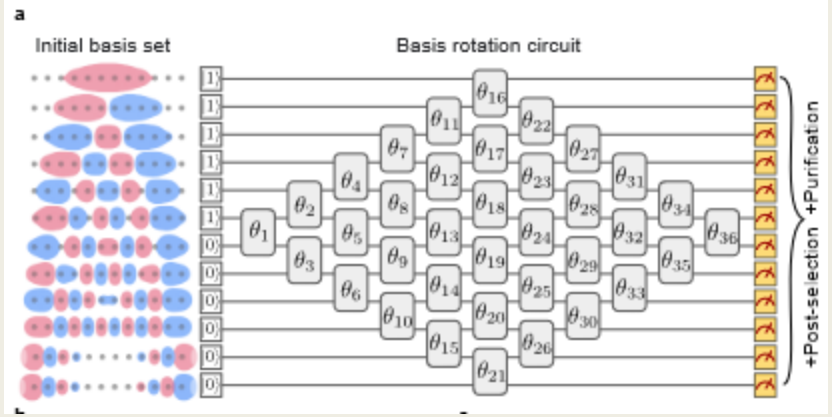

Fig. 1.a. [1]

- Hartree-Fock wavefunction on a QC
- Needs fewer shots than VQE to optimize and measure energy
  - ☺ *Measurement of only* $a_i^\dagger a_j$
  - ☺ *Error mitigation schemes*
    - Post selection
    - Positive trace
    - McWeeny purification
  - ☺ *Optimization with only* $a_i^\dagger a_j$ *and* $\mathcal{H}$
- ☹ HF wave function is not so close to the ground state

QSCI

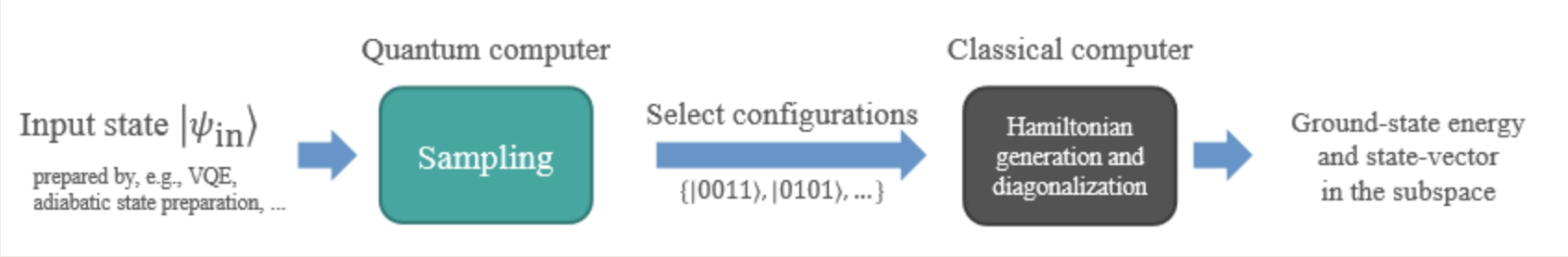

FIG.1.[2]

- A kind of Configuration Interaction(CI)
  - CISD contains HF, single and double
- QSCI contains the basis QC often emits
  - *Diagonalize Hamiltonian within the spanned basis*
- No need for the exact coefficient of each basis
  - ☺*No need to measure it exactly*
- It just needs what basis seems important.
  - ☺*Robust to noise*
  - ☺*Fewer shots than measuring energy*
- ☹ No criteria to optimize wave functions

Pros and Cons of HF and QSCI

- HF ansatz is
  - ☺ *easy to optimize*
  - ☹ *inaccurate wavefunction*
  - ☹ *still a bit noisy energy estimation*
- QSCI is
  - ☺ *exact wavefunction within the spanned space*
  - ☺ *exact energy*
  - ☹ *no general optimization scheme*

Combination of HF and QSCI

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  - ☺ *exact energy within the spanned space*
  - ☹ *no general optimization scheme*
- ☺Each solves the missing part of the other!
- HF wavefunction is
  - *not so accurate but enough to sample the important basis*

What is Quantum advantage?

- HF calculation itself is easy (N: number of electrons)
- $$\begin{pmatrix} b_1^\dagger \\ b_2^\dagger \\ \dots \\ b_{2N}^\dagger \end{pmatrix} = \begin{pmatrix} u_{11} & u_{12} & \dots & u_{1\,2N} \\ u_{21} & u_{22} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ u_{2N1} & u_{2N2} & \dots & u_{2N2N} \end{pmatrix} \begin{pmatrix} a_1^\dagger \\ a_2^\dagger \\ \vdots \\ a_{2N}^\dagger \end{pmatrix}$$

- HF wavefunction: $b_N^\dagger \dots b_2^\dagger b_1^\dagger |0..00>$
  $= \left(u_{N1}a_1^\dagger \dots u_{N2N}a_{2N}^\dagger\right)\left(u_{N-1,1}a_1^\dagger \dots u_{N-1,2N}a_{2N}^\dagger\right) \dots (u_{11}a_1^\dagger \dots u_{12N}a_{2N}^\dagger)|0\dots00>$
  $= c_{00..1111..1}|00..1111..1> + \dots + c_{111..100..00}|111..100..00>$
- To obtain some of the largest coefficient (will be) hard classically but is easy for Quantum computer
  - *Classically*

references

- [1] Google AI Quantum and Collaborators*†, et al. "Hartree-Fock on a superconducting qubit quantum computer." *Science* 369.6507 (2020): 1084-1089.

- [2] Kanno, Keita, et al. "Quantum-Selected Configuration Interaction: classical diagonalization of Hamiltonians in subspaces selected by quantum computers." *arXiv preprint arXiv:2302.11320* (2023).