Finding Near-Optimal Quantum State with Restricted Particle-Preserving Ansatz

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Overview

1. I decided to use ion-trap type computers.
2. I limited the search space based on the number of electrons.
3. I reduced the search space by freezing some qubits.
4. I mitigated depolarizing noises by preprocessing.
5. I extended the Nakanishi-Fujii-Todo method into multiple angle variables.

The idea

Why not superconducting type?

- The measurement results obtained from superconducting (SC) type computers were too noisy and biased.
  - The error rate of SC-type computers was set 10x higher than ion-trap (IT) type.
- In addition, SC-type computers have limited qubit connectivity, which requires additional multi-qubit gates for circuit compilation.
  - Swapping adjacent qubits requires 3 native CNOT gates.
  - Remote CNOT gate requires 4 native CNOT gates.

Limiting the search space

After running some naive algorithms, I found it difficult to reach the optimal state in a large search space such as $\mathbb{C}^{256}$. So I limited the search space based on the ideas below:

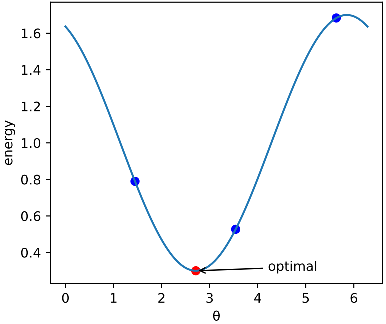
1. Fixing the number of electrons.
   - Each basis contains four “0”s and four “1”s.
2. Freezing some qubits.
   - A site with a low energy level should be occupied with two electrons.
   - A site with a high energy level should be empty.
   - Freezing two sites shrinks the search space from $\mathbb{C}^{256}$ to $\mathbb{C}^{16}$.

Sequential Minimal Optimization (Nakanishi et al., PRR, 2020)

- Fixing all parameters except θ_i, the cost function $\langle\psi(\boldsymbol{\theta})|\,\hat{H}\,|\psi(\boldsymbol{\theta})\rangle$ can be described as

$$f(\theta_i) = a\cos\theta_i + b\sin\theta_i + c. \qquad (1)$$

- After identifying the landscape $f(\theta_i)$ from a few (at least three) measurements, we can easily calculate the optimal parameter.



Improving Measurement

Noise Analysis

In the IT-type simulator, the noise parameters are

- $t_1 = 10, t_2 = 1, t_{\text{gate}} = 10^{-4}$ [sec]
- $p_{\text{dep,single}} = 10^{-5}, p_{\text{dep,double}} = 10^{-3}$
- $p_{\text{meas}} = 10^{-3}$

Thus, the magnitude of each noise can be estimated as

- Amplitude damping: $t_{\text{gate}} \cdot O(10) \cdot t_1^{-1} = O(10^{-4})$
- Phase damping: $t_{\text{gate}} \cdot O(10) \cdot t_2^{-1} = O(10^{-3})$
- Depolarizing noise: $p_{\text{dep,single}} \cdot O(10 \sim 100) + p_{\text{dep,double}} \cdot O(10) = O(10^{-2})$
- Measurement noise: $p_{\text{meas}} \cdot O(1 \sim 8) = O(10^{-3} \sim 10^{-2})$

Mitigating Depolarizing Noise (Urbanek et al., PRL, 2021)

- Under the depolarizing noise, the expected value of the observable $\hat{O}$ is

$$\mathrm{tr}(\hat{O}\rho) = (1-p)\langle\psi|\,\hat{O}\,|\psi\rangle + \frac{p}{2^n}\mathrm{tr}(\hat{O}), \tag{2}$$

  where $\langle\psi|\,\hat{O}\,|\psi\rangle$ is what we want to obtain.

- Because $\frac{\mathrm{tr}(\hat{O})}{2^n} = c$ (the coefficient corresponding to the identity) can be explicitly obtained from the observable, we get

$$\langle\psi|\,\hat{O}\,|\psi\rangle = \frac{1}{1-p}\left(\mathrm{tr}(\hat{O}\rho) - c\right) + c. \tag{3}$$

Mitigating Bit-Flip Noise

- Let p, q as the probability of measuring $|0\rangle\,, |1\rangle$.
- When measuring $\hat{O} = Z^{\otimes k}$ under bit-flip error e, the actual probability p', q' will be

$$\begin{pmatrix} p' \\ q' \end{pmatrix} = \begin{pmatrix} 1-e & e \\ e & 1-e \end{pmatrix}^k \begin{pmatrix} p \\ q \end{pmatrix}, \tag{4}$$

  which changes the observed value from $p - q$ into $p' - q' = (1-2e)^k (p-q)$.
- Hence, we can mitigate bit-flip error by multiplying the factor $(1-2e)^{-k}$.

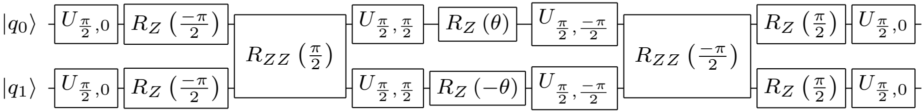
Implementation details

Givens rotation gate

- Givens rotation gate $G(\theta)$ applies $R(\theta)$ on the center of the 4x4 matrix.

$$G(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & -\sin(\theta) & 0 \\ 0 & \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{5}$$

- $G(\theta)$ can be implemented as below:

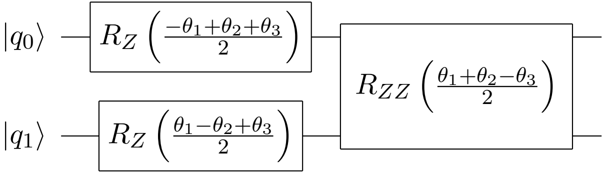


Phase rotation gate

- Phase rotation gate $P(\theta_1, \theta_2, \theta_3)$ applies a diagonal unitary matrix.
  - Note that the global phase can be ignored.

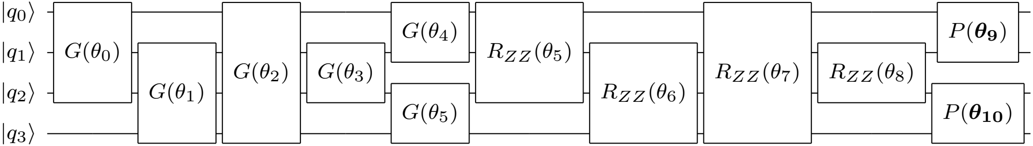
$$P(\theta_1, \theta_2, \theta_3) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{i\theta_1} & 0 & 0 \\ 0 & 0 & e^{i\theta_2} & 0 \\ 0 & 0 & 0 & e^{i\theta_3} \end{pmatrix} \tag{6}$$

- $P(\theta_1, \theta_2, \theta_3)$ can be implemented as below:



Particle-preserving ansatz

- By combining Givens rotation and phase rotation gates, we can build a circuit that preserves the number of particles.
- In the case of 4 qubits, for example, the particle-preserving ansatz looks like



Extension of the NFT method

- It is well known that the NFT method can be applied to optimize R_X, R_Y, R_Z gates.
- Is it applicable for other rotation gates such as $G(\theta)$, $R_{ZZ}(\theta)$, and $P(\theta_1, \theta_2, \theta_3)$?
- I found that $G(\theta)$ and $R_{ZZ}(\theta)$ can be optimized in the same way as R_X, R_Y, R_Z gates, whereas the landscape of $P(\theta_1, \theta_2, \theta_3)$ is

$$
\begin{aligned}
f(\theta_1, \theta_2, \theta_3) = & A_{12} \cos(\theta_1 - \theta_2) + A_{13} \cos(\theta_1 - \theta_3) + A_{23} \cos(\theta_2 - \theta_3) \\
& + B_{12} \sin(\theta_1 - \theta_2) + B_{13} \sin(\theta_1 - \theta_3) + B_{23} \sin(\theta_2 - \theta_3) \\
& + A_1 \cos(\theta_1) + A_2 \cos(\theta_2) + A_3 \cos(\theta_3) \\
& + B_1 \sin(\theta_1) + B_2 \sin(\theta_2) + B_3 \sin(\theta_3) + C,
\end{aligned} \tag{7}
$$

which requires at least 13 measurement results to optimize them simultaneously.