Trotter Circuit Optimization

through Adiabatic computation

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Part I

QUBO PROBLEMS IN CIRCUIT OPTIMIZATION

To simulate time-evolving process such as adiabatic quantum process, we approximate continuous process with discrete steps.
We call the discretized approximation as **Trotter** formula.

$$\exp(-i\mathcal{H}t) \approx \Pi_i^n \exp\left(-i\mathcal{H}_i \frac{t}{n}\right) \tag{1}$$

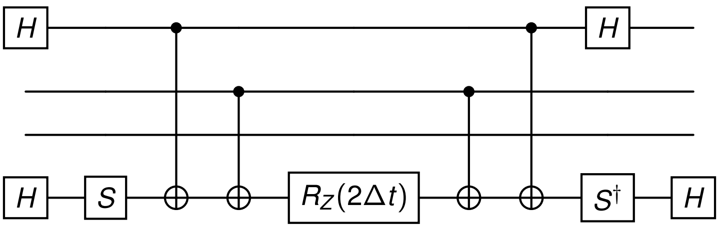
where, n is a trotter steps.
As we increase the step number n, we get more precise unitary trnasformation.

Lie-Trotter Formula and Circuit

Trotterization

Practically, each terms of Hamiltonian are described with **Pauli string**. A single Pauli string, for example *XZIY*, Hamiltonian has a well known corresponding circuit.

$$\exp(-i\Delta t(X \otimes Z \otimes I \otimes Y)) \tag{2}$$



Optimization of Hamiltonian

Optimization of evolution circuit is a combination of two parts.

- Mutually Commuting Partition
- Pauli-Frame

Optimization of Hamiltonian

Mutually Commuting Partition

Pauli strings are always anti-commute or commute each other.
For given two Pauli strings, P_i, P_j,

$$\text{either } [P_i, P_j] = 0 \text{ or } \{P_i, P_j\} = 0 \tag{3}$$

where, [ ] is a commutator, and { } is an anti-commutator.
If all Pauli-terms of Hamiltonain are mutually commute each other, Eq(1) becomes an unitary operator of total Hamiltonain evolution of time t.

$$\exp(-i\mathcal{H}t) = \Pi_i^n \exp\left(-i\mathcal{H}_i t\right) \tag{4}$$

1. We must know all commuting relation of the given Pauli-stirng set.
2. How to make a mutually partitions of the given set?

Optimization of Hamiltonian

Mutually Commuting Partition

To make a mutually commuting partition, we have to know all commuting relationships of the given Pauli-terms of Hamiltonian. We can check the commutation with General commutativity(GC), see Gokhale et al., 2020.

If a system is n qubits system and there are m number of Pauli-terms, total operation would be, roughly,

$$\binom{m}{2} * n = O(m^2 n) \tag{5}$$

Unfortunately, $\max(m) = 2^n$ for n-qubit system Hamiltonian, it could be expoentially growth.

Optimization of Hamiltonian

Mutually Commuting Partition

Chapuis et al., 2018 suggested acceleration of commuting term determination.
They decompose single Pauli-string into X and Z families.

- X-family: $IIIX, XIXI, IIXI, XXII, IXXX, \ldots$
- Z-family: $IIIZ, ZIZI, IIZI, ZZII, IZZZ, \ldots$

$$YZIX = XIIX \cdot ZZII = x_i \cdot z_j \tag{6}$$

$$[P_i, P_j] = [x_k z_l, x_m, z_n] = \begin{cases} 0 & if [z_l, x_m] = [x_k, z_n] \\ -2P_iP_j & otherwise \end{cases} \tag{7}$$

Optimization of Hamiltonian

Mutually Commuting Partition

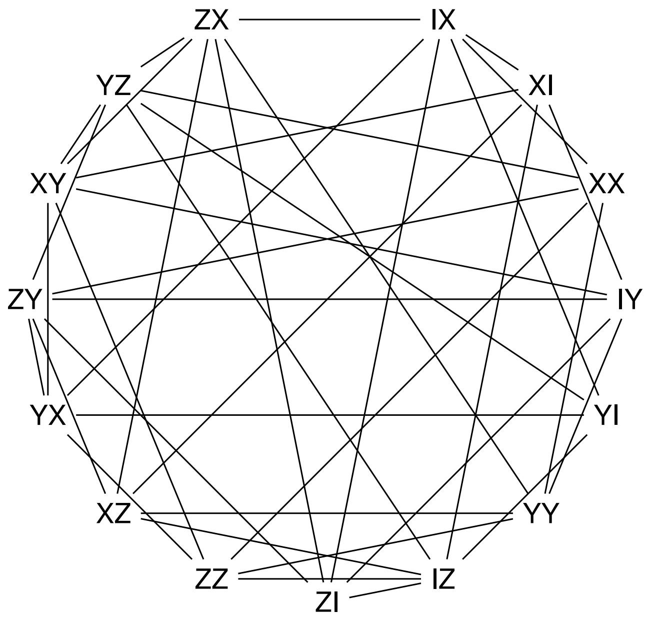
Now, if we have compatible grpah of Pauli-set, we can extract mutually commuting partition by solving a sequential Max-Clique problem of the commute graph.
It is well known NP-complete problem, from 21-complete problems. See Karp, 1972.
Kurita et al., 2023 suggested Ising formulation for finding Max-clique finding problem of compatible graph.

$$\mathcal{H} = -\mu_0 \sum Z_i + \mu_1 \sum h_{ij} Z_i Z_j \tag{8}$$

where, $h_{ij} = 0$ if $Z_i - Z_j$ edge weight is 0 otherwise 1, $\mu_0 = 1, \mu_1 = 2$ in Kurita et al..

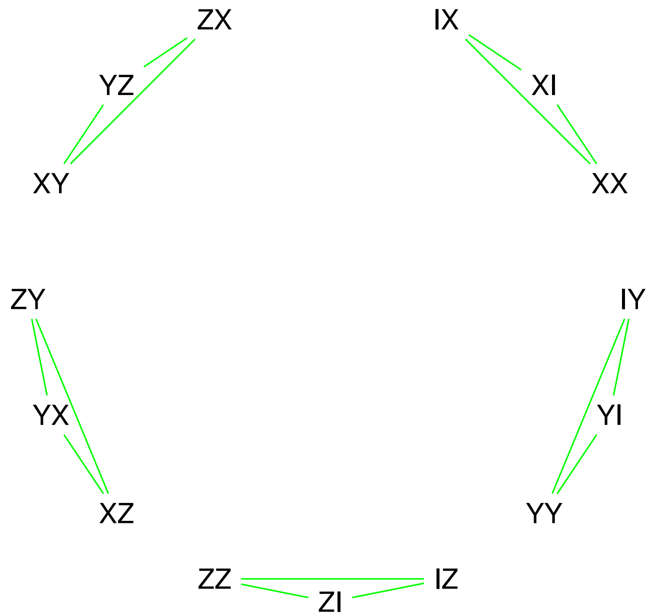
Optimization of Hamiltonian

Mutually Commuting Partition



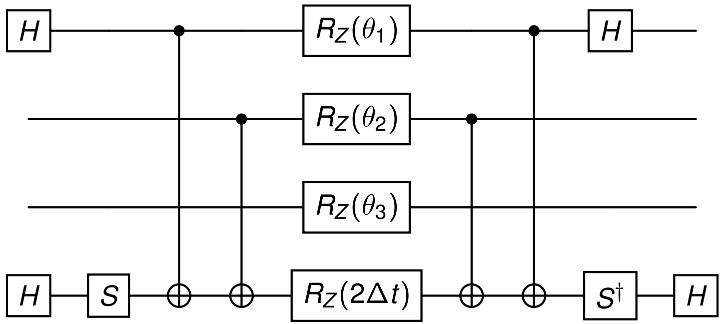
Optimization of Hamiltonian

Mutually Commuting Partition



Optimization of Hamiltonian

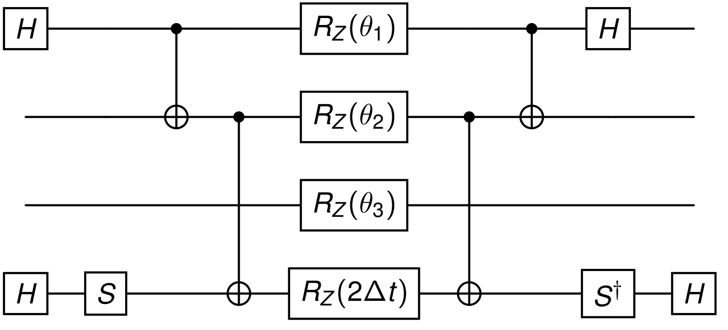
Pauli Frame



$$\mathcal{H} = tXZIY + \theta_1 XIII + \theta_2 IZII + \theta_3 IIII$$

Optimization of Hamiltonian

Pauli Frame



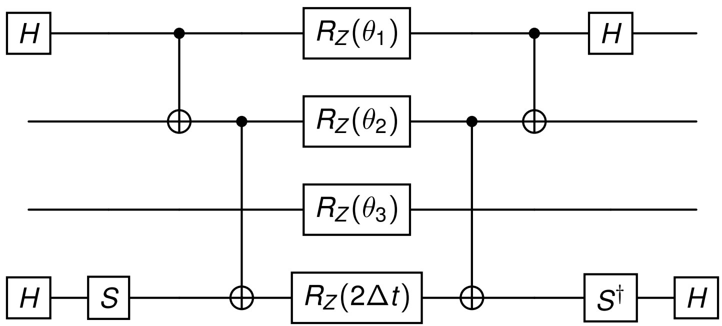
$$\mathcal{H} = tXZIY + \theta_1 XIII + \theta_2 XZII + \theta_3 IIII$$

Optimization of Hamiltonian

Pauli Frame

Schmitz et al., 2023 analyzed and Pauli-Frame method and optimized circuit with minimum cost of *CNOT*, *H*, *S* operations to

$$\begin{array}{cc} Z_1 & X_1 \\ Z_2 & X_2 \\ Z_3 & X_3 \\ Z_4 & X_4 \end{array} \rightarrow_{H_2, H_4 - S_4} \begin{array}{cc} X_1 & Z_1 \\ Z_2 & Z_2 \\ Z_3 & X_3 \\ Y_4 & Z_4 \end{array} \rightarrow_{CNOT1,2} \begin{array}{cc} X_1 & Z_1 \\ X_1 Z_2 & Z_1 X_2 \\ Z_3 & X_3 \\ Y_4 & X_4 \end{array} \rightarrow_{CNOT2,4} \begin{array}{cc} X_1 & Z_1 \\ X_1 Z_2 & Z_1 X_2 \\ Z_3 & X_3 \\ X_1 Z_2 Y_4 & Z_1 X_2 Z_4 \end{array} \tag{9}$$



$$\mathcal{H} = tXZIY + \theta_1 XIII + \theta_2 XZII + \theta_3 IIII$$

Degenerate Reducing of Mutually Hamiltonian

If there are two max clique on graph, sharing same number of nodes, the next Hamiltonian pick one of them randomly.

$$\mathcal{H} = -\mu_0 \sum Z_i + \mu_1 \sum h_{ij} Z_i Z_j \tag{10}$$

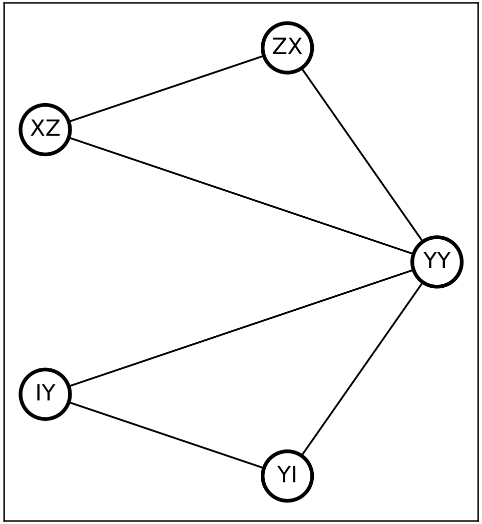
Eventhough, they are same in commutation graph, frame change cost can be different.
In this project, we only consider H, S costs. The weight of each Pauli-terms would be calculated with function $w(,)$, such that

- $w(,) = 0$: (X, X), (Y, Y), (Z, Z), (Z, I)
- $w(,) = 1$: (X, Z),(X, Y),(X, I)
- $w(,) = 2$: (Y, I), (Y, Z)

For N-qubit system, extended weight function $W(,)$ is defined as,

$$W(S_i, S_j) := \frac{1}{N} \sum_{k=1}^{N} w((S_i)_k, (S_j)_k) \tag{11}$$

Degenerate Reducing of Mutually Hamiltonian



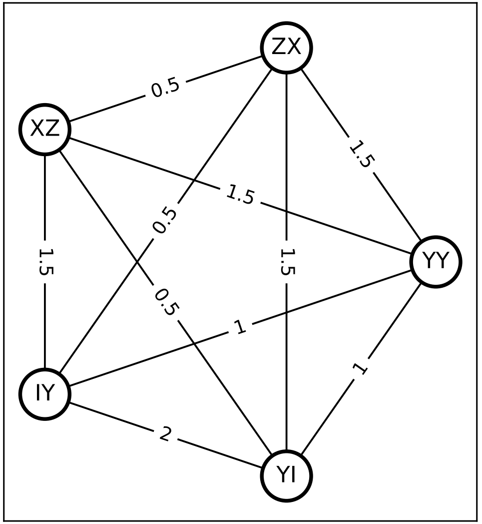


Figure. Compatible and basis transform weight graph example. Left graph is a compatible graph of 5 Pauli basis of 2 qubits system and edges are indicating commutation relationship. Right graph is a basis transform weight graph of the same Pauli-basis set of the left.

Degenerate Reducing of Mutually Hamiltonian

We can redefine a Hamiltonian for optimization,

$$\mathcal{H} = -\mu_0 \sum Z_i + \mu_1 \sum_{i<j} h_{ij} Z_i Z_j + \mu_2 \sum_{i<j} w_{ij} Z_i Z_j \tag{12}$$

To avoid the degeneration of energy and to conserve max and commuting condition, the coefficients, μ_0, μ_1, μ_2 have next relationship.
For N qubits system,

$$\|\mu_1\| > N\|\mu_0\| \; \|\mu_0\| > \frac{1}{2}N(N-1)\|\mu_2\| \tag{13}$$

Degenerate Reducing of Mutually Hamiltonian

Full procedure of algorithm.

1. Find a compatible graph of the given Hamiltonian
2. Calculate weigtht between Pauli-strings with Eq(11)
3. Find a min-number of mutually commuting partition, $p_1, p_2, \ldots,$ using **adiabatic computer**.
4. Find a shortest hamilton path of each local partition p_i, <- reduced problem, you can use classic algorithm.
5. Connecting p_i in order to following 4 step result.

Optimization Example

HeH+ molcular hamiltonian

Pennylane HeH+ molcule Hamiltonian:
4 qubits are required and consist of 25 Pauli-terms.
'ZXZX','IYIY','ZYZY','IZIZ','XZXZ','XIXI','YZYZ','YIYI','ZIZI', ,'IIIZ', 'ZZII', 'IZZI', 'ZIIZ', 'IZII', 'IIZI', 'ZIII', 'IIZZ', ,'XZXI', 'YZYI', 'XXYY', 'YXXY', 'YYXX', 'XYYX', 'IYZY', 'IXZX'

Optimization Example

HeH+ molcular Hamiltonian

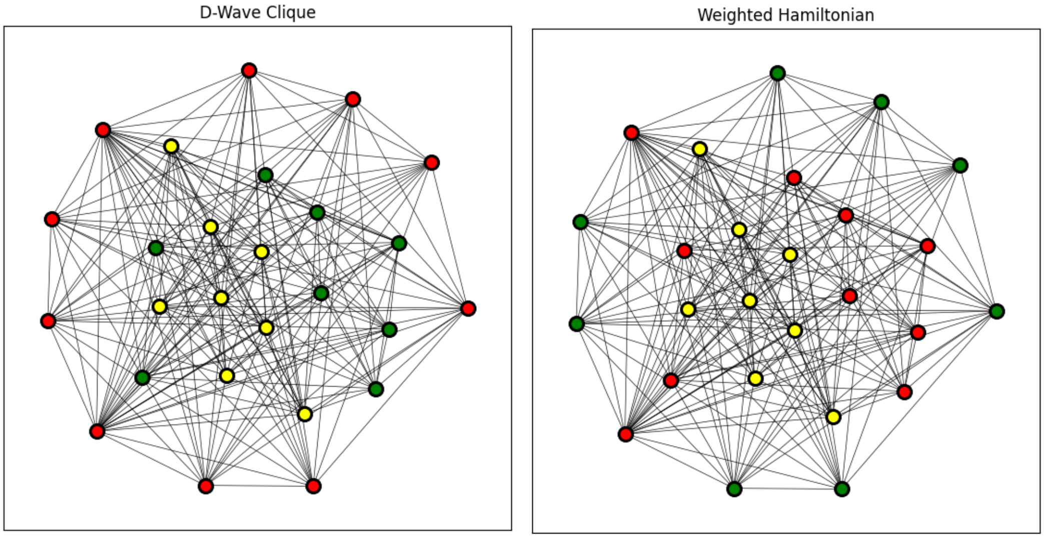


Figure. Commuting Partition HeH+ Hamiltonian Pauli-terms. Left: Ising formula solution of D-Wave. Right: Basis cost term weight added optimization.

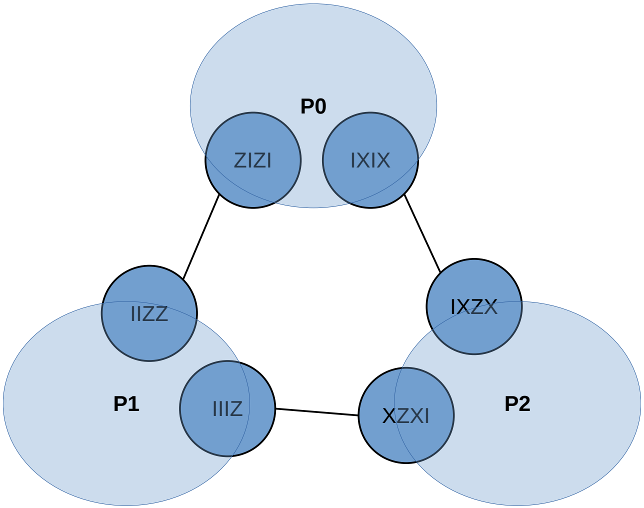
Optimization Example

HeH+ molcular hamiltonian

The optimization result is 3 number of partition.
p_0 ['ZXZX','IYIY','ZYZY','IZIZ','XZXZ','XIXI','YZYZ','YIYI','ZIZI']
p_1 ['IIIZ', 'ZZII', 'IZZI', 'ZIIZ', 'IZII', 'IIZI', 'ZIII', 'IIZZ']
p_2 ['XZXI', 'YZYI', 'XXYY', 'YXXY', 'YYXX', 'XYYX', 'IYZY', 'IXZX']

Optimization Example

HeH+ molcular hamiltonian



Optimization Example

HeH+ molcular hamiltonian

Compare to Pennylane ApproxTimeEvovle() circuit

```
gates: 270
depth: 169
shots: Shots(total=None)
gate_types:
{'RZ': 106, 'CNOT': 84, 'RX': 80}
gate_sizes:
{1: 186, 2: 84}
```

```
gates: 137
depth: 107
shots: Shots(total=None)
gate_types:
{'Hadamard': 16, 'CNOT': 74, 'RZ': 25, 'S': 11, 'Adjoint(S)': 11}
gate_sizes:
{1: 63, 2: 74}
```

Figure. Left: Pennylane ApproxTimeEvolve() trotter number =1 circuit. Right: Optimized evolve circuit.

References I

Chapuis, G., Djidjev, H. N., Hahn, G., & Rizk, G. (2018, April). **Finding Maximum Cliques on the D-Wave Quantum Annealer [arXiv:1801.08649 [quant-ph]].**

Gokhale, P., Angiuli, O., Ding, Y., Gui, K., Tomesh, T., Suchara, M., Martonosi, M., & Chong, F. T. (2020). $O(N^3)$ **Measurement cost for variational quantum eigensolver on molecular hamiltonians.** *IEEE Transactions on Quantum Engineering*, *1*, 1–24. https://doi.org/10.1109/TQE.2020.3035814

Karp, R. M. (1972). **Reducibility among combinatorial problems.** In R. E. Miller, J. W. Thatcher, & J. D. Bohlinger (Eds.), *Complexity of computer computations: Proceedings of a symposium on the complexity of computer computations, held march 20–22, 1972, at the ibm thomas j. watson research center, yorktown heights, new york, and sponsored by the office of naval research, mathematics program, ibm world trade corporation, and the ibm research mathematical sciences department* (pp. 85–103). Springer US. https://doi.org/10.1007/978-1-4684-2001-2_9

Kurita, T., Morita, M., Oshima, H., & Sato, S. (2023). **Pauli string partitioning algorithm with the ising model for simultaneous measurements [PMID: 36653017].** *The Journal of Physical Chemistry A*, *127*(4), 1068–1080. https://doi.org/10.1021/acs.jpca.2c06453

Schmitz, A. T., Sawaya, N. P. D., Johri, S., & Matsuura, A. Y. (2023, May). **Graph Optimization Perspective for Low-Depth Trotter-Suzuki Decomposition [arXiv:2103.08602 [cond-mat, physics:math-ph, physics:physics, physics:quant-ph]].**