Trotter Circuit Optimization

through Adiabatic computation

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Part I

QUBO PROBLEMS IN CIRCUIT OPTIMIZATION

Lie-Trotter Formula and Circuit

Trotterization

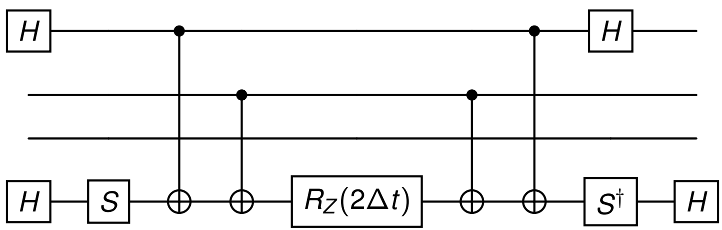
To simulate time-evolving process such as adiabatic quantum process, we approximate continuous process with discrete steps.
We call the discretized approximation as **Trotter** formula.

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

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

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),
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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.

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

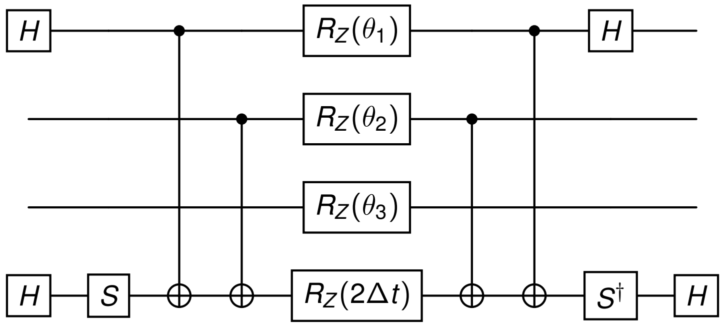
Now, if we have compatible grpah of Pauli-set, we can extract mutually commuting partition by solving a sequential Max-Clique problem of the commute graph.
It is well known NP-complete problem, from 21-complete problems. See Karp, 1972.
Kurita et al., 2023 suggested Ising formulation for finding Max-clique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

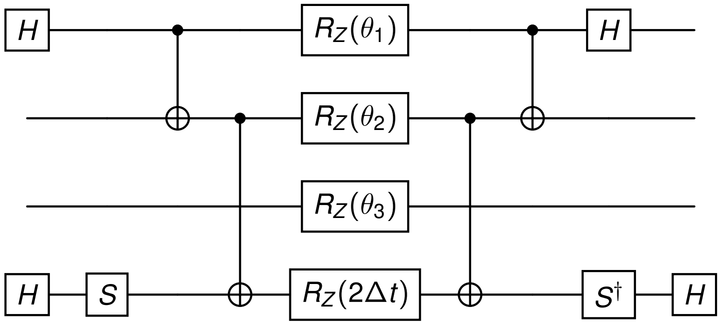
Pauli Frame



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

OPTIMIZATION OF HAMILTONIAN

PAULI FRAME



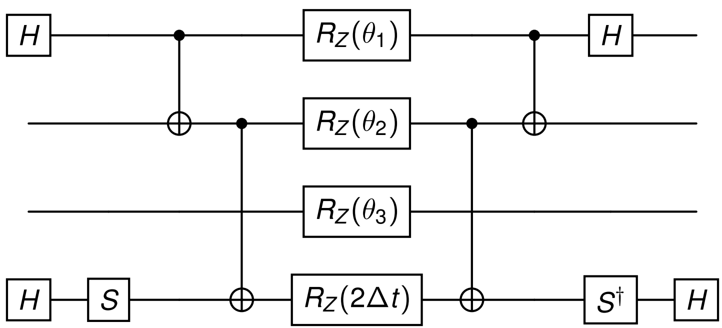
$$\mathcal{H} = tXZIY + \theta_1 XIII + \theta_2 XZII + \theta_3 IIII$$

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

$$
\begin{array}{cc} Z_1 & X_1 \\ Z_2 & X_2 \\ Z_3 & X_3 \\ Z_4 & X_4 \end{array}
\rightarrow_{H_2, H_4 - S_4}
\begin{array}{cc} X_1 & Z_1 \\ Z_2 & Z_2 \\ Z_3 & X_3 \\ Y_4 & Z_4 \end{array}
\rightarrow_{CNOT 1,2}
\begin{array}{cc} X_1 & Z_1 \\ X_1 Z_2 & Z_1 X_2 \\ Z_3 & X_3 \\ Y_4 & X_4 \end{array}
\rightarrow_{CNOT 2,4}
\begin{array}{cc} X_1 & Z_1 \\ X_1 Z_2 & Z_1 X_2 \\ Z_3 & X_3 \\ X_1 Z_2 Y_4 & Z_1 X_2 Z_4 \end{array}
\tag{9}
$$



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

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

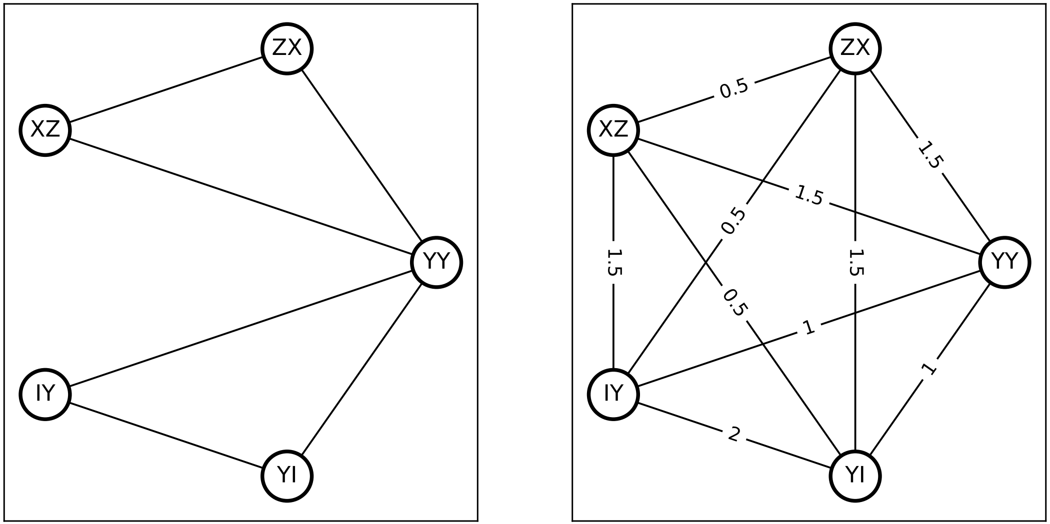


Figure. Compatible and basis transform weight graph example. Left graph is a compatible graph of 5 Pauli basis of 2 qubits system and edges are indicating commutation relationship. Right graph is a basis transform weight graph of the same Pauli-basis set of the left.

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

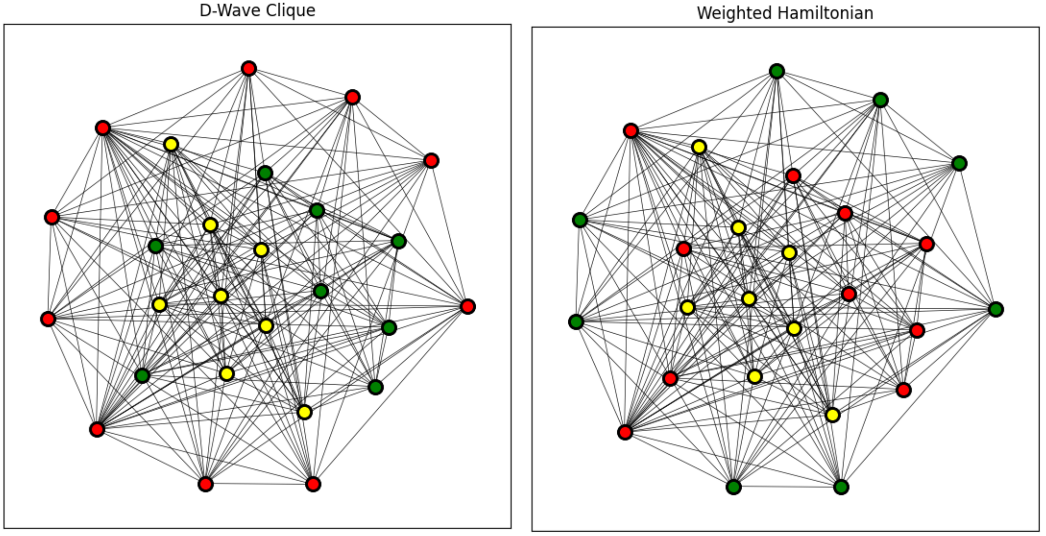


Figure. Commuting Partition HeH+ Hamiltonian Pauli-terms. Left: Ising formula solution of D-Wave. Right: Basis cost term weight added optimization.

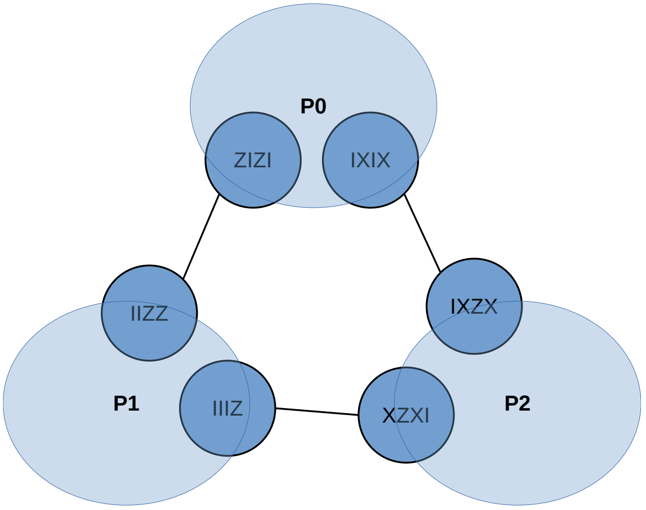
Optimization Example

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.

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