Symmetry Adapted way for the efficient Trotter decomposition

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In this report, we simulate the time evolution of the $N = 3$ Heisenberg model by Tritterization on `ibmq_jakarta`, based on the circuit level approach (without pulse). Focusing on the symmetry of the Hamiltonian of the Heisenberg model, we construct and Trotterize an effective Hamiltonian on $(N-1)$-qubit space which is encoded from the N particle Heisenberg model. We show this Trotterization of effective Hamiltonian is equivalent to changing the axis of the Trotterization of the original Hamiltonian. This encoding framework makes it possible to reduce the number of CNOT gates for one Trotter step from 6 to 4 in general, and when $N = 3$, the circuit depth and the number of CNOT gates becomes constant for any trotter steps. Combining with several error mitigation techniques, we finally achieve fidelity 0.98 ± 0.001 on `fake_jakarta` simulator, and 0.94 ± 0.001 on `ibmq_jakarta` real quantum device, for the given problem setting.

I. INTRODUCTION

Before getting into the details, we will briefly review our method and results here. First, we solved the problem by circuit level optimization WITHOUT using Qiskit pulse.

Toward this, we focus on the symmetry to embed the N site Heisenberg model into $N-1$-qubit system.

The theoretical insight of the effective Hamiltonian of the Heisenberg model is mainly done by Naoki Negishi. The incorporation of the error mitigation and the code implementation is mainly done by Bo Yang.

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II. THEORETICAL FOUNDATION

The XXX Heisenberg 3-spins Hamiltonian H_{Heis} is commutable with both the products of σ_μ^i, $(\mu \in \{x, y, z\})$ for all sites as

$$[H_{\text{Heis}}, \sigma_\mu^1 \sigma_\mu^2 \sigma_\mu^3] = 0. \tag{1}$$

This Hamiltonian can be decomposed as a direct sum of the subspace

$$H_{\text{Heis}} \in \mathcal{H}_{\text{odd}} \oplus \mathcal{H}_{\text{even}}, \tag{2}$$

and $\mathcal{H}_{\text{odd,even}}$ is the the subspace composed by the eigen states of $\sigma_z^1 \sigma_z^2 \sigma_z^3$ equal to $-1, 1$, that is

$$\mathcal{H}_{\text{odd}} = \{|100\rangle, |010\rangle, |001\rangle, |111\rangle\} \tag{3}$$
$$\mathcal{H}_{\text{even}} = \{|110\rangle, |101\rangle, |011\rangle, |000\rangle\}. \tag{4}$$

Because of the Eq.(1) in $\mu = x$ case, any eigen vector of H_{Heis} in the subspace $\mathcal{H}_{\text{odd}}$, defined as $|\text{odd}\rangle$ having the eigen energy E, and the vector $\sigma_x^1 \sigma_x^2 \sigma_x^3 |\text{odd}\rangle \in \mathcal{H}_{\text{even}}$ is degenerated, and we can say that any states between $|\text{odd}\rangle \in \mathcal{H}_{\text{odd}}$ and $\sigma_x^1 \sigma_x^2 \sigma_x^3 |\text{odd}\rangle \in \mathcal{H}_{\text{even}}$ are identified. In our strategy, we introduced effective Hamiltonian H_{eff} which gives the same time evolution for any initial state, reducing 2-spins state as $|ab\rangle_{\text{eff}}$ by identifying $|\text{odd}\rangle$ and $\sigma_x^1 \sigma_x^2 \sigma_x^3 |\text{odd}\rangle$ as

$$|000\rangle, |111\rangle \sim |00\rangle_{\text{eff}} \tag{5}$$
$$|011\rangle, |100\rangle \sim |01\rangle_{\text{eff}} \tag{6}$$
$$|110\rangle, |001\rangle \sim |10\rangle_{\text{eff}} \tag{7}$$
$$|101\rangle, |010\rangle \sim |11\rangle_{\text{eff}}, \tag{8}$$

where the symbol "$\sim$" represents equivalent relation. The time-dependent Schrödinger equation (TDSE) is governed by H_{eff} as

$$i\partial_t |\psi(t)\rangle_{\text{eff}} = H_{\text{eff}} |\psi(t)\rangle_{\text{eff}}, \tag{9}$$

and H_{eff} is constructed as

$$H_{\text{eff}} = \sigma_x^1 + \sigma_x^2 + \sigma_z^1 + \sigma_z^2 - (\sigma_z^1\sigma_x^2 + \sigma_x^1\sigma_z^2), \tag{10}$$

consistently equal to the TDSE under the H_{Heis} in the 3-spins system. $\psi(t)$ is the wavefunction.

In addition, making the two kinds of projection operators $P_{+,-}$ to the subspace $\mathcal{H}_{\text{even,odd}}$, respectively, we can rewrite H_{Heis} as

$$H_{\text{Heis}} = \sum_{i\in\{+,-\}} P_i^\dagger H_{\text{eff}}^{13} P_i, \tag{11}$$

where H_{eff}^{13} is given by Eq.(10) substituting $\boldsymbol{\sigma}^2 \to \boldsymbol{\sigma}^3$. Thus time propagation under the effective Hamiltonian is equivalent to that of the Hisenberg Hamiltonian, so we do not modified the specified Hamiltonian in this contest. The projection operator satisfies the following relations,

$$P_+ \in \mathcal{H}_{\text{even}}, P_- \in \mathcal{H}_{\text{odd}} \tag{12}$$

$$P_+P_-^\dagger = P_-P_+^\dagger = P_+^\dagger P_- = P_-^\dagger P_+ = 0 \tag{13}$$

$$P_+^\dagger P_+ = I_+ \in \mathcal{H}_{\text{even}} \tag{14}$$

$$P_-^\dagger P_- = I_- \in \mathcal{H}_{\text{odd}} \tag{15}$$

$$H_{\text{eff}}^{13} \in \mathcal{H}_{\text{odd}} \oplus \mathcal{H}_{\text{even}}, \tag{16}$$

where $I_{+,-}$ is identity operator in the subspace $\mathcal{H}_{\text{even,odd}}$, respectively. Because $P_+^\dagger H_{\text{eff}}^{13} P_+$ and $P_-^\dagger H_{\text{eff}}^{13} P_-$ are commutable, the time evolution operator $\exp(-iH_{\text{Heis}}t)$ can be exactly separated into two parts,

$$\exp(-iH_{\text{Heis}}t) = \exp(-iP_-^\dagger H_{\text{eff}}^{13} P_- t)\exp(-iP_+^\dagger H_{\text{eff}}^{13} P_+ t) \tag{17}$$

$$\begin{aligned} &= \{P_+^\dagger P_+ + P_-^\dagger \exp(-iH_{\text{eff}}^{13}t)P_-\} \\ &\times \{P_-^\dagger P_- + P_+^\dagger \exp(-iH_{\text{eff}}^{13}t)P_+\} \\ &= \sum_{i\in\{+,-\}} P_i^\dagger \exp(-iH_{\text{eff}}^{13}t)P_i. \end{aligned} \tag{18}$$

Therefore, the time propagation is described by $\exp(-iH_{\text{eff}}^{13}t)$. We Trotterize this time evolution operator into

$$\begin{aligned} &\exp(-iH_{\text{eff}}^{13}t) \\ &= \exp\left[-it\left\{(\sigma_x^1 + \sigma_z^2 - \sigma_x^1\sigma_z^2) + (\sigma_x^2 + \sigma_z^1 - \sigma_x^2\sigma_z^1)\right\}\right] \\ &= \lim_{n\to\infty}\left[e^{\frac{-it}{n}(\sigma_x^1+\sigma_z^2)} e^{\frac{it}{n}(\sigma_x^1\sigma_z^2+\sigma_x^2\sigma_z^1)} e^{\frac{-it}{n}(\sigma_x^2+\sigma_z^1)}\right]^n. \end{aligned} \tag{19}$$

Both of the first and third Trotter block can be given by local rotation-Z and rotation-X gates for each qubit. The second Trotter block is represented as 4×4 matrix given by

$$\begin{aligned} &\exp\left[\frac{it}{n}(\sigma_x^1\sigma_z^2 + \sigma_z^1\sigma_x^2)\right] \\ &= \begin{pmatrix} \cos^2\frac{t}{n} & i\sin\frac{t}{n}\cos\frac{t}{n} & i\sin\frac{t}{n}\cos\frac{t}{n} & \sin^2\frac{t}{n} \\ i\sin\frac{t}{n}\cos\frac{t}{n} & \cos^2\frac{t}{n} & -\sin^2\frac{t}{n} & -i\sin\frac{t}{n}\cos\frac{t}{n} \\ i\sin\frac{t}{n}\cos\frac{t}{n} & -\sin^2\frac{t}{n} & \cos^2\frac{t}{n} & -i\sin\frac{t}{n}\cos\frac{t}{n} \\ \sin^2\frac{t}{n} & -i\sin\frac{t}{n}\cos\frac{t}{n} & -i\sin\frac{t}{n}\cos\frac{t}{n} & \cos^2\frac{t}{n} \end{pmatrix} \end{aligned} \tag{20}$$

This matrix is given by a 2-qubit circuit as the figure below (FIG.1).

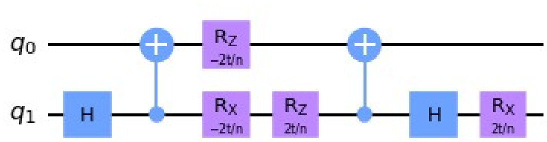

FIG. 1. The quantum gate of the second Trotter block given by Eq.(26)

Including with the first and third trotter blocks in Eq.(19) into the second, the unit of the Trotter step is represented as FIG.2.

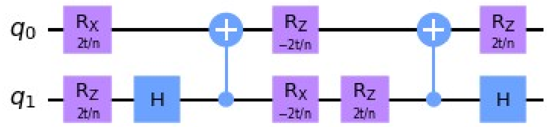

FIG. 2. The quantum gate of the Trotter unit given by Eq.(25)

The last task is the encoding and decoding of the initial and final state, respectively. In our method, we identify the 8 states in 3-spin states with the product between no time-evolving one particle state $|a\rangle_{\text{stat}}$ and time-evolving two-particle state $|bc\rangle_{\text{eff}}$under H_{eff}^{23} given by Eq.(16), as follows.

$$\begin{aligned}
U_{\text{enc}}\,|000\rangle &= |000\rangle = |0\rangle_{\text{stat}}\,|00\rangle_{\text{eff}} \\
U_{\text{enc}}\,|011\rangle &= |001\rangle = |0\rangle_{\text{stat}}\,|01\rangle_{\text{eff}} \\
U_{\text{enc}}\,|110\rangle &= |010\rangle = |0\rangle_{\text{stat}}\,|10\rangle_{\text{eff}} \\
U_{\text{enc}}\,|101\rangle &= |011\rangle = |0\rangle_{\text{stat}}\,|11\rangle_{\text{eff}} \\
U_{\text{enc}}\,|111\rangle &= |100\rangle = |1\rangle_{\text{stat}}\,|00\rangle_{\text{eff}} \\
U_{\text{enc}}\,|100\rangle &= |101\rangle = |1\rangle_{\text{stat}}\,|01\rangle_{\text{eff}} \\
U_{\text{enc}}\,|001\rangle &= |110\rangle = |1\rangle_{\text{stat}}\,|10\rangle_{\text{eff}} \\
U_{\text{enc}}\,|010\rangle &= |111\rangle = |1\rangle_{\text{stat}}\,|11\rangle_{\text{eff}}
\end{aligned}$$

where U_{enc} is the unitary operator to promote encoding, and the decoder of that is given by $U_{\text{enc}}^{\dagger}$. By the encoding and decoding, the circuit for the general solution of the time evolution under H_{Heis} can be represented as FIG.3

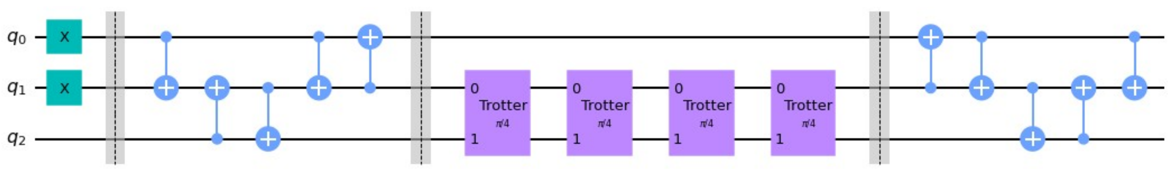

FIG. 3. The circuit gives the general solution of the time evolution by using Trotterization in this approach. Note that the number of Trotter steps on this figure is $n = 4$ case.

III. STRATEGIES: REDUCING CNOT GATE IN ENCODING AND DECODING

We made the general method of the time evolution under H_{Heis}, meaning that, ideally, the circuit in FIG.3 guarantees the exact time evolution in any initial state under $n \to \infty$. However, because the quantum gate of the encoding and decoding need to set 5 CNOT gates for each when we use ibm-jakarta, the noises are not perfectly removed for the high state tomography fidelity. In this section, we show the strategies to get much higher fidelity by reducing CNOT gates in encoding and decoding process by adapting the initial state conditions and time duration.

A. Considering initial condition

In this contest, the initial state is chosen as not entangled state, $|011\rangle$. This means that the encoding process never required CNOT gate in this method. Thus, it is only need to consider the decoding process. Analitically, the time propagation under H_{Heis} for the initial state of $|011\rangle$ is closed in the subspace $\mathcal{H}_{\text{even}}$. Thus we need to consider the decoding process as 4 states given by

$$\begin{aligned}
|000\rangle &= U_{\text{enc}}^{\dagger} |000\rangle \\
|011\rangle &= U_{\text{enc}}^{\dagger} |001\rangle \\
|110\rangle &= U_{\text{enc}}^{\dagger} |010\rangle \\
|101\rangle &= U_{\text{enc}}^{\dagger} |011\rangle .
\end{aligned}$$

This decoding process is given by 2 CNOT gates only, then the circuit in this strategy is given by FIG.5

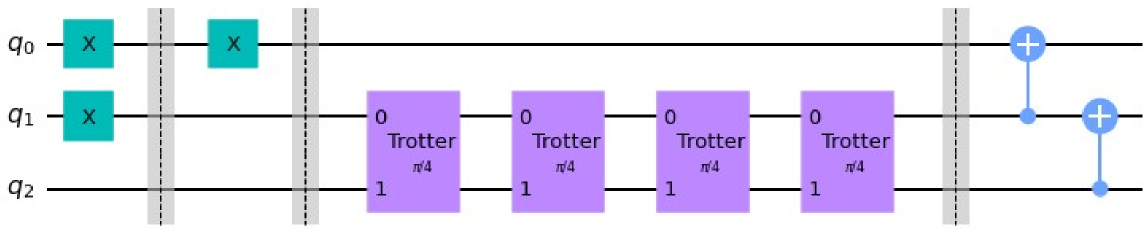

FIG. 4. The circuit giving the specific solution of the time evolution by using Trotterization of the H_{Heis} in this approach considering initial condition and subspace. Note that the number of Trotter steps on this figure is $n = 4$ case.

B. Considering time duration

If the Hamiltonian of the system is time independent, the time evolution is described by the eigen energies E_i and vectors $|i\rangle$ as $|\psi(t)\rangle = \sum_i c_i e^{iE_i t} |i\rangle$. If the initial wavefunction is composed by more three eigen states, the state vector $\psi(t)$ cannot return to the initial state $\psi(0)$. However, in the case of any gaps of the eigen energies $\Delta_{ij} = E_i - E_j$ is given by the integer multiplication of a certain real value ϵ, that is $\Delta_{ij} \in \epsilon\mathbb{Z}$ for any i and j, the state completely return to the initial state in $t \in \frac{2\pi}{\epsilon}\mathbb{Z}$. In the case of H_{Heis}, we can proof $\Delta_{ij} \in 2\mathbb{Z}$ without diagonalization of 8×8 matrix. By introducing total Pauli matrix vector $\boldsymbol{\sigma}^{\text{tot}}$ defined as

$$\boldsymbol{\sigma}^{\text{tot}} = \boldsymbol{\sigma}^1 + \boldsymbol{\sigma}^2 + \boldsymbol{\sigma}^3, \tag{21}$$

the Hamiltonian is reconstructed as

$$\begin{aligned}
H_{\text{Heis}} &= \frac{1}{2}(\boldsymbol{\sigma}^{\text{tot}})^2 - \boldsymbol{\sigma}^1 \cdot \boldsymbol{\sigma}^3 - \frac{1}{2}\sum_i (\sigma^i)^2 \\
&= \frac{1}{2}(\boldsymbol{\sigma}^{\text{tot}})^2 - \boldsymbol{\sigma}^1 \cdot \boldsymbol{\sigma}^3 - \frac{9}{2} \\
&= \frac{1}{2}(\boldsymbol{\sigma}^{\text{tot}})^2 - \frac{1}{2}(\boldsymbol{\sigma}^1 + \boldsymbol{\sigma}^3)^2 - \frac{3}{2}
\end{aligned} \tag{22}$$

And we can show the commutation relation as

$$[H_{\text{Heis}}, \boldsymbol{\sigma}^{\text{tot}}] = 0. \tag{23}$$

Therefore, the eigen state of this system also can be that of total spin square operator $(\boldsymbol{\sigma}^{\text{tot}})^2$. The eigen value of the operator can be written as,

$$\langle(\sigma^{\text{tot}})^2\rangle = S^{\text{tot}}(S^{\text{tot}} + 2) \tag{24}$$

where S^{tot} =3 or =1. The residual second term in Eq.(22) is also the summated spin square operator between $i = 1$ and $= 3$ state, and the eigen value is also known that it is given by Eq.(24) with $S^{\text{tot}} = 2$ or $= 0$. Then, substituting $(\boldsymbol{\sigma}^{\text{tot}})^2$ =15 or =3, and $(\boldsymbol{\sigma}^1 + \boldsymbol{\sigma}^3)^2$ =8 or =0, respectively, we can say that the eigen energy of the system is in even number. $\Delta_{ij} \in 2\mathbb{Z}$ guarantees that the state after the time duration $t = \pi$ in this system perfectly returns to initial state ($t = 0$) in any initial condition. It means that regarding the decoding process as inverse operation of encoding process is arrowed in $t \in \pi\mathbb{Z}$ case. In the case of the initial state equal to $|011\rangle$, the circuit can be represented by FIG.5. In such case, we can encode and decode without CNOT gate.

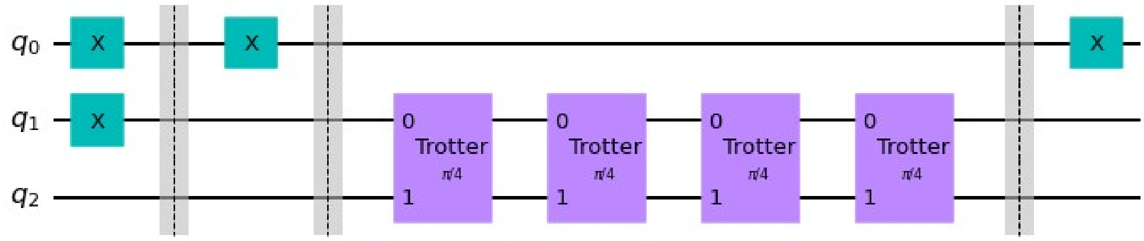

FIG. 5. The circuit giving the specific solution of the time evolution by using Trotterization of the H_{Heis} in this approach considering initial condition, subspace and time dulation $t \in \pi\mathbb{Z}$. Note that the number of Trotter steps on this figure is $n = 4$ case.

IV. ERROR MITIGATION

V. RUNNING ON SIMULATOR

The numerical simulation is conducted on both the `qasm_simulator` and the `fake_jakarta`.
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VI. RUNNING ON REAL DEVICE

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ACKNOWLEDGMENTS

Thank you!

[1] N. F. Berthusen, T. V. Trevisan, T. Iadecola, and P. P. Orth, Quantum dynamics simulations beyond the coherence time on nisq hardware by variational trotter compression (2021).

Appendix A: Soruce Code

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