Quantum Hackaton 2021: Hamiltonian Simulation Final Project Report

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Abstract

In this report, we describe our achievements and challenges on the assigned problems of hamiltonian simulation. First, we utilized Trotterization to simulate 2 qubit Heisenberg model and obtained the temporal evolution of the expectation value of $\langle Z_1 \rangle$ with random initial condition by using the IBMQ computing system. Next, Truncated Taylor Quantum Simulator(TQS) is used to perform the same task. By comparing the results from both methods, we discuss the efficiency of Quantum computing methods.

0 Preliminary studies

0.1 Difficulties in Quantum Simulations

The dynamics of a quantum system is governed by the time-dependent Schrödinger equation, $i\hbar\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$. When an arbitrary state $|\alpha\rangle$ changes under a time displacement $t_0 \to t$, this is related to the so-called time-evolution operator $\mathcal{U}(t,\, t_0)$: $|\alpha,\ t_0; t\rangle = \mathcal{U}(t, t_0)|\alpha,\ t_0\rangle$. The time-evolution operator can be expressed as follows:

$$\mathcal{U}(t, t_0) = \exp\left\{\frac{-iH(t-t_0)}{\hbar}\right\} \tag{1}$$

When we use one qubit, we should consider the two states $|0\rangle$ and $|1\rangle$, and 2^n hamiltonian for n qubits. This leads to a problem that we have to deal with a $2^n \times 2^n$ matrix. Moreover, when the number of qubits is doubled, the matrix's size becomes $2^{2n} \times 2^{2n}$ and an exponential growth can be observed. In classical computers, performing such quantum dynamics requires a deadly amount of computational cost and this makes the difficulty in quantum simulations.

0.2 Trotterization

In general, the hamiltonian of a quantum system consists of a sum of individual hamiltonians as $H = \sum_{i=1}^{l} H_i$. From the Baker-Campbell-Hausdorff(BCH) formula, the Trotterization formula reads as

$$e^{-iHt} = (e^{-iH_1 t/r} ... e^{-iH_l t/r})^r + O(2) \tag{2}$$

where r is finite[1]. In the limit of $r \to \infty$, the $O(2)$ term vanishes. However, this limit can not be reached due to the lack of quantum simulations, Trotterization makes it possible to effectively simulate non-commuting hamiltoninas by repeatedly switching the individual hamiltonians for a small period of time, t/r.

By selecting a large value of r, or an infinitesimal time slice t/r, higher order errors can be dropped and we can focus only on the lowest order. However, Trotter error still exists. Moreover, high order errors sometimes cannot be ignored since there terms can be dominant for specific time slices. At this point, calculating the deserving amount of time slices for Trotterization is still infeasible, due to the lack of computing resources. In order to cope with this shortage, various improved algorithms were suggested[1, 2, 5].

Also quantum localization bounds Trotter errors in digital quantum simulation[3]. In Quantum many-body systems, the interactions inside make localization. For qubits, this localization changes Trotterization conditions as time evolves. The best way to mitigate the error is to protect a single qubit by more than 1000 other qubits. But it requires a considerable resource which can not be implemented in the current state. Thus, it is a key point to make qubits which do not or less interact with other qubits while they must be easily distinguishable. We conjecture that the errors can be reduced by utilizing both the distinguishability and the interaction properties of qubits.

0.3 TQS

As mentioned above, Trotterization method has inevitable errors which originate from truncation. Besides, in this project, we will show a newly introduced algorithm for quantum dynamics simulation. Truncated Taylor quantum simulator (TQS) is rather like an optimization problem although it gives the time evolution for a given intial state. Introducing cumulative K-moment states as the basis of ansatz of time evolved initial states, this approach requires us to maximize the *Fidelity* under certain constraint.

In detail, let us discuss the cumulative K-moment states, $\mathbb{CS}_K$ first. Given that our Hamiltonian is

$$\hat{H} = \frac{1}{2}\,\hat{X}_0 \otimes \hat{X}_1 + \hat{Y}_0 \otimes \hat{Y}_1 + \hat{Z}_0 \otimes \hat{Z}_1\,, \tag{3}$$

we have three tensored Pauli matrices,

$$\mathbb{I}_0 \otimes \mathbb{I}_1\,, \quad \hat{X}_0 \otimes \hat{X}_1\,, \quad \hat{Y}_0 \otimes \hat{Y}_1\,, \quad \hat{Z}_0 \otimes \hat{Z}_1\,. \tag{4}$$

For some arbitrary initial state $|\psi\rangle$, we have

- 0 - moment state $\mathbb{S}_0$

$$|\psi\rangle$$

- 1st moment state $\mathbb{S}_1$

$$\{\hat{X}_0 \otimes \hat{X}_1\ |\psi\rangle\ , \hat{Y}_0 \otimes \hat{Y}_1\ |\psi\rangle\ , \hat{Z}_0 \otimes \hat{Z}_1\ |\psi\rangle\}$$

- and so on ...

Hence, cumulative 1st moment state is the union of $\mathbb{S}_0$ and $\mathbb{S}_1$. Likewise K-th cumulative moment state is the union of $\mathbb{S}_0$, $\mathbb{S}_1$, $\cdots$ $\mathbb{S}_K$. In our case, it is enough to think cumulative 1st moment state $\mathbb{CS}_1$,

$$\{|\psi\rangle\ , \hat{X}_0 \otimes \hat{X}_1\ |\psi\rangle\ , \hat{Y}_0 \otimes \hat{Y}_1\ |\psi\rangle\ , \hat{Z}_0 \otimes \hat{Z}_1\ |\psi\rangle\}\,, \tag{5}$$

or,

$$\{|\chi_0\rangle\ , |\chi_1\rangle\ , |\chi_2\rangle\ , |\chi_3\rangle\}\,. \tag{6}$$

Above states constitutes basis of ansatz of initial state and time evolved state of initial states,

$$|\psi(\alpha(t))\rangle = \alpha_0(t)\ |\chi_0\rangle + \alpha_1(t)\ |\chi_1\rangle + \alpha_2(t)\ |\chi_2\rangle + \alpha_3(t)\ |\chi_3\rangle\ . \tag{7}$$

where t is an initial time.

After some small time Δt, time evolved initial state becomes

$$\begin{aligned} U(\Delta t)\ |\psi(t)\rangle &\approx (I - i\,\Delta t\,\hat{H})\ |\psi(t)\rangle \\ &= |\psi(\alpha(t+\Delta t)\rangle \\ &= \frac{V(\Delta t)\ |\psi(\alpha(t))\rangle}{\sqrt{\langle\psi(t)|\ V^\dagger(\Delta t)\,V(\Delta t)\,|\psi(\alpha(t))\rangle}}\,. \end{aligned} \tag{8}$$

Note that the matrix $V(t)$ grows exponentially as the size of system grows. That's why we implement quantum computer when we execute quantum dynamics simulation. Since the time evolution operators requires too much resources in classical computer, it cannot afford to run a quantum dynamics of many body system. Here, we introduce a variational parameter α and we update this parameter after each time slice. Then time evolved states are depend on the updated variational parameters. Our job is now to determine this variational parameters with proper constraints.

Now let us see how to determine variational parameters α. Although $V(t)$ is already an approximation of time evolution operator, still it gives rather exact time evolved state $|\psi(\alpha(t+\Delta t)\rangle$, due to the small size of time slice Δt. However in general, because of its tremendous size, we cannot directly utilize $V(\Delta t)$. Therefore we introduce α-updated state $\psi(\alpha')$ and gauge this parameters by measuring distance from 'almost exact' time evolution $|\psi(\alpha(t+\Delta t))\rangle$ or fidelity between $\psi(\alpha')$ and $|\psi(\alpha(t+\Delta t))\rangle$. Namely,

$$\begin{aligned} F(\alpha') &= |\,\langle\psi(\alpha')|\psi(\alpha(t+\Delta t)\rangle\,|^2 \\ &= \frac{|\,\langle\psi(\alpha')|\,V(\Delta t)\,|\psi(\alpha)\rangle\,|^2}{\langle\psi(\alpha)|\,V^\dagger(\Delta t)\,V(\Delta t)\,|\psi(\alpha)\rangle}\,. \end{aligned} \tag{9}$$

Above fidelity can be written as

$$F(\alpha') = \langle\psi(\alpha')|\,W_\phi\,|\psi(\alpha'\rangle\ , \tag{10}$$

where

$$W_\phi = \frac{|\phi\rangle\,\langle\phi|}{\langle\phi|\phi\rangle}\,, \quad |\phi\rangle = V(\Delta t)\ |\psi(\alpha)\rangle\ . \tag{11}$$

Since we want $\psi(\alpha')$ is as close to $|\psi(\alpha(t+\Delta t)\rangle$ as possible, we have to choose α' such that maximizes $F(\alpha')$. Further, $|\psi(\alpha')\rangle$ should be normalized. Hence quantum dynamics simulation is reduced to optimization problem,

$$\begin{aligned} &\max_{\alpha'}\ \langle\psi(\alpha')|\ W_\phi\,|\psi(\alpha')\rangle \\ &\text{such that}\ \ \langle\psi(\alpha'|\psi(\alpha')\rangle = 1\,. \end{aligned} \tag{12}$$

Given that our ansatz,

$$|\psi(\alpha')\rangle = \alpha'_0\ |\chi_0\rangle + \alpha'_1\ |\chi_1\rangle + \alpha'_2\ |\chi_2\rangle + \alpha'_3\ |\chi_3\rangle\ , \tag{13}$$

above constraint is reduced to

$$\alpha'^*_n\,\mathcal{E}_{nm}\,\alpha'_m = 1 \tag{14}$$

where

$$\mathcal{E}_{nm} = \langle\chi_n|\chi_m\rangle \tag{15}$$

From our randomized state $|\xi\rangle$,

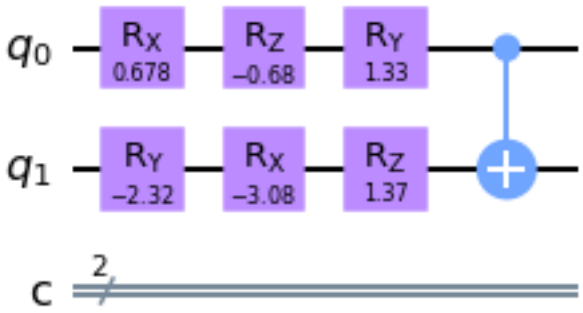

Figure 1: Randomized initial state

above inner product can be calculated via a complex conjugation of left state on the quantum circuit.

For some unitary U_m, and U_n,

$$|\chi_m\rangle = U_m\ |00\rangle\ , \quad |\chi_n\rangle = U_n\ |00\rangle\ . \tag{16}$$

This indicates that $\mathcal{E}_{nm} = \langle\chi_n|\chi_m\rangle$ is a $|00\rangle$ component of $U_n^\dagger U_m\,|00\rangle$. For example, consider $\langle\chi_0|\chi_1\rangle$. Say, $|\chi_0\rangle = U_0\ |00\rangle$. Then $|\chi_1\rangle$ is,

$$|\chi_1\rangle = \hat{X}_0 \otimes \hat{X}_1\, U_0\ |00\rangle\ , \tag{17}$$

and the inner product between two states is

$$\langle\chi_1|\chi_0\rangle = \langle 00|\ U_0^\dagger\,(\hat{X}_0 \otimes \hat{X}_1)\,U_0\ |00\rangle\ . \tag{18}$$

Thanks to the orthogonality of two-qubit states, (18) is square root of amplitude of $|00\rangle$ component of Fig. 2.

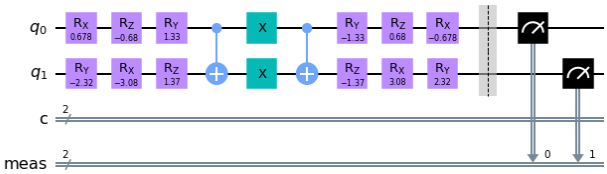

Figure 2: Relevent circuit for $\langle\chi_0|\chi_1\rangle$

Finally we have obtained,

$$\mathcal{E} = \begin{pmatrix} 1. & 0.678233 & 0.51961524 & 0.70781353 \\ 0.678233 & 1. & 0.70285134 & 0.53572381 \\ 0.51961524 & 0.70285134 & 1. & 0.70427267 \\ 0.70781353 & 0.53572381 & 0.70427267 & 1. \end{pmatrix} \tag{19}$$

Likewise, the fidelity matrix W_ϕ in our optimization problem can be expressed as

$$W_\phi = \frac{G\,\alpha\,\alpha^\dagger\,G^\dagger}{\alpha^\dagger\,\mathcal{E}\,\alpha} \tag{20}$$

where,

$$\langle\phi|\phi\rangle \approx \alpha^\dagger \mathcal{E}\, \alpha\,, \quad G_{mn} = (\mathcal{E}_{mn} - i\,\Delta t \mathcal{D}_{mn})\,, \quad \mathcal{D}_{mn} = \langle\chi_m|\,\hat{H}\,|\chi_n\rangle\ . \tag{21}$$

In short, our optimization problem can be seen as

$$\begin{aligned} &\max_{\alpha'} \alpha', W_\alpha \alpha' \\ &\text{such that } \alpha'^* \,\mathcal{E}\, \alpha' = 1\,. \end{aligned} \tag{22}$$

The expectation value of Hamiltonian can easily be computed by convert each Pauli matrices into qubit representation; for example,

$$\langle \hat{X}\,\hat{X}\rangle = \langle\chi_n|00\rangle\,\langle 11|\chi_m\rangle + \langle\chi_n|01\rangle\,\langle 10|\chi_m\rangle + \langle\chi_n|10\rangle\,\langle 01|\chi_m\rangle + \langle\chi_n|11\rangle\,\langle 00|\chi_m\rangle\ . \tag{23}$$

By counting shots in quantum measurement, we can determine each piece. We have obtained

$$\mathcal{D} = \begin{pmatrix} 0.47750756 & 0.44257414 & 0.43913715 & 0.48028896 \\ 0.44257414 & 0.49367551 & 0.49231906 & 0.44384673 \\ 0.43913715 & 0.49231906 & 0.4927895 & 0.44167669 \\ 0.48028896 & 0.44384673 & 0.44167669 & 0.4837155 \end{pmatrix}\ . \tag{24}$$

Note that quantum computer's job is only restricted to derive a matrix $\mathcal{E}$ and $\mathcal{D}$. Optimization problem can be solved by classical computer.

1 Problem 1: Trotterization

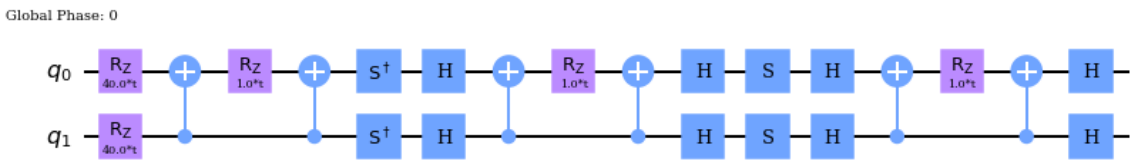

Figure 3: Quantum circuit for the hamiltonian $H = \frac{1}{2}X_0X_1 + \frac{1}{2}Y_0Y_1 + \frac{1}{2}Z_0Z_1 + \frac{1}{2}(Z_0 + Z_1)$.

In Fig. 3, we plot the quantum circuit of the given hamiltonian, $H = \frac{1}{2}X_0X_1 + \frac{1}{2}Y_0Y_1 + \frac{1}{2}Z_0Z_1 + \frac{1}{2}(Z_0 + Z_1)$. With this quantum circuit, the temporal evolution of the expectation values, $\langle Z_{0,1}\rangle$, $\langle X_{0,1}\rangle$, and $\langle Y_{0,1}\rangle$ are plotted by using the classical computer in Fig. 4 and Fig. 5. Randomized states were used as initial states. To be specific, we used $0.175|00\rangle + 0.040|01\rangle + 0.736|10\rangle + 0.653|11\rangle$ as the initial state to plot the results in Fig. 4 and $0.508|00\rangle + 0.405|01\rangle + 0.314|10\rangle + 0.692|11\rangle$ to plot the results in Fig. 5. Oscillatory behaviors can be easily observed. The red and blue line depicts the measurement from q_0 and q_1 respectively. Due to the existence of the field term in the hamiltonian, $\frac{1}{2}(Z_1 + Z_2)$, non-linear behaviors could be found in the X-axis and Y-axis.

In order to compare the results from classical computing(CC) and quantum computing(QC), we both plot the expectation values on Z-axis in Fig. 6 (a). The differences between them are also plotted in Fig. 6 (b).

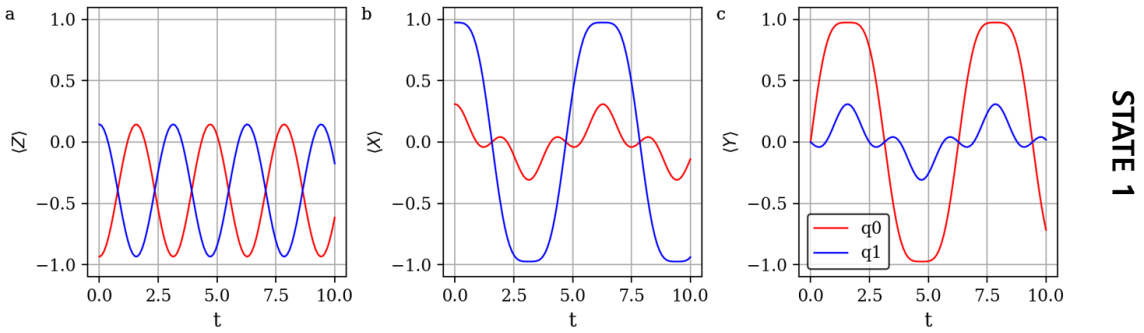

Figure 4: Plot of the expectation values versus time for an initial state $0.175|00\rangle + 0.040|01\rangle + 0.736|10\rangle + 0.653|11\rangle$.

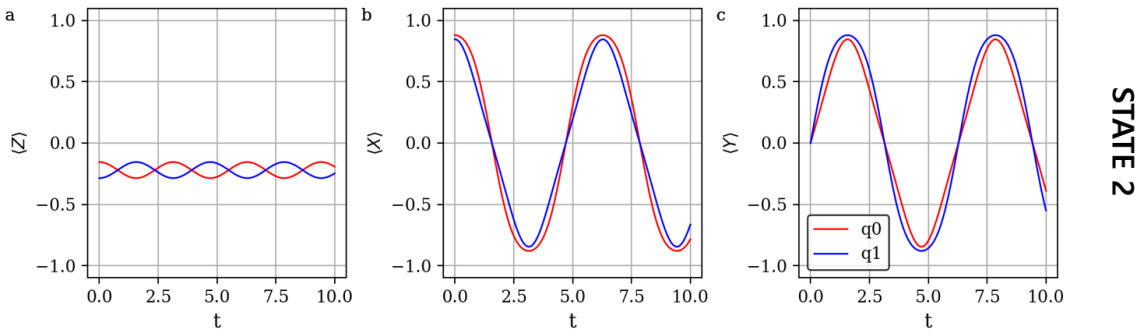

Figure 5: Plot of the expectation values versus time for an initial state $0.508|00\rangle + 0.405|01\rangle + 0.314|10\rangle + 0.692|11\rangle$.

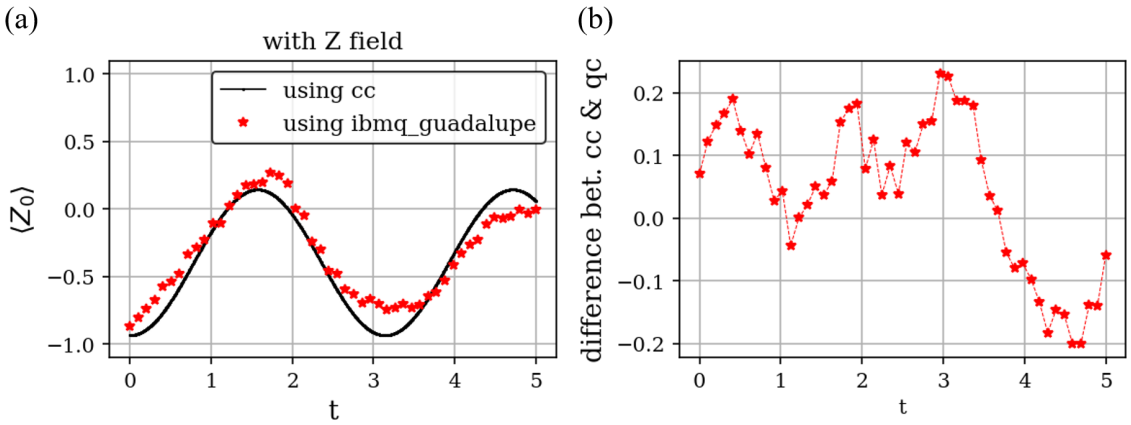

Figure 6: Plot of (a) the results from Classical Computing(CC) and Quantum Computing(QC) and (b) the difference between CC and QC.

2 Problem 2: TTQS

As we have seen above, quantum computer only used in generating basis states for ansatz and calculating $\mathcal{E}$ and $\mathcal{D}$ matrices. Along with (19), (24) and optimization problem (22), we have obtained Fig. 7. One can refer FIG. 1. in [4] for smoother optimization.

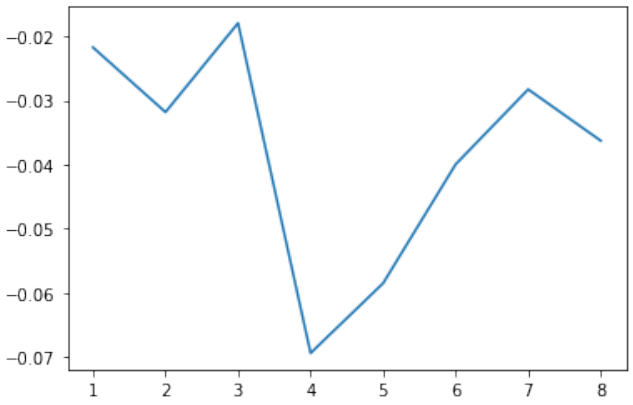

Figure 7: Expectation value of Z_1 , optimized with Adam optimizer

3 Conclusion

In this article, we report the results of solving hamiltonian simulation via IBMQ computing resource. We successively implemented the trotterization methods for quantum simulations and the expectations values were well-measured. On the contrary, utilizing TTQS in our simulation was quite challenging. Even though we devoted most of our efforts to understand the ground knowledge of the algorithm, implementing this in Qiskit was quite hard. However, we believe that this cherish experience would lead us to a new world of quantum information and quantum computing.

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