# Simulation of three-spin evolution under XX Hamiltonian on quantum processor of IBM-Quantum Experience 

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#### Abstract

We simulate the evolution of three-node spin chain on the quantum processor of IBM Quantum Experience using the diagonalization of $X X$-Hamiltonian and representing the evolution operator in terms of CNOT operations and one-qubit rotations. We study the single excitation transfer from the first to the third node and show the significant difference between calculated and theoretical values of state transfer probability. Then we propose a method reducing this difference by applying the two-parameter transformation including the shift and scale of the calculated probabilities. We demonstrate the universality of this transformation inside of the class of three-node evolutionary systems governed by the $X X$-Hamiltonian.


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## I. INTRODUCTION

Development of quantum information is stimulated by amazing advantages of quantum devices in comparison with their classical counterparts. In particular, many well-known quantum algorithms have appeared [1]. Although they are written for an ideal quantum processor, these algorithms present a constitutional part of general progress in quantum computation. Among others we mention Shor algorithm [2] for factorizing integers and Deutsch-Jozsa algorithm [3] demonstrating quantum speedup. There are also algorithms allowing to perform set of algebraic operations [4]. Most famous algorithm of this kind was proposed by A.Harrow, A.Hassidim and S.Lloyd (HHL algorithm) [5-7] for solving systems of linear equations. This algorithm includes the algorithm of Hamiltonian simulation [8, 9] and phase estimation [10, 11] based on the quantum Fourier transform [1, 12]. An essential part of those algorithm is a preparing particular input states which is a particular problem requiring a special approach [13, 14].

However, the implementation of those algorithms on the real quantum processor faces large problems because of calculation errors. The fact is that contemporary quantum processors are far from the ideal ones. Operation of these processors unavoidably generates quantum noise which creates a serious obstacle for nowaday application of quantum algorithms in practice. It is known that quantum noise is mostly generated by two-qubit operations, such as CNOT which is widely used in all algorithms to entangle different qubits. Therefore the problem to compensate the effect of quantum noise is of a principal meaning. We study this problem simulating the quantum state evolution governed by the $X X$-Hamiltonian.

To simulate the spin-chain evolution under certain Hamiltonian on a quantum processor one can formally appeal to the Trotter method [1, 15, 16]. This method was intensively studied and considerable results were obtained [16, 17]. However, Trotterization involves numerous two-qubit operations which result in large calculation errors.

Therefore the alternative methods for simulating spin-evolution are of interest [18]. As a simple example of such alternative, the evolution operator for a two-qubit system governed by the $X X$-Hamiltonian was represented in terms of CNOT operations and one-qubit rotations in Refs. 15,19$]$.

We develop a method of simulating the spin-evolution based on diagonalization of the

Hamiltonian, so that the time-dependent part of evolution operator becomes diagonal. The obvious disadvantage of this method is that it is not completely quantum one but involves the classical operation of Hamiltonian diagonalization at the first stage of calculation. However, the simplicity of realization of the diagonal evolution in comparison with the nondiagonal one is very promising.

Here we consider the evolution of short two- and three-qubit spin systems based on the diagonalization of the $X X$-Hamiltonian

$$
\begin{equation*}
H=U \Lambda U^{+}, \tag{1}
\end{equation*}
$$

where $\Lambda$ is the matrix of eigenvalues and $U$ is the matrix of eigenvectors of the Hamiltonian. Therefore the evolution operator $V$ can be written as

$$
\begin{equation*}
V(t)=e^{-i H t}=U e^{-i \Lambda t} U^{+} \tag{2}
\end{equation*}
$$

Thus, the evolution is hidden into the diagonal operator $e^{-i \Lambda t}$.
Below we propose the scheme including the CNOT operations and one-qubit rotations which realize both the unitary transformation $U$ and the diagonal evolution $e^{-i \Lambda t}$ in (22) and which can be executed on a quantum processor. Then we simulate the propagation of the one-qubit excitation from the first to the third node and compare the probability of the excited state transfer calculated on a quantum processor with the theoretical value of this probability. As expected, the deviation is significant. But using the special transformation of the calculated probability we can significantly improve the result. Such transformation is a principal subject of our paper.

The paper is organized as follows. In Sec.II, we consider the two-spin chain governed by the $X X$-Hamiltonian and give diagonal representation of the evolution operator in terms of CNOT operations and one-qubit rotations. Then, in Sec.III, we give detailed description of the three-spin alternating chain governed by the $X X$-Hamiltonian under approximation of nearest-neighbor interactions. For different values of alternation parameter, we consider the probability of the excited state transfer from the first to the third spin and compare the theoretically predicted value of this probability with the value found on the quantum processor. We also consider a two-parametric transformation reducing the difference between the two above values. We demonstrate certain universality of that transformation by applying it to the three-node alternating chain governed by the $X X$-Hamiltonian with all-node interactions. Conclusions are given in Sec.IV.

## II. TWO-SPIN CHAIN

We start with the evolution of a dimer under the $X X$ Hamiltonian

$$
\begin{equation*}
H_{2}=D\left(I_{x 1} I_{x 2}+I_{y 1} I_{y 2}\right) \tag{3}
\end{equation*}
$$

(where $D$ is a coupling constant, $I_{x i}$ and $I_{y i}$ are the $x$ - and $y$-projections of the angular momentum of the $i$ th spin) and simulate it on the quantum processor. For this purpose we diagonalise Hamiltonian (3):

$$
\begin{equation*}
H_{2}=U_{12} \Lambda_{12} U_{12}^{+} \tag{4}
\end{equation*}
$$

where $U_{12}$ and $\Lambda_{12}$ are, respectively, the matrices of eigenvectors and eigenvalues,

$$
U_{12}=\left(\begin{array}{cccc}
1 & 0 & 0 & 0  \tag{5}\\
0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\
0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 1
\end{array}\right), \quad \Lambda_{12}=D \tilde{\Lambda}_{12}, \quad \tilde{\Lambda}_{12}=\operatorname{diag}(0,2,-2,0)
$$

Evolution operator (22) in the diagonalised form reads

$$
\begin{equation*}
V(t)=U_{12} e^{-i \tilde{\Lambda}_{12} \tau} U_{12}^{+}, \quad \tau=D t \tag{6}
\end{equation*}
$$

where $\tau$ is the dimensionless time.
It is remarkable that the operator $U_{12}$ can be written in terms of CNOT operations and one-qubit $y$-rotations as follows:

$$
\begin{equation*}
U_{12}=C_{21} R_{y 2}\left(\frac{\pi}{4}\right) C_{12} R_{y 2}\left(-\frac{\pi}{4}\right) C_{21} \tag{7}
\end{equation*}
$$

where $R_{y j}$ is the $y$-rotation of the $j$ th spin over the angle $\phi$ :

$$
\begin{equation*}
R_{y j}(\phi)=e^{-i I_{y j} \phi} \tag{8}
\end{equation*}
$$

while $C_{i j}$ and $C_{j i}$ written in the basis

$$
\begin{equation*}
(00),(0 j),(i 0),(i j) \tag{9}
\end{equation*}
$$

read respectively

$$
C_{i j}=\left(\begin{array}{llll}
1 & 0 & 0 & 0  \tag{10}\\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{array}\right), \quad C_{j i}=\left(\begin{array}{llll}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0
\end{array}\right)
$$



FIG. 1: Simplest one-parameter two-qubit operator $U_{i j}$ conserving the excitation number in a system.

The operator $U_{12}$ is a particular case of the operator

$$
\begin{equation*}
U_{i j}(\chi)=C_{j i} R_{y j}(\chi) C_{i j} R_{y j}(-\chi) C_{j i}, \tag{11}
\end{equation*}
$$

introduced in Ref. 20] as a simplest two-qubit operator conserving the number of excited spins in a system (i.e., commuting with the $z$-projection of the total spin momentum $I_{z}$ ) and representable in terms of CNOT operations and one-qubit $y$-rotations, Fig [1. Namely this operator will be used as a structural block for constructing the eigenvector matrix for the 3 -qubit systems below.

In turn, the diagonal operator $e^{-i \tilde{\Lambda}_{12} \tau}$ can be written as a composition of two one-qubit $z$-rotations,

$$
\begin{align*}
& e^{-i \tilde{\Lambda}_{12} \tau}=R_{z 1}(2 \tau) R_{z 2}(-2 \tau)  \tag{12}\\
& R_{z i}(\phi)=e^{-i I_{z i} \phi} \tag{13}
\end{align*}
$$

which can be simply simulated on a quantum processor.
The two-qubit systems have been studied, for instance, in [15, 19], therefore we do not consider them here. Notice also that our two-qubit evolution operator (6) includes 6 CNOT operations which is rather big number of two-qubit operations. But the constructed unitary block $U_{i j}$ (11) preserves the excitation number and can be used in systems of higher dimension, which is shown below in Sec III for a three-spin system.

## III. THREE-SPIN CHAIN

We consider the evolution of three-spin system under the $X X$-Hamiltonian using both approximation of nearest neighbor interactions and all spin interactions. We show difference and similarity in simulation schemes for each of these cases on a quantum computer.

## A. Nearest neighbor approximation

First we consider the three-node chain governed by the $X X$-Hamiltonian using the nearest neighbor approximation with two different coupling constants (an alternating chain),

$$
\begin{equation*}
H_{3}=D\left(I_{x 1} I_{x 2}+I_{y 1} I_{y 2}+d\left(I_{x 2} I_{x 3}+I_{y 2} I_{y 3}\right)\right) . \tag{14}
\end{equation*}
$$

where $d$ is the alternation parameter ( $d=1$ for the homogeneous chain). We can diagonalise this Hamiltonian,

$$
\begin{equation*}
H_{3}=U_{123} \Lambda_{123} U_{123}^{+} \tag{15}
\end{equation*}
$$

Then the evolution operator (2) reads

$$
\begin{equation*}
V(t)=U_{123} e^{-i \tilde{\Lambda}_{123}} U_{123}^{+}, \quad \tau=D t \tag{16}
\end{equation*}
$$

Here $U_{123}$ and $\Lambda_{123}$ are the matrices of eigenvectors and eigenvalues respectively. We do not give the explicit form for $U_{123}$, but represent the matrix $U_{123}$ in terms of CNOT operations and one-qubit $y$-rotations as follows:

$$
\begin{equation*}
U_{123}=S W A P_{23} V_{123}^{(1)} U_{12} U_{23} V_{123}^{(2)} S W A P_{23} \tag{17}
\end{equation*}
$$

Here $S W A P_{23}=C_{23} C_{32} C_{23}$, the operators $V_{123}^{(i)}, i=1,2$, are the diagonal, and $V_{123}^{(1)}$ is representable in terms of CNOT operations and z-rotations,

$$
\begin{equation*}
V_{123}^{(1)}=R_{z 1}\left(\frac{\pi}{2}\right) C_{32} R_{z 2}\left(\frac{\pi}{2}\right) C_{32} . \tag{18}
\end{equation*}
$$

while the operator $V_{123}^{(2)}$,

$$
\begin{equation*}
V_{123}^{(2)}=\operatorname{diag}(-i, 1,1, i, 1, i, i, 1) \tag{19}
\end{equation*}
$$

commutes with $S W A P_{23}$,

$$
\begin{equation*}
\left[V_{123}^{(2)}, S W A P_{23}\right]=0 \tag{20}
\end{equation*}
$$

and therefore disappears from Hamiltonian (15). Each of the operators $U_{12}$ and $U_{23}$ in (17) is of form (11) with a particular choice of the parameter $\chi$. In the operator $U_{23}$, we take $\chi=\frac{\pi}{4}$, so that

$$
\begin{equation*}
U_{23}=C_{32} R_{y 3}\left(\frac{\pi}{4}\right) C_{23} R_{y 3}\left(-\frac{\pi}{4}\right) C_{32} \tag{21}
\end{equation*}
$$



FIG. 2: Simulation of diagonal part $e^{-i \tilde{\Lambda} \tau}$ of the three-qubit evolution operator in terms of CNOT operations and one-qubit $z$-rotations.

Written in the matrix form, this operator coincides with the operator $U_{12}$ (5) in Sec. III. The parameter $\chi$ in the operator $U_{12}$ in (17) is defined by the alternation parameter $d$,

$$
\begin{align*}
U_{12} & =C_{21} R_{y 2}(\chi) C_{12} R_{y 2}(-\chi) C_{21},  \tag{22}\\
U_{12} & =\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & \sin \chi & \cos \chi & 0 \\
0 & \cos \chi & -\sin \chi & 0 \\
0 & 0 & 0 & 1
\end{array}\right), d=\tan \chi .
\end{align*}
$$

Since $d>0$, we consider $0<\chi<\frac{\pi}{2}$. In a particular case of homogeneous chain $d=1$ and $\chi=\frac{\pi}{4}$. Therefore the operators $U_{23}$ and $U_{12}$ become equivalent two-qubit operators, each coincides with the operator $U_{12}$ in Sec. III, but is applied to different pairs of qubits.

Finally, the eigenvalue matrix $\Lambda_{123}$ reads

$$
\begin{equation*}
\Lambda_{123}=D \tilde{\Lambda}_{123}, \quad \tilde{\Lambda}_{123}=\operatorname{diag}(0,-\lambda, \lambda, 0,0, \lambda,-\lambda, 0), \quad \lambda=\frac{\sqrt{1+d^{2}}}{2}=\frac{1}{2 \cos \chi} \tag{23}
\end{equation*}
$$

Then the diagonal part of the evolution operator $e^{-i \tilde{\Lambda}_{123} \tau}$ can be represented in terms of CNOT operations and $z$-rotations as follows, see Fig. 2 ,

$$
\begin{equation*}
e^{-i \tilde{\Lambda}_{123} \tau}=C_{12} R_{z 2}(-\lambda \tau) C_{12} C_{13} R_{z 3}(\lambda \tau) C_{13} \tag{24}
\end{equation*}
$$

1. Probability of excited state transfer: theoretical results versus simulation on quantum processor

We study the probability of the excited state transfer from the first to the third spin, i.e., the initial state of the three-qubit chain reads $|100\rangle$. This state governed by the Hamiltonian


FIG. 3: Simulation of the excited state evolution along the three-spin chain on the quantum processor. The probability $\bar{p}(25)$ of the excitation transfer is an output. Here

$$
\chi=\tan ^{-1} d
$$

(14), (15) evolves as follows:

$$
\begin{align*}
|\psi(\tau)\rangle= & U_{123} e^{-i \tilde{\Lambda}_{123} \tau} U_{123}^{+}|100\rangle=\cos \chi \sin \chi(\cos (\lambda \tau)-1)|001\rangle-  \tag{25}\\
& i \cos \chi \sin (\lambda \tau)|010\rangle+\left(\cos ^{2} \chi(\cos (\lambda \tau)-1)+1\right)|100\rangle
\end{align*}
$$

This evolution can be simulated on a quantum processor with the scheme in Fig.3. The probability of the excited state transfer to the third spin is following:

$$
\begin{equation*}
p=|\langle 001 \mid \psi(\tau)\rangle|^{2}=\frac{1}{4} \sin ^{2}(2 \chi)(\cos (\lambda \tau)-1)^{2} \tag{26}
\end{equation*}
$$

Namely this probability is measured at the third qubit $q_{2}$ as an output, as shown in Fig. 3 , We implement our quantum protocol on the 5 -qubit quantum processor ibmq_lima of IBM Quantum Experience using $2^{13}$ shots and averaging over 5 runs.

Having probability obtained both with analytical formulas (25) and (26), and as the result of calculation on the quantum processor, we discuss a method for reducing the discrepancy between those two values. We emphasize that the scheme in Fig.3 serves to describe the evolution of any initial state at the input site of the scheme. Of course, it can be simplified for transfer just single excited state. We do not consider such simplification.

Thus, the results of calculation on quantum processor of IBM QE exhibit significant difference in comparison with the theoretical results, as shown in Fig_4, where theoretically calculated $p$ is represented by the solid line, while the probabilities calculated on the quantum processor are represented by circles for a set of values of the alternation parameter $d: d=$ $1,0.8,0.6,0.4,0.2$. On this figure, the largest difference is revealed for small values of $p(\tilde{p}>p)$ as well as for large values of $p(\tilde{p}<p)$, whereas $\tilde{p} \approx p$ for intermediate values. This observation can be clarified as follows. If the theoretical probability to detect the


FIG. 4: Probability of the excited state transfer from the 1st to the 3rd spin of the alternating chain governed by the $X X$-Hamiltonian, approximation of nearest-node interactions. Different plates correspond to different values of the alternation parameter $d$, $d=1$ corresponds to the homogeneous chain. We present the theoretically calculated probability $p$ (solid lines), probability calculated on the quantum processor $\tilde{p}$ (circles), corrected probabilities $\bar{p}$ (squares) and $p^{(f)}$ (stars), cross means probability measured at the quantum processor at $\tau=0$, see text.
excitation at a given qubit is negligible $(p \rightarrow 0)$, then measured probability is increased due to the noise of quantum gates. On the contrary, if the theoretical probability is significant ( $p \sim 1$ ), then the same noise decreases the measured value of this probability. Thus, there are two counteracting noise effects: increasing small probability of excitation registration and decreasing large value of this probability. As the result of this counteracting, the intermediate values of probability remains almost correct. If that is the basic reason of the above observed difference between $p$ and $\tilde{p}$, then we can try to eliminate (or at least reduce) it by the regular method. One of such methods might be analogous to the geometrical homotetic transformation. For that, one needs to fix the homotetic center (i.e., such value $p_{0}$ that $\left.p_{0}=\tilde{p}_{0}\right)$ and calculate the homotetic coefficient. This approach requires additional detailed exploration of the relations between the theoretically predicted and measured probabilities so that we postpone it. Instead, we suggest a simpler method which nevertheless gives a quite acceptable result.

It is interesting to note that the difference between the calculated value $\tilde{p}(\tau)$ and theoretical one $p(\tau)$ can be reduced by the combination of two operations: the shift over the value $s$ and scale by the factor $k$ defined as follows:

$$
\begin{align*}
& s=\tilde{p}(\varepsilon)-p(\varepsilon), \quad \varepsilon=0.001 \ll 1,  \tag{27}\\
& k=p_{\max } / \tilde{p}_{\max } .
\end{align*}
$$

Here $\tau_{\max }$ is a time instant of maximum of $p(\tau): p_{\max }=p\left(\tau_{\max }\right)$, and $\tilde{p}_{\max }=\tilde{p}\left(\tau_{\max }\right)$. Thus, we obtain the corrected function $\bar{p}$,

$$
\begin{equation*}
\bar{p}=k(\tilde{p}-s), \tag{28}
\end{equation*}
$$

shown in Fig 4 by squares. We see that most squares belong to the solid curve representing the theoretical probability of the excited state transfer.

We shall clarify the reason of setting $\tau=\varepsilon$ instead of $\tau=0$ in the definition of the shift $s$, Eq. (27). The matter is that the quantum processor can automatically simplify the simulation scheme canceling the combinations of the form $A A^{+}$, where $A$ is a unitary transformation. Therefore, if $\tau=0$, then the evolution operator $V$ becomes the identity $E$ : $V(0)=U_{123} U_{123}^{+}=E$. Therefore the scheme in (3) is drastically simplified up to the scheme in Fig.5, Thus, setting $\tau=0$ we examine a trivial scheme and the measured probability is different, see crosses in Fig.4. The minor deviation $\varepsilon$ from $\tau=0$ turns on all operators

## Initial state ${ }_{1}^{1}$ Measure



FIG. 5: Scheme in Fig 3 trivialized at $\tau=0$.

| $d$ | 1 | 0.8 | 0.6 | 0.4 | 0.2 | mean |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $s$ | 0.1211 | 0.1400 | 0.1352 | 0.1091 | 0.0827 | 0.1176 |
| $k$ | 1.5145 | 1.5475 | 1.5924 | 1.3873 | 1.3761 | 1.4836 |

TABLE I: Shifts $s$ and scale factors $k$ for set of values of the alternation parameter $d$. The last column presents the mean values $\bar{s}$ ans $\bar{k}$.
in Fig 3. The shifts $s$ and scale factors $k$ for different values of the alternation parameter $d$ are collected in Table (1) Remember, that the analogous transformation of the computed probabilities with the purpose to fit the theoretical results was proposed in [17] to correct errors of implementation of the Trotter method of Hamiltonian simulation on a quantum processor.

Table $\square$ shows that the spread of shifts $s$ and scales $k$ found for different experiments is not significant, especially for $d>0.2$. This motivates us to introduced the mean values $\bar{s}$ and $\bar{k}$ for these shifts and scales (arithmetical averages),

$$
\begin{equation*}
\bar{s}=0.1176, \quad \bar{k}=1.4836, \tag{29}
\end{equation*}
$$

and use this values to correct the probabilities calculated on quantum processor in all experiments with the scheme in Fig.3. Thus, we propose to use the corrected probability $p^{(f)}$,

$$
\begin{equation*}
p^{(f)}=\bar{k}(\tilde{p}-\bar{s}), \tag{30}
\end{equation*}
$$

instead of $\bar{p}$ given in (28). In fact, the probability $p^{(f)}$ shown in Fig.4 by stars only slightly differs from the probability $\bar{p}$ shown by squares, except the case $d=0.2$. The last fact is in accordance with the observation made in [20], where the corrected quantity well agrees with the theoretical value for the case when the measured probability exceeds $\sim 0.2$.

Below we use the calculated $\bar{s}$ and $\bar{k}$ to find corrected probabilities of the excited state transfer along the three-node chains with all-node interactions governed by the XXHamiltonian.

## B. $X X$-Hamiltonian with all-node interactions

The 3-qubit $X X$-Hamiltonian involving interactions among all-nodes reads:

$$
\begin{align*}
& H_{3}=D_{12}\left(I_{x 1} I_{x 2}+I_{y 1} I_{y 2}\right)+D_{23}\left(I_{x 2} I_{x 3}+I_{y 2} I_{y 3}\right)+D_{13}\left(I_{x 1} I_{x 3}+I_{y 1} I_{y 3}\right),  \tag{31}\\
& D_{i j}=\frac{\gamma^{2} \hbar^{3}}{r_{i j}},
\end{align*}
$$

where $\gamma$ is the gyromagnetic ratio, $\hbar$ is the Planck constant, $r_{i j}$ is the distance between the $i$ th and $j$ th nodes. The diagonalization of this Hamiltonian is given by formula (15) with different $U_{123}$ and $\lambda_{123}$. Unlike the case of nearest neighbor approximation, the representation of the evolution of the homogeneous spin chain in terms of CNOT operations and one-qubit rotations can not be considered as a limit $d \rightarrow 1$ of the similar representation for the alternating chain. It seamed out that $d \neq 1$ requires additional operator $U$ of form (11) and consequently includes more CNOT operators. Therefore, we consider the homogeneous and alternating chains separately.

## 1. Homogeneous chain

For the homogeneous chain we set $D_{12}=D_{23}=D$ and use the dimensionless time $\tau=D t$. We have

$$
\begin{align*}
U_{123}= & S W A P_{23} V_{123}^{(1)} U_{12} U_{23} V_{123}^{(2)} S W A P_{23},  \tag{32}\\
& V_{123}^{(1)}=R_{z 1}\left(\frac{\pi}{2}\right) C_{32} R_{z 2}\left(\frac{\pi}{2}\right) C_{32}, \\
& V_{123}^{(2)}=\operatorname{diag}(-i, 1,1, i, 1, i, i, 1),
\end{align*}
$$

where $V_{123}^{(2)}$ commutes with $S W A P_{23}$ and therefore disappears from Hamiltonian (31). Next, we find

$$
\begin{align*}
& U_{12}=C_{21} R_{y 2}\left(\chi_{1}\right) C_{12} R_{y 2}\left(-\chi_{1}\right) C_{21},  \tag{33}\\
& U_{23}=C_{32} R_{y 3}\left(\chi_{2}\right) C_{23} R_{y 3}\left(-\chi_{2}\right) C_{32},
\end{align*}
$$

where

$$
\begin{equation*}
\chi_{1}=\frac{\pi}{4}, \chi_{2}=\arccos \left(\frac{16}{\sqrt{513-3 \sqrt{57}}}\right) \approx 0.7633 \tag{34}
\end{equation*}
$$

Finally,

$$
\begin{align*}
& \Lambda_{123}=D_{12} \operatorname{diag}\left(0, \lambda_{1}, \lambda_{2},-\lambda_{3},-\lambda_{3}, \lambda_{2}, \lambda_{1}, 0\right)  \tag{35}\\
& \lambda_{1}=\frac{1}{32}(1-3 \sqrt{57}), \lambda_{2}=\frac{1}{32}(1+3 \sqrt{57}), \lambda_{3}=\frac{1}{16},
\end{align*}
$$

so that the diagonal part of the evolution operator reads:

$$
\begin{equation*}
e^{-i \tilde{\Lambda}_{123} \tau}=C_{21} R_{z 1}\left(\lambda_{1} \tau\right) C_{21} C_{32} R_{z 2}\left(-\lambda_{3} \tau\right) C_{32} C_{13} R_{z 3}\left(\lambda_{2} \tau\right) C_{13} . \tag{36}
\end{equation*}
$$

The evolution of the first excited spin is described by the formula

$$
\begin{align*}
|\psi(t)\rangle= & U_{123} e^{-i \tilde{\Lambda}_{123} \tau} U_{123}^{+}|100\rangle=\frac{1}{2}\left(\sin ^{2} \chi_{2} e^{-i \lambda_{1} \tau}+\cos ^{2} \chi_{2} e^{-i \lambda_{2} \tau}-e^{i \lambda_{3} \tau}\right)|001\rangle+  \tag{37}\\
& \gamma_{1}(\tau)|010\rangle+\gamma_{2}(\tau)|100\rangle
\end{align*}
$$

where we do not give explicite form for $\gamma_{i}, i=1,2$. Then the probability of the excited state transfer is defined by Eq.(26).

We notice that the representation of the evolution operator in terms of CNOT operations and one-spin rotations coincides with such representation of the evolution operator for $X X$ Hamiltonian under the approximation of nearest-neighbor interactions described in Sec. IIIA. Therefore, the corrected probability $p^{(f)}$ (30) can be found with the same mean values $\bar{s}$ and $\bar{k}$, see Table II. The scheme of implementation of such state transfer on the quantum processor coincides with one given in Fig 3 with the only difference in the $\tau$-dependent operator $\exp \left(-i \tilde{\Lambda}_{123} \tau\right)$ which now is given in Eq.(36) and includes one more rotation and two additional CNOT operators in comparison with Eq.(24).

In Fig.[6, we see that the stars $p^{(f)}$ very closely approach the theoretical curve, similar to Fig.4. This confirms the applicability of the corrected probability $p^{(f)}$ to this case of Hamiltonian.

## 2. Alternating chain with $d=1 / 2$.

In this section we consider an example of state transfer, for which the scheme of its implementation on the quantum processor differs from one considered in Fig 3, but nevertheless


FIG. 6: Probability of the excited state transfer from the 1st to the 3rd spin of the homogeneous chain governed by the $X X$-Hamiltonian, interactions among all nodes are included. We present the theoretically calculated probability $p$ (solid lines), probability calculated on the quantum processor $\tilde{p}$ (circles), corrected probabilities $\bar{p}$ (squares) and $p^{(f)}$
(stars), cross means probability measured at the quantum processor at $\tau=0$. To construct $\bar{p}$ we use $s=0.1357$ and $k=1.5541$ in Eq.(27).
the corrected probability $p^{(f)}$ with the parameter $\bar{s}$ and $\bar{k}$ from Table I also significantly improves the result.

We use Hamiltonian (31), dimensionless time $\tau=D_{12} t$ and alternation constant $d=\frac{D_{23}}{D_{12}}$. For certainty, we set $d=1 / 2$. In Eq.(15) we have

$$
\begin{align*}
U_{123}= & S W A P_{23} V_{123}^{(1)} U_{12} V_{123}^{(2)} U_{23} U_{31} V_{123}^{(3)} S W A P_{23} .  \tag{38}\\
V_{123}^{(1)} & =R_{z 1}\left(\frac{\pi}{2}\right) C_{23} R_{z 3}\left(\frac{\pi}{2}\right) C_{23},  \tag{39}\\
V_{123}^{(2)} & =C_{12} R_{z 2}(\pi) C_{12} \\
V_{123}^{(3)} & =\operatorname{diag}(-1,-i,-i, 1, i,-1,-1,-i) .
\end{align*}
$$

Obviously, $V_{123}^{(3)}$ commutes with $S W A P_{23}:\left[V_{123}^{(3)}, S W A P_{23}\right]=0$. Therefore this diagonal operator disappears from Hamiltonian (31). Next,

$$
\begin{align*}
& U_{12}=C_{21} R_{y 2}\left(\chi_{1}\right) C_{12} R_{y 2}\left(-\chi_{1}\right) C_{21},  \tag{40}\\
& U_{23}=C_{32} R_{y 3}\left(\chi_{2}\right) C_{23} R_{y 3}\left(-\chi_{2}\right) C_{32}, \\
& U_{31}=C_{13} R_{y 1}\left(\chi_{3}\right) C_{31} R_{y 1}\left(-\chi_{3}\right) C_{13},
\end{align*}
$$

where

$$
\begin{equation*}
\chi_{1}=3.5541, \chi_{2}=0.7712, \chi_{3}=1.6380 \tag{41}
\end{equation*}
$$



FIG. 7: Probability of the excited state transfer from the 1st to the 3rd spin of the alternating spin chain, $d=0.5$, governed by the $X X$-Hamiltonian, interactions among all nodes are included. We present the theoretically calculated probability $p$ (solid lines), probability calculated on the quantum processor $\tilde{p}$ (circles), corrected probabilities $\bar{p}$ (squares) and $p^{(f)}$ (stars). To construct $\bar{p}$ we use $s=0.1276$ and $k=1.6046$ in Eq.(27).

Finally,

$$
\begin{align*}
& \Lambda_{123}=D_{12} \operatorname{diag}\left(0,-\lambda_{1}, \lambda_{2},-\lambda_{3},-\lambda_{3}, \lambda_{2},-\lambda_{1}, 0\right),  \tag{42}\\
& \lambda_{1}=0.5426, \lambda_{2}=0.5772, \lambda_{3}=0.0346
\end{align*}
$$

So that the diagonal part of the evolution operator reads:

$$
\begin{equation*}
e^{-i \tilde{\Lambda}_{123} \tau}=C_{21} R_{z 1}\left(-\lambda_{1} \tau\right) C_{21} C_{32} R_{z 2}\left(-\lambda_{3} \tau\right) C_{32} C_{13} R_{z 3}\left(\lambda_{2} \tau\right) C_{13} \tag{43}
\end{equation*}
$$

and structurally coincides with Eq.(36).
The evolution of the initial excited state reads as follows:

$$
\begin{align*}
& |\psi(\tau)\rangle=U_{123} e^{-i \tilde{\Lambda}_{123} \tau} U_{123}^{+}|100\rangle=\left(\frac{e^{i \lambda_{1} \tau}}{2} \sin 2 \chi_{1} \sin ^{2} \chi_{2}-\right.  \tag{44}\\
& e^{-i \lambda_{2} \tau}\left(\cos \chi_{1} \cos \chi_{3}-\sin \chi_{1} \cos \chi_{2} \sin \chi_{3}\right)\left(\sin \chi_{1} \cos \chi_{3}+\cos \chi_{1} \cos \chi_{2} \sin \chi_{3}\right)- \\
& \left.e^{i \lambda_{3} \tau}\left(\sin \chi_{1} \sin \chi_{3}-\cos \chi_{1} \cos \chi_{2} \cos \chi_{3}\right)\left(\cos \chi_{1} \sin \chi_{3}+\sin \chi_{1} \cos \chi_{2} \cos \chi_{3}\right)\right)|001\rangle+ \\
& \gamma_{1}(\tau)|010\rangle+\gamma_{2}(\tau)|100\rangle,
\end{align*}
$$

where we do not give explicite form for $\gamma_{i}, i=1,2$. Again, the probability of the excited state transfer is defined by Eq. (26).

We emphasize that the structure of the formulas for $U_{123}$ (38) and $e^{-i \tilde{\Lambda}_{123} \tau}$ (43) differ from the structure of the analogous operators for the case of approximation of nearest-neighbor
approximations, see Eqs.(17) and (24). In fact, the unitary operator $U_{123}$ in (38) includes three operators of form (11) $\left(U_{12}, U_{23}\right.$ and $\left.U_{31}\right)$ instead of two such operators in Eq.(17), while the form of the operator $e^{-i \tilde{\Lambda}_{123} \tau}$ coincides with the form of this operator in Eq.(36). The scheme in Fig 3 does not fit this example. Nevertheless, the corrected probability $p^{(f)}$ with the parameters $\bar{s}$ and $\bar{k}$ from Table [1] (stars in Fig[7) fits rather well the theoretical curve (solid line in Fig.77), just demonstrating a certain universality of the proposed correction method.

## IV. CONCLUSION

Although the existing quantum processors are very noisy and usually give the results with large error, there are some methods to overcome this problem at least partially. One of such methods is a two-parametric recovering transformation combining properly adjusted shift and scale of measured probabilities [17]. We show that, for a given scheme implemented on a quantum processor, there is such transformation of the measured probability from $\tilde{p}$ to $p^{(f)}$ that the latter does not significantly differ from the theoretically predicted value $p$. At that, the most important factor responsible for applicability of a recovery transformation with a particular values of parameters is the number of CNOT operations included in the evolutionary operator under consideration.

We simulate the evolution of the three-node spin chain governed by the XX-Hamiltonian on the quantum processor using diagonalization of the Hamiltonian thus avoiding Trotterization. The diagonalization allows to present the time-dependent part of the evolution operator in the diagonal form. We represent both the matrix of eigenvectors and the (time-dependent) diagonal part of the evolution operator in terms of CNOT operations and one-qubit rotations. We show that there is the recovering transformation (28) with particular values of parameters $\bar{s}$ and $\bar{k}$ that improves results of calculations. Having constructed the parameters $\bar{s}$ and $\bar{k}$ for the alternating three-node chain governed by the $X X$-Hamiltonian under approximation of nearest-node interactions we then demonstrate its applicability to the case of the $X X$-Hamiltonian with all-node interactions just confirming certain universality of the considered correction method. This method is applicable if the measured probability $\gtrsim 0.2$. Otherwise the error still remains significant, as shown in the last plate of $\operatorname{Fig}[4(d=0.2)$.

Thus, we propose the scheme simulating three-qubit evolution governed by the $X X$ Hamiltonian and avoiding Trotterization. This scheme is based on blocks $U_{i j}$ of form (11) having an important property of conserving the excitation number in a system. Extension of such scheme to systems of larger dimension would be of interest for simulating spin dynamics on a quantum processor.

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Conflict of interest The authors declare that they have no conflict of interest.
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