Generalization of CNOT-based Discrete Circular Quantum Walk: Simulation and Effect of Gate Errors

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Abstract—We investigate the counterparts of random walk in universal quantum computing and their implementation using standard quantum circuits. Quantum walk have been recently well investigated for traversing graphs with certain oracles. We focus our study on traversing a 1-D graph, namely a circle, and show how to implement discrete circular quantum walk in quantum circuits built with universal CNOT and single qubit gates. We review elementary quantum gates and circuit decomposition and propose a a generalized version of the all CNOT based quantum discrete circular walk. We simulated these circuits on an IBM quantum supercomputer London IBM-Q with 5 qubits. This quantum computer has non perfect gates based on superconducting qubits, therefore we analyze the impact of errors on the fidelity of the Walker circuit.

Index Terms—CNOT gate, quantum computing, Quantum random walk

I. INTRODUCTION

Like any other generalized tool in the field of quantum computing, there exists a quantum version of random walk, a useful mathematical tool to model graphs such as Markov chains. Basic concepts of quantum walk can be found in [1]. Quantum walk are used in computer science and are fundamental for building quantum routers. The best examples of quantum algorithms based on quantum walk are the searching in an unsorted list, searching in an hypercube, element distinctness problem, triangle problems etc ... [2]. Circuit implementations of quantum walk along a circle, a 2D hypercycle, a twisted toroidal lattice graph, a complete circle and a glued tree are presented in [3]. Other research has addressed physical realization of quantum walk algorithms[4]. We distinguish two models of quantum walk: (1). The discrete quantum walk, where we require a coin qubit, a walker qubits and a unitary evolution operator and (2). Continuous quantum walk, where an evolution operator is applied with no restrictions and the time evolution of the walker is given through the Schrödinger equation [1]. In this paper, we address the circuit implementation of all CNOT based Circular Quantum Discrete Random Walk (CQDRW) along a circle and we simulate them on an IBMQ machine. In this work, we use the London 5 qubits IBM-Q to simulate a 4 qubits CQDRW.

This paper is organized into four sections: we start section 2 by reviewing some single quantum gates and the CNOT in order to recall their universality. We also show how to decompose $C^m NOT$ into elementary gates, specifically $C^2 NOT$ and $C^3 NOT$. We show that their simulation on the IBM composer and their implementation on London IBMQ have different outputs due to errors of the gates. Section 3 presents the CNOT based circuits for building CQDRW in a general context. The specific simulation results for the 4 qubits walker is presented in section 4. We focus on comparing the composer simulation and the device execution to study the impact of errors gates mainly due to CNOT’s. The analysis is done by calculating the fidelity parameter. We conclude with other possible 2-D quantum walk implementation and some techniques to reduce the set of obtained errors.

II. ELEMENTARY GATES FOR BUILDING QUANTUM CIRCUITS

A. Universality of the CNOT and the single qubit gates

Single qubit gates are the basic elements for building quantum circuit. We address in this work the Identity gate ($I_2$), the Hadamard gate ($H$), the negation gate ($\sigma_x$), the rotation by $\theta$ around $\hat{y}$ ($R_y(\theta)$), the rotation by $\alpha$ around $\hat{z}$ ($R_z(\alpha)$), the $\delta$-phase shift gate ($\Phi(\delta)$) and the $T(\varphi)$ gate, having the following transforms [5], [6], [7]:

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1)$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (2)$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (3)$$
The $\sigma_x$ gate is also known as the NOT transform as illustrated by figure 1. The Controlled-NOT (CNOT) gate is a two qubits gate, it performs $\sigma_x$ on the target qubit if and only if the control qubit is in the state $|1\rangle$, it has the following transform:

$$U_{\text{CNOT}} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}$$  (8)

The set of single qubit gates and CNOT gate are universal for building any quantum circuit. Specifically, any unitary gate acting on multiple qubit circuit can be implemented with single qubit gates and CNOT gates. Following paragraphs, we show how to decompose certain circuits into a set of single qubit and CNOT gates.

The NOT controlled by two quits is known as the Toffoli gate, having the following transform:

$$U_{\text{Toffoli}} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}$$  (9)

Further generalization of the NOT gate, controlled by n qubits all in the state $|1\rangle$, is referred as $C^n\text{NOT}$ gate. When the NOT gate is controlled by the n qubits all in the state $|0\rangle$, it is denoted $C^n_0\text{NOT}$ and it’s control qubits are represented by the empty circle (figure 1).

The matrix transforms of the the $C^n\text{NOT}$ and the $C^n_0\text{NOT}$ are obtained as follows:

$$U_{\text{CNOT}} = \begin{pmatrix}
I_2 & O & \cdots & O \\
O & I_2 & \cdots & \cdots \\
\vdots & \vdots & \ddots & \vdots \\
O & \cdots & I_2 & O \\
\cdots & \cdots & \cdots & O \\
O & \cdots & \cdots & O \\
0 & \cdots & I_2 & O \\
0 & \cdots & O & I_2
\end{pmatrix} = \begin{pmatrix}
I_{2^n+1-2} & O \\
O & \sigma_x
\end{pmatrix}$$  (10)

$$U_{\text{CNOT}} = \begin{pmatrix}
\sigma_x & O & \cdots & O \\
O & I_2 & \cdots & \cdots \\
\vdots & \vdots & \ddots & \vdots \\
O & \cdots & I_2 & O \\
\cdots & \cdots & \cdots & O \\
O & \cdots & \cdots & O \\
0 & \cdots & I_2 & O \\
0 & \cdots & O & I_2
\end{pmatrix} = \begin{pmatrix}
\sigma_x & O \\
O & I_{2^n+1-2}
\end{pmatrix}$$  (11)

where $I_{2^n+1-2}$ is a $(2^n+1-2) \times (2^n+1-2)$ identity matrix.

Many works have addressed circuit implementation of quantum algorithms, such as database search algorithms, while using $C^n\text{NOT}$ and $C^n_0\text{NOT}$ gates [8], [9], but IBMQ uses only single qubit operations and multiple CNOTs to implement the circuits. Therefore, we show in figure 2 the technique used to build equivalent $C^n\text{NOT}$ based implementation of $C^n_0\text{NOT}$ gates [10].

Following the general decomposition method described in [11], [12], we illustrate in stage 2 of figure 3a the CNOT based implementation of the Toffoli gate, while the $T$ and $T^\dagger$ transforms refer to $T(\pi/4)$ and $T(-\pi/4)$ of equation 7, respectively.

![Figure 1: Controlled NOT gates](image1.png)

![Figure 2: Equivalent CNOT based implementation of C^n_0 NOT gates](image2.png)

![Figure 3: Decomposition of the Toffoli gate and result of simulation in the IBMQ composer for one input |110\rangle](image3.png)
For any circuit to be simulated, IBMQ sets all input qubits automatically to 0. In our case, the input of the decomposed Toffoli gate is set by default to $|000\rangle$. To observe the output of the decomposed Toffoli, we consider only the input state $|000\rangle$ to this end, we add the two NOT gates in stage 1 of figure 3a (represented by X gate in IBMQ), and we illustrate the correct output $|111\rangle$ in figure 3b as obtained after simulation on the composer.

To observe the result after execution on the real IBMQ device, a transpiled circuit is automatically generated as given by figure 4a. The transpiled circuit performs some approximations and simplifications based on optimizations techniques to generate transpiled circuits that are equivalent to the original circuit. For these approximations, all single qubits transforms given by equation 1 to equation 7 are compiled down to physical gates based on superconducting qubits, denoted $U_1$, $U_2$ and $U_3$, and given as follows:

$$U_1(\lambda) = U_3(0, 0, \lambda) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix} \tag{12}$$

$$U_2(\phi, \lambda) = U_3(\pi/2, \phi, \lambda) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -e^{i\lambda} \\ e^{i\phi} & e^{i\lambda+\phi} \end{pmatrix} \tag{13}$$

$$U_3(\theta, \phi, \lambda) = \begin{pmatrix} \cos(\theta/2) & -e^{i\lambda}\sin(\theta/2) \\ e^{i\phi}\sin(\theta/2) & e^{i\lambda+\phi}\cos(\theta/2) \end{pmatrix} \tag{14}$$

From equations 12, 13 and 14, we deduce that the two NOTs gates illustrated in stage 1 of figure 3a are implemented by $U_3(\pi, 0, \pi)$, while the Hadamard gate of equation 2 is obtained by $U_2(0, \pi)$.

For the same input state $|110\rangle$ applied to the composer, we illustrate in figure 4b the output after execution on the IBMQ device. We observe a success probability of 57.202 % for obtaining the correct output $|111\rangle$, and various errors for the other output states $|000\rangle$, $|001\rangle$, $|010\rangle$, $|011\rangle$, $|100\rangle$, $|101\rangle$ and $|110\rangle$.

Following the same steps sussed to decompose the Toffoli gate \cite{11, 12}, we decomposed the $C^3 NOT$ gate and it is illustrated in figure 5a. The equivalent circuit in this figure is composed by 20 CNOTs and 16 single qubits gates. The rotation gates given in stages 2, 8, 10, 16, 18, 24 and 26 of figure 5a are all identical and equal to $R_y(\pi/8)$. The single qubit gates given in stages 4, 6, 12, 14, 20, 22 and 28 of figure 5a are equal to $R_y(-\pi/8)$, the single qubit gate of stage 1 is $R_z(\pi/2)$ and it is $R_z(-\pi/2)$ for stage 30.

For an input state $|1110\rangle$, we observe with 100 % success the correct output $|1111\rangle$ in the composer (figure 5b). But for the according transpiled circuit (figure 6a), we observe the correct output only with 0.238 of success probability (figure 6b), this is basically due to the error rate of the single qubit gates and the CNOT gates, which are in the range $[3.455 \times 10^{-4}, 1.058 \times 10^{-3}]$ and $[9.144 \times 10^{-3}, 1.381 \times 10^{-2}]$, respectively, according to IBMQ real device (London) \cite{13}.
The N qubits system of a CQDRW at a specific position $P_k$, and after performing $m$ steps, is described by the state $|\text{Walker}_k|^m$:

$$|\text{Walker}_k|^m = |P_k\rangle \otimes |c\rangle = |p_{N-2}^k p_{N-1}^k \ldots p_0^k\rangle \otimes |c\rangle$$  \hspace{1cm} (17)

The walker can go one step backward or one step forward, depending on the state of the coin, being in $|0\rangle$ or $|1\rangle$, respectively. When the coin is in the state $|c\rangle = |0\rangle$, an operator denoted $\text{DEC}$ is applied to $|P_k\rangle$ and we obtain:

$$\text{DEC} |P_k\rangle = |P_{k-1}\rangle$$  \hspace{1cm} (18)

When the coin is in the state $|c\rangle = |1\rangle$, an operator denoted $\text{INC}$ is applied to $|P_k\rangle$ and we obtain:

$$\text{INC} |P_k\rangle = |P_{k+1}\rangle$$  \hspace{1cm} (19)

Let us suppose the N qubits system with the CQDRW being at a specific position $P_k$ and a coin initially at the state $|c\rangle = |0\rangle$, then equation (17) becomes:

$$|\text{Walker}_k|^0 = |P_{k}\rangle \otimes |0\rangle = |p_{N-2}^k p_{N-1}^k \ldots p_0^k\rangle \otimes |0\rangle$$  \hspace{1cm} (20)

A single step of the walker consists of applying $H$ transform to the coin, and then apply the appropriate $\text{DEC}$ or $\text{INC}$ operator depending on the state of the coin. $|\text{Walker}_k|^0$ of equation (20) becomes $|\text{Walker}_k|^1$:

$$= \frac{1}{\sqrt{2}} (|\text{DEC} |P_{k}\rangle \otimes |0\rangle + |\text{INC} |P_{k}\rangle \otimes |1\rangle)$$  \hspace{1cm} (21)

A second step of the walker transforms equation (21) to the following:

$$|\text{Walker}_k|^1 \rightarrow |\text{Walker}_k|^2 = \frac{1}{\sqrt{2}} \left( |\text{DEC} |P_{k-1}\rangle \otimes |0\rangle + |\text{INC} |P_{k-1}\rangle \otimes |1\rangle\right) + \left( |\text{DEC} |P_{k+1}\rangle \otimes |0\rangle - |\text{INC} |P_{k+1}\rangle \otimes |1\rangle\right)$$  \hspace{1cm} (22)

According to equation (22) after two steps, $|\text{Walker}_k|^0$ has walked to the positions $|P_{k-2}\rangle$, $|P_{k+2}\rangle$ and returned to initial position $|P_k\rangle$, with probability amplitude equal to $1/\sqrt{2}$, $-1/\sqrt{2}$ and $1/\sqrt{2}$, respectively. For $m > 2$, we need to apply each time the transform $H$ of equation (2) and then we apply the appropriate $\text{DEC}$ or $\text{INC}$ operator depending on the state of the coin $|c\rangle$. Therefore, the general state of the N qubits CQDRW, being initially at a position $P_k$ among $2^{N-1}$ positions in a circle, and after performing $m$ steps is expressed as:

$$|\text{Walker}_k|^m = \sum_{i=0}^{2^{m-1}} \alpha_i |P_i\rangle \otimes |c\rangle$$  \hspace{1cm} (23)

where $\alpha_i$ is the probability amplitude of being in the position $|P_i\rangle$ after applying the Hadamard operator $m$ times.
A $C^n NOT$ and a $C_0^0 NOT$ based implementation of the N qubits walker, including DEC and INC possible realization is illustrated in figure 7.

![Figure 7: $C^n NOT$ and a $C_0^0 NOT$ based implementation of N qubits CQDRW](image)

Introducing all transformation rules presented in section 2 permits us to transform the circuit of figure 7 into a generalized single qubit and CNOT based implementation of any N qubits CQDRW.

IV. SIMULATION RESULTS

In order to study the impact of the errors of the CNOT gates on the success probability of correctly realizing the circular quantum discrete walk, we take as an example of $N = 4$ (figure 8a). An equivalent $C^3 NOT$, $C^2 NOT$ and CNOT based implementation of figure 8a is given by figure 8b. It is worth mentioning that minimization rules detailed in [10], [15] permit us to reduce the size of the circuit as given by figure 8c, but since the aim of this paper is to study the impact of the errors of the CNOT gates, we simulate the implementation of figure 8b, where we introduce the decomposition of the $C^2 NOT$ and $C^3 NOT$, as illustrated by figures 4a and 5a, respectively.

In the specific case of $N = 4$, and for an initial position $P_0$ and a coin set to $|c\rangle = |0\rangle$, the initial state of the 4 qubits quantum walker is expressed as:

$$|Walker_0\rangle^0 = |P_0\rangle \otimes |0\rangle = |p_0^0 p_0^0 p_0^0 p_0^0 \rangle \otimes |0\rangle$$

(24)

After one step, $|Walker_0\rangle^0$ moves to $|Walker_0\rangle^1$ as:

$$|Walker_0\rangle^0 \rightarrow |Walker_0\rangle^1 = \frac{1}{\sqrt{2}} \left( |111\rangle \otimes |0\rangle + |001\rangle \otimes |1\rangle \right)$$

(25)

The state of the walker given by equation 25 describes exactly the result obtained after simulation of the circuit on IBMQ (figure 9a). But on the real IBMQ device (figure 9b), $|Walker_0\rangle^0$ of equation 24 becomes:

$$|Walker_0\rangle^0 \rightarrow |Walker_0\rangle^1 = \sqrt{0.1466} |111\rangle \otimes |0\rangle + \sqrt{0.0311} |001\rangle \otimes |1\rangle$$

(26)

According to equation 26 and figure 9b, we have only 0.03 and 0.14 success probabilities for ending correctly in the positions $|001\rangle$ and $|111\rangle$, after just one step of the walker. To measure the performance of the 4 qubits CQDRW over all possible initial states, we refer to the fidelity denoted $F_{Walker}$ and given by:

$$F_{Walker} = \langle \Psi_{in} | U_{Walker}^{-1} \rho_{Walker} U_{Walker} | \Psi_{in} \rangle$$

(27)
where the upper line indicates that the fidelity is obtained according to the average over all 8 possible initial positions states \( |\Psi_{in}\rangle = \{|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle\}. \( p_n \) is given by \( p_n = \langle \Psi_{out}|\Psi_{out}\rangle \), with \( |\Psi_{out}\rangle \) is the state at the output of the IBMQ transpiled 4 qubits CQDRW circuit for the specific \( |\Psi_{in}\rangle \) input. The transform \( U_{\text{walker}} \) is a \( 16 \times 16 \) matrix representing the ideal transform of the 4 qubits CQDRW, and obtained through Matlab simulation.

The fidelity obtained by IBMQ real device is only 17.42\%. This low value is basically due to the 87 CNOTs making up the circuit (figure 8). If we consider the error of each CNOT gate as being equal to \( 1.38 \times 10^{-2} \) [13], the success probability of each CNOT is around 0.9862, and if we neglect the errors due to the single qubits operations and the decoherence, the total success probability of the entire circuit is approximately \( \approx (0.9862)^{87} = 29.85 \% \), which is near the fidelity value obtained in our simulation.

For higher number of steps \( m > 1 \), the simulation of the 4 qubits CQDRW would have necessitate larger circuits and a huge number of gates. Therefore, we consider the abstract probabilistic CNOT model of equation [15] and we vary randomly all \( \varepsilon = (\varepsilon_j)_{1 \leq j \leq 12} \) in a realistic range of errors \( 10^{-5} \ldots 10^{-2} \). The results of the MATLAB simulation of the fidelity of the walker depending on these errors and on the number of steps \( m = [1..50] \) (figure 10).

![Figure 10: Fidelity of the 4 qubits CQDRW depending on the errors of the CNOT and the number of steps](image)

According to figure [10] the fidelity value of 17.42 \% obtained by IBMQ after one step, is obtained for a CNOT error around \( 10^{-2} \), which is in the error range declared by the manufacturer. It is seen from figure [10] that reaching reasonable fidelity values around 80\% or more, the error of the CNOT should be less than \( 10^{-3} \), which leads us to conclude that actual state of the art devices are still not yet ready for simulating real quantum algorithms.

### V. Conclusion

We investigated the CQDRW both theoretically and practically and presented a CNOT based implementation of the CQDRW in a N qubits system. We showed through simulation on the IBMQ that the 4 qubits CQDRW system could not exceed the fidelity value of 17\%. We underlined the source of the errors is related to the number of CNOT gates used in the circuit and to the decoherence. We simulated the CQDRW for large number of steps and showed that the error of the CNOT should be lower than \( 10^{-4} \) to have acceptable fidelity values. IBMQs resources constraints limited our work to 4 qubits and informally speaking, larger CQDRW in a 5 qubits system or 2D hyper cubic quantum walks requires decompostion of the \( C^4 NOT \) with more CNOTs, which will cause more and more errors. Our simulation proves that working with superconducting qubits has the major drawback of high probability of the errors. This work could be extended by proposing quantum error correcting codes used to reduce the total errors of the entire circuit.

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