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CIRCUIT DESIGN FOR CONTINUOUS TIME QUANTUM WALKS ON CYCLE GRAPH AND ITS EXPERIMENTAL DEMONSTRATION IN IBM QUANTUM COMPUTER

ANJISHNU ADHIKARI*
Departmentof Physics, Indian Institute of Space Science and Technology, Valiamala Thiruvananthapuram, Kerala, 695547, India

BIKASH K. BEHERA† and PRASANTA K. PANIGRAHI‡
Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, 741246 Mohanpur, West Bengal, India

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Continuous-time quantum walk (CTQW) and its experimental realization are of great interest due to its profound application starting from graph matching to quantum search algorithms. Here, we propose quantum circuits for CTQW on cycle graph with 2, 4, and 8 vertices at any time t for given different initial conditions. We present a comparative study of theoretical probability distribution, simulated and implemented output after executing the quantum circuits on the real quantum chip, "ibmq_16_melbourne" provided by IBM quantum experience platform and thus experimentally verify our quantum circuits and provide a demonstration of CTQW on mentioned graphs.

Keywords: Continuous-time quantum walks, cycle graph, ibmq_16_melbourne, IBM quantum experience

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1. Introduction

Quantum walks (QW) represent propagation of a quantum particle over a discrete set of positions or states. These are quantum analogues of classical quantum walks which behave in a different way as compared to the classical ones. If we consider random walk on a line then at each discrete instant of time, the walker can move to the left or right if he gets head or tail after tossing. However, in quantum walks, the evolution is controlled by a quantum coin (e.g. Hadamard coin) which can be superposition of head and tail states rather than a classical coin, thus it evolves in a superposition of states of possible positions. As the dynamics is discrete in time, this model is named as *discrete-time quantum walks* (DTQW) introduced by Aharonov *et al.* [1] and Meyer [2] independently. A detailed review and application of discrete-time quantum walks can be found in the Ref. [3] by Chandrashekar. A different model, *continuous-time quantum walks* (CTQW) where the walker moves continuously with respect to time, was introduced by Farhi and Guttman [4] as generalizations of diffusion-type

*anjishnu.sc17b143@ug.iist.ac.in
†bkb18rs025@iiserkol.ac.in
‡pprasanta@iiserkol.ac.in

differential equations, where they used complex amplitude and unitary dynamics instead of probability and Markovian dynamics.

Over the past decade there have been several schemes for implementation as well as experimental realization of quantum walks, using a variety of quantum, classical and hybrid systems including Nuclear Magnetic Resonance quantum information processor [5], cavity QED [6, 7], ion traps [8, 9, 10], coupled waveguide [11], optical traps [12], optical networks [13] and quantum dots [14, 15] to name a few. Quantum walks form a versatile structures for studying multitudinous physical processes like biological systems [16], satisfiability problems in computer science [17], topological systems in physics [18], proposing quantum algorithms [19, 20], transport on networks [21, 22], group matching [23] and performing universal computation [24] etc.

CTQW are important in models of coherent transport on complex networks [25], transfer of information in complex system in the context of perfect state transfer [26]. CTQW are also closely related to the so-called quantum graphs [27, 28, 29, 30] and also Grover search algorithm [31, 32]. Recently, topological quantum walks have been realized using the IBM-Q five-qubit quantum computer [33]. D. Solenov *et al.* theoretically investigated continuous-time quantum walks on a uniform cycle graph [34]. However, quantum circuit for experimental implementation of CTQW on cycle graph has not been suggested before. Experimental implementation and verification are unexplored in a quantum computer. Here, we follow the mathematical treatment of A. Ahmadi *et al.* [35] where they showed that CTQW on well-behaved graphs like cycle graphs do not exhibit uniform mixing and the equations they used are close to the analysis of Moore and Russell [36]. However, we make the assumptions according to our convenience and propose quantum circuits, design them the IBM-Q 14-qubit quantum computer and verify the predicted theoretical investigations with the experimental results.

IBM Quantum Experience, an online platform which has gained popularity by freely availing the 5-qubit and 14-qubit quantum chips to the research community and making easily accessible through QISKit. A number of quantum computational and information processing tasks have been experimentally realized on the real quantum chips. The works include in the field of quantum simulation [37, 38, 39, 40, 41], quantum machine learning [42, 43], quantum error correction [44, 45, 46, 47], quantum information theory [48, 49, 50], quantum cryptography [51], quantum algorithms [52, 53], quantum optimization problems [54], quantum games [55, 56, 57], designing quantum communication devices [58, 59] are tested on the real chips and feasible results are obtained.

Our organization of the paper is as follows. Firstly, we introduce quantum walks on cycle graph and our scheme for implementation in a proper way in Section 2. In Section 3, we propose quantum circuits for 3 types of cycle graphs. Then in Section 4, we present the experimental realization of quantum walk in the IBM 14-qubit quantum computer. Finally, we conclude in Section 5 by summarizing and providing future directions of our work.

2. Scheme of Quantum Walks in Cycle Graph

Assume $G = (V, E)$ is a simple, undirected, connected, d-regular n-vertex graph. Let A be the adjacency matrix of G that can be represented as

$$A_{jk} = \begin{cases} 1 & \text{if } (j,k) \in E \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

Transition matrix can be defined as $H = \frac{A}{d}$ (the Hamiltonian of the quantum system). Assume the initial amplitude wave function of the particle is $|\psi_0\rangle$. The the amplitude wave function at time t, will be governed by Schrödinger's equation, as

$$i\hbar \frac{d}{dt}|\psi_t\rangle = H|\psi_t\rangle \tag{2}$$

Now if we assume $\hbar d = 1$ then our Hamiltonian is effectively same as the adjacency matrix. Because if we plot graph or practically implement this, then the scaling factor simply scales the time axis.

$$|\psi_t\rangle = e^{-iHt}|\psi_0\rangle \tag{3}$$

From Ref. [35], the above equations can be found as mentioned before. Now consider a cycle graph with n vertices (say) C_n then for 2, 4, and 8 vertices we can map the states generated by 1, 2, and 3 qubits respectively to produce $|i\rangle$ ($0 \leq i \leq n-1$ and $i \in \mathbb{N}$) states in the system. The mapping for all types of cycle graphs are given in the following, e.g., for C_8, $|000\rangle \to |0\rangle$, $|001\rangle \to |1\rangle$, $|010\rangle \to |2\rangle$, $|011\rangle \to |3\rangle$, $|100\rangle \to |4\rangle$ etc. Similarly for C_4, $|00\rangle \to |0\rangle$, $|01\rangle \to |1\rangle$, $|10\rangle \to |2\rangle$, $|11\rangle \to |3\rangle$, for C_2 $|0\rangle \to |0\rangle$, $|1\rangle \to |1\rangle$. Adjacency matrices for C_8, C_4 and C_2 graphs are given in the following Eqs. (4), (5) and (6) respectively.

$$A_{C_8} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{4}$$

$$A_{C_4} = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \tag{5}$$

$$A_{C_2} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{6}$$

The unitary evolution operator, e^{-iHt} for C_2, C_4, and C_8 graphs are given in Equations (7), (8) and (9) respectively.

$$U_{C_2} = \begin{bmatrix} \cos t & -i\sin t \\ -i\sin t & \cos t \end{bmatrix} \tag{7}$$

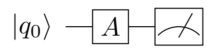

Fig. 1. **Quantum circuit for C_2 graph**. The qubit, $|q_0\rangle$ is taken for the system. An unitary evolution operator, A (U_{C_2}) is then applied on the system.

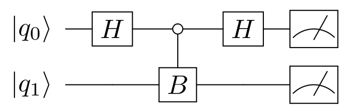

Fig. 2. **Quantum circuit for C_4 graph**. Two qubits, $|q_0\rangle$ and $|q_1\rangle$ are taken as the system. An unitary evolution operator (U_{C_4}), consisting Hadamard (H_0), anti-controlled-B_{01}, and Hadamard (H_0) gates, is then applied on the system.

$$U_{C_4} = \begin{bmatrix} \frac{\cos 2t}{2} + \frac{1}{2} & \frac{-i\sin 2t}{2} & \frac{\cos 2t}{2} - \frac{1}{2} & \frac{-i\sin 2t}{2} \\ \frac{-i\sin 2t}{2} & \frac{\cos 2t}{2} - \frac{1}{2} & \frac{-i\sin 2t}{2} & \frac{\cos 2t}{2} + \frac{1}{2} \\ \frac{\cos 2t}{2} - \frac{1}{2} & \frac{-i\sin 2t}{2} & \frac{\cos 2t}{2} + \frac{1}{2} & \frac{-i\sin 2t}{2} \\ \frac{-i\sin 2t}{2} & \frac{\cos 2t}{2} + \frac{1}{2} & \frac{-i\sin 2t}{2} & \frac{\cos 2t}{2} - \frac{1}{2} \end{bmatrix} \tag{8}$$

$$U_{C_8} = \begin{bmatrix}
\frac{\cos(2t)}{4} + \frac{\cos(\sqrt{2}t)}{2} + \frac{1}{4} & -\frac{i\sin(2t)}{4} - \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{1}{4} & -\frac{i\sin(2t)}{4} + \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{\cos(\sqrt{2}t)}{2} + \frac{1}{4} & -\frac{i\sin(2t)}{4} + \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{1}{4} & -\frac{i\sin(2t)}{4} - \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} \\
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\frac{\cos(2t)}{4} - \frac{1}{4} & -\frac{i\sin(2t)}{4} - \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} + \frac{\cos(\sqrt{2}t)}{2} + \frac{1}{4} & -\frac{i\sin(2t)}{4} - \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{1}{4} & -\frac{i\sin(2t)}{4} + \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{\cos(\sqrt{2}t)}{2} + \frac{1}{4} & -\frac{i\sin(2t)}{4} + \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} \\
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\frac{\cos(2t)}{4} - \frac{\cos(\sqrt{2}t)}{2} + \frac{1}{4} & -\frac{i\sin(2t)}{4} + \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{1}{4} & -\frac{i\sin(2t)}{4} - \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} + \frac{\cos(\sqrt{2}t)}{2} + \frac{1}{4} & -\frac{i\sin(2t)}{4} - \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{1}{4} & -\frac{i\sin(2t)}{4} + \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} \\
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\frac{\cos(2t)}{4} - \frac{1}{4} & -\frac{i\sin(2t)}{4} + \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{\cos(\sqrt{2}t)}{2} + \frac{1}{4} & -\frac{i\sin(2t)}{4} + \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{1}{4} & -\frac{i\sin(2t)}{4} - \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} + \frac{\cos(\sqrt{2}t)}{2} + \frac{1}{4} & -\frac{i\sin(2t)}{4} - \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} \\
-\frac{i\sin(2t)}{4} - \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{1}{4} & -\frac{i\sin(2t)}{4} + \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{\cos(\sqrt{2}t)}{2} + \frac{1}{4} & -\frac{i\sin(2t)}{4} + \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} - \frac{1}{4} & -\frac{i\sin(2t)}{4} - \frac{i\sqrt{2}\sin(\sqrt{2}t)}{4} & \frac{\cos(2t)}{4} + \frac{\cos(\sqrt{2}t)}{2} + \frac{1}{4}
\end{bmatrix} \tag{9}$$

3. Quantum Circuit for Demonstrating Quantum Walks on Cycle Graph

Now for a given initial state, $|\psi_0\rangle$ we can have different probability amplitudes at different time instances. The quantum state at time t, $|\psi(t)\rangle$ is calculated by multiplying e^{-iHt} matrix of corresponding graph with qubit image of $|i\rangle$ state, in other words it will be i^{th} column of e^{-iHt} matrix. Probability of $|i\rangle^{th}$ state at any instant of time is given by;

$$P_i = |\langle i|\psi(t)\rangle|^2 \tag{10}$$

Considering all possible initial states, the quantum circuits for C_2, C_4, and C_8 graphs are given in Figures 1, 2 and 3, where the matrix form of A, B, C, D, and E gates are given in Equations (11), (12), (14), (15), and (16) respectively, and H is the Hadamard gate.

3.1. *Construction of quantum circuit from $|\psi(t)\rangle$*

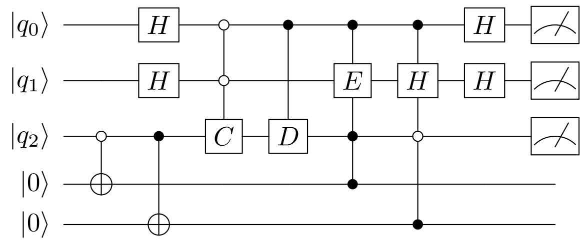

Fig. 3. **Quantum circuit for C_8 graph**. Three qubits, $|q_0\rangle$, $|q_1\rangle$ and $|q_2\rangle$ represent the system. Then two ancillary qubits prepared in $|0\rangle$ states are then taken to construct the unitary evolution operator U_{C_8}.

The unitary evolution operator for C_2 graph, U_{C_2} can be prepared using the $U3$ gate available in the IBM-Q interface (Ref. [60]). The general form of the gate can be given as, $U3(\theta,\phi,\lambda) = [cos(\theta/2), -e^{i\lambda}sin(\theta/2); e^{i\phi}sin(\theta/2), e^{i(\lambda+\phi)}cos(\theta/2)]$, where the above operation is designed with the following parameters, $\theta = 2t$, $\phi = -\pi/2$ and $\lambda = \pi/2$, i.e., $U_{C_2} = A = U3(2t, -\pi/2, \pi/2)$, whose form is presented below.

$$A = \begin{bmatrix} \cos t & -i\sin t \\ -i\sin t & \cos t \end{bmatrix} \tag{11}$$

In case of C_4 graph, the unitary evolution operator, U_{C_4} is prepared by implementing Hadamard (H_0), anti-controlled-B_{01}, and Hadamard (H_0) gates, where H_0 means the application of Hadamard operation on the q_0 qubit. Anti-controlled-B_{01} implies the application of B operator (Eq. (12)) on the q_1 qubit, only when the q_0 qubit is in the state $|0\rangle$. As there is no anti-controlled-B_{01} operator available, we decompose the operator into controlled-Not ($CNOT$) gates and other phase gates such as $U1$ and $U3$ gates available at IBM-Q platform ([60]). As $U3$ gate has been discussed before, the form of U1 gate can be written as, $U1(\theta) = [1, 0; 0, e^{\theta}]$.

$$B = \begin{bmatrix} \cos 2t & -i\sin 2t \\ -i\sin 2t & \cos 2t \end{bmatrix} \tag{12}$$

Because, any unitary operation can be written as,

$$U = e^{i\alpha}PXQXR \text{ and } PQR = I \tag{13}$$

where X is Pauli-X gate and P, Q, R have to be determined. Detailed calculation and controlled operations can be found in Ref. [61]. In our case, for B unitary operation, $P = e^{i\pi/4}U3(2t, -\pi/8, 0)$, $Q = U3(2t, \pi, -\pi)$, $R = e^{-i\pi/4}U1(\pi/8)$. The anti-controlled-B_{01} operation is then applied with the application of two $CNOT$ gates and the above P, Q, and R gates. For C_8 graph, the quantum circuit for the unitary evolution operator, U_{C_8} (Fig. 3), is designed using single and multiple controlled and anti-controlled unitary operations such as C, D, E and H operations. The matrix forms of the above operations, C, D and E are given in the following Equations (14), (15), and (16) respectively.

$$C = \begin{bmatrix} \cos 2t & -i\sin 2t \\ -i\sin 2t & \cos 2t \end{bmatrix} \tag{14}$$

$$D = \begin{bmatrix} \cos\sqrt{2}t & -i\sin\sqrt{2}t \\ -i\sin\sqrt{2}t & \cos\sqrt{2}t \end{bmatrix} \tag{15}$$

$$E = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \tag{16}$$

We decompose the anti-anti-control-C_{012} operation by the method given in Ref. [61]. We take two ancilla qubits, then from two working qubits we impose Toffoli gate on the ancillas. From the ancilla, control-C is then drawn to the target qubit and again Toffoli gate is applied to retrieve back the states of ancilla. All these operations need not be broken into $CNOT$, Hadamard, phase, $\pi/8$ gates, because in QISKit, Toffoli gate can be directly applied. Only we have to decompose the control-C_{12} operation using the Eq. (13), where $P = e^{i\pi/4}U3(2t, -\pi/8, 0)$, $Q = U3(2t, \pi, -\pi)$, and $R = e^{-i\pi/4}U1(\pi/8)$. The same process is followed in case of other control-control operations of E, D, and H unitary operations in circuit as required. In case of control-D_{02}, the operators are calculated to be, $P = e^{i\pi/4}U3(2t, -\pi/8, 0)$, $Q = U3(2t, \pi, -\pi)$, $R = e^{-i\pi/4}U1(\pi/8)$. Controlled-D is similarly decomposed into the unitary operators, as $P = e^{i\pi/4}U3(\sqrt{2}t, -\pi/8, 0)$, $Q = U3(\sqrt{2}t, \pi, -\pi)$, $R = e^{-i\pi/4}U1(\pi/8)$ gates. Controlled-$E = U3(\pi/2, 0, 0)$ operator is directly prepared with the help of QISKit. Same logic is applied to the control-Hadamard operation to design the quantum circuits for it.

4. Experimental Realization of Quantum Walk in IBM Quantum Computer

Our proposed circuit is not restricted to any particular initial condition. So it can be simulated and executed for given any initial condition. Consider a particular initial condition, $|\psi_0\rangle = |0\rangle$, for which the quantum walks can be simulated in qasm simulator as well as the quantum circuits can be executed in the "ibmq_16_melbourne" processor using QISKit. In our case, the initial states, $|0\rangle$, $|00\rangle$ and $|000\rangle$ are considered for C_2, C_4 and C_8 graphs respectively. Starting from $t = 0$, we implement the quantum circuit by increasing time upto $t = 4.5$, $t = 3.14$, $t = 6.3$ in 0.02 interval for C_8, C_4, and C_2 graphs respectively. For each of these time instances, we plot the probability distribution. We simulate the quantum circuits in the qasm simulator using QISKit for C_8, C_4, and C_2 graphs. The circuit is then implemented in the IBM real quantum processor "ibmq_16_melbourne" for C_4 and C_2 graphs. In case of C_8 graph, the simulated and implemented outputs i.e., the probability of different states are found to be far away from each other due to large gate errors and limitation of number of shots. A large error arises due to the use of large number of gates and the shots are the number of times with which we perform the measurement. Graphs representing the probability of different states for simulation and run are given in Figures 4, 5, 6, 7, 8, and 9. Here, theoretically $|\psi(t)\rangle$ for C_2 graph is given as,

$$|\psi(t)\rangle = \begin{bmatrix} \cos t \\ -i\sin t \end{bmatrix} \tag{17}$$

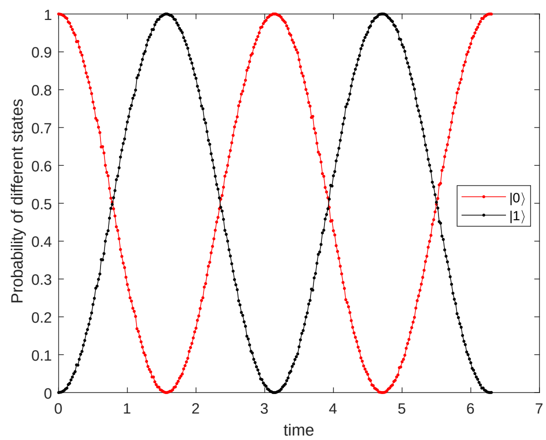

Fig. 4. Simulation output of quantum walk on C_2 graph

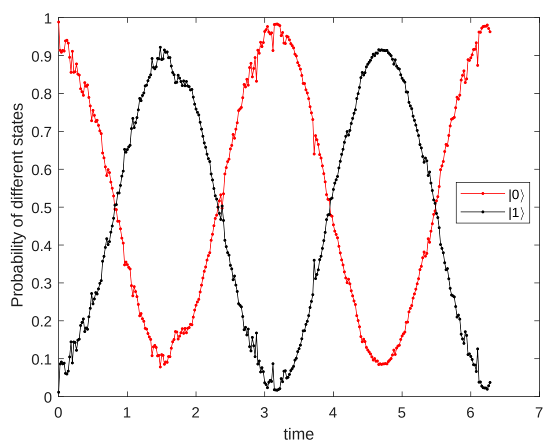

Fig. 5. Implementation output of quantum walk on C_2 graph

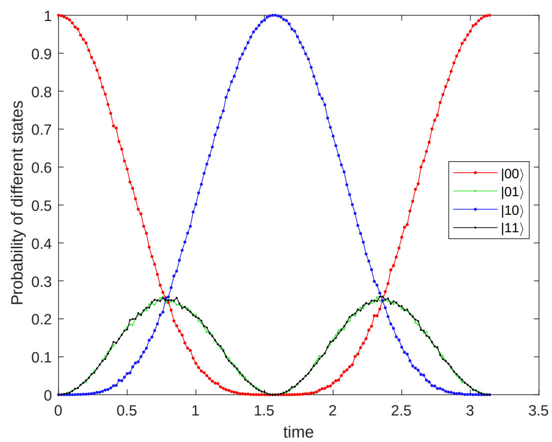

Fig. 6. Simulation output of quantum walk on C_4 graph

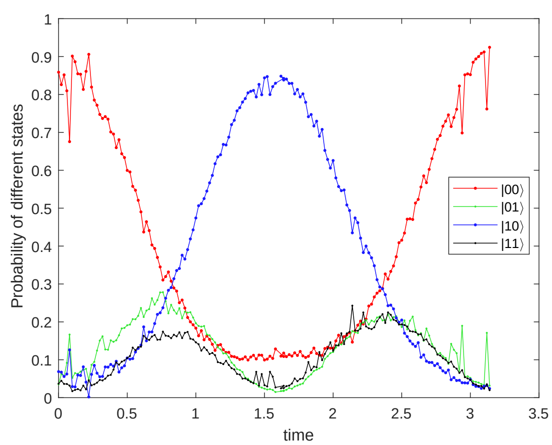

Fig. 7. Implementation output of quantum walk on C_4 graph.

From Eq. (17), it is clear that for other graphs like C_4, C_8, $|\psi(t)\rangle$ will be the column vector consisting of only first column of their corresponding unitary evolution operators, e.g., U_{C_4} and U_{C_8} respectively. Mathematically, Eq. (17) depicts that for $|0\rangle$ and $|1\rangle$ states, the corresponding probabilities will be $\cos^2 t$ and $\sin^2 t$. The simulation and implementation of Figures 4 and 5 are consistent with this. However, due to gate error in the real processor, the probabilities show a little deviation from the simulational results. As the probabilities are periodic with period $\pi \approx 3.14$, so it is guaranteed that all the data are consistent with each other for any time t. For C_4 graph also, simulation (Fig. 6) almost exactly matches with the mathematical calculation. But due to gate error in the real chip, implementation data (Fig. 7) deviates from the simulation. Here the probabilities have maximum period of π. All the outputs are observed to agree with each other for any time.

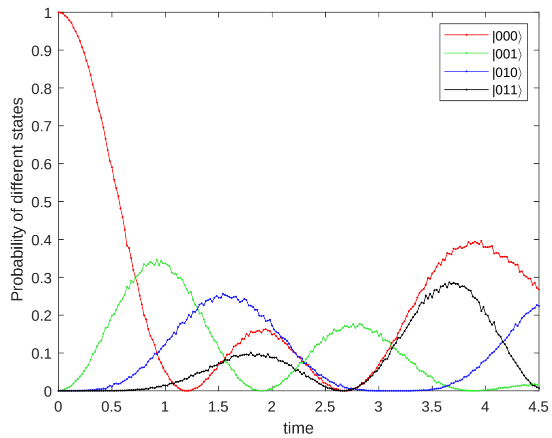

Fig. 8. Simulation data of quantum walk on C_8 graph for $|0\rangle$ to $|3\rangle$ states.

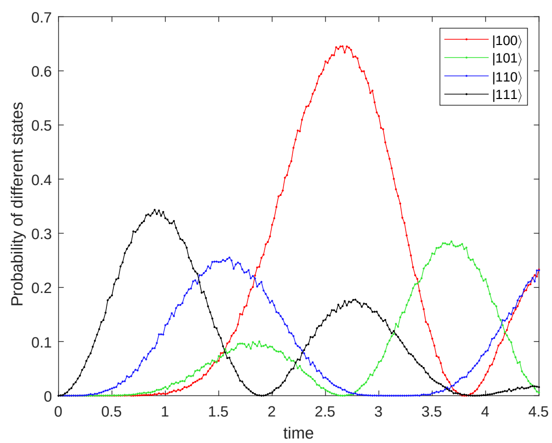

Fig. 9. Simulation data of quantum walk on C_8 graph for $|4\rangle$ to $|7\rangle$ states.

As mentioned before, due to large gate error in case of C_8 graphs, the implementation data is not shown here. All the probabilities are not periodic though we expect that mathematically calculated values match with the simulated data (Figs. 8 and 9) for arbitrary time.

5. Conclusion

To conclude, we have proposed here quantum circuits as well as implemented those for CTQW on cycle graph for 2, 4, and 8 vertices. Our quantum circuits are experimentally demonstrated by successfully designing those on the 14-qubit real quantum chip. As mentioned before, though there were theoretical investigations on the CTQW on cycle graph, implementation of those on a quantum computer were not provided. Here, we both propose and experimentally verify the quantum circuits. It has been observed that for C_2 and C_4 graphs, the theoretical investigations match with the experimental simulation of quantum circuits. There have been a good agreement of the simulational data with the experimental run data for the case of C_2 and C_4 graphs.However, as the number of vertices increases, the complexity of the unitary evolution operator increases very rapidly. Hence, for C_8 graph, due to the use of a large number of gates, a large errors were encountered in the experiment. In future, a generalized quantum circuit can be proposed for cycle graphs with any number of vertices and experimental also can be verified with the current quantum computer architecture. In near future, it can have powerful application in the field of graph matching or developing quantum search algorithms.

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