Quantum Random Walk

Chen-Yun Chang,[1] Hao-Rong Yang,[2] Yu-Tai Lin,[2] Ming-Yun Yang,[1] and Pin-Yu Huang[1]

[1] *Department of Physics, National Tsing Hua University*
[2] *Department of Physics, National Changhua University of Education*

Abstract. We discuss the difference between quantum random walk and classical random walk, and use IBMQ simulator to simulate quantum random walk. We set the different initial states and the number of steps to be independent variables, and observe the results which not appears at classical random walk. Last but not least, we have some short description of the potential applications to quantum random walk.
Keywords: quantum random walk, searching algorithm, quantum computing.

I. INTRODUCTION

A. The difference between classical random walk and quantum random walk in one-dimensional case

In mathematics, classical random walk is derived from a sequence of Bernoulli trials and known as a stochastic process, which the objects wander away from the origin and can continue forever, i.e., it is unbounded. Sometimes, if the walker can not go outside due to the boundaries, the walk is view as restricted. On the other hand, quantum Random Walk shows the superposition of classical random walk. The main structure of 1D quantum random walk includes: a walker, shift operator S and coin operator C. The shift operators S and coin operators C operate the walker's position state and the coin state, respectively. The two operations are repeated without measuring. The measurement is preformed only when the whole walking process is done. Figure 1 is the comparison between the probabilities of two random walks. In the below content, we give the explanations about the difference.

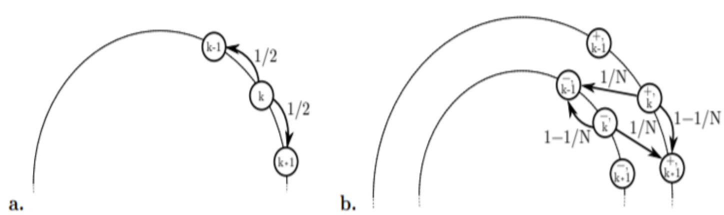


FIG. 1. Probabilities difference between (a) classical random walk and (b) quantum walk[1].

B. Classical random walk

Suppose $X_1, X_2, ..., X_n$ are a set of random from Ber(p), then

$$\sum_{i=1}^{n} X_i \to \text{Bin}(n, p).$$

If $X \to \text{Bin}(n, p)$, then $E(X) = np, \text{Var}(X) = np(1 - p)$. By Central limiting theorem,

$$\frac{\sum_{i=1}^{n} X_i - np}{\sqrt{np(1-p)}} \xrightarrow{d} N(0, 1),$$

so statistically the walker's departure from the center is proportional to the square root of the step number:

$$\sigma^2 \sim n.$$

We list the probability table about position n and steps t in Table I. Note that $p = 1/2$.

t \ n	-4	-3	-2	-1	0	1	2	3	4
0					1				
1				$\frac{1}{2}$		$\frac{1}{2}$			
2			$\frac{1}{4}$		$\frac{1}{2}$		$\frac{1}{4}$		
3		$\frac{1}{8}$		$\frac{3}{8}$		$\frac{3}{8}$		$\frac{1}{8}$	
4	$\frac{1}{16}$		$\frac{1}{4}$		$\frac{3}{8}$		$\frac{1}{4}$		$\frac{1}{16}$

TABLE I. The the probability table of 1D classical random walk. n is the number that labels the position.

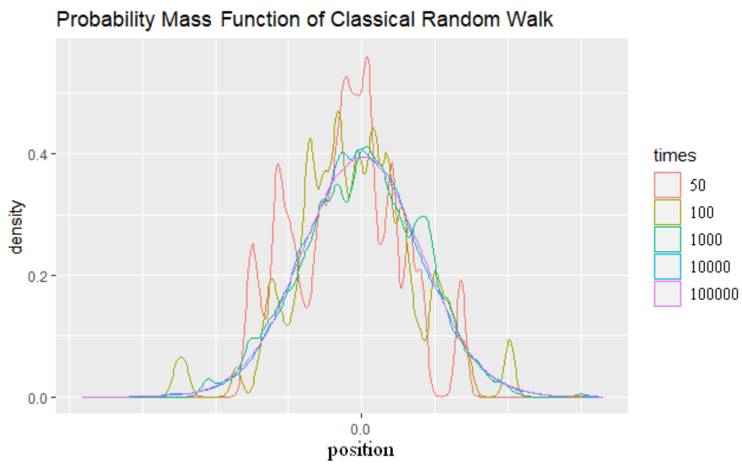


FIG. 2. Probability mass function of classical random walk.

C. Quantum random walk

In 1D quantum random walk, we define two Hilbert space:

$$H = H_C \otimes H_P,$$

where $H_C = \{|\uparrow\rangle, |\downarrow\rangle\}$ is coin space, $H_C = \{|n\rangle\}$ is position space, and $\otimes$ is Kronecker product. The total time evolution operator is given by

$$U = S \cdot (C \otimes I) \tag{1}$$

The shift operator S is defined as

$$S := \sum_n (|\uparrow\rangle \langle\uparrow| \otimes |n+1\rangle \langle n| + |\downarrow\rangle \langle\downarrow| \otimes |n-1\rangle \langle n|) \tag{2}$$

The coin we focus on is Hadamard coin, which can be represented in form of:

$$C = H = \frac{1}{\sqrt{2}}(|\uparrow\rangle \langle\uparrow| + |\uparrow\rangle \langle\downarrow| + |\downarrow\rangle \langle\uparrow| - |\downarrow\rangle \langle\downarrow|). \tag{3}$$

Now, we propagate the system for several time steps with the following initial condition

$$\begin{aligned} |\psi(0)\rangle &= |\psi(0)\rangle_c \otimes |\psi(0)\rangle_p \\ &= \left[\frac{1}{\sqrt{2}}(|\downarrow\rangle + i|\uparrow\rangle)\right] \otimes |0\rangle, \end{aligned}$$

t \ n	-4	-3	-2	-1	0	1	2	3	4
0					1				
1				$\frac{1}{2}$		$\frac{1}{2}$			
2			$\frac{1}{4}$		$\frac{1}{2}$		$\frac{1}{4}$		
3		$\frac{1}{8}$		$\frac{3}{8}$		$\frac{3}{8}$		$\frac{1}{8}$	
4	$\frac{1}{16}$		$\frac{3}{8}$		$\frac{1}{8}$		$\frac{3}{8}$		$\frac{1}{16}$

TABLE II. In this table, t is the number of steps of quantum random walk with symmetric coin, n is the number that labels the position. There is a significant difference with respect to classical random walk after 4 steps.

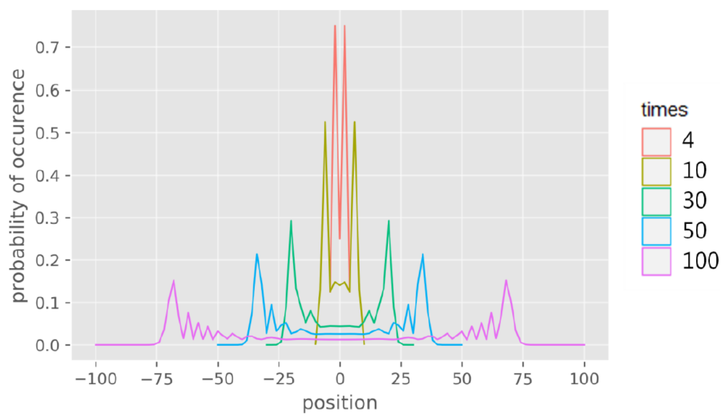


FIG. 3. Probability Mass Function of Quantum Random Walk

and obtain

$$|\psi(1)\rangle = U|\psi(0)\rangle = SC|\psi(0)\rangle = \frac{1}{2}[(1+i)|\uparrow\rangle \otimes |1\rangle - (1-i)|\downarrow\rangle \otimes |-1]\rangle,$$

$$|\psi(2)\rangle = U|\psi(1)\rangle = \frac{1}{2\sqrt{2}}\{(1+i)|\uparrow\rangle \otimes |2\rangle + [(1+i)|\downarrow\rangle - (1-i)|\uparrow\rangle \otimes |0\rangle] - (1-i)|\downarrow\rangle \otimes |-2\rangle\},$$

$$\vdots$$

We can then list the probability about position n and steps t as in Table II. With the symmetric coin, as seen in the example, we obtain a symmetric distribution since "fair" coin that treats left and right in the same way. It's not hard to find that

$$\sigma^2 \sim n^2,$$

that is, quantum random walk moves faster than classical random walk.

II. WHY DO WE NEED QUANTUM

For some oracular problems, quantum walks provide an exponential speedup over any classical algorithm and is helpful in many practical problems. For instance, in database searching problems, the probability of quantum random walk can spread faster and wider than the classical random walk, which suggests that it may achieve to the target with less cost. We will give further discussion in Section V.

III. METHOD

A. Operators & Gates

To simulate the 1D Quantum random walk, we need to build up the oracle for the two operators. In the following content, we will first briefly introduce the required quantum gates and then explain how to construct the oracles.

TABLE III. The states of qubit go through controlled NOT gate.

Before		After	
Control	Target	Control	Target
$\|0\rangle$	$\|0\rangle$	$\|0\rangle$	$\|0\rangle$
$\|0\rangle$	$\|1\rangle$	$\|0\rangle$	$\|1\rangle$
$\|1\rangle$	$\|0\rangle$	$\|1\rangle$	$\|1\rangle$
$\|1\rangle$	$\|1\rangle$	$\|1\rangle$	$\|0\rangle$

1. Hadamard gate

When qubit goes through Hadamard gate, it will become superposition state. It acts on a single qubit to rotate a π-angle about the axis $\frac{\hat{x}+\hat{z}}{\sqrt{2}}$. It can be represented by the matrix:

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

It maps the basis states

$$|0\rangle \mapsto \frac{|0\rangle + |1\rangle}{\sqrt{2}} \quad \text{and} \quad |1\rangle \mapsto \frac{|0\rangle - |1\rangle}{\sqrt{2}}.$$

2. Controlled NOT gate

It is a reversible gate, which can produce entanglement. It flips the target qubit if and only if the control qubit is $|1\rangle$. A CNOT gate can be represented with the matrix:

$$\text{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

Table III provides the truth table of CNOT operations.

B. 1D quantum random walk circuit

We set 3 bits to represent the position, so there are a total of 8 positions from 000 to 111 as shown in Figure 4 and can be expanded to Figure 5. The reading method is (q_3, q_2, q_1), for example, when $q_1 = 0, q_2 = 0, q_3 = 1$, it means that is at position 100.

In Figure 6, q_0 is the coin, q_3, q_2, and q_1 represent the position. There are two circuits, which are drawn by black boxes. We name the left box the plus-one-operator, which means moving the position one step clockwise in Figure 4. For example, when the qubit is at the position of 011, and then pass through once the plus-one-operator, the position will become 100. On the contrary, we name the right box the minus-one operator. Its function is to move the position one step counterclockwise. The coin is set as the controlled qubit in the circuit. When the coin is 1, the plus-one-circuit will be executed, and the minus-one-circuit will not be executed, and vice versa. After the coin state passing through a Hadamard gate, the coin state becomes a superposition of $|0\rangle$ and $|1\rangle$, and the whole system going through the plus-one-operator and the minus-one operator to finish the circuit of quantum random walk with one step.

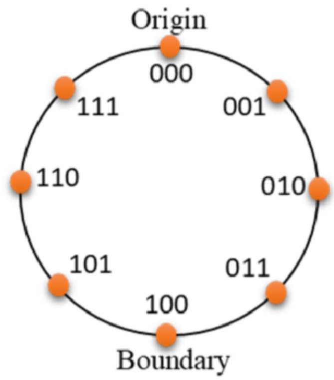


FIG. 4. 8 positions from 000 to 111.

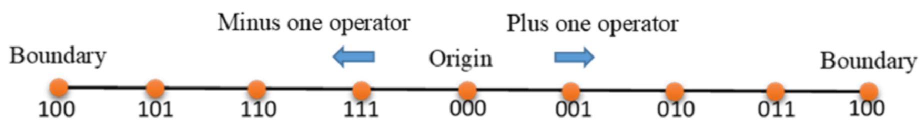


FIG. 5. 8 positions from 000 to 111 on a straight line.

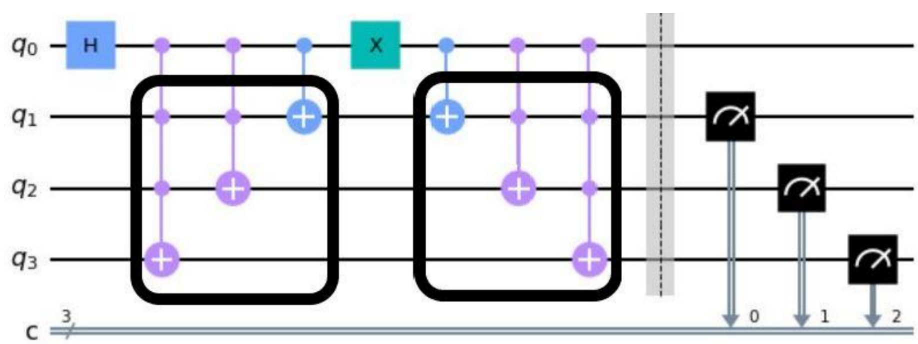


FIG. 6. Four qubits quantum random walk circuit.

IV. RESULT

A. Simulation results

We use IBMQ's `qasm_simulator` to execute the program and obtain Figure 7. After a coin tossed, the position is 001 and 111 from the origin 000, and the probability are of occupying them are identical: $1/2$. We change the initial state of the coin toss, and then toss the coin four times to record the simulated position probability. According to the Figure 8 and Figure 9, we can find that the initial coin state affects the result of the final probability distribution. If the initial coin state is a superposition state, it will end up with a symmetrical distribution. However, if the initial coin state is leftward, the final probability distribution will be leftward, and vice versa.

B. Analysis

We change the number of steps and record the simulated position probability. The results of this simulation are in line with the original three expectations. First, we know that after quantum random walk, the probability of the position staying at both sides of the origin is the greatest rather than the origin, which shows very different results to classical random walk.

Second, the final position of the result is related to the initial state of the input coin. The most probable position

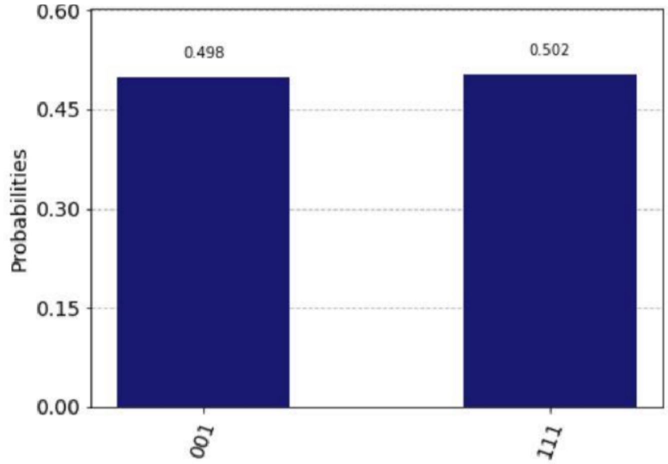


FIG. 7. The position probability distribution of 1024 repeated measurements with `qasm_simulator`. The probability of 001 and 111 are 50%.

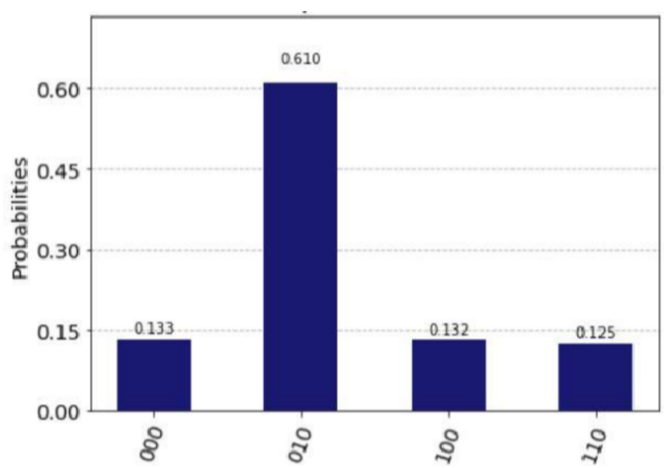


FIG. 8. Location probability distribution where coin initial state is $|0\rangle$. The most probable position is 010.

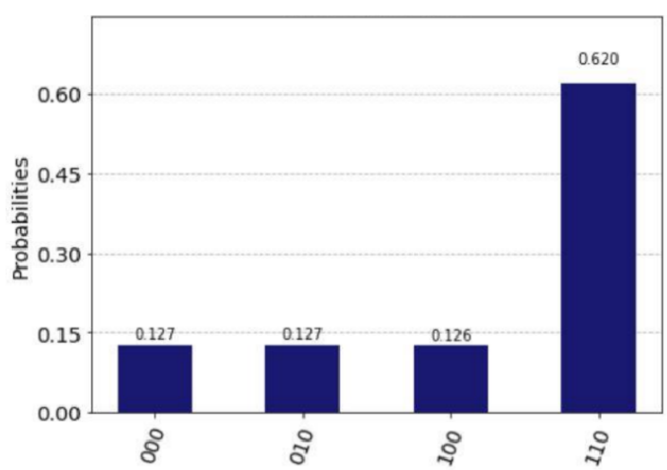


FIG. 9. Location probability distribution where coin initial state is $|1\rangle$. The most probable position is 110.

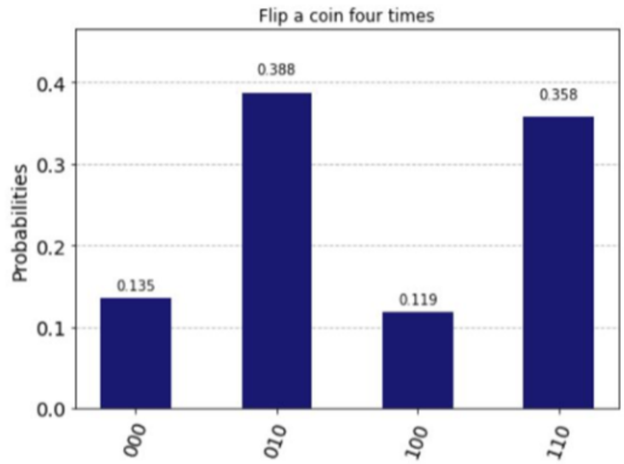


FIG. 10. Location probability distribution where coin initial state is $\frac{|0\rangle - i|1\rangle}{\sqrt{2}}$. The most probable positions are 010 and 110.

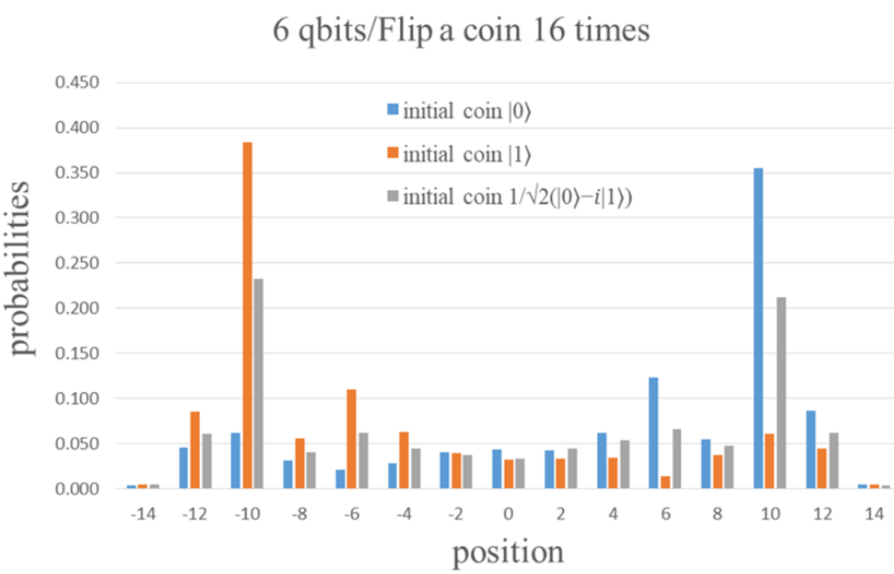
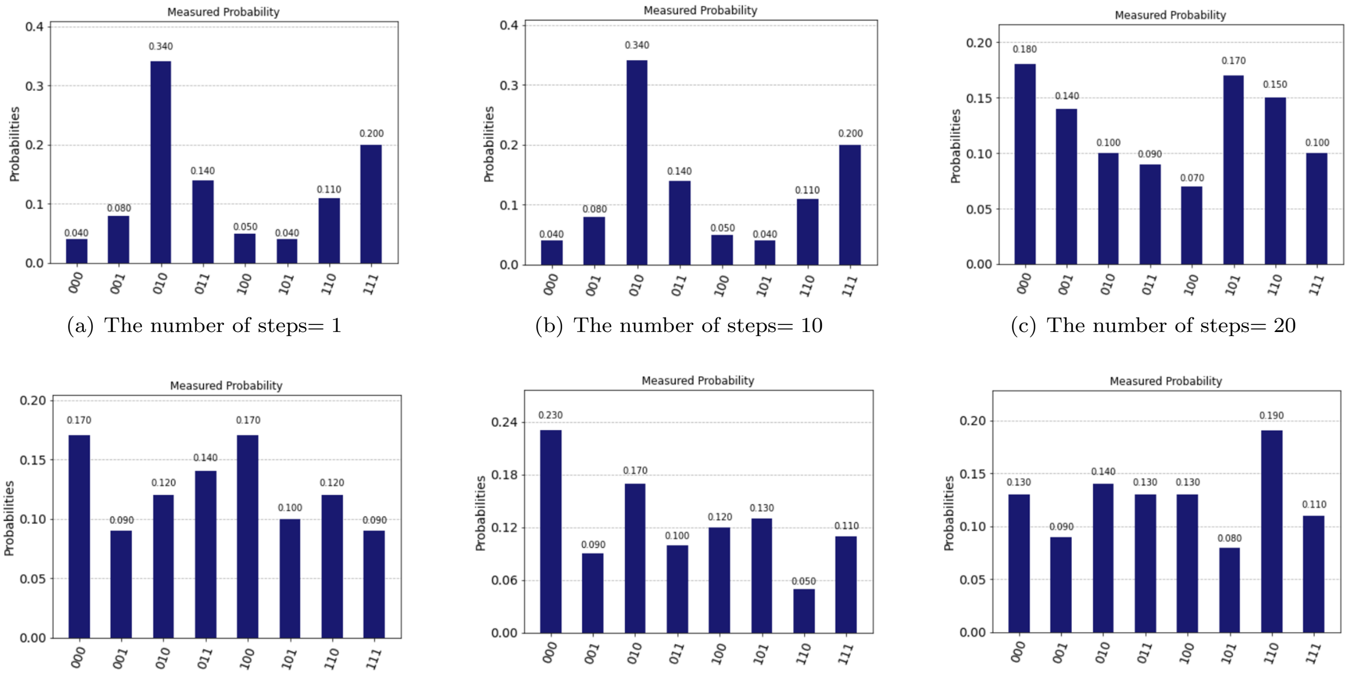


FIG. 11. The probability of different initial states. The total steps $T = 16$.

between initial state 0 and 1 will appear at the same distance but opposite position. Because of the Hadamard matrix, which cancels out some of the amplitudes of the coin, the most probable position is only one rather than two. As a result, the probabilities after n steps are heavily skewed to the other side. As shown in Figure 8, when the initial state of the coin is 0, the most probable position is 010, and the probability is 0.610. As shown in Figure 9, when the initial state of the coin is 0, the most probable position is 110, and the probability is 0.620. As shown in Figure 10, when the initial state of the coin is $\frac{|0\rangle - i|1\rangle}{\sqrt{2}}$, the most probable positions are 010 and 110, and the probabilities are 0.388 and 0.358. In Figure 11, we simulate the quantum random walk with 5 qubits as the position register, i.e., totally 32 nodes and a coin qubit. We can easily observe how the initial coin state affects the final probability distribution in position.

Last but not least, in this circuit, we need to avoid the occurrence of number of steps (T) greater than number of nodes (N). If we are lucky to go in a certain direction, we will hit the boundary in the process of walking. To avoid this, we may restrict $T \leq N$, which means to limit the coin toss to less than four times, because if we keep moving in the same direction for four steps, we will hit the boundary and cause the measurement result to be inaccurate, as shown in Figure 12.



(a) The number of steps= 1

(b) The number of steps= 10

(c) The number of steps= 20

(d) The number of steps= 30

(e) The number of steps= 40

(f) The number of steps= 500

FIG. 12. The simulated position probability of different steps.

V. DISCUSSION

We had shown that quantum random walks display different behavior than their classical counterparts. Consequently, it may lead to some applications due to the promising features:

1. Element distinctness:
   Previous studies such as Ref. [2] and Ref. [3] have used quantum walk to produce search algorithms on d-dimensional lattices (d≥2) which is faster than the naive application of Grover's search.

2. Database searching [4]:
   Quantum Walk provides a unitary evolution of the quantum amplitude distribution, such that the amplitude at each vertex gets redistributed over itself and its neighbours at every time step. With quantum superposition allowing simultaneous exploration of multiple possibilities.

3. Art:
   The sculpture, Quantum cloud, in Figure 13, were arranged using a computer model with a random walk algorithm starting from points on the surface of an enlarged figure based on the body that forms a residual outline at the centre of the sculpture.

VI. CONCLUSION

Quantum random walk shows very different results to the classical random walk. Quantum walk provides a speedup over the classical algorithms. From the simulation of quantum circuit, we observe the phenomenon of quantum random walk such as the probability of the position staying at both sides of the origin is the greatest, the final position of the result is related to the initial state of the input coin, and we need to avoid the occurrence of number of steps greater than number of nodes. We also know that results can be applied to element distinctness, database searching, and art. Quantum random walk is not only speedup the classical random walk, it gives us new perceptions to calculation and still have many potential application.

In Section I C we have shown that the distribution of quantum random walk is based on the calculation of matrix S, C, and the initial qubit state. In section 4, we compare the results to theoretical ones. Here is the discussion

FIG. 13. British sculptor Antony Gormley's "Quantum Cloud"[5]

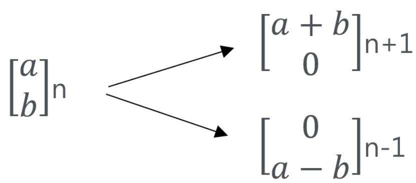


FIG. 14. Tree structure after one step

about how we derive the theoretical probability distribution of quantum random walk after n steps with arbitrarily initial state, like what we show in Figure 3. We simplify the notation of calculation and find the recursion pattern of theoretical probability distribution.

Appendix A: Visualize calculation

In Section I C we knew we can propagate the system by operation of SC matrix such that this multiplication is the propagator U. U matrix times an arbitrary initial state $(a\left|\downarrow\right\rangle + b\left|\uparrow\right\rangle) \otimes \left|n\right\rangle$ which a and b are complex numbers, give us the equation,

$$\begin{aligned} SC(a\left|\downarrow\right\rangle + b\left|\uparrow\right\rangle) \otimes \left|n\right\rangle &= \frac{1}{\sqrt{2}}((a-b)\left|\downarrow\right\rangle \otimes \left|n-1\right\rangle + (a-b)\left|\uparrow\right\rangle) \otimes \left|n+1\right\rangle \\ &= \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ a-b \end{bmatrix} \otimes \left|n-1\right\rangle + \frac{1}{\sqrt{2}} \begin{bmatrix} a+b \\ 0 \end{bmatrix} \otimes \left|n+1\right\rangle . \end{aligned}$$

Here, we express the coin state of qubits with matrix notation. For simplicity, we also omit the Kronecker product and ket:

$$\frac{1}{\sqrt{2}} \left(\begin{bmatrix} 0 \\ a-b \end{bmatrix} n-1 + \begin{bmatrix} a+b \\ 0 \end{bmatrix} n+1 \right).$$

Next, we put the propagation process into tree structure (ignoring the multiplication of $2^{-0.5}$ term every step).

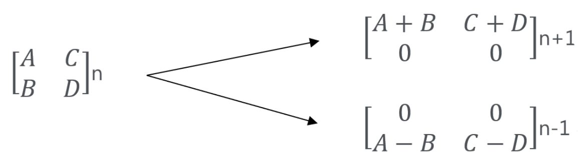


FIG. 15. Tree structure after one step in matrix form

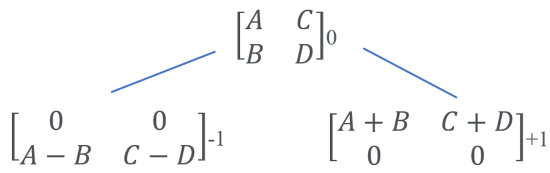


FIG. 16. Two stages triangle

Appendix B: Pascal's triangle in quantum random walk

With the tree structure to describe the propagation of quantum random walk, we can derive the recursion rule of possibility distribution by constructing a "quantum pascal's triangle". First, we expand the complex numbers a and b:

$$\begin{bmatrix} a \\ b \end{bmatrix} n = \begin{bmatrix} A + Ci \\ B + Di \end{bmatrix} n$$

Second, since the calculation between complex numbers here is similar to vectors, for simplicity, we note them as vectors which means the coin state of qubit now is represented by a matrix with four real numbers:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} n$$

Thus, the tree structure rule in Figure 14 becomes Figure 15. Now we would like to construct the so-called *quantum pascal's triangle* by this rule. We set initial position at the orgin and coin with arbitrary parameters A, B, C, and D. After first step, the triangle becomes Figure 16. Next, by the second stage of the triangle, we try to build the third stage. Since we know the tree structure rule, it is easy to get the first term and the third term. While the second term is more complex, it is the result of using tree structure rule two times. One is propagated from the $+1$ position which move backward, and the other is from -1 position which move forward, as Figure 17 shows. By adding two terms, we can have the third stage of the triangle as Figure 18. By the tree structure rule, we can compute any stage that is wanted.

Every term in the triangle represents a possible position after corresponding step, with its coin state attached, i.e., The third term of fifth stage represents the coin state after five steps at position 0. Finally, we calculate the possibilities of each position. Since four elements in coin state matrix belongs to two complex number originally, the probability of an arbitrary coin state is proportional to the sum of square of each element (because there are $2^{-0.5}$ terms we ignore at first). Note as

$$\left\| \begin{bmatrix} A & B \\ C & D \end{bmatrix} n \right\| = A^2 + B^2 + C^2 + D^2,$$

we can view it as the norm of four dimension vector in Euclidean space. For n stage in the triangle, the possibilities of each term is its norm divided by 2^n, which comes from C gate.

Quantum pascal's triangle give us a way to explain and compute the theoretical probability distribution of quantum random walk after n steps. The formulas in triangle also imply some significant different between quantum random walk and classical random walk, i.e., In quantum random walk, the distribution is affected by initial state. In other word, every event of flipping a quantum coin is not independent.

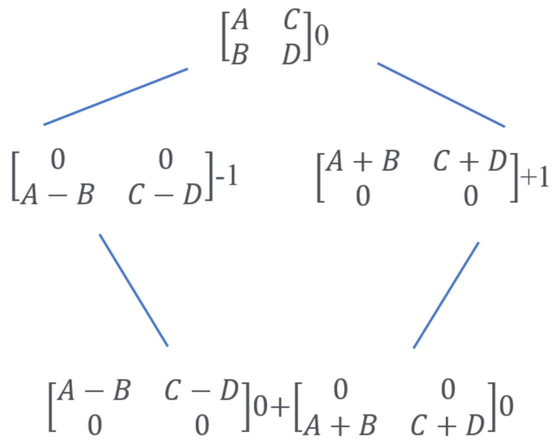


FIG. 17. The combination of two terms from second stage.

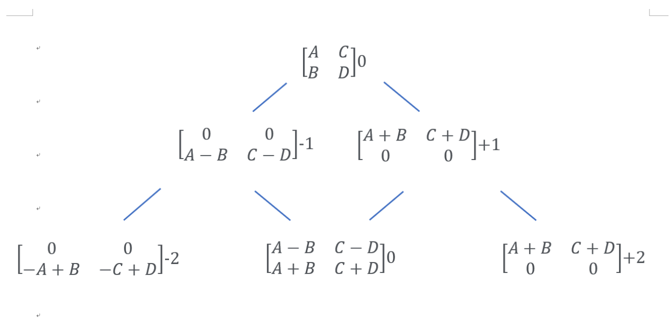


FIG. 18. Three stages triangle.

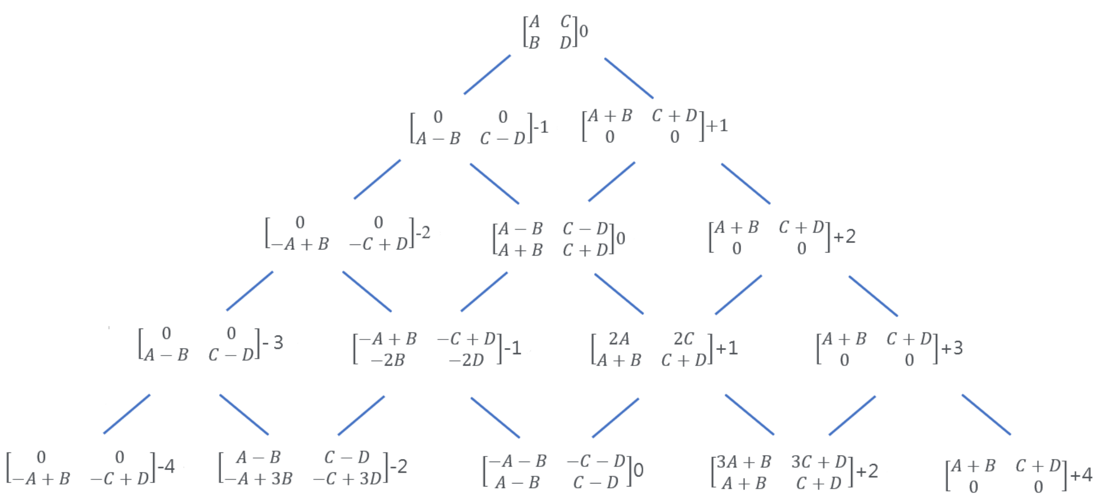


FIG. 19. Five stages triangle.

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