Computational power of single qubit discrete-time quantum walk

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ABSTRACT

Quantum walk has been regarded as a primitive to universal quantum computation. By using the operations required to describe the single particle discrete-time quantum walk on a position space we demonstrate the realization of the universal set of gates on two- and three-qubit system. The idea is to reap the effective Hilbert space of the single qubit and the position space on which it evolves in superposition of position space in order to realize multi-qubit states and universal set of quantum gates on them. Realization of many non-trivial gates in the form of engineering arbitrary states is simpler in the proposed quantum walk model when compared to the circuit based model of computation. We will also discuss the scalability of the model and some propositions for using lesser number of qubits in realizing larger qubit systems.

1 Introduction

Quantum walk\textsuperscript{1–5}, a quantum mechanical analogue of classical random walk has been a basis for many quantum algorithms\textsuperscript{6–10} and schemes for quantum simulations\textsuperscript{11–16}. The dynamics of quantum walk has been described in several ways, however, broadly they can be classified under the two of the most distinct and prominent ones, the continuous-time and discrete-time quantum walks. Engineering quantum gates and realizing universal quantum computation has been shown using both these forms of quantum walks\textsuperscript{17–19}. This means that any problem that can be solved on a quantum computer can also be solved using quantum walks. The one dimensional discrete-time quantum walk has also been used to engineer arbitrary qudit states\textsuperscript{20}. It has been experimentally implemented on linear optical system which uses the orbital angular momentum degree of freedom of single photon states to represent the particle\textsuperscript{21}. The idea is to increase the control over the dynamics of walk by using appropriate evolution operators and thus driving the particles’ state towards the desired qudit state. Theoretically, this technique can be used to prepare any high-dimensional quantum state and experimentally, a six-dimensional qudit state has been prepared and measured. All this highlights the versatility of quantum walks. The scheme for quantum computation presented here is based on controlled dynamics of the walk with the help of appropriate position dependent evolution operators and has a scope of designing an architecture for quantum processor using quantum walks. Experimental demonstration of an eighteen-qubit entangled state (2\textsuperscript{18} possible states) from six individual photons by simultaneously using three degrees of freedom\textsuperscript{22} and demonstration of flexible two-qubit quantum computation from a single photon\textsuperscript{23}, highlight the potential power of associated Hilbert space with the photon in realizing higher number of qubits. This, along with the ability to engineer the quantum walk dynamics serve as a strong motivation for us to explore a resourceful way to use lesser number of qubits to realize an entangled state of a bigger system. Thus, in this work, we particularly explore the power of single qubit discrete-time quantum walk in realizing a multi-qubit computational model.

One of the main criteria for a system to be considered as a suitable candidate for universal quantum computation is its potential to realised universal set of quantum gates. A set of gates is called universal for quantum computation if it can reproduce an approximation of any \(n \geq 1\)-qubit unitary operator to an arbitrary accuracy on a quantum circuit. In general, the universal set of gates are \(\{P,H,CNOT\}\)\textsuperscript{24}, where phase (\(P\)) and Hadamard (\(H\)) are single qubit gates and controlled-NOT (\(CNOT\)) is a two qubit gate.

Quantum computing has been shown on both forms of quantum walks, i.e., continuous-time\textsuperscript{17} and discrete-time quantum walks\textsuperscript{18}, where the position space of the quantum walker represents quantum wires. They give a way of programming a quantum computer rather than modelling or mimicking one and hence do not represent the potential towards physical architecture. On the other hand our model, based on the discrete-time quantum walk, gives a physical building block to model a quantum computer on different lattice based or photonic systems. The scheme presented here maps the position basis state to the qubit state and
then performs quantum computation by mimicking gates using evolution unitaries. In this work we consider a single physical qubit with positional degrees of freedom to mimic the computational basis of a multi-qubit system. By using a set of operations used to describe the dynamics of quantum walk we show the realization of universal set of gates and a controlled-Z gate on two- and three-qubit systems using the single particle quantum walk in a position space consisting of two and four points, respectively (Sec. 2). In our scheme, the ability of the walker to hop between different points in the position space in superposition makes the realization of many non-trivial gates much simpler when compared to the circuit model of computation. We demonstrate this by presenting the scheme for realization of a simple three qubit circuit and creation of a GHZ-state. Scalability of the model, its practical relevance and some propositions for using lesser number of qubits in realizing larger qubit system are presented in Sec. 3.4. We conclude with our remarks in Sec. 4.

2 Quantum computation via discrete-time quantum walk

2.1 Discrete-time quantum walk

The dynamics of the one dimensional discrete-time quantum walk on a line are described by a walker with two internal degrees of freedom, which is defined on a combined Hilbert space $\mathcal{H}_w = \mathcal{H}_c \otimes \mathcal{H}_p$. The coin Hilbert space, $\mathcal{H}_c = \text{span}\{|0\rangle, |1\rangle\}$ represents the internal coin states and position Hilbert space, $\mathcal{H}_p = \text{span}\{|l\rangle\}$, $l \in \mathbb{Z}$ represents the number of position states available to the walker.

Evolution of each step in the walk is defined by the action of the unitary quantum coin operation followed by the position shift operation. The general form of the quantum coin operator is a non-orthogonal unitary $U$ which acts only on the coin space, and is given by,

$$\hat{C}(\tau, \xi, \zeta, \theta) = e^{i\tau} \begin{bmatrix} e^{i\xi \cos(\theta)} & e^{i\xi \sin(\theta)} \\ e^{-i\xi \sin(\theta)} & -e^{-i\xi \cos(\theta)} \end{bmatrix}. \quad (1)$$

The position shift operators $\hat{S}_-$ and $\hat{S}_+$ translate the walker to the left and right, respectively, conditioned on the internal state of the walker. They are of the form,

$$\hat{S}_-^k = \sum_{l,l' \in \mathbb{Z}} |k\rangle \langle k| \otimes |l-1\rangle \langle l| + |j \neq k\rangle \langle j| \otimes |l\rangle \langle l|,$$

$$\hat{S}_+^l = \sum_{l,l' \in \mathbb{Z}} |k \neq j\rangle \langle k| \otimes |l+1\rangle \langle l| + |j \rangle \langle j| \otimes |l\rangle \langle l|. \quad (2)$$

Here, $|k\rangle$ and $|j\rangle$ are the basis states of coin Hilbert space $\mathcal{H}_c$, i.e., $|k\rangle, |j\rangle \in \{|0\rangle, |1\rangle\}$. The operator $W_{z} = (\hat{S}_-^1 \hat{C}(\tau, \xi, \zeta, \theta_2) \otimes \mathbb{I}_p)(\hat{S}_+^0 \hat{C}(\tau, \xi, \zeta, \theta_2) \otimes \mathbb{I}_p)$ implements one step of split-step quantum walk $^{13,26}$ and the operator $W_d = (\hat{S}_-^1 \hat{C}(\tau, \xi, \zeta, \theta) \otimes \mathbb{I}_p)$ implements one step of directed quantum walk (conditioned on the state $|1\rangle$) $^{27-29}$, a variant of discrete-time quantum walk which results in non-zero probability at all of the position space it spans through while walking. The set of operators $\{\hat{S}_z^0, \hat{S}_z^1, \hat{C}(\tau, \xi, \zeta, \theta)\}$ along with the identity operator $\hat{1} = \mathbb{I}$ can be considered a generic set of operators that describes the quantum walk. We will use this set of operators for the realization of the universal quantum gates on a two- and three-qubit system by mapping the position space to the computational basis.

2.2 Universal quantum gates

The universal set of quantum gates for quantum computation comprises of two single qubit gates– Phase gate ($P$) and Hadamard gate ($H$) and one two-qubit gate– controlled-NOT gate ($CNOT$), i.e.,

$$U = \{P, H, CNOT\}$$

$$= \left\{ \begin{bmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \right\}. \quad (3)$$
The action of phase gate is given by, \( P |0\rangle = |0\rangle \) and \( P |1\rangle = e^{i\theta} |1\rangle \). The action of Hadamard gate is given by \( H |0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \) and \( H |1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \). Similarly, the action of CNOT gate is given by, \( CNOT |00\rangle = |00\rangle \), \( CNOT |01\rangle = |01\rangle \), \( CNOT |10\rangle = |11\rangle \), and \( CNOT |11\rangle = |10\rangle \), where the first qubit is the control bit and the second qubit is the target bit.

### 3 Results

#### 3.1 Quantum walk set-up for computation on two and three qubit system

The quantum walk based quantum computation scheme proposed herein uses a directed shift operation with a position dependent coin operator to realize the gate operation. To perform the operations of universal set of gates on two qubit system, the walker will execute a quantum walk on an open graph of two vertices such that walker itself will act as first qubit with two internal degrees of freedom, \( \text{span}\{ |0\rangle , |1\rangle \} \) representing the state of the first qubit. The second qubit will be represented by the position space on which the walk is performed as shown in the Fig. 1-(b). Similarly, for three qubit case, first qubit is represented by the walker’s internal degree of freedom and the remaining two qubits states are mapped on the position space. The position space is a two dimensional closed graph with four vertices and four edges, \( \text{span}\{ |00\rangle , |01\rangle , |11\rangle , |10\rangle \} \) as shown in the Fig. 1-(c), on which gate operations are performed.

In the previously known schemes \(^{17,18}\), position space (computational basis state) was used as a quantum ‘wire’ and gates required for universality were then attached to these wires. The flow of the computation from input to output was represented as a quantum walk on these wires. The computational basis states thus represented wires rather than qubits and thus these models did not admit a physical architecture straightaway. In the scheme presented here, however, the computation basis represents the
qubit and the universal gates are mimicked with the help of controlled evolution operators. As a consequence, the proposed scheme is closer to physical architecture. Direction of the flow (role of wire), is given by the shift operators (evolution operator) of directed quantum walk type. This scheme has a scope of being used for quantum computation on a system with access to position basis states e.g., photonic or lattice based system. Quantum walks in position space with sufficient control over dynamics have already been experimentally implemented for different purposes and it favours our scheme to be used in future for quantum computation due to the fact that it is simpler and straightforward.

3.2 Quantum gates on discrete-time quantum walk

Below we describe the mapping of the single particle quantum walk system to the computational basis of the two-qubit and three-qubit system. The arrow shows the forward (positive) direction of the walker. We further present the appropriate combination of shift and coin operations that describes the quantum walk and effectively implements the universal set of gates on the computational basis. In order to realize the two-qubit gates using single walker quantum walk, the mapping of the physical system to the gate implementation is done by using the walker’s coin space as the first qubit and the two points in the position as the second qubit. Similarly, mapping for the three-qubit system is done using a single particle on a four points in position space. Since we shall use only a single qubit in our scheme, most of the operations described in the rest of this work are essentially position-specific operations in the walker’s Hilbert space.

3.2.1 Phase Gate

To implement a phase gate on a quantum walk system we need only a position dependent coin operation and thus the shift operator takes the form of identity operator. For both the two-qubit and three-qubit systems, when the computational basis of the quantum walker in position space is in the desired two- or three-qubit-state, phase gate on the first (real) qubit (walker) can be applied by using phase operator as quantum coin operation, and identity operator in the position space,

$$ P = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix} \otimes \mathbb{I}_p. $$

(4)
Applying a phase operator to the second and third qubits requires the implementation of two different types of position specific identity operator separated by a phase,

$$\Phi = e^{i\phi} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes I_p \quad \text{and} \quad I = I \otimes I_p.$$  \hspace{1cm} (5)

In Fig. 2 we illustrate the mapping of two points in position space to the computation basis of the second qubit in the two-qubit system. The position dependent coin operator on the real qubit, i.e., $I$ and $\Phi$ on the space labeled $|0 \rangle$ and $|1 \rangle$, respectively, will implement the phase gate on the second qubit. Similarly, in Fig. 3, we illustrate the mapping of four points in position space to the computation basis of the second and third qubits in the three-qubit system. The position dependent coin operators $I$ and $\Phi$ on the relevant points in the position space, as shown in Fig. 3 will implement the phase gate on the second and third qubits.

### 3.2.2 Hadamard Gate

Hadamard operation on the first qubit, i.e., the coin state of the walker is given by the evolution operation,

$$W = I(\hat{C}(0,0,0,0,\pi/4) \otimes I_p) \equiv \hat{H}_1.$$  \hspace{1cm} (6)

Which is a coin operator $\hat{C}(0,0,0,0,\pi/4)$ as in equation (1) on the state of the walker followed by identity operation on position space in place of a shift operation. The subscripts of $\hat{H}$ represents the qubit on which the Hadamard operation is performed. Hadamard operation on second and third qubits in this computational basis using the single walker quantum walk can be performed by evolving the coin state of the walker in superposition of position space using the different combination of shift operators $\{S^k, S^l\}$ as given in equation (2), where $\{|k\rangle, |j\rangle\}$ are the states of the coin space, Pauli operators $\sigma_x$ and $\sigma_z$, and Hadamard operation $\hat{H}$ on the coin space of the walker. The quantum walk operations to realize Hadamard operation on second and third qubit in computational basis take the form,

$$W^0_+ |k\rangle \otimes |m\rangle = \left[ \sigma^m_x S^k_+ (\sigma_z \otimes I) \right]$$
$$W^1_+ |k\rangle \otimes |m\rangle = \left[ \sigma^m_x S^k_+ (\sigma_z \otimes I) \right]$$
$$W^0_- |j\rangle \otimes |n\rangle = \left[ \sigma^n_x S^l_- (\sigma_z \otimes I) \right]$$
$$W^1_- |j\rangle \otimes |n\rangle = \left[ \sigma^n_x S^l_- (\sigma_z \otimes I) \right]$$  \hspace{1cm} (7)

where, $\sigma^m_x = \sigma_x \otimes |m\rangle \langle m| + \mathbb{I} \otimes \sum_{l \neq m} |l\rangle \langle l|$ is the initial position state of the walker. In the equation (7), Hadamard operator is the coin operation on the first qubit for all initial states of the multi-qubit system followed by the conditional shift operator on position space.

Figs. 4 and 5 shows the mapping of the points in position to the computational basis on the second qubit of two-qubit system,
Figure 4. Schematic illustration of Hadamard operation on the computational basis of a two-qubit system using the $W$ operator (equation (6)) on a single particle quantum walk on two-point position space. On the first qubit it is the Hadamard operation and on the second qubit Hadamard operation is realized using the $\sigma_x$ and $I$ operators.

Figure 5. Schematic illustration of the Hadamard operation on the computational basis of the three-qubit system using position dependent quantum walk operators. The form $W$ of the operators involved in realization of Hadamard operation on second and third qubit are in equation (7).
When second qubit is the control and third qubit is the target in the computational basis of the three-qubit system, the position basis state is the coin basis state of the real qubit, given as $|l\rangle$ where $l$ is the position basis state and $|k\rangle$ is the coin basis state.

Similarly, as shown in the Fig. 5, one can realize the Hadamard operation on the second qubit from the two-qubit system.

$$
H_2 |k00\rangle \rightarrow W^{(k \mod 2)}_+ (\hat{H} \otimes I) |k, l = 0\rangle,
$$

$$
H_2 |k01\rangle \rightarrow W^{(k \mod 2)}_ (\hat{H} \otimes I) |k, l = 1\rangle,
$$

$$
H_2 |k11\rangle \rightarrow W^{((k+1) \mod 2)}_+ (\hat{H} \otimes I) |k, l = 2\rangle,
$$

$$
H_2 |k10\rangle \rightarrow W^{((k+1) \mod 2)}_ (\hat{H} \otimes I) |k, l = 3\rangle
$$

and

$$
H_3 |k00\rangle \rightarrow W^{(k \mod 2)}_+ (\hat{H} \otimes I) |k, l = 0\rangle,
$$

$$
H_3 |k01\rangle \rightarrow W^{((k+1) \mod 2)}_ (\hat{H} \otimes I) |k, l = 1\rangle,
$$

$$
H_3 |k11\rangle \rightarrow W^{((k+1) \mod 2)}_+ (\hat{H} \otimes I) |k, l = 2\rangle,
$$

$$
H_3 |k10\rangle \rightarrow W^{((k+1) \mod 2)}_ (\hat{H} \otimes I) |k, l = 3\rangle
$$

where $|k\rangle$ is the coin basis state of the real qubit, given as $\text{span} \{ |0\rangle, |1\rangle \}$. Here $l$ are the labels to the points in the position space in a clockwise direction, as illustrated in Fig. 1-(c).

### 3.2.3 Controlled-NOT Gate

This gate can be engineered by evolving the state of the walker using evolution operator which consists of identity coin operator followed by a position dependent shift operator. The shift operator can be either $S^x_1$ or $S^z_1$ as given in equation (2) when the coin space is the control and position space (corresponding computational basis) is the target. But when the real qubit, i.e., coin space is the target, and position space is the control qubit, then the position-dependent coin operation $\hat{C}(0, 0, \pi/2) \equiv \sigma_x$ followed by the identity shift operator will give controlled-NOT operation implementation on computational basis using single walker. This is schematically illustrated for the two-qubit system in Fig. 6.

When second qubit is the control and third qubit is the target in the computational basis of the three-qubit system, the position dependent conditional shift operator $S^x_1 S^z_1$ and $S^z_1 S^z_1$ on the position space with identity operator on coin space implements the CNOT gate. A similar architecture may be designed for third qubit as control and second as target. These implementations and the corresponding single particle quantum walk operators are schematically illustrated in Fig. 7.

### 3.2.4 Toffoli Gate

This gate can only be realized for a system with three or more qubits. We demonstrate a possible realization of this gate for a three-qubit system. When the first and second qubits are the controls and the third is the target, realization of this gate simply requires conditional shift operations, given by the shift operator $S^z_1$, as defined in equation (2). The shift operators are to be applied on certain position basis states only, and other position basis states are simply operated upon by the identity operator. The corresponding scheme is schematically illustrated in Fig. 8.

The Fredkin gate is a controlled swap operation, and closely resembles the Toffoli gate in its implementation. In case when the first or third qubit are the target and other one is the control qubit, these operations for its realization can be worked out exactly the same way as described for the corresponding Toffoli gate.

### 3.2.5 Controlled-Z gate

In a two-qubit system, controlled-Z gate is closely related to the phase gate, and is implemented exactly like the phase gate applied to the second qubit in the position space, as illustrated in Fig. 2. The only distinction in the realization of these two gates is that in the controlled-Z gate, the parameter $\phi$ is fixed, so that $\phi = \pi$.

In a three-qubit system, this gate can be implemented by using the position dependent application of the phase operator $P$ on some position basis states and identity operator on the others. It is also observed that the implementation of this gate is symmetric, i.e., the implementation of the gate between the $i^{th}$ and $j^{th}$ qubits is the same as the implementation between the $j^{th}$ and $i^{th}$ qubits, where $i, j = 1, 2, 3$, and $i \neq j$. As in the case of a two-qubit system, the parameter $\phi$ is fixed to $\pi$.

In case the gate is applied between the second and third qubits, the scheme can be implemented by using just two kinds of
Figure 6. Schematic illustration of the controlled-NOT gate on the computational basis of two-qubit system using a single particle quantum walk on two point position space using position-dependent coin operation on the real qubit. Form of the shift operator $S^1_\pm$ is given in equation (2).

Figure 7. Schematic illustration of the controlled-NOT gate on the computational basis of three-qubit system using position-dependent quantum walk operators. Form of the shift operator $S^1_\pm$ is given in equation (2).
The identity operators, separated by a phase of $\pi$. The identity with the phase $e^{i\pi I \otimes I_p}$ is applied only to one position state, whereas all the other states are acted upon by the identity operator $I \otimes I_p$. This is schematically illustrated in Fig. 9.

3.3 Circuit implementation on quantum walk based computation setup

Any two or three qubit circuit can be implemented very easily on this scheme. In Fig. 10, a simple three qubit circuit and the quantum walk scheme to implement those same gates to get the same output result is shown. The input state for this circuit is $|\Psi\rangle_{in} = |000\rangle$ and the output is $|\Psi\rangle_{out} = \frac{1}{2} \left( |000\rangle + |011\rangle + |100\rangle + |111\rangle \right)$. The quantum walk-based scheme can implement the circuit shown in three steps. The first step would be the coin operator followed by shift operator of the form $W^0$ to get Hadamard on the second qubit, the second step would be coin operation $\hat{C}(0, 0, 0, \pi/4)$ followed by identity shift operation to get Hadamard on first qubit and the third step would be identity on coin state followed by position dependent shift operation $S_1^+ S_1^- S_0^+$ on position state $|10\rangle$ to get CNOT-operation, where the coin operator $\hat{C}$ has been defined in equation (1), the $S_1^+$ in equation (2) and $W^0$ in equation (8).

The scheme can help in reducing the time complexity for some circuits. One example is the circuit for preparing GHZ state, the complexity reduces by one step. Fig. 11 shows a three qubit circuit to create a GHZ-state and simplified implementation on quantum walk scheme. Notice that unlike the circuit model, which requires the application of three gates, the quantum walk can achieve the output in only two steps.

The quantum walk operation for creation of GHZ in computational basis is quite straightforward. For instance, a walker prepared in the state $|000\rangle$, upon being subjected to two steps of quantum walk can create a GHZ state. The first step would be the coin operator $\hat{C}(0, 0, 0, \pi/4)$ followed by $S_1^+$ shift operator and the second step would be identity on coin state followed by
Figure 10. Quantum circuit on three qubit system and equivalent quantum walk scheme to implement same circuit is illustrated. Red circle represents $|0\rangle$ of the real particle and green circle represents $|1\rangle$ of the real particle. The input state is $|\Psi_{in}\rangle = |000\rangle$ and output state is a superposition of four states $|\Psi_{out}\rangle = \frac{1}{2} (|000\rangle + |011\rangle + |100\rangle + |111\rangle)$. $CNOT_{23}$ is a position dependent shift operation given by $\hat{S}_0\hat{S}_1^i$ at position $|01\rangle$ and identity at other states.

Figure 11. Quantum circuit to create GHZ-state on three qubit system and equivalent quantum walk scheme to obtain GHZ-state is illustrated. Red circle represents $|0\rangle$ of the real particle and green circle represents $|1\rangle$ of the real particle. Here the QW-based scheme is more simplified compared to quantum circuit implementation. The input state is $|\Psi_{in}\rangle = |000\rangle$ and output state is a GHZ-state $|\Psi_{out}\rangle = \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle)$.
Figure 12. An illustration of scaling of three-qubit equivalent system to N-qubit system. Multiple closed graphs of four vertices equivalent to two qubit can be used to extended the quantum walk based universal quantum computer physically. Red solid circle is represents $|0\rangle$ of the real particle.

$S_1^+$ shift operator, where the coin operator $\hat{C}$ has been defined in equation (1) and the $S_1^+$ in equation (2). The sequence of steps, when executed will create the state $\frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$.

### 3.4 Scalability of the scheme

The scheme can be scaled up to larger number of qubit by multiple ways. Basic structure should follow Fig. 1 which systematically demonstrates the mapping of real qubit and its presence in superposition of position space to the multi-qubit computational basis. Extending the same scheme to higher dimensions to represent larger qubit systems is one way of extending the scheme to multi-qubit computation is one straight forward option. A single walker can perform universal computation on multi-qubit system with the help of multiple closed graphs of four vertices in tensor product as shown in Fig. 12. With an increase in number of qubits, different levels of two-qubit equivalent graphs can be added to the system. Each level communicates with different levels with the help of appropriate unitary evolution operators which are the extension of the operators presented for one-dimensional walk in Section 2. For example, if a gate is implemented on the fourth qubit, then walk is performed by the real qubit on the second level of the graph. In such case, we will apply identity on every other level and perform walk on the second level. E.g., if Hadamard operation is applied on the fourth qubit of the five qubit system, one will need two levels of closed graph such that the qubit state is given by $|\phi_2\rangle \otimes |\phi_1\rangle \otimes |\phi_2\rangle$. If the initial state of the walker is $|00000\rangle$ then the equivalent state on quantum walk scheme would be $|0\rangle \otimes |00\rangle \otimes |00\rangle$, then applying $H_2$ from equation (8) on the second level and identity on the first level will give Hadamard operation on fourth qubit,

$$H_2 |0000\rangle = (I_1 \otimes W^0)(H_1 \otimes I_1 \otimes I_2).$$

(10)

Similarly, in this way, this scheme can be used to implement multi-qubit computation using quantum walk. However, this scaling scheme is not unique and we can have different other possibilities of scaling on this scheme of computation. Some of the other possibilities are given in Figs. 13 and 14.

Scaling onto a four-qubit system can be realized by either considering two qubit quantum walkers on a four point position space, or a single quantum walker on an eight point position space as shown in Fig. 14 and Fig. 13, respectively. Similarly, a
Figure 13. Illustration of an extension of position space mapping of three-qubit system to four-qubit system by connecting two three-qubit models position state by two edges. This is one of the many ways to multiply qubits for quantum walk based computational scheme.

Figure 14. An illustration of the implementation of a three-qubit (eight point) position space for higher-qubit operations.

A five-qubit system may be realized by a system of two quantum walkers on an eight point position space. In a system described as such, there will be two real qubits and three qubits will be realized by superposition in the position space. An alternate realization of a five-qubit state can also be a three-particle quantum walk on a four point position state. A subtle point to be made in using the eight point position space with each vertex connected to three other vertices is that the set of shift operators required needs to be expanded to include operators that make the walker choose a certain path. This is required because the set of universal gates can only act on a maximum of two qubit states at a time and thus, each point in the position space must be connected to either one or two other points. Therefore, on an eight point position space, the shift operator at each position must have three different variants which at a time can create the required superposition between two points in position space. Different architectures with well connected or limited connection can be further engineered to expand the scheme. The configuration of the position space, connectivity and the ability to define the shift operators to transfer the real qubit across position plays a crucial role in defining the operations of the larger qubits system.

4 Discussion and Conclusion

By using the provision of engineering the presence of a single particle (walker) in superposition of position space using discrete-time quantum walk, we have demonstrated the realization of universal quantum gates in a multi-qubit system. The main idea in this work is to demonstrate the effective use of controlled evolution of particle on the position space and mapping the states of the system to the computational basis. We have presented different constructions to show that the scheme can be scaled up to realize higher number of computational basis but an efficient scaling scheme needs some work. Scaling using combination of extended position space and a real qubit can be used to realize large dimensional computation basis. For larger computational basis, if only one real qubit is considered, the position space required quickly scales up. Therefore, a scheme
of multi particle quantum walk on extended position space could be more effective way to scale up scheme. Although the realization of Hadamard operation on computational basis looks a bit involved in the presented scheme, we can see that the gates like CNOT and Toffoli are more easily realizable. While this work presents some tasks realizable by this framework, they are by no means exhaustive, and only provide a small glimpse into the possibilities of this scheme. With many experimental implementations of quantum walks in lattice based and photonic systems being reported, the idea from our scheme might motivate a new quantum computer architecture based on hopping of quantum particle in superposition of position space (lattice). Our scheme exploring the power of single qubit in superposition of position space can immediately drive towards controlled engineering of quantum states and quantum simulations of sizable quantum system using fewer qubits.

Quantum walks have been implemented on ion-traps \cite{30-33}, photonic systems \cite{34-37} and trapped atoms \cite{38,39}. Quantum walk on a well-defined quantum systems with access to one dimensional closed graphs will be well suited to realize two and three qubit systems presented in this work. The experimental set-up for scaling needs multiple levels of one-dimensional closed graph to map to the many-particle states and position dependent evolution operators to implement quantum gates. Implementing any gate requires only few steps of quantum walk which are realizable but implementing a complete circuit requires number of steps almost equivalent to the number of gates in the circuit. This implies that the scheme presented by us can be very well be used for quantum computation of small circuits implemented on near-term quantum devices. Limitations with realizability of the required shift operators could be seen as an equivalent to the restricted connectivity we are seeing in the current available quantum processors. Increasing the size of the Hilbert Space accessible without increasing the number of real qubits required for implementation is the key in the demonstrated protocol.

5 Methods

In the quantum walk scheme, gate operation is performed with the help of the evolution operations and initial state can be defined by the initial state of the quantum walker. The direction of the quantum walk during the circuit operation is defined by the directed walk evolution operator. The walker remains at the initial position state with certain probability based on the form of coin operator, and moves with certain probability in either forward or backward direction based on the shift operation given by equation (2).

References

1. Riazanov, G. V. The feynman path integral for the dirac equation. *Sov. J. Exp. Theor. Phys.* 6, 1107, DOI: http://www.jetp.ac.ru/cgi-bin/r/index/r33/6/p1437?a=list (1958).
2. Feynman, R. P. Quantum mechanical computers. *Found. physics* 16, 507–531, DOI: http://link.springer.com/article/10.1007 (1986).
3. Aharonov, Y., Davidovich, L. & Zagury, N. Quantum random walks. *Phys. Rev. A* 48, 1687, DOI: http://dx.doi.org/10.1103/PhysRevA.48.1687 (1993).
4. Meyer, D. A. From quantum cellular automata to quantum lattice gases. *J. Stat. Phys.* 85, 551–574, DOI: https://link.springer.com/article/10.1007/BF02199356 (1996).
5. Farhi, E. & Gutmann, S. Quantum computation and decision trees. *Phys. Rev. A* 58, 915, DOI: https://doi.org/10.1103/PhysRevA.58.915 (1998).
6. Yin, Y., Katsanos, D. E. & Evangelou, S. N. Quantum walks on a random environment. *Phys. Rev. A* 77, 022302, DOI: https://doi.org/10.1103/PhysRevA.77.022302 (2008).
7. Kempe, J. Quantum random walks: an introductory overview. *Contemp. Phys.* 44, 307–327, DOI: http://www.tandfonline.com/doi/abs/10.1080/0010751031000110776 (2003).
8. Venegas-Andraca, S. E. Quantum walks: a comprehensive review. *Quantum Inf. Process.* 11, 1015–1106, DOI: https://link.springer.com/article/10.1007%2Fs11128-012-0432-5 (2012).
9. Nayak, A. & Vishwanath, A. Quantum walk on the line. *arXiv preprint quant-ph/0010117* DOI: https://arxiv.org/abs/quant-ph/0010117 (2000).
10. Inui, N., Konno, N. & Segawa, E. One-dimensional three-state quantum walk. *Phys. Rev. E* 72, 056112, DOI: https://doi.org/10.1103/PhysRevE.72.056112 (2005).
11. Mohseni, M., Rebentrost, P., Lloyd, S. & Aspuru-Guzik, A. Environment-assisted quantum walks in photosynthetic energy transfer. *The J. chemical physics* 129, 11B603, DOI: https://aip.scitation.org/doi/10.1063/1.3002335 (2008).
12. Godoy, S. & Fujita, S. A quantum random-walk model for tunneling diffusion in a 1d lattice. a quantum correction to fick’s law. *The J. chemical physics* 97, 5148–5154, DOI: https://aip.scitation.org/doi/10.1063/1.463812 (1992).
13. Kitagawa, T., Rudner, M. S., Berg, E. & Demler, E. Exploring topological phases with quantum walks. *Phys. Rev. A* **82**, 033429, DOI: https://journals.aps.org/pra/abstract/10.1103/PhysRevA.82.033429 (2010).

14. Chandrashekar, C. M. Disordered-quantum-walk-induced localization of a bose-einstein condensate. *Phys. Rev. A* **83**, 022320, DOI: https://journals.aps.org/pra/abstract/10.1103/PhysRevA.83.022320 (2011).

15. Chandrashekar, C. M. Two-component dirac-like hamiltonian for generating quantum walk on one-, two-and three-dimensional lattices. *Sci. reports* **3**, 1–10, DOI: https://www.nature.com/articles/srep02829 (2013).

16. Mallick, A., Mandal, S. & Chandrashekar, C. M. Neutrino oscillations in discrete-time quantum walk framework. *The Eur. Phys. J. C* **77**, 1–11, DOI: https://link.springer.com/article/10.1140%2Fepjc%2Fs10052-017-4636-9 (2017).

17. Childs, A. M. Universal quantum computation by quantum walk. *Phys. review letters* **102**, 180501, DOI: https://doi.org/10.1103/PhysRevLett.102.180501 (2009).

18. Lovett, N. B., Cooper, S., Everitt, M., Trevers, M. & Kendon, V. Universal quantum computation using the discrete-time quantum walk. *Phys. Rev. A* **81**, 042330, DOI: https://doi.org/10.1103/PhysRevA.81.042330 (2010).

19. Hoyer, S. & Meyer, D. A. Faster transport with a directed quantum walk. *Phys. Rev. A* **79**, 024307, DOI: https://doi.org/10.1103/PhysRevA.79.024307 (2009).

20. Travaglione, B. C. & Milburn, G. J. Implementing the quantum random walk. *Phys. Rev. A* **65**, 032310, DOI: https://doi.org/10.1103/PhysRevA.65.032310 (2002).

21. Schmitz, H. et al. Quantum walk of a trapped ion in phase space. *Phys. review letters* **103**, 090504, DOI: https://doi.org/10.1103/PhysRevLett.103.090504 (2009).

22. Schreiber, A. et al. Photons walking the line: a quantum walk with adjustable coin operations. *Phys. review letters* **104**, 050502, DOI: https://doi.org/10.1103/PhysRevLett.104.050502 (2010).

23. Peruzzo, A. et al. Quantum walks of correlated photons. *Science* **329**, 1500–1503, DOI: 10.1126/science.1193515 (2010).
37. Xue, P., Qin, H., Tang, B. & Sanders, B. C. Observation of quasiperiodic dynamics in a one-dimensional quantum walk of single photons in space. *New J. Phys.* **16**, 053009, DOI: https://iopscience.iop.org/article/10.1088/1367-2630/16/5/053009/meta (2014).

38. Karski, M. *et al.* Quantum walk in position space with single optically trapped atoms. *Science* **325**, 174–177, DOI: 10.1126/science.1174436 (2009).

39. Preiss, P. M. *et al.* Strongly correlated quantum walks in optical lattices. *Science* **347**, 1229–1233, DOI: 10.1126/science.1260364 (2015).

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**Author contributions statement**

C.M.C. designed the study, and S.S. and P.C. carried out the further work under the guidance of C.M.C. and prepared the figures. S.S., P.C., A.S. and C.M.C. together wrote the manuscript.

**Data Availability**

All data generated or analysed during this study are included in this article itself.

**Competing Interests**

The authors declare no competing interests.