Universal quantum entangling gates are a crucial building block in the large-scale quantum computation and quantum communication, and it is an important task to find simple ways to implement them. Here an effective quantum circuit for the implementation of a controlled-NOT (CNOT) gate is constructed by introducing a non-computational quantum state in the auxiliary space. Furthermore, the method is extended to the construction of a general n-control-qubit Toffoli gate with (2n − 1) qubit–qudit gates and (2n − 2) single-qudit gates. Based on the presented quantum circuits, the polarization CNOT and Toffoli gates with linear optics are designed by operating on the spatial-mode degree of freedom of photons. The proposed optical schemes can be achieved with a higher success probability and no extra auxiliary photons are needed.

1. Introduction

Multi-qubit quantum entangling gates have complex structures and play an important role in quantum computing, quantum algorithms, quantum communication, cryptography, etc. In theory, multi-qubit quantum gates can be realized by sequences of two-qubit gates and single-qubit gates in a quantum circuit model. The cost (also called complexity) of the quantum circuits usually is measured by the number of the two-qubit entangled gates involved in the quantum circuit, because they introduce more imperfections and more demands than the single-qubit gates. However, when the cost of a quantum circuit is high, it is difficult to perform the experiments because of the low computing fidelity and limited coherence time. Moreover, the cost of a universal quantum circuit increases exponentially with the accumulation of the number of qubits. The theoretical lower bound for simulating an n-qubit universal quantum circuit is (4^n − 3n − 1)/4 controlled-NOT (CNOT) gates in a qubit system. Hence, it is crucial to find an effective method for building a universal quantum circuit in the simplest possible way.

Several matrix decomposition techniques have been introduced to optimize a large-scale quantum circuit. Two-qubit universal quantum circuits have also been constructed with the lowest cost (resources) in qubit systems. However, there is still a gap between the current best result and the theoretical lower bound for a multi-qubit universal quantum circuit. Fortunately, Ralph et al. found that the quantum circuit may be optimized further by using higher-dimensional Hilbert spaces, and this proposal was later experimentally demonstrated in optical and superconducting systems. Following this, Liu et al. reduced the cost of the n-qubit universal circuit to (5/16) × 4^n − (5/4) × 2^n + 2n CNOT gates when n was even and (5/16) × 4^n − 2^n + 2(n − 1) CNOTs when n was odd. Liu et al. simplified a Fredkin gate from eight CNOTs to five CNOTs or three qubit–qudit gates. In addition, higher-dimensional quantum systems have also been studied and applied in quantum computing, quantum communication, and quantum metrology.

The Toffoli (controlled-controlled-NOT) gate, a three-qubit conditional operation, is one of the most popular universal multi-qubit quantum gates. It is also an essential component in complex quantum algorithms and quantum error correction and quantum fault tolerance. In 1995, Barenco et al. proposed a concrete construction of a three-qubit Toffoli gate with five two-qubit entangled gates. When two-qubit gates are restricted to CNOT gates, the optimal cost of a Toffoli gate increases to six. In 2013, Yu et al. confirmed that the minimum resource for simulating a three-qubit Toffoli gate is...
Figure 1. Synthesis of a CNOT gate. The single-qutrit \( X_A \) gate implements the transformation \( |1\rangle \rightarrow |2\rangle \). The controlled node \( \otimes \) is turned on for the input \(|0\rangle\) or \(|1\rangle\). That is, a swap operation is applied to \( c \) and \( t \), and if and only if, the control qubit \( c \) is in the state \(|0\rangle\) or \(|1\rangle\). \( H \) is a single-qubit Hadamard gate to achieve operations \(|0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\) and \(|1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)\). \( \sigma_x \) completes \( \sigma_x|0\rangle = |0\rangle \) and \( \sigma_x|1\rangle = -|1\rangle \).

is five two-qubit gates. In 2020, Kiktenko et al.\(^{[65]}\) constructed a generalized \( m \)-qubit Toffoli gate with \((2m - 3)\) CNOTs based on qutrits. Independent of the standard decomposition-based approach, the realization of Toffoli gate has been proposed theoretically and implemented experimentally in superconducting circuits,\(^{[35,59]}\) linear optics,\(^{[34,42,66-68]}\) trapped ions,\(^{[69]}\) atoms\(^{[70,71]}\) and quantum dots.\(^{[72]}\)

Ralph et al.\(^{[31,34]}\) first proposed an interesting scheme for synthesizing a Toffoli gate using three qubit–qudit CNOT gates and two single-qutrit \( X_a \) gates. The main idea of the works in Refs. \([33,34]\) was to extend temporally the higher-dimensional subspaces on one of the controlled qubit carriers and then perform corresponding logical operations. Using the same method as Refs. \([33,34]\), in this paper, we propose an alternative scheme to implement the CNOT and Toffoli gates based on the partial-swap (P-SWAP) gates using higher-dimensional spaces. Specifically, \((2n - 1)\) qubit–qudit and \((2n - 2)\) single-qutrit gates are required to implement an \( n \)-control-qubit Toffoli gate. In addition, using the spatial-mode degree of freedom (DOF) of the single-photon, we design a feasible optical architecture for implementing CNOT and Toffoli gates with linear optics. Our proposals have several other advantages: i) Our optical implementation of the CNOT gate does not require an extra entangled photon pair or a single-photon, and the success probability of the gate is enhanced. ii) Linear optical Toffoli gates can be constructed with a higher success probability than other existing optical schemes.\(^{[33,34,73]}\) iii) Our schemes are simple and feasible with the current technology.

2. Construction of CNOT and Toffoli Gates with Higher-Dimensional Spaces

2.1. Synthesis of a CNOT Gate Using Qutrits

A CNOT gate with two P-SWAP gates using qutrits is shown in Figure 1. The qubit qutrits are encoded on two computational states, \(|0\rangle\) and \(|1\rangle\). The single-qutrit \( X_A \) gate provides a 3D subspace on the control qubit. In the following, we describe the construction process of our protocol in detail.

Suppose that the state of the system is initially

\[
|\phi_0\rangle = \alpha_1|0\rangle|0\rangle + \alpha_2|0\rangle|1\rangle + \alpha_3|1\rangle|0\rangle + \alpha_4|1\rangle|1\rangle
\]

where \( \alpha_i \) (\( i = 1, 2, 3, 4 \)) are complex coefficients that satisfy the normalization condition \( \sum_{i=1}^{4} |\alpha_i|^2 = 1 \). Subscripts \( c \) and \( t \) denote the control and target qubits, respectively.

First, qubit \( c \) undergoes a single-qutrit gate \( X_a \), which introduces an ancillary state \(|2\rangle\) on \( c \) and completes the transformations \(|1\rangle \leftrightarrow |2\rangle \) and \(|0\rangle \leftrightarrow |0\rangle\). After the \( X_A \) gate and a Hadamard \((H)\) gate are applied to \( c \) and \( t \), the initial state \(|\phi_0\rangle\) is changed to

\[
|\phi_1\rangle = \frac{1}{\sqrt{2}} \left[ \alpha_1|0\rangle(|0\rangle + |1\rangle) + \alpha_2|0\rangle(|0\rangle - |1\rangle) + \alpha_3|2\rangle(|0\rangle + |1\rangle) + \alpha_4|2\rangle(|0\rangle - |1\rangle) \right]
\]

Second, a P-SWAP gate is applied to \( c \) and \( t \), and it transforms \(|\phi_1\rangle\) into

\[
|\phi_2\rangle = \frac{1}{\sqrt{2}} \left[ \alpha_1(|0\rangle + |1\rangle)|0\rangle + \alpha_2(|0\rangle - |1\rangle)|0\rangle + \alpha_3|2\rangle(|0\rangle + |1\rangle) + \alpha_4|2\rangle(|0\rangle - |1\rangle) \right]
\]

Here, the P-SWAP gate performs a swap operation only between two computational states \(|0\rangle\) and \(|1\rangle\), that is,

\[
\begin{align*}
|00\rangle & \rightarrow |00\rangle, \\
|01\rangle & \rightarrow |10\rangle, \\
|10\rangle & \rightarrow |01\rangle, \\
|11\rangle & \rightarrow |11\rangle,
\end{align*}
\]

Third, a \( \sigma_x \) operation acts on \( t \) to change \(|\phi_2\rangle\) to

\[
|\phi_3\rangle = \frac{1}{\sqrt{2}} \left[ \alpha_1(|0\rangle + |1\rangle)|0\rangle + \alpha_2(|0\rangle - |1\rangle)|0\rangle + \alpha_3|2\rangle(|0\rangle + |1\rangle) + \alpha_4|2\rangle(|0\rangle - |1\rangle) \right]
\]

Finally, after the P-SWAP gate, the \( X_A \) gate and \( H \) operation are applied to \( c \) and \( t \) again, \(|\phi_3\rangle\) is changed to

\[
|\phi_4\rangle = \alpha_1|0\rangle|0\rangle + \alpha_2|0\rangle|1\rangle + \alpha_3|1\rangle|1\rangle + \alpha_4|1\rangle|0\rangle
\]

From Equations (1)–(6), one can see that a CNOT gate is completed by Figure 1, and such a construction can be achieved in linear optics with a high success probability and without additional photons (see Section 3).

2.2. Construction of the Toffoli Gates with Higher-Dimensional Spaces

2.2.1. Synthesis of Three-Qubit Toffoli Gate Using Qutrits

Based on the CNOT and P-SWAP gates, the process for implementing a three-qubit Toffoli gate with 4D space is presented in Figure 2.
Figure 2. Simplified synthesis of a three-qubit Toffoli gate with two P-SWAP and one CNOT gates. As shown in Figure 1, the operations in the dotted rectangle are a CNOT gate.

Considering an arbitrary normalization three-qubit initial state

\[
|\psi_0\rangle = \alpha_1|0_1\rangle|0_2\rangle|0_3\rangle + \alpha_2|0_1\rangle|0_2\rangle|1_3\rangle + \alpha_3|1_1\rangle|0_2\rangle|0_3\rangle + \alpha_4|1_1\rangle|0_2\rangle|1_3\rangle
\]

(7)

First, the \( X_a \) gate acts on \( c_2 \) to achieve \( |1_1\rangle \rightarrow |2_1\rangle \) and \( |0_2\rangle \rightarrow |0_2\rangle \). After the first P-SWAP gate is executed on \( c_1 \) and \( c_2 \), \(|\psi_0\rangle\) becomes

\[
|\psi_1\rangle = \alpha_1|0_1\rangle|0_2\rangle|0_3\rangle + \alpha_2|0_1\rangle|0_2\rangle|1_3\rangle + \alpha_3|1_1\rangle|0_2\rangle|0_3\rangle + \alpha_4|1_1\rangle|0_2\rangle|1_3\rangle + \alpha_5|0_1\rangle|1_2\rangle|0_3\rangle + \alpha_6|0_1\rangle|1_2\rangle|1_3\rangle + \alpha_7|1_1\rangle|1_2\rangle|0_3\rangle + \alpha_8|1_1\rangle|1_2\rangle|1_3\rangle
\]

(8)

Second, a CNOT gate is applied to \( c_1 \) and \( t \) (which can be achieved by the circuit in the dotted rectangle), resulting in

\[
|\psi_2\rangle = \alpha_1|0_1\rangle|0_2\rangle|0_3\rangle + \alpha_2|0_1\rangle|0_2\rangle|1_3\rangle + \alpha_3|1_1\rangle|0_2\rangle|0_3\rangle + \alpha_4|1_1\rangle|0_2\rangle|1_3\rangle + \alpha_5|0_1\rangle|1_2\rangle|0_3\rangle + \alpha_6|0_1\rangle|1_2\rangle|1_3\rangle + \alpha_7|1_1\rangle|1_2\rangle|0_3\rangle + \alpha_8|1_1\rangle|1_2\rangle|1_3\rangle
\]

(9)

Finally, the P-SWAP and \( X_2 \) gates are applied again. The two operations induce \(|\psi_3\rangle\) as the final state

\[
|\psi_3\rangle = \alpha_1|0_1\rangle|0_2\rangle|0_3\rangle + \alpha_2|0_1\rangle|0_2\rangle|1_3\rangle + \alpha_3|1_1\rangle|0_2\rangle|0_3\rangle + \alpha_4|1_1\rangle|0_2\rangle|1_3\rangle + \alpha_5|0_1\rangle|1_2\rangle|0_3\rangle + \alpha_6|0_1\rangle|1_2\rangle|1_3\rangle + \alpha_7|1_1\rangle|1_2\rangle|0_3\rangle + \alpha_8|1_1\rangle|1_2\rangle|1_3\rangle
\]

(10)

From Equations (7)–(10), one can see that a three-qubit Toffoli gate can be simulated using three nearest-neighbor qubit–qudit gates and two single-qudit gates.

2.2.2. Synthesis of \( n \)-Control-Qubit Toffoli Gate Using Qudits

Using a higher-dimensional space, the method can be applied to any multi-qubit Toffoli gate. As shown in Figure 3, an \( n \)-control-qubit Toffoli gate is constructed with \((2n - 1)\) qubit–qudit and \((2n - 2)\) single-qudit gates, which flips the target qubit states \( |0\rangle \) and \(|1\rangle \) if and only if the \( n \) control-qubits are all \(|1\rangle \). Here, single-qudit gates \( X_0, X_1, \ldots, X_n \) create multi-level qudits on \( c_n \) and complete transformations \(|0_0\rangle \leftrightarrow |2_0\rangle, |1_1\rangle \leftrightarrow |3_1\rangle, |0_2\rangle \leftrightarrow |4_2\rangle, \ldots, |0_n\rangle \leftrightarrow |2_n\rangle, |1_n\rangle \leftrightarrow |3_n\rangle, |0_0\rangle \leftrightarrow |4_0\rangle, \ldots, |1_n\rangle \leftrightarrow |3_n\rangle \) when \( n \) is even or \(|0_n\rangle \leftrightarrow |2_n\rangle, |1_n\rangle \leftrightarrow |3_n\rangle, |0_0\rangle \leftrightarrow |4_0\rangle, \ldots, |1_n\rangle \leftrightarrow |3_n\rangle \) when \( n \) is odd. These single-qudit gates can temporarily expand the 2D space of \( c_i \) to an \((n+1)\)-dimensional subspace. All CNOT and P-SWAP gates act on computational states \(|0\rangle \) and \(|1\rangle \). The synthesis requires only \( O(n) \) qubit–qudit gates and the low-cost advantage is more evident in our scheme as the number of qubits increases.

3. Implementation of CNOT and Toffoli Gates with Linear Optics

3.1. Implementation of a Post-Selected P-SWAP Gate with Linear Optics

In the previous section, we proposed the simulation of CNOT and Toffoli gates based on P-SWAP gates and auxiliary higher-dimensional spaces. In an optical system, two computational states can be encoded on the polarization DOF of a single photon in the spatial-mode \( i \), that is, \(|0\rangle \equiv |H_i\rangle \) and \(|1\rangle \equiv |V_i\rangle \). Here, \( H \) and \( V \) represent the horizontal and vertical polarized components, respectively. The higher-dimensional state can be encoded on the \( V \)-polarized component in a new spatial-mode \( i' \), that is, \(|2\rangle \equiv |V_{i'}\rangle \). The qudit operation \( X_{i'} \) can be achieved by employing a polarizing beam splitter (PBS), which reflects the \( V \)-polarized component and transmits the \( H \)-polarized component, respectively. Before describing the implementation of the CNOT gate,
we first detail the step-by-step construction of the P-SWAP gate with linear optical elements.

As shown in Figure 4, the injected photon 1 is divided into $H$-polarized component and $V$-polarized component by a PBS. The $H$-polarized component passes into the spatial-mode $1_{in}$, which is encoded on $|H\rangle_{1_{in}} \equiv |0\rangle$ (and $V$-polarized component in the spatial-mode $1_{in}$ is encoded on $|V\rangle_{1_{in}} \equiv |1\rangle$), while the $V$-polarized component is reflected into another spatial-mode $1_{in}$, which is encoded on $|V\rangle_{1_{in}} \equiv |2\rangle$. The photon 2 from the spatial-mode $2_{in}$ is encoded on $|H\rangle_{2_{in}} \equiv |0\rangle$ (and $V$-polarized component in the spatial-mode $2_{in}$ is encoded on $|V\rangle_{2_{in}} \equiv |1\rangle$). A general injected photon state can be considered as

\[
|\varphi_{0}\rangle = \left( a_{1_{in}} \hat{a}_{H_{in}}^\dagger + a_{2_{in}} \hat{a}_{H_{in}}^\dagger + a_{3_{in}} \hat{a}_{V_{in}}^\dagger + a_{4_{in}} \hat{a}_{V_{in}}^\dagger \right) |\text{vac}\rangle.
\]

Here $|\text{vac}\rangle$ is the state vector of vacuum.

First, PBS$_1$ and PBS$_2$ transmit the $H$-photons into modes 1 and 3 to interact with half-wave plates HWP$^{45^\circ}$ and HWP$^{22.5^\circ}$ and reflect the $V$-photons into modes 2 and 4 to interact with HWP$^{45^\circ}$ and HWP$^{67.5^\circ}$. Here, HWP$^{45^\circ}$ is a half-wave plate set to $45^\circ$ and achieves the qubit-flip operation $\hat{a}_{H} \rightarrow \hat{a}_{V}$. HWP$^{22.5^\circ}$ completes the transformations

\[
\hat{a}_{H} \overset{\text{HWP}^{22.5^\circ}}{\rightarrow} \frac{1}{\sqrt{2}}(\hat{a}_{H}^\dagger + \hat{a}_{V}^\dagger), \quad \hat{a}_{V} \overset{\text{HWP}^{22.5^\circ}}{\rightarrow} \frac{1}{\sqrt{2}}(\hat{a}_{H}^\dagger - \hat{a}_{V}^\dagger)
\]

HWP$^{67.5^\circ}$ results in

\[
\hat{a}_{H} \overset{\text{HWP}^{67.5^\circ}}{\leftrightarrow} \frac{1}{\sqrt{2}}(\hat{a}_{H}^\dagger + \hat{a}_{V}^\dagger), \quad \hat{a}_{V} \overset{\text{HWP}^{67.5^\circ}}{\leftrightarrow} \frac{1}{\sqrt{2}}(\hat{a}_{H}^\dagger - \hat{a}_{V}^\dagger)
\]

The above operations, PBS$_1$ $\rightarrow$ HWP$^{45^\circ}$ (HWP$^{45^\circ}$) and PBS$_2$ $\rightarrow$ HWP$^{22.5^\circ}$ (HWP$^{67.5^\circ}$) cause $|\varphi_{0}\rangle$ to become

\[
|\varphi_{1}\rangle = \frac{1}{\sqrt{2}} \left[ a_{1_{in}} \hat{a}_{V_{in}}^\dagger (\hat{a}_{H_{in}}^\dagger + \hat{a}_{V_{in}}^\dagger) + a_{2_{in}} \hat{a}_{H_{in}}^\dagger (\hat{a}_{H_{in}}^\dagger + \hat{a}_{V_{in}}^\dagger) \right. \\
+ a_{3_{in}} \hat{a}_{V_{in}}^\dagger (\hat{a}_{V_{in}}^\dagger + \hat{a}_{V_{in}}^\dagger) + a_{4_{in}} \hat{a}_{H_{in}}^\dagger (\hat{a}_{V_{in}}^\dagger + \hat{a}_{V_{in}}^\dagger) \bigg] |\text{vac}\rangle.
\]

Second, photons in mode $1'_{in}$ are then split into modes $1'$ and $1''_{in}$ by a balanced polarization beam splitter (BS), that is, $\hat{a}_{1'_{in}} \overset{\text{BS}}{\leftrightarrow} \frac{(\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger)}{\sqrt{2}}$. Photons emitted from modes 2 and 4 (1 and 3) are split into modes 5 and 6 (7 and 8) by PBS$_1$ (PBS$_2$) and followed by HWP$^{22.5^\circ}$ (HWP$^{67.5^\circ}$). These elements change $|\varphi_{1}\rangle$ as

\[
|\varphi_{2}\rangle = \frac{1}{2\sqrt{2}} \left[ a_{1_{in}} (\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger) (-\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger) + a_{2_{in}} (\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger) \right. \\
+ a_{3_{in}} (\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger) (\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger) \bigg] |\text{vac}\rangle.
\]

Third, PBS$_3$ (PBS$_4$) induces photons into modes 9 and 10 (11 and 12). Photons in modes 10 and 12 will undergo HWP$^{45^\circ}$. Thus, the state of the system evolves as

\[
|\varphi_{3}\rangle = \frac{1}{2\sqrt{2}} \left[ a_{1_{in}} (\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger) (-\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger) + a_{2_{in}} (\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger) \right. \\
+ a_{3_{in}} (\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger) (\hat{a}_{1'_{in}}^\dagger + \hat{a}_{1''_{in}}^\dagger) \bigg] |\text{vac}\rangle.
\]
The state $|\varphi_{3}\rangle$ also has the form

$$|\varphi_{3}\rangle = |\varphi_{1}\rangle + |\varphi_{2}\rangle + |\varphi_{4}\rangle + |\varphi_{5}\rangle$$

$$+ \frac{1}{2\sqrt{2}} \left[ \alpha_{s}(\hat{a}_{\delta_{1}}^{\dagger} + \hat{a}_{\delta_{12}}^{\dagger})(-\hat{a}_{\delta_{1}}^{\dagger} + \hat{a}_{\delta_{12}}^{\dagger})
+ \alpha_{s}(-\hat{a}_{\delta_{1}}^{\dagger} \hat{a}_{\delta_{12}}^{\dagger} + \hat{a}_{\delta_{1}}^{\dagger} \hat{a}_{\delta_{12}}^{\dagger} - \hat{a}_{\delta_{1}}^{\dagger} \hat{a}_{\delta_{12}}^{\dagger} + \hat{a}_{\delta_{1}}^{\dagger} \hat{a}_{\delta_{12}}^{\dagger})
+ \alpha_{s}(-\hat{a}_{\delta_{12}}^{\dagger} \hat{a}_{\delta_{12}}^{\dagger} + \hat{a}_{\delta_{12}}^{\dagger} \hat{a}_{\delta_{12}}^{\dagger} - \hat{a}_{\delta_{12}}^{\dagger} \hat{a}_{\delta_{12}}^{\dagger} + \hat{a}_{\delta_{12}}^{\dagger} \hat{a}_{\delta_{12}}^{\dagger})
+ \alpha_{s}(\hat{a}_{\delta_{1}}^{\dagger} + \hat{a}_{\delta_{12}}^{\dagger})(\hat{a}_{\delta_{1}}^{\dagger} - \hat{a}_{\delta_{12}}^{\dagger}) + \alpha_{s}(\hat{a}_{\delta_{12}}^{\dagger} + \hat{a}_{\delta_{12}}^{\dagger})(\hat{a}_{\delta_{12}}^{\dagger} - \hat{a}_{\delta_{12}}^{\dagger})
+ \alpha_{s}(\hat{a}_{\delta_{12}}^{\dagger} + \hat{a}_{\delta_{12}}^{\dagger})(\hat{a}_{\delta_{1}}^{\dagger} + \hat{a}_{\delta_{12}}^{\dagger}) \right] |\text{vac}\rangle$$

(17)

Here the four orthogonal states $|\varphi_{1}\rangle$, $|\varphi_{2}\rangle$, $|\varphi_{4}\rangle$, and $|\varphi_{5}\rangle$ are given by

$$|\varphi_{1}\rangle = \frac{1}{2\sqrt{2}} \left[ \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{12}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} \right] |\text{vac}\rangle$$

(18)

$$|\varphi_{2}\rangle = \frac{1}{2\sqrt{2}} \left[ \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{12}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} \right] |\text{vac}\rangle$$

(19)

$$|\varphi_{4}\rangle = \frac{1}{2\sqrt{2}} \left[ \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{12}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} \right] |\text{vac}\rangle$$

(20)

$$|\varphi_{5}\rangle = \frac{1}{2\sqrt{2}} \left[ \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{1}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} + \alpha_{s}\hat{a}_{\delta_{12}}^{\dagger}\hat{a}_{\delta_{12}}^{\dagger} \right] |\text{vac}\rangle$$

(21)

Based on Equations (18)–(21), a post-selected P-SWAP gate can be operated correctly in the coincidence basis where the photons act as their own qubits. This means the success of the gate is heralded by a detection of an outgoing single photon in the desired output ports of the gate (see Table 1).

i) If desired coincidence detections of the output modes are 9, 1', and 12 (outputs 1, 10, and 11 are discarded), the state $|\varphi_{3}\rangle$ will collapse into $|\varphi_{1}\rangle$, and the P-SWAP gate is completed.

ii) If desired coincidence detections of the output modes are 10, 1', and 12 (outputs 1, 9, and 11 are discarded), the state $|\varphi_{3}\rangle$ will collapse into $|\varphi_{2}\rangle$, and the P-SWAP gate is completed.

iii) If desired coincidence detections of the output modes are 9, 1', and 11 (outputs 1, 10, and 12 are discarded), the state $|\varphi_{3}\rangle$ will collapse into $|\varphi_{4}\rangle$. And then, a phase flip operation, $\hat{a}_{\delta_{1}}^{\dagger} \rightarrow -\hat{a}_{\delta_{1}}^{\dagger}$, should be applied to complete the P-SWAP gate. Such feed-forward operation $\sigma_{1}$ can be easily achieved by setting an HWP$^{\pi/2}$ in output mode 1'. The feed-forward operations can be determined by post-selection principle, moreover, the spatial-mode-based feed-forward operations have been experimentally demonstrated recently.[74–77]

iv) If desired coincidence detections of the output modes are 10, 1', and 11 (outputs 1, 9, and 12 are discarded), the state $|\varphi_{3}\rangle$ will collapse into $|\varphi_{5}\rangle$. And then, an HWP$^{\pi/2}$ is set in spatial mode 1' to complete the P-SWAP gate.

Putting all the pieces together one can find that the quantum circuit shown in Figure 4 completes a linear optical P-SWAP gate in the coincidence basis with a success probability of $4 \times 1/8 = 1/2$. The success (or the output modes) of the scheme can be heralded by using the success instances in the post-selection in the applications.

### 3.2. Implementation of a Post-Selected CNOT Gate with Linear Optics

As shown in Figure 5, a post-selected CNOT gate based on P-SWAP gate can be realized in the coincidence basis with linear optical elements. PBS plays a role in the qutrit $X_{3}$ to provide an additional spatial mode. The operation in the blue dotted rectangle corresponds to a P-SWAP gate in Figure 4.

![Table 1. Coincident expectation outgoing values for six logic basis inputs.](image)

| Input | $\alpha_{912}$ | $\alpha_{1012}$ | $\alpha_{1212}$ | $\alpha_{912}$ | $\alpha_{1012}$ | $\alpha_{1212}$ |
|-------|---------------|---------------|---------------|---------------|---------------|---------------|
| $a_{9}$ | 1/8           | 0             | 0             | 0             | 0             | 0             |
| $a_{10}$ | 0            | 1/8           | 0             | 0             | 0             | 0             |
| $a_{12}$ | 0            | 0             | 1/8           | 0             | 0             | 0             |
| $a_{9}$ | 0            | 0             | 0             | 1/8           | 0             | 0             |
| $a_{10}$ | 0            | 0             | 0             | 0             | 1/8           | 0             |
| $a_{12}$ | 0            | 0             | 0             | 0             | 0             | 1/8           |

![Figure 5. Implementation of a linear optical CNOT gate. The operation in the dotted rectangle is a P-SWAP gate in Figure 4. Input–output ports pairs mapping (1\text{in}, 1'\text{in}, 2\text{in}) → (9, 1', 12) and (1\text{in}, 1'\text{in}, 2\text{in}) → (10, 1', 12) are necessary for the leftmost P-SWAP gate. The output photons from ports (9, 1', 12) and (10, 1', 12) of the leftmost P-SWAP gate as inputs will route to the next operations. Ports mapping (1\text{in}, 1'\text{in}, 2\text{in}) → (9, 1', 12), (1\text{in}, 1'\text{in}, 2\text{in}) → (10, 1', 12), (1\text{in}, 1'\text{in}, 2\text{in}) → (9, 1', 11), and (1\text{in}, 1'\text{in}, 2\text{in}) → (10, 1', 11) are employed for the rightmost P-SWAP gate. The output photon pairs emitted from ports (9, 12), (10, 12), (9, 11), and (10, 11) complete the CNOT operation with a success probability of 1/8.](image)
First, after the two photons are injected into modes 1 and 2, the input state of the system is given by

\[ |X_0\rangle = \left( a_1^\dagger \hat{a}_{H_1}^\dagger + a_2 \hat{a}_{H_1}^\dagger + a_3 \hat{a}_{V_1}^\dagger + a_4 \hat{a}_{V_1}^\dagger \right) |\text{vac}\rangle \] (22)

Second, photons 1 and 2 execute a PBS_1 and an HWP^{22,5}, respectively, to pass through the leftmost P-SWAP gate. The output ports of the leftmost P-SWAP gate are modes 9, 1', and 12 (or 10, 1', and 12), which as an input will be led to the next HWP^{22} and the rightmost P-SWAP gate. PBS_1, HWP^{22,5}, and the leftmost P-SWAP gate change \(|X_0\rangle\) into \(|X_{9,1',12}\rangle\) or \(|X_{10,1',12}\rangle\). Here,

\[ |X_{9,1',12}\rangle = \frac{1}{4} \left[ a_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{12}}^\dagger + a_2 \hat{a}_{H_{10}}^\dagger + a_3 \hat{a}_{V_{10}}^\dagger + a_4 \hat{a}_{V_{10}}^\dagger \right] |\text{vac}\rangle \] (23)

\[ + a_3 \hat{a}_{V_{12}}^\dagger \hat{a}_{V_{12}}^\dagger + a_4 \hat{a}_{V_{12}}^\dagger \hat{a}_{V_{12}}^\dagger \right) |\text{vac}\rangle \] (24)

Third, HWP^{22} acts on mode 12 to complete \(\hat{a}_{H_{12}}^\dagger \to \hat{a}_{H_{12}}^\dagger\) and \(\hat{a}_{V_{12}}^\dagger \to -\hat{a}_{V_{12}}^\dagger\). The second P-SWAP gate produces eight desired outcomes of the system, that is,

i) If the desired coincidence detections of the output modes in the second P-SWAP gate are 9, 1', and 12, the state \(|X_{9,1',12}\rangle\)

\[ + a_3 \hat{a}_{V_{12}}^\dagger \hat{a}_{V_{12}}^\dagger \right) |\text{vac}\rangle \] (25)

ii) If the desired coincidence detections of the output modes in the second P-SWAP gate are 10, 1'', and 12, the state \(|X_{10,1'',12}\rangle\)

\[ |X_{10,1'',12}\rangle = \frac{1}{8} \left[ a_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{12}}^\dagger + a_2 \hat{a}_{H_{12}}^\dagger + a_3 \hat{a}_{V_{12}}^\dagger + a_4 \hat{a}_{V_{12}}^\dagger \right] |\text{vac}\rangle \] (26)

iii) If the desired coincidence detections of the output modes in the second P-SWAP gate are 9, 1', and 11, the state \(|X_{9,1',11}\rangle\)

\[ l_1 l_2 l_3 \]

\[ \chi_{10} = \left( a_1^\dagger \hat{a}_{H_1}^\dagger + a_2 \hat{a}_{H_1}^\dagger + a_3 \hat{a}_{V_1}^\dagger + a_4 \hat{a}_{V_1}^\dagger \right) |\text{vac}\rangle \] (22)

\[ + a_3 \hat{a}_{V_{12}}^\dagger \hat{a}_{V_{12}}^\dagger \right) |\text{vac}\rangle \] (27)

iv) If the desired coincidence detections of the output modes in the second P-SWAP gate are 10, 1'', and 11, the state \(|X_{10,1'',11}\rangle\)

\[ |X_{10,1'',11}\rangle = \frac{1}{8} \left[ a_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{11}}^\dagger + a_2 \hat{a}_{H_{11}}^\dagger + a_3 \hat{a}_{V_{11}}^\dagger + a_4 \hat{a}_{V_{11}}^\dagger \right] |\text{vac}\rangle \] (28)

Fourth, as shown in Figure 5, PBS_1 leads the photons in modes 9 (i.e., \(\hat{a}_{V_9}^\dagger |\text{vac}\rangle\)) and 1' (i.e., \(\hat{a}_{V_{1'}}^\dagger |\text{vac}\rangle\)) into one output mode, and combines the photons in modes 10 (i.e., \(\hat{a}_{V_{10}}^\dagger |\text{vac}\rangle\)) and 1'' (i.e., \(\hat{a}_{V_{1''}}^\dagger |\text{vac}\rangle\)) into one output mode. After PBS_2 and HWP^{22,5}:

i) Equation (25) evolves into twofold output state

\[ |X_{9,12}\rangle = \frac{1}{8} \left( a_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{12}}^\dagger + a_2 \hat{a}_{H_{12}}^\dagger + a_3 \hat{a}_{V_{10}}^\dagger + a_4 \hat{a}_{V_{12}}^\dagger \right) |\text{vac}\rangle \] (29)

The CNOT gate is completed. ii) Equation (26) evolves into twofold output state

\[ |X_{10,12}\rangle = \frac{1}{8} \left( a_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{12}}^\dagger + a_2 \hat{a}_{H_{12}}^\dagger + a_3 \hat{a}_{V_{12}}^\dagger \right) |\text{vac}\rangle \] (30)

The CNOT gate is completed. iii) Equation (27) evolves into twofold output state

\[ |X_{9,1'}\rangle = \frac{1}{8} \left( a_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{1'}}^\dagger + a_2 \hat{a}_{H_{1'}}^\dagger + a_3 \hat{a}_{V_{10}}^\dagger \right) |\text{vac}\rangle \] (31)

And then an HWP^{22} is set in the output mode 9 to complete the CNOT gate. iv) Equation (28) evolves into twofold output state

\[ |X_{10,1''}\rangle = \frac{1}{8} \left( a_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{1''}}^\dagger + a_2 \hat{a}_{H_{1''}}^\dagger + a_3 \hat{a}_{V_{12}}^\dagger \right) |\text{vac}\rangle \] (32)

And then an HWP^{22} is set in the output mode 10 to complete the CNOT gate.

Based on above orthogonal twofold states \(|X_{9,12}\rangle\), \(|X_{10,12}\rangle\), \(|X_{9,1'}\rangle\), \(|X_{10,1'}\rangle\), and \(|X_{10,1''}\rangle\), one can find that after the feed-forward operations are only applied to the rightmost P-SWAP gate, an optical post-selected CNOT gate can be operated correctly with a success probability of 8 x 1/64 = 1/8. Remarkably, additional entangled photon pairs or single photons are necessary for previous schemes, but are not required for our CNOT gate. In addition, the success probability of the gate is improved on the results without an auxiliary photon. We also note that other method for implementing linear optical CNOT gate with additional DOFs has been demonstrated experimentally.

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3.3. Implementation of a Post-Selected Toffoli Gate with Linear Optics

We propose the implementation of a Toffoli gate based on the designed P-SWAP and CNOT gates. As shown in Figure 6, three photons are injected into modes 1, 2, and 3, simultaneously, the initial state is given by

$$|\Xi_0\rangle = \left( a_1^\dagger a_2^\dagger a_3^\dagger a_1 a_2 a_3 \right) |\text{vac}\rangle$$

First, after photons go through the PBS1 and the leftmost P-SWAP gate, if the output modes of the leftmost P-SWAP gate are 9, 1', and 12, (10, 1', and 12) and we can obtain two desired states,

$$|\Xi_{1a}\rangle = \frac{1}{2\sqrt{2}} \left( a_1 a_2^\dagger a_3 a_1 a_2 a_3 + a_2 a_1^\dagger a_3^\dagger a_1 a_2 a_3 \right) |\text{vac}\rangle$$

$$|\Xi_{1b}\rangle = \frac{1}{2\sqrt{2}} \left( a_1^\dagger a_2 a_3 a_1 a_2^\dagger a_3 + a_2^\dagger a_1 a_3^\dagger a_1^\dagger a_2 a_3 \right) |\text{vac}\rangle$$

Second, the states described by Equations (34) and (35) are employed as the initial states for the next CNOT gate acting on photons 1 and 3. If the output photons emitted from path pairs (9, 11), (9, 12), (10, 11), or (10, 12), which can yield 16 desired states $|\Xi_{9,9}\rangle_i$ (twofold) and $|\Xi_{10,10}\rangle_i$ (twofold). Here, $|\Xi_{9,9}\rangle_i$ and $|\Xi_{10,10}\rangle_i$ with $i \in \{9, 10\}$ are described by

$$|\Xi_{9,9}\rangle_i = \frac{1}{16\sqrt{2}} \left( a_1 a_2^\dagger a_3^\dagger a_1 a_2 a_3 + a_2 a_1^\dagger a_3 a_1 a_2 a_3 \right) |\text{vac}\rangle$$

$$|\Xi_{10,10}\rangle_i = \frac{1}{16\sqrt{2}} \left( a_1 a_2 a_3^\dagger a_1^\dagger a_2^\dagger a_3 + a_2^\dagger a_1 a_3 a_1 a_2 a_3 \right) |\text{vac}\rangle$$

Third, above 16 states are introduced as the initial states for the rightmost P-SWAP gate acting on photons 1 and 2. If coincidence detection mode pairs are (9, 1), and (9, 1', 11), or (10, 1', 12), or (10, 1', 11), and 11, we can obtain 64 desired states $|\Xi_{12,9,k}\rangle_i$, $|\Xi_{12,10,k}\rangle_i$, and $|\Xi_{11,10,k}\rangle_i$. Here, eightfold states $|\Xi_{12,9,k}\rangle_i$, $|\Xi_{12,10,k}\rangle_i$, $|\Xi_{11,10,k}\rangle_i$ with $k \in \{11, 12\}$ are described by

$$|\Xi_{12,9,k}\rangle_i = \frac{1}{64} \left( a_1 a_2 a_3 a_1 a_2 a_3 + a_2 a_1 a_3 a_1 a_2 a_3 \right) |\text{vac}\rangle$$

$$|\Xi_{12,10,k}\rangle_i = \frac{1}{64} \left( a_1 a_2 a_3 a_1 a_2 a_3 + a_2 a_1 a_3 a_1 a_2 a_3 \right) |\text{vac}\rangle$$

$$|\Xi_{11,10,k}\rangle_i = \frac{1}{64} \left( a_1 a_2 a_3 a_1 a_2 a_3 + a_2 a_1 a_3 a_1 a_2 a_3 \right) |\text{vac}\rangle$$
Finally, as shown in Figure 6, the photons emitted from modes 9 (i.e., $\hat{a}^\dagger_{11\text{vac}}(\text{vac})$) and 10 (i.e., $\hat{a}^\dagger_{10\text{vac}}(\text{vac})$) are combined into the same output mode by PBS$_2$. The photons emitted from modes 10 (i.e., $\hat{a}^\dagger_{10\text{vac}}(\text{vac})$) and 1$^\circ$ ($\hat{a}^\dagger_{1\text{vac}}(\text{vac})$) are also led to the same output mode by PBS$_2$. Therefore, after PBS$_2$, i) Equation (38) evolves into eightfold output state

$$\Xi_{11,10,k}^2 = \frac{1}{64} \left( \alpha_1 \hat{a}^\dagger_{11\text{H}_1} \hat{a}^\dagger_{10\text{H}_1} \hat{a}^\dagger_{10\text{H}_2} + \alpha_2 \hat{a}^\dagger_{11\text{H}_1} \hat{a}^\dagger_{10\text{H}_2} \hat{a}^\dagger_{10\text{H}_1} \hat{a}^\dagger_{10\text{H}_2} \right) |\text{vac}\rangle$$

(41)

And then an HWPO$^0$ is set in the output mode 10 to complete the three-photon Toffoli gate.

Based on above orthogonal eightfold states described by Equations (42)–(45), one can find that our proposal can be achieved in the coincidence basis with a higher success probability ($64 \times 1/64^2 = 1/64$) than the simplified CNOT-based one (1/72)$^{13,34}$ and the one without a decomposition-based approach (1/133).$^{73}$ In addition, optical single-qudit operation ensembles $X_n, X_{n-1}, \ldots, X_0$ can be achieved by employing a sequence of PBSs, and the linear optical n-control-photon Toffoli gate can be implemented in principle (see Figure 7).

### 4. Discussion and Conclusion

The optimal cost of a Toffoli gate is six CNOT gates using the standard decomposition-based approach in qubit systems.$^{62}$ The theoretical lower bound of a Toffoli gate is five two-qubit gates in qubit system.$^{63}$ Ralph et al.$^{13}$ first reduced the cost of a Toffoli gate to three qubit–qudit CNOT gates by introducing a qudit. Using the same idea as the works in Refs. [33, 34], we designed an alternative the quantum circuit to implement the Toffoli gate with a higher success probability based on the P-SWAP gates, which required the same number of qubit–qudit gates as the protocols in Refs. [33, 34]. The required qubit–qudit entangled gates are all nearest neighbors in our construction of the three-qubit Toffoli gate. Note that the nearest-neighbor quantum gate where each qudit interacts only with its nearest neighbors requires less resource overhead than the long-range one. For example, a long-range CNOT gate acting on the first qubit and the third qubit is constructed by four nearest-neighbor CNOT gates.$^{86}$ In addition, $(2n-1)$ qubit–qudit gates and $(2n-2)$ single-qudit gates can simulate an n-control-qubit Toffoli gate in higher-dimensional spaces.

Linear optics has inherent probability characteristics for the implementation of controlled quantum gates. With the help of an additional entangled photon pair$^{75,78}$ or a single photon,$^{79}$ optical CNOT gate with a success probability of 1/4 or 1/8 can be realistically implemented. Without auxiliary photons, CNOT gate with a success probability of 1/9 has been experimentally demonstrated in linear optics.$^{81-84}$ Remarkably, the success probability of our P-SWAP-based CNOT gate is enhanced to 1/8 without additional photons. Moreover, the success probability of our P-SWAP-based Toffoli gate (1/64) is higher than the CNOT-based protocols (1/72)$^{13,34}$ and it is also higher than the no-decomposition-based one (1/133).$^{73}$

The multi-level system is essential to realize our schemes. In optical system, we can encode polarization DOF of photons as two computational qubits and spatial-mode DOF as the qudit (extra level). We can also encode these levels on orbital angular
momentum of photons. Besides, diamond nitrogen-vacancy defect center[87,88] and superconducting system[89,90] can also provide available multiple levels to implement the universal quantum gates due to their long coherence time and flexible manipulation.

In summary, by introducing higher-dimensional spaces, we proposed simplified CNOT and Toffoli gates. A three-qubit Toffoli gate can be simulated with two P-SWAP, one CNOT, and two single-qutrit gates. $(2n - 1)$ qubit–qudit gates and $(2n - 2)$ single-qudit gates are sufficient for constructing an $n$-control-qubit Toffoli gate. Following the simplified synthesis, as a feasible example, linear optics architectures for implementing CNOT and Toffoli gates were designed with a higher success probability.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

Keywords

higher-dimensional space, linear optics, quantum computation, quantum circuits, quantum gates

Figure 7. Implementation of an $(n + 1)$-photon Toffoli gate.
