Implementation of CNOT and Toffoli gates with higher-dimensional spaces

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Abstract

Minimizing the number of necessary two-qubit gates is an important task in quantum information processing. By introducing non-computational quantum states in auxiliary spaces, we construct effective circuits for the controlled-NOT (CNOT) gate and the $n$-control-qubit Toffoli gate with $(2^n - 1)$ qubit-qudit gates and $(2^n - 2)$ single-qudit gates. We propose the polarization CNOT and Toffoli gates based on the designed quantum circuits in linear optics by operating on the spatial-mode degree of freedom of photons. Our optical schemes can be achieved with a higher success probability and no extra auxiliary photons are needed.

Contents

1 Introduction

2 Construction of CNOT and Toffoli gates with higher-dimensional spaces
   2.1 Synthesis of a CNOT gate using qutrits
   2.2 Construction of Toffoli gates with higher-dimensional spaces
      2.2.1 Synthesis of a three-qubit Toffoli gate using qutrits
      2.2.2 Synthesis of $n$-control-qubit Toffoli gate using qudits

3 Implementation of CNOT and Toffoli gates with linear optics
   3.1 Implementation of a P-SWAP gate with linear optics
   3.2 Implementation of a CNOT gate with linear optics
   3.3 Implementation of a Toffoli gate with linear optics
1 Introduction

Multi-qubit quantum gates have complex structures and play an important role in quantum computing [1], quantum algorithms [2–5], cryptography [6], etc. [7]. The most popular paradigm for implementing a quantum gate is the quantum circuit model [1,8]. Quantum circuits can be realized by sequences of two-qubit gates and single-qubit gates in principle [1]. 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 qubit system [9]. 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 [10–16]. Two-qubit universal quantum circuits have also been constructed with the lowest cost (resources) in qubit systems [9,17–19]. However, there is still a gap between the current best result [13] and the theoretical lower bound [9] for a multi-qubit universal quantum circuit. Fortunately, Ralph et al. [20] found that the quantum circuit may be optimized further by using higher-dimensional Hilbert spaces, and this proposal was later experimentally demonstrated in optical [21] and superconducting systems [22]. Following this, Liu et al. [23,24] reduced the cost of the $n$-qubit universal circuit to $(5/16) \times 4^n - (5/4) \times 2^n + 2n$ CNOT gates when $n$ was even and $(5/16) \times 4^n - 2^n + 2(n - 1)$ CNOTs when $n$ was odd. Liu et al. simplified a Fredkin gate from eight CNOTs to five CNOTs [25] or three qubit-qudit gates [26]. In addition, higher-dimensional quantum systems have also been studied [27,28] and applied in quantum computing [29,32], quantum communication [33,40], and quantum metrology [41].

The Toffoli (controlled-NOT-NOT) gate, a three-qubit conditional operation, is one of the most popular universal multi-qubit quantum gates [42]. It is also an essential component in complex quantum algorithms [2–5], quantum error correction [13,44], and quantum fault tolerance [45,46]. In 1995, Barenco et al. [1] 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 [47]. In 2013, Yu et al. [48,49] confirmed that the minimum resource for simulating a three-qubit Toffoli gate is five two-qubit gates. In 2020, Kiktenko et al. [50] constructed a generalized $m$-qubit Toffoli gate with $(2m - 3)$ CNOTs based on qudits. Independent of the standard decomposition-based approach, Toffoli gates have been implemented experimentally in superconducting circuits [22,44], linear optics [21,29,51,53], trapped ions [54], atoms [55,56], and quantum dots [57].
Ralph et al. [20, 21] 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. [20, 21] was to extend temporarily the higher-dimensional subspaces on one of the controlled qubit carriers and then perform corresponding logical operations. Using the same method as Refs. [20, 21], in this paper, we propose an alternative scheme to implement the CNOT and Toffoli gates based on the partial-swap (P-SWAP) gates by using higher-dimensional spaces. Specifically, $(2^n - 1)$ qubit-qudit and $(2^n - 2)$ single-qudit 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 [20, 21, 58]. (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 qudits

A CNOT gate with two P-SWAP gates using qudits is shown in Fig. 1. The gate qudits are encoded on two computational states, $|0\rangle$ and $|1\rangle$. The single-qudit $X_A$ gate provides a three-dimensional subspace on the control qubit. In the following, we describe the construction process of our protocol in detail.

Figure 1: Synthesis of a CNOT gate. The single-qudit $X_A$ gate implements the transformation $|1\rangle \leftrightarrow |2\rangle$. The controlled node $\odot$ is turned on for the input $|0\rangle$ or $|1\rangle$. That is, a swap operation is applied to $c$ and $t$, if and only if, the control qubit $c$ is in the state $|0\rangle$ or $|1\rangle$. $H$ is a single-qubit Hardmard gate to achieve operations $|0\rangle \leftrightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $|1\rangle \leftrightarrow \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. $\sigma_z$ completes $\sigma_z|0\rangle = |0\rangle$ and $\sigma_z|1\rangle = -|1\rangle$.

Suppose that the state of the system is initially

$$|\phi_0\rangle = \alpha_1|0_c\rangle|0_t\rangle + \alpha_2|0_c\rangle|1_t\rangle + \alpha_3|1_c\rangle|0_t\rangle + \alpha_4|1_c\rangle|1_t\rangle.$$  

(1)

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 qudits, respectively.

First, qubit $c$ undergoes a single-qudit gate $X_A$, which introduces an ancillary state $|2\rangle$ on $c$ and completes the transformations $|1_c\rangle \leftrightarrow X_A|1_c\rangle$ and $|0_c\rangle \leftrightarrow X_A|0_c\rangle$. 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

\[
|\phi_1\rangle = \frac{1}{\sqrt{2}} [\alpha_1 |0_c\rangle |0_t\rangle + \alpha_2 |0_c\rangle |1_t\rangle + \alpha_3 |2_c\rangle |0_t\rangle + \alpha_4 |2_c\rangle |1_t\rangle].
\] (2)

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

\[
|\phi_2\rangle = \frac{1}{\sqrt{2}} [\alpha_1 |0_c\rangle + |1_c\rangle] |0_t\rangle + \alpha_2 |0_c\rangle - |1_c\rangle |0_t\rangle
+ \alpha_3 |2_c\rangle |0_t\rangle + \alpha_4 |2_c\rangle |1_t\rangle].
\] (3)

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

\[
\begin{align*}
|00\rangle & \xrightarrow{\text{P-SWAP}} |00\rangle, & |01\rangle & \xrightarrow{\text{P-SWAP}} |10\rangle, \\
|10\rangle & \xrightarrow{\text{P-SWAP}} |01\rangle, & |11\rangle & \xrightarrow{\text{P-SWAP}} |11\rangle, \\
|20\rangle & \xrightarrow{\text{P-SWAP}} |20\rangle, & |21\rangle & \xrightarrow{\text{P-SWAP}} |21\rangle.
\end{align*}
\] (4)

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

\[
|\phi_3\rangle = \frac{1}{\sqrt{2}} [\alpha_1 |0_c\rangle + |1_c\rangle] |0_t\rangle + \alpha_2 |0_c\rangle - |1_c\rangle |0_t\rangle
+ \alpha_3 |2_c\rangle |0_t\rangle + \alpha_4 |2_c\rangle |1_t\rangle].
\] (5)

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

\[
|\phi_4\rangle = \alpha_1 |0_c\rangle |0_t\rangle + \alpha_2 |0_c\rangle |1_t\rangle + \alpha_3 |1_c\rangle |1_t\rangle + \alpha_4 |1_c\rangle |0_t\rangle.
\] (6)

Note that Eq. (6) is a CNOT gate, and such a construction can be achieved in linear optics with a high success probability and without additional photons (see Sec. 3).

### 2.2 Construction of Toffoli gates with higher-dimensional spaces

#### 2.2.1 Synthesis of a three-qubit Toffoli gate using qutrits

Based on the designed CNOT and P-SWAP gates, the process for implementing a three-qubit Toffoli gate with four-dimensional space is presented in Fig. 2.

Considering an arbitrary normalization three-qubit initial state

\[
|\psi_0\rangle = \alpha_1 |0_{c1}\rangle |0_{c2}\rangle |0_t\rangle + \alpha_2 |0_{c1}\rangle |0_{c2}\rangle |1_t\rangle + \alpha_3 |0_{c1}\rangle |1_{c2}\rangle |0_t\rangle + \alpha_4 |0_{c1}\rangle |1_{c2}\rangle |1_t\rangle
+ \alpha_5 |1_{c1}\rangle |0_{c2}\rangle |0_t\rangle + \alpha_6 |1_{c1}\rangle |0_{c2}\rangle |1_t\rangle + \alpha_7 |1_{c1}\rangle |1_{c2}\rangle |0_t\rangle + \alpha_8 |1_{c1}\rangle |1_{c2}\rangle |1_t\rangle.
\] (7)

First, the \(X_A\) gate acts on \(c_2\) to achieve \(|1_{c2}\rangle \xrightarrow{X_A} |2_{c2}\rangle\) and \(|0_{c2}\rangle \xrightarrow{X_A} |0_{c2}\rangle\). After the first P-SWAP gate is executed on \(c_1\) and \(c_2\), \(|\psi_0\rangle\) becomes

\[
|\psi_1\rangle = \alpha_1 |0_{c1}\rangle |0_{c2}\rangle |0_t\rangle + \alpha_2 |0_{c1}\rangle |0_{c2}\rangle |1_t\rangle + \alpha_3 |0_{c1}\rangle |2_{c2}\rangle |0_t\rangle + \alpha_4 |0_{c1}\rangle |2_{c2}\rangle |1_t\rangle
+ \alpha_5 |0_{c1}\rangle |1_{c2}\rangle |0_t\rangle + \alpha_6 |0_{c1}\rangle |1_{c2}\rangle |1_t\rangle + \alpha_7 |1_{c1}\rangle |2_{c2}\rangle |0_t\rangle + \alpha_8 |1_{c1}\rangle |2_{c2}\rangle |1_t\rangle.
\] (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

\[
|\psi_2\rangle = \alpha_1|0_{c_1}\rangle|0_{c_2}\rangle|0_t\rangle + \alpha_2|0_{c_1}\rangle|0_{c_2}\rangle|1_t\rangle + \alpha_3|0_{c_1}\rangle|2_{c_2}\rangle|0_t\rangle + \alpha_4|0_{c_1}\rangle|2_{c_2}\rangle|1_t\rangle \\
+ \alpha_5|1_{c_1}\rangle|1_{c_2}\rangle|0_t\rangle + \alpha_6|0_{c_1}\rangle|1_{c_2}\rangle|1_t\rangle + \alpha_7|1_{c_1}\rangle|2_{c_2}\rangle|1_t\rangle + \alpha_8|1_{c_1}\rangle|2_{c_2}\rangle|0_t\rangle. \tag{9}
\]

Finally, the P-SWAP and \( X_A \) gates are applied again. The two operations induce \( |\psi_2\rangle \) as the final state

\[
|\psi_3\rangle = \alpha_1|0_{c_1}\rangle|0_{c_2}\rangle|0_t\rangle + \alpha_2|0_{c_1}\rangle|0_{c_2}\rangle|1_t\rangle + \alpha_3|0_{c_1}\rangle|1_{c_2}\rangle|0_t\rangle + \alpha_4|0_{c_1}\rangle|1_{c_2}\rangle|1_t\rangle \\
+ \alpha_5|1_{c_1}\rangle|0_{c_2}\rangle|0_t\rangle + \alpha_6|1_{c_1}\rangle|0_{c_2}\rangle|1_t\rangle + \alpha_7|1_{c_1}\rangle|1_{c_2}\rangle|1_t\rangle + \alpha_8|1_{c_1}\rangle|1_{c_2}\rangle|0_t\rangle. \tag{10}
\]

From Eqs. (9) and (10), one can see that a three-qubit Toffoli gate can be simulated using three nearest-neighbor qubit-qudit gates and two single-qutrit 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 Fig. 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 \( X_a, X_b, \ldots, X_n \) create multi-level qudits on \( c_n \) and complete transformations \(|0_{c_n}\rangle \leftrightarrow |2_{c_n}\rangle, |1_{c_n}\rangle \leftrightarrow |3_{c_n}\rangle, |0_{c_n}\rangle \leftrightarrow |4_{c_n}\rangle, \ldots, |0_{c_n}\rangle \leftrightarrow |n_{c_n}\rangle \) when \( n \) is even or \(|0_{c_n}\rangle \leftrightarrow |2_{c_n}\rangle, |1_{c_n}\rangle \leftrightarrow |3_{c_n}\rangle, |0_{c_n}\rangle \leftrightarrow |4_{c_n}\rangle, \ldots, |1_{c_n}\rangle \leftrightarrow |n_{c_n}\rangle \) when \( n \) is odd. These single-qudit gates can temporally expand the two-dimensional space of \( c_n \) 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 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, \( |0\rangle \equiv |H\rangle_i \) and \( |1\rangle \equiv |V\rangle_i \). 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, $|2\rangle \equiv |V\rangle_{i'}$. The qutrit operation $X_A$ 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 Fig. 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 $|V\rangle_{2_{in}} \equiv |1\rangle$. A general injected photon state can be considered as

$$|\varphi_0\rangle = (\alpha_1 \hat{a}_{H_{1_{in}}}^{\dagger} \hat{a}_{H_{2_{in}}}^{\dagger} + \alpha_2 \hat{a}_{H_{1_{in}}}^{\dagger} \hat{a}_{V_{2_{in}}}^{\dagger} + \alpha_3 \hat{a}_{V_{1_{in}}}^{\dagger} \hat{a}_{H_{2_{in}}}^{\dagger} + \alpha_4 \hat{a}_{V_{1_{in}}}^{\dagger} \hat{a}_{V_{2_{in}}}^{\dagger} + \alpha_5 \hat{a}_{V_{1'_{in}}}^{\dagger} \hat{a}_{H_{2_{in}}}^{\dagger} + \alpha_6 \hat{a}_{V_{1'_{in}}}^{\dagger} \hat{a}_{V_{2_{in}}}^{\dagger})|\text{vac.}\rangle.$$  

(11)

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 degrees and achieves the qubit-flip operation $\hat{a}_H^{\dagger} \leftrightarrow \hat{a}_V^{\dagger}$. HWP$^{22.5^\circ}$ completes the transformations

$$\hat{a}_H^{\dagger} \xrightarrow{\text{HWP}^{22.5^\circ}} \frac{1}{\sqrt{2}}(\hat{a}_H^{\dagger} + \hat{a}_V^{\dagger}), \quad \hat{a}_V^{\dagger} \xrightarrow{\text{HWP}^{22.5^\circ}} \frac{1}{\sqrt{2}}(\hat{a}_H^{\dagger} - \hat{a}_V^{\dagger}).$$  

(12)

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

$$\hat{a}_H^{\dagger} \xrightarrow{\text{HWP}^{67.5^\circ}} \frac{1}{\sqrt{2}}(-\hat{a}_H^{\dagger} + \hat{a}_V^{\dagger}), \quad \hat{a}_V^{\dagger} \xrightarrow{\text{HWP}^{67.5^\circ}} \frac{1}{\sqrt{2}}(\hat{a}_H^{\dagger} + \hat{a}_V^{\dagger}).$$  

(13)

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

$$|\varphi_1\rangle = \frac{1}{\sqrt{2}}[\alpha_1 \hat{a}_{V_{1_{in}}}^{\dagger} (\hat{a}_{H_{3}}^{\dagger} + \hat{a}_{V_{3}}^{\dagger}) + \alpha_2 \hat{a}_{V_{1_{in}}}^{\dagger} (\hat{a}_{H_{4}}^{\dagger} + \hat{a}_{V_{4}}^{\dagger}) + \alpha_3 \hat{a}_{H_{2}}^{\dagger} (\hat{a}_{H_{3}}^{\dagger} + \hat{a}_{V_{3}}^{\dagger}) + \alpha_4 \hat{a}_{H_{2}}^{\dagger} (\hat{a}_{H_{4}}^{\dagger} + \hat{a}_{V_{4}}^{\dagger}) + \alpha_5 \hat{a}_{V_{1'_{in}}}^{\dagger} (\hat{a}_{H_{3}}^{\dagger} + \hat{a}_{V_{3}}^{\dagger}) + \alpha_6 \hat{a}_{V_{1'_{in}}}^{\dagger} (\hat{a}_{H_{4}}^{\dagger} + \hat{a}_{V_{4}}^{\dagger})]|\text{vac.}\rangle.$$  

(14)

Second, photons in mode $1'_{in}$ are then split into modes 1’ and 1” by a balanced polarization beam splitter (BS), i.e., $\hat{a}_{V_{1'_{in}}}^{\dagger} \xrightarrow{\text{BS}} (\hat{a}_{V_{1'}^{\dagger}}^{\dagger} + \hat{a}_{V_{1''}^{\dagger}}^{\dagger})/\sqrt{2}$. Photons emitted from modes 2 and 4 (1 and 3) are split into modes 5 and 6 (7 and 8) by PBS$_3$ (PBS$_4$) and followed by HWP$^{22.5^\circ}$ (HWP$^{67.5^\circ}$). These elements change $|\varphi_1\rangle$ as

$$|\varphi_2\rangle = \frac{1}{2\sqrt{2}}[\alpha_1 (\hat{a}_{H_{2}}^{\dagger} + \hat{a}_{V_{2}}^{\dagger}) (-\hat{a}_{H_{2}}^{\dagger} + \hat{a}_{V_{2}}^{\dagger} + \hat{a}_{H_{8}}^{\dagger} + \hat{a}_{V_{8}}^{\dagger}) + \alpha_2 (\hat{a}_{H_{7}}^{\dagger} + \hat{a}_{V_{7}}^{\dagger}) (\hat{a}_{H_{7}}^{\dagger} + \hat{a}_{V_{7}}^{\dagger} + \hat{a}_{H_{6}}^{\dagger} + \hat{a}_{V_{6}}^{\dagger}) + \alpha_3 (\hat{a}_{H_{6}}^{\dagger} + \hat{a}_{V_{6}}^{\dagger}) (-\hat{a}_{H_{7}}^{\dagger} + \hat{a}_{V_{7}}^{\dagger} + \hat{a}_{H_{6}}^{\dagger} + \hat{a}_{V_{6}}^{\dagger}) + \alpha_4 (\hat{a}_{H_{6}}^{\dagger} + \hat{a}_{V_{6}}^{\dagger}) (-\hat{a}_{H_{8}}^{\dagger} + \hat{a}_{V_{8}}^{\dagger} + \hat{a}_{H_{6}}^{\dagger} + \hat{a}_{V_{6}}^{\dagger}) + \alpha_5 (\hat{a}_{V_{1'}^{\dagger}}^{\dagger} + \hat{a}_{V_{1''}^{\dagger}}^{\dagger}) (-\hat{a}_{H_{2}}^{\dagger} + \hat{a}_{V_{2}}^{\dagger} + \hat{a}_{H_{8}}^{\dagger} + \hat{a}_{V_{8}}^{\dagger}) + \alpha_6 (\hat{a}_{V_{1'}^{\dagger}}^{\dagger} + \hat{a}_{V_{1''}^{\dagger}}^{\dagger}) (\hat{a}_{H_{2}}^{\dagger} + \hat{a}_{V_{2}}^{\dagger} + \hat{a}_{H_{8}}^{\dagger} - \hat{a}_{V_{8}}^{\dagger})]|\text{vac.}\rangle.$$  

(15)
Third, PBS$_5$ (PBS$_6$) 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

$$|\varphi_3\rangle = \frac{1}{2\sqrt{2}} \left[ \alpha_1 (\hat{a}^\dagger_{H_{11}} + \hat{a}^\dagger_{H_{12}})(-\hat{a}^\dagger_{H_{11}} + \hat{a}^\dagger_{H_{12}} + \hat{a}^\dagger_{H_9} + \hat{a}^\dagger_{H_{10}}) \\
+ \alpha_2 (\hat{a}^\dagger_{V_{10}} + \hat{a}^\dagger_{V_{12}})(\hat{a}^\dagger_{V_{10}} + \hat{a}^\dagger_{V_{9}} - \hat{a}^\dagger_{V_{11}}) \\
+ \alpha_3 (\hat{a}^\dagger_{V_{12}} + \hat{a}^\dagger_{V_{11}})(-\hat{a}^\dagger_{H_{11}} + \hat{a}^\dagger_{H_{12}} + \hat{a}^\dagger_{H_9} + \hat{a}^\dagger_{H_{10}}) \\
+ \alpha_4 (\hat{a}^\dagger_{V_{12}} + \hat{a}^\dagger_{V_{11}})(\hat{a}^\dagger_{V_{10}} + \hat{a}^\dagger_{V_{9}} + \hat{a}^\dagger_{V_{12}} - \hat{a}^\dagger_{V_{11}}) \\
+ \alpha_5 (\hat{a}^\dagger_{V_{12}} + \hat{a}^\dagger_{V_{11}})(-\hat{a}^\dagger_{H_{11}} + \hat{a}^\dagger_{H_{12}} + \hat{a}^\dagger_{H_9} + \hat{a}^\dagger_{H_{10}}) \\
+ \alpha_6 (\hat{a}^\dagger_{V_{12}} + \hat{a}^\dagger_{V_{11}})(\hat{a}^\dagger_{V_{10}} + \hat{a}^\dagger_{V_{9}} + \hat{a}^\dagger_{V_{12}} - \hat{a}^\dagger_{V_{11}})] |\text{vac.}\rangle. \right.$$ (16)

The state $|\varphi_3\rangle$ also has the form

$$|\varphi_3\rangle = |\varphi_4\rangle + |\varphi_2\rangle + |\varphi_3\rangle_1 + |\varphi_3\rangle_2$$ (17)

$$+ \frac{1}{2\sqrt{2}} \left[ \alpha_1 (\hat{a}^\dagger_{H_{11}} + \hat{a}^\dagger_{H_{12}})(-\hat{a}^\dagger_{H_{11}} + \hat{a}^\dagger_{H_{12}}) \\
+ \alpha_2 (-\hat{a}^\dagger_{H_{11}} \hat{a}^\dagger_{V_{11}} + \hat{a}^\dagger_{H_{11}} \hat{a}^\dagger_{V_{12}} - \hat{a}^\dagger_{V_{11}} \hat{a}^\dagger_{H_{12}} + \hat{a}^\dagger_{V_{12}} \hat{a}^\dagger_{H_{12}}) \\
+ \alpha_3 (-\hat{a}^\dagger_{H_{11}} \hat{a}^\dagger_{V_{11}} + \hat{a}^\dagger_{V_{11}} \hat{a}^\dagger_{V_{12}} - \hat{a}^\dagger_{V_{11}} \hat{a}^\dagger_{H_{12}} + \hat{a}^\dagger_{V_{12}} \hat{a}^\dagger_{H_{12}}) \\
+ \alpha_4 (\hat{a}^\dagger_{V_{12}} + \hat{a}^\dagger_{V_{11}})(\hat{a}^\dagger_{V_{12}} - \hat{a}^\dagger_{V_{11}}) \\
+ \alpha_5 (\hat{a}^\dagger_{V_{12}} + \hat{a}^\dagger_{V_{11}})(\hat{a}^\dagger_{H_9} + \hat{a}^\dagger_{H_{10}}) \\
+ \alpha_6 (\hat{a}^\dagger_{V_{12}} + \hat{a}^\dagger_{V_{11}})(\hat{a}^\dagger_{V_{6}} + \hat{a}^\dagger_{V_{10}})] |\text{vac.}\rangle. \right.$$ (18)

Here the four orthogonal states $|\varphi_4\rangle$, $|\varphi_2\rangle$, $|\varphi_3\rangle_1$, and $|\varphi_3\rangle_2$ are given by

$$|\varphi_4\rangle = \frac{1}{2\sqrt{2}} \left( \alpha_1 \hat{a}^\dagger_{H_9} \hat{a}^\dagger_{H_{12}} + \alpha_2 \hat{a}^\dagger_{V_{10}} \hat{a}^\dagger_{H_{12}} + \alpha_3 \hat{a}^\dagger_{H_9} \hat{a}^\dagger_{V_{12}} + \alpha_4 \hat{a}^\dagger_{V_{9}} \hat{a}^\dagger_{V_{12}} \\
+ \alpha_5 \hat{a}^\dagger_{V_{11}} \hat{a}^\dagger_{H_{12}} + \alpha_6 \hat{a}^\dagger_{V_{10}} \hat{a}^\dagger_{V_{12}}) |\text{vac.}\rangle. \right.$$ (19)

$$|\varphi_2\rangle = \frac{1}{2\sqrt{2}} \left( \alpha_1 \hat{a}^\dagger_{H_9} \hat{a}^\dagger_{H_{12}} + \alpha_2 \hat{a}^\dagger_{V_{10}} \hat{a}^\dagger_{H_{12}} + \alpha_3 \hat{a}^\dagger_{H_9} \hat{a}^\dagger_{V_{12}} + \alpha_4 \hat{a}^\dagger_{V_{10}} \hat{a}^\dagger_{V_{12}} \\
+ \alpha_5 \hat{a}^\dagger_{V_{11}} \hat{a}^\dagger_{H_{12}} + \alpha_6 \hat{a}^\dagger_{V_{10}} \hat{a}^\dagger_{V_{12}}) |\text{vac.}\rangle. \right.$$ (20)

$$|\varphi_3\rangle_1 = \frac{1}{2\sqrt{2}} \left( \alpha_1 \hat{a}^\dagger_{H_9} \hat{a}^\dagger_{H_{11}} + \alpha_2 \hat{a}^\dagger_{V_{10}} \hat{a}^\dagger_{H_{11}} + \alpha_3 \hat{a}^\dagger_{H_9} \hat{a}^\dagger_{V_{11}} + \alpha_4 \hat{a}^\dagger_{V_{9}} \hat{a}^\dagger_{V_{11}} \\
- \alpha_5 \hat{a}^\dagger_{V_{11}} \hat{a}^\dagger_{H_{11}} - \alpha_6 \hat{a}^\dagger_{V_{10}} \hat{a}^\dagger_{V_{11}}) |\text{vac.}\rangle. \right.$$ (21)

$$|\varphi_3\rangle_2 = \frac{1}{2\sqrt{2}} \left( \alpha_1 \hat{a}^\dagger_{H_9} \hat{a}^\dagger_{H_{11}} + \alpha_2 \hat{a}^\dagger_{V_{10}} \hat{a}^\dagger_{H_{11}} + \alpha_3 \hat{a}^\dagger_{H_9} \hat{a}^\dagger_{V_{11}} + \alpha_4 \hat{a}^\dagger_{V_{10}} \hat{a}^\dagger_{V_{11}} \\
- \alpha_5 \hat{a}^\dagger_{V_{11}} \hat{a}^\dagger_{H_{11}} - \alpha_6 \hat{a}^\dagger_{V_{10}} \hat{a}^\dagger_{V_{11}}) |\text{vac.}\rangle. \right.$$
Based on Eqs. (18-21), one can see that there are four desired coincidence outcomes for the construction of the post-selection P-SWAP gate (see Tab. 1).

(i) When one chooses the event that photons come from output mode pairs (9, 12) and (1', 12), the state $|\varphi_3\rangle$ will collapse into $|\varphi_4\rangle$, and the P-SWAP gate is completed.

(ii) When one chooses the event that photons come from output mode pairs (10, 12) and (1'', 12), the state $|\varphi_3\rangle$ will collapse into $|\varphi_5\rangle$, and the P-SWAP gate is completed.

(iii) When one chooses the event that photons come from output mode pairs (9, 11) and (1', 11), the state $|\varphi_3\rangle$ will collapse into $|\varphi_3\rangle$. And then, a phase flip operation, $a_{V_1'} \rightarrow -a_{V_1'}$, should be applied to complete the P-SWAP gate. Such feed-forward operation can be achieved by setting an HWP$^{0\circ}$ in spatial mode 1'. The spatial-based classical feed-forward operations has been experimentally demonstrated recently [59, 62].

(iv) When one chooses the event that photons come from output mode pairs (10, 11) and (1'', 11), the state $|\varphi_3\rangle$ will collapse into $|\varphi_2\rangle$. And then, an HWP$^{90\circ}$ 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 Fig. 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.

| Table 1: Coincident expectation outgoing values for six logic basis inputs. |
|---------------------------------------------------------------|
| Input | $\hat{a}_{H_0}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_0}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ |
|-------|----------------|----------------|----------------|----------------|----------------|----------------|
| $\hat{a}_{H_0}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_0}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{V_1}$ |
| $\hat{a}_{H_11}$ | $\hat{a}_{V_0}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ |
| $\hat{a}_{V_0}$ | $\hat{a}_{H_11}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ |
| $\hat{a}_{V_1}$ | $\hat{a}_{H_11}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ |
| $\hat{a}_{V_0}$ | $\hat{a}_{H_11}$ | $\hat{a}_{V_0}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ |
| $\hat{a}_{V_1}$ | $\hat{a}_{H_11}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ | $\hat{a}_{V_1}$ | $\hat{a}_{H_12}$ |

3.2 Implementation of a CNOT gate with linear optics

As shown in Fig. 5 a P-SWAP-based CNOT gate can be realized in the coincidence basis with linear optical elements. PBS plays a role in the qutrit $X_A$ to provide an additional spatial mode. The operation in the black dotted rectangle corresponds to a P-SWAP gate in Fig. 4.

First, after the two photons are injected into modes 1 and 2, the input state of the system is given by

$$|\chi_0\rangle = (\alpha_1 \hat{a}_{H_1} \hat{a}_{H_2} + \alpha_2 \hat{a}_{H_1} \hat{a}_{V_2} + \alpha_3 \hat{a}_{V_1} \hat{a}_{H_2} + \alpha_4 \hat{a}_{V_1} \hat{a}_{V_2}) |\text{vac.}\rangle.$$  (22)

Second, photons 1 and 2 execute a PBS1 and an HWP$^{22.5\circ}$, respectively, to pass through the first P-SWAP gate. After the photons interact with the first P-SWAP gate, the outing
photons emitted from spatial mode pairs \((9, 12)\) and \((1', 12)\), or \((10, 12)\) and \((1'', 12)\) (as an input) will be led to the next HWP\(^{0\circ}\) and the rightmost P-SWAP gate. PBS\(_1\), HWP\(^{22.5\circ}\), and the leftmost P-SWAP gate change \(|\chi_0\rangle\) into \(|\chi_{9,1',12}\rangle\) or \(|\chi_{10,1'',12}\rangle\). Here,

\[
|\chi_{9,1',12}\rangle_1 = \frac{1}{4} \left[ \alpha_1 (a_{H9}^+ + a_{V9}^+) a_{H12}^+ + \alpha_2 (a_{H9}^+ - a_{V9}^+) a_{H12}^+ \\
+ \alpha_3 a_{V1'}^+ (a_{H12}^+ + a_{V12}^+) + \alpha_4 a_{V1'}^+ (a_{H12}^+ - a_{V12}^+) \right] |\text{vac.}\),
\]

\[
|\chi_{10,1'',12}\rangle_1 = \frac{1}{4} \left[ \alpha_1 (a_{H10}^+ + a_{V10}^+) a_{H12}^+ + \alpha_2 (a_{H10}^+ - a_{V10}^+) a_{H12}^+ \\
+ \alpha_3 a_{V1''}^+ (a_{H12}^+ + a_{V12}^+) + \alpha_4 a_{V1''}^+ (a_{H12}^+ - a_{V12}^+) \right] |\text{vac.}\).
\]

Third, HWP\(^{0\circ}\) acts on mode 12 to complete \(a_{H12}^+ \rightarrow a_{H12}^+\) and \(a_{V12}^+ \rightarrow -a_{V12}^+\). The second P-SWAP gate produces eight desired outcomes of the system, that is, (i) when the outing photons emitted from spatial mode pairs \((9, 12)\) and \((1', 12)\), the state \(|\chi_{9,1',12}\rangle_1\) and \(|\chi_{10,1'',12}\rangle_1\) both become

\[
|\chi_{9,1',12}\rangle_2 = \frac{1}{8\sqrt{2}} \left[ \alpha_1 a_{H9}^+ (a_{H12}^+ + a_{V12}^+) + \alpha_2 a_{H9}^+ (a_{H12}^+ - a_{V12}^+) \\
+ \alpha_3 a_{V1'}^+ (a_{H12}^+ + a_{V12}^+) + \alpha_4 a_{V1'}^+ (a_{H12}^+ + a_{V12}^+) \right] |\text{vac.}\).
\]

(ii) When the outing photons emitted from spatial mode pairs \((10, 12)\) and \((1'', 12)\), the state \(|\chi_{9,1',12}\rangle_1\) and \(|\chi_{10,1'',12}\rangle_1\) both become

\[
|\chi_{10,1'',12}\rangle_2 = \frac{1}{8\sqrt{2}} \left[ \alpha_1 a_{H10}^+ (a_{H12}^+ + a_{V12}^+) + \alpha_2 a_{H10}^+ (a_{H12}^+ - a_{V12}^+) \\
+ \alpha_3 a_{V1''}^+ (a_{H12}^+ + a_{V12}^+) + \alpha_4 a_{V1''}^+ (a_{H12}^+ + a_{V12}^+) \right] |\text{vac.}\).
\]

(iii) When the outing photons emitted from spatial mode pairs \((9, 11)\) and \((1'', 11)\), the state \(|\chi_{9,1',12}\rangle_1\) and \(|\chi_{10,1'',12}\rangle_1\) both become

\[
|\chi_{9',1''}\rangle_2 = \frac{1}{8\sqrt{2}} \left[ \alpha_1 a_{H9}^+ (a_{H11}^+ + a_{V11}^+) + \alpha_2 a_{H9}^+ (a_{H11}^+ - a_{V11}^+) \\
- \alpha_3 a_{V1'}^+ (a_{H11}^+ + a_{V11}^+) - \alpha_4 a_{V1'}^+ (a_{H11}^+ + a_{V11}^+) \right] |\text{vac.}|.
\]
(iv) When the outing photons emitted from spatial mode pairs (10, 11) and (1′′, 11), the state $|\chi_{10,1''11}\rangle_1$ and $|\chi_{10,1'12}\rangle_1$ both become

$$|\chi_{10,1''11}\rangle_2 = \frac{1}{8\sqrt{2}}[\alpha_1 \hat{a}_{H_{10}}^\dagger (\hat{a}_{H_{11}}^\dagger + \hat{a}_{V_{11}}^\dagger) + \alpha_2 \hat{a}_{H_{10}}^\dagger (\hat{a}_{H_{11}}^\dagger - \hat{a}_{V_{11}}^\dagger)
- \alpha_3 \hat{a}_{V_{10}}^\dagger (\hat{a}_{H_{11}}^\dagger - \hat{a}_{V_{11}}^\dagger) - \alpha_4 \hat{a}_{V_{10}}^\dagger (\hat{a}_{H_{11}}^\dagger + \hat{a}_{V_{11}}^\dagger)]|\text{vac.}\rangle.$$  

(28)

Fourth, as shown in Fig. 5, PBS$_2$ leads the photons in modes 9 (i.e., $\hat{a}_{H_{9}}^\dagger |\text{vac.}\rangle$) 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., $\hat{a}_{H_{10}}^\dagger |\text{vac.}\rangle$) and 1′′ (i.e., $\hat{a}_{V_{1}}^\dagger |\text{vac.}\rangle$) into one output mode. After PBS$_2$ and HWP$^{22.5\circ}$, (i) when the photons emitted from output pair (9, 12), we obtain the two-fold output state

$$|\chi_{9,12}\rangle_3 = \frac{1}{8}(\alpha_1 \hat{a}_{H_{9}}^\dagger \hat{a}_{H_{12}}^\dagger + \alpha_2 \hat{a}_{H_{9}}^\dagger \hat{a}_{V_{12}}^\dagger + \alpha_3 \hat{a}_{V_{9}}^\dagger \hat{a}_{V_{12}}^\dagger + \alpha_4 \hat{a}_{V_{9}}^\dagger \hat{a}_{H_{12}}^\dagger)|\text{vac.}\rangle.$$  

(29)

The CNOT gate is completed.

(ii) When the photons emitted from output pair (10, 12), we obtain the two-fold output state

$$|\chi_{10,12}\rangle_3 = \frac{1}{8}(\alpha_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{12}}^\dagger + \alpha_2 \hat{a}_{H_{10}}^\dagger \hat{a}_{V_{12}}^\dagger + \alpha_3 \hat{a}_{V_{10}}^\dagger \hat{a}_{V_{12}}^\dagger + \alpha_4 \hat{a}_{V_{10}}^\dagger \hat{a}_{H_{12}}^\dagger)|\text{vac.}\rangle.$$  

(30)

The CNOT gate is completed.

(iii) When the photons emitted from output pair (9, 11), we obtain the two-fold output state

$$|\chi_{9,11}\rangle_3 = \frac{1}{8}(\alpha_1 \hat{a}_{H_{9}}^\dagger \hat{a}_{H_{11}}^\dagger + \alpha_2 \hat{a}_{H_{9}}^\dagger \hat{a}_{V_{11}}^\dagger - \alpha_3 \hat{a}_{V_{9}}^\dagger \hat{a}_{V_{11}}^\dagger - \alpha_4 \hat{a}_{V_{9}}^\dagger \hat{a}_{H_{11}}^\dagger)|\text{vac.}\rangle.$$  

(31)

And then an HWP$^{0\circ}$ is set in the output mode 9 to complete the CNOT gate.

(iv) When the photons emitted from output pair (10, 11), we obtain the two-fold output state

$$|\chi_{10,11}\rangle_3 = \frac{1}{8}(\alpha_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{11}}^\dagger + \alpha_2 \hat{a}_{H_{10}}^\dagger \hat{a}_{V_{11}}^\dagger - \alpha_3 \hat{a}_{V_{10}}^\dagger \hat{a}_{V_{11}}^\dagger - \alpha_4 \hat{a}_{V_{10}}^\dagger \hat{a}_{H_{11}}^\dagger)|\text{vac.}\rangle.$$  

(32)

And then an HWP$^{0\circ}$ is set in the output mode 10 to complete the CNOT gate.

Based on above orthogonal two-fold states $|\chi_{9,12}\rangle_3$, $|\chi_{10,12}\rangle_3$, $|\chi_{9,11}\rangle_3$, and $|\chi_{10,11}\rangle_3$, one can find that after the feed-forward operations are only applied to the rightmost P-SWAP gate, an optical post-selection CNOT gate can be completed with a success probability of $8 \times 1/64 = 1/8$. Remarkably, additional entangled photon pairs or single photons are necessary for previous schemes [59, 61, 63, 64], 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 [65, 67].

### 3.3 Implementation of a 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 Fig. 6, three photons are injected into modes 1, 2, and 3, simultaneously, the initial state is given by

$$|\Xi_0\rangle = (\alpha_1 \hat{a}_{H_{1}}^\dagger \hat{a}_{H_{2}}^\dagger \hat{a}_{H_{3}}^\dagger + \alpha_2 \hat{a}_{H_{1}}^\dagger \hat{a}_{H_{2}}^\dagger \hat{a}_{V_{3}}^\dagger + \alpha_3 \hat{a}_{H_{1}}^\dagger \hat{a}_{V_{2}}^\dagger \hat{a}_{H_{3}}^\dagger + \alpha_4 \hat{a}_{H_{1}}^\dagger \hat{a}_{V_{2}}^\dagger \hat{a}_{V_{3}}^\dagger + \alpha_5 \hat{a}_{V_{1}}^\dagger \hat{a}_{H_{2}}^\dagger \hat{a}_{H_{3}}^\dagger + \alpha_6 \hat{a}_{V_{1}}^\dagger \hat{a}_{H_{2}}^\dagger \hat{a}_{V_{3}}^\dagger + \alpha_7 \hat{a}_{V_{1}}^\dagger \hat{a}_{V_{2}}^\dagger \hat{a}_{H_{3}}^\dagger + \alpha_8 \hat{a}_{V_{1}}^\dagger \hat{a}_{V_{2}}^\dagger \hat{a}_{V_{3}}^\dagger)|\text{vac.}\rangle.$$  

(33)
First, after photons go through the PBS\(_1\) and the leftmost P-SWAP gate, when the outing photons emitted from path pairs (9, 12) and (1', 12), or (10, 12) and (1'', 12), we can obtain two desired states,

\[
|\Xi_{1a}\rangle = \frac{1}{2\sqrt{2}} \left( \alpha_1 \hat{a}_{H_{12}}^\dagger \hat{a}_H^\dagger \hat{a}_3^\dagger + \alpha_2 \hat{a}_{H_{12}}^\dagger \hat{a}_H^\dagger \hat{a}_3^\dagger + \alpha_3 \hat{a}_{V_{12}}^\dagger \hat{a}_{H_3}^\dagger + \alpha_4 \hat{a}_{H_{12}}^\dagger \hat{a}_{V_1}^\dagger \hat{a}_{V_3}^\dagger + \alpha_5 \hat{a}_{V_{12}}^\dagger \hat{a}_{V_9}^\dagger \hat{a}_{H_3}^\dagger + \alpha_6 \hat{a}_{H_{12}}^\dagger \hat{a}_{V_9}^\dagger \hat{a}_{V_3}^\dagger + \alpha_7 \hat{a}_{V_{12}}^\dagger \hat{a}_{V_{12}}^\dagger \hat{a}_{H_3}^\dagger + \alpha_8 \hat{a}_{V_{12}}^\dagger \hat{a}_{V_{12}}^\dagger \hat{a}_{V_3}^\dagger \right) |\text{vac.}\rangle,
\]

(34)

\[
|\Xi_{1b}\rangle = \frac{1}{2\sqrt{2}} \left( \alpha_1 \hat{a}_{H_{12}}^\dagger \hat{a}_{H_{10}}^\dagger \hat{a}_H^\dagger + \alpha_2 \hat{a}_{H_{12}}^\dagger \hat{a}_{H_{10}}^\dagger \hat{a}_3^\dagger + \alpha_3 \hat{a}_{H_{12}}^\dagger \hat{a}_{V_{12}}^\dagger \hat{a}_{H_3}^\dagger + \alpha_4 \hat{a}_{H_{12}}^\dagger \hat{a}_{V_1}^\dagger \hat{a}_{V_3}^\dagger + \alpha_5 \hat{a}_{H_{12}}^\dagger \hat{a}_{V_{10}}^\dagger \hat{a}_H^\dagger + \alpha_6 \hat{a}_{H_{12}}^\dagger \hat{a}_{V_{10}}^\dagger \hat{a}_3^\dagger + \alpha_7 \hat{a}_{V_{12}}^\dagger \hat{a}_{V_{12}}^\dagger \hat{a}_{H_3}^\dagger + \alpha_8 \hat{a}_{V_{12}}^\dagger \hat{a}_{V_{12}}^\dagger \hat{a}_{V_3}^\dagger \right) |\text{vac.}\rangle,
\]

(35)

Second, the states described by Eqs. (34) and (35) are considered as the inputs for the next CNOT gate acting on photon 1 and photon 3. When the outing photons emitted from path pairs (9, 11), (9, 12), (10, 11), or (10, 12), which can yield 16 desired states \(|\Xi_{i,9,k}\rangle_1\) (two-fold) and \(|\Xi_{i,10,k}\rangle_1\) (two-fold). Here, \(|\Xi_{i,9,k}\rangle_1\) and \(|\Xi_{i,10,k}\rangle_1\) with \(i \in \{9, 10\}\) and \(k \in \{11, 12\}\) are described by

\[
|\Xi_{i,9,k}\rangle_1 = \frac{1}{\sqrt{6}} \left( \alpha_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{10}}^\dagger \hat{a}_H^\dagger + \alpha_2 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{10}}^\dagger \hat{a}_3^\dagger + \alpha_3 \hat{a}_{H_{10}}^\dagger \hat{a}_{V_1}^\dagger \hat{a}_{V_3}^\dagger + \alpha_4 \hat{a}_{H_{10}}^\dagger \hat{a}_{V_1}^\dagger \hat{a}_{V_3}^\dagger + \alpha_5 \hat{a}_{H_{10}}^\dagger \hat{a}_{V_9}^\dagger \hat{a}_H^\dagger + \alpha_6 \hat{a}_{H_{10}}^\dagger \hat{a}_{V_9}^\dagger \hat{a}_3^\dagger + \alpha_7 \hat{a}_{V_{10}}^\dagger \hat{a}_{V_{10}}^\dagger \hat{a}_{H_3}^\dagger + \alpha_8 \hat{a}_{V_{10}}^\dagger \hat{a}_{V_{10}}^\dagger \hat{a}_{V_3}^\dagger \right) |\text{vac.}\rangle,
\]

(36)

\[
|\Xi_{i,10,k}\rangle_1 = \frac{1}{6\sqrt{2}} \left( \alpha_1 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{12}}^\dagger \hat{a}_H^\dagger + \alpha_2 \hat{a}_{H_{10}}^\dagger \hat{a}_{H_{12}}^\dagger \hat{a}_3^\dagger + \alpha_3 \hat{a}_{H_{10}}^\dagger \hat{a}_{V_{12}}^\dagger \hat{a}_{H_3}^\dagger + \alpha_4 \hat{a}_{H_{10}}^\dagger \hat{a}_{V_{12}}^\dagger \hat{a}_{V_3}^\dagger + \alpha_5 \hat{a}_{H_{10}}^\dagger \hat{a}_{V_{10}}^\dagger \hat{a}_H^\dagger + \alpha_6 \hat{a}_{H_{10}}^\dagger \hat{a}_{V_{10}}^\dagger \hat{a}_3^\dagger + \alpha_7 \hat{a}_{V_{10}}^\dagger \hat{a}_{V_{10}}^\dagger \hat{a}_{H_3}^\dagger + \alpha_8 \hat{a}_{V_{10}}^\dagger \hat{a}_{V_{10}}^\dagger \hat{a}_{V_3}^\dagger \right) |\text{vac.}\rangle.
\]

(37)

Third, above 16 states are considered as inputs for the rightmost P-SWAP gate acting on photon 1 and photon 2. When the photon emitted from path pairs (9, 12) and (1', 12), or (9, 11) and (1', 11), or (10, 12) and (1'', 12), or (10, 11) and (1'', 11), we can obtain 64 desired states \(|\Xi_{12,9,k}\rangle_2, |\Xi_{12,10,k}\rangle_2, |\Xi_{11,9,k}\rangle_2\) and \(|\Xi_{11,10,k}\rangle_2\). Here, eight-fold states \(|\Xi_{12,9,k}\rangle_2,\)
\[ |\Xi_{12,10,k}\rangle_2, |\Xi_{11,9,k}\rangle_2, \text{ and } |\Xi_{11,10,k}\rangle_2 \text{ with } k \in \{11,12\} \text{ are described by} \]
\[
|\Xi_{12,9,k}\rangle_2 = \frac{1}{64} \left[ \alpha_1 \hat{a}_{H_1}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_2 \hat{a}_{H_12}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_3 \hat{a}_{H_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_4 \hat{a}_{H_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_5 \hat{a}_{V_12}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_6 \hat{a}_{V_12}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_7 \hat{a}_{V_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{V_k}^{\dagger} + \alpha_8 \hat{a}_{V_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{H_k}^{\dagger} \right] \text{vac.},
\]
\[
|\Xi_{12,10,k}\rangle_2 = \frac{1}{64} \left[ \alpha_1 \hat{a}_{H_1}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_2 \hat{a}_{H_12}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_3 \hat{a}_{H_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_4 \hat{a}_{H_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_5 \hat{a}_{V_12}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_6 \hat{a}_{V_12}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_7 \hat{a}_{V_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{V_k}^{\dagger} + \alpha_8 \hat{a}_{V_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{H_k}^{\dagger} \right] \text{vac.},
\]
\[
|\Xi_{11,9,k}\rangle_2 = \frac{1}{64} \left[ \alpha_1 \hat{a}_{H_1}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_2 \hat{a}_{H_11}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
- \alpha_3 \hat{a}_{H_11}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{H_k}^{\dagger} - \alpha_4 \hat{a}_{H_11}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_5 \hat{a}_{V_11}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_6 \hat{a}_{V_11}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
- \alpha_7 \hat{a}_{V_11}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{V_k}^{\dagger} - \alpha_8 \hat{a}_{V_11}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{H_k}^{\dagger} \right] \text{vac.},
\]
\[
|\Xi_{11,10,k}\rangle_2 = \frac{1}{64} \left[ \alpha_1 \hat{a}_{H_1}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_2 \hat{a}_{H_11}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
- \alpha_3 \hat{a}_{H_11}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{H_k}^{\dagger} - \alpha_4 \hat{a}_{H_11}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_5 \hat{a}_{V_11}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_6 \hat{a}_{V_11}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
- \alpha_7 \hat{a}_{V_11}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{V_k}^{\dagger} - \alpha_8 \hat{a}_{V_11}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{H_k}^{\dagger} \right] \text{vac.}.
\]

Finally, as shown in Fig. 6, the photons emitted from modes 9 (i.e., \(\hat{a}_{H_9}\) |vac.\)) and 1’ (i.e., \(\hat{a}_{V_9}\) |vac.\)) are combined into the same output mode by PBS2. The photons emitted from modes 10 (i.e., \(\hat{a}_{H_{10}}\) |vac.\)) and 1'' (\(\hat{a}_{V_{10}}\) |vac.\)) are also led to the same output mode by PBS2. Therefore, after PBS2, (i) when the photons emitted from output pairs (12, 9, k) with \(k \in \{11,12\}\), simultaneously, we obtain the eight-fold state
\[
|\Xi_{12,9,k}\rangle_3 = \frac{1}{64} \left[ \alpha_1 \hat{a}_{H_12}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_2 \hat{a}_{H_12}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_3 \hat{a}_{H_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_4 \hat{a}_{H_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_5 \hat{a}_{V_12}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{H_k}^{\dagger} + \alpha_6 \hat{a}_{V_12}^{\dagger} \hat{a}_{H_9}^{\dagger} \hat{a}_{V_k}^{\dagger} \\
+ \alpha_7 \hat{a}_{V_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{V_k}^{\dagger} + \alpha_8 \hat{a}_{V_12}^{\dagger} \hat{a}_{V_9}^{\dagger} \hat{a}_{H_k}^{\dagger} \right] \text{vac.}.
\]

The three-photon Toffoli gate is completed.
neously, we obtain the eight-fold state

\[ |\Xi_{12,10,k}^\pm\rangle_3 = \frac{1}{64} \left[ \alpha_1 \hat{a}_{H_1} \hat{a}_{H_9} \hat{a}_{H_k} + \alpha_2 \hat{a}_{H_1} \hat{a}_{H_9} \hat{a}_{V_k} + \right. \\
- \alpha_3 \hat{a}_{H_1} \hat{a}_{V_9} \hat{a}_{H_k} - \alpha_4 \hat{a}_{H_1} \hat{a}_{V_9} \hat{a}_{V_k} + \right. \\
+ \alpha_5 \hat{a}_{V_1} \hat{a}_{H_9} \hat{a}_{H_k} + \alpha_6 \hat{a}_{V_1} \hat{a}_{H_9} \hat{a}_{V_k} - \alpha_7 \hat{a}_{V_1} \hat{a}_{V_9} \hat{a}_{H_k} - \alpha_8 \hat{a}_{V_1} \hat{a}_{V_9} \hat{a}_{V_k} \left. \right] \text{[vac.]}.
\]

The three-photon Toffoli gate is also completed.

(iii) When the photons emitted from outport pairs \((11,9,k)\) with \(k \in \{11,12\}\), simultaneously, we obtain the eight-fold state

\[ |\Xi_{11,9,k}^\pm\rangle_3 = \frac{1}{64} \left[ \alpha_1 \hat{a}_{H_1} \hat{a}_{H_9} \hat{a}_{H_k} + \alpha_2 \hat{a}_{H_1} \hat{a}_{H_9} \hat{a}_{V_k} + \right. \\
- \alpha_3 \hat{a}_{H_1} \hat{a}_{V_9} \hat{a}_{H_k} - \alpha_4 \hat{a}_{H_1} \hat{a}_{V_9} \hat{a}_{V_k} + \right. \\
+ \alpha_5 \hat{a}_{V_1} \hat{a}_{H_9} \hat{a}_{H_k} + \alpha_6 \hat{a}_{V_1} \hat{a}_{H_9} \hat{a}_{V_k} - \alpha_7 \hat{a}_{V_1} \hat{a}_{V_9} \hat{a}_{H_k} - \alpha_8 \hat{a}_{V_1} \hat{a}_{V_9} \hat{a}_{V_k} \left. \right] \text{[vac.]}.
\]

And then an HWP\(^{0\circ}\) is set in the output mode 9 to complete the three-photon Toffoli gate.

(iv) When the photons emitted from outport pairs \((11,10,k)\) with \(k \in \{11,12\}\), simultaneously, we obtain the eight-fold state

\[ |\Xi_{11,10,k}^\pm\rangle_3 = \frac{1}{64} \left[ \alpha_1 \hat{a}_{H_1} \hat{a}_{H_9} \hat{a}_{H_k} + \alpha_2 \hat{a}_{H_1} \hat{a}_{H_9} \hat{a}_{V_k} + \right. \\
- \alpha_3 \hat{a}_{H_1} \hat{a}_{V_9} \hat{a}_{H_k} - \alpha_4 \hat{a}_{H_1} \hat{a}_{V_9} \hat{a}_{V_k} + \right. \\
+ \alpha_5 \hat{a}_{V_1} \hat{a}_{H_9} \hat{a}_{H_k} + \alpha_6 \hat{a}_{V_1} \hat{a}_{H_9} \hat{a}_{V_k} - \alpha_7 \hat{a}_{V_1} \hat{a}_{V_9} \hat{a}_{H_k} - \alpha_8 \hat{a}_{V_1} \hat{a}_{V_9} \hat{a}_{V_k} \left. \right] \text{[vac.]}.
\]

And then an HWP\(^{0\circ}\) is set in the output mode 10 to complete the three-photon Toffoli gate.

Based on above orthogonal eight-fold states described by Eqs. (43,44,45), one can find that our proposal can be achieved with a higher success probability \((64 \times 1/64^2 = 1/64)\) than the simplified CNOT-based one \((1/72)\) \([20,21]\) and the one without a decomposition-based approach \((1/133)\) \([58]\). In addition, optical single-qudit operation ensembles \(X_a, X_b, \cdots, X_n\) can be achieved by employing a sequence of PBSs, and the linear optical \(n\)-control-photon Toffoli gate can be implemented in principle (see Fig. 7).

4 Discussion and Conclusion

The optimal cost of a Toffoli gate is six CNOT gates using the standard decomposition-based approach in qubit system \([47]\). The theoretical lower bound of a Toffoli gate is five two-qubit gates in qubit system \([48]\). Ralph et al. \([20]\) first reduced the cost of a Toffoli gate to three qubit-qudit CNOT gates by introducing a qutrit. Using the same idea as the works in Refs. \([20,21]\), we designed an alternative the quantum circuit to implement the Toffoli gate with
Figure 7: Implementation of an \((n + 1)\)-photon Toffoli gate.

A higher success probability based on the P-SWAP gates, which required the same number of qubit-qudit gates as the protocols in Refs. \[20, 21\]. 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 qubit 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 \[68\]. 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 \[60\, 63\] or a single photon \[64\], 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 \[65\, 67\]. 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 \((1/72)\) \[20\, 21\] and it is also higher than the no-decomposition-based one \((1/133)\) \[58\].

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 \[69\, 70\] and superconducting system \[71\, 72\] 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-qudit gates. \(2(n - 1)\) qubit-qudit gates and \(2(n - 2)\) 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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