The duality of a single particle with an \( n \)-dimensional internal degree of freedom*

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The wave–particle duality of a single particle with an \( n \)-dimensional internal degree of freedom is re-examined theoretically in a Mach–Zehnder interferometer. The famous duality relation \( D^2 + V^2 \leq 1 \) is always valid in this situation, where \( D \) is the distinguishability and \( V \) is the visibility. However, the sum of the particle information and the wave information, \( D^2 + V^2 \), can be smaller than one for the input of a pure state if this initial pure state includes the internal degree of freedom of the particle, while the quantity \( D^2 + V^2 \) is always equal to one when the internal degree of freedom of the particle is excluded.

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1. Introduction

The principle of complementarity, proposed by Bohr in 1928,[1] lies at the heart of quantum mechanics. Complementarity emphasizes equally real but mutually exclusive properties, such as those in the wave–particle duality. For two complementary properties, an observation of either one precludes the simultaneous observation of the other. Young’s double-slit experiment provides a good example of wave–particle duality.[2–5] Besides the all-or-nothing cases, some intermediate situations actually exist,[3–10] with partial which-path knowledge and reduced interference visibility. An inequality, \( D^2 + V^2 \leq 1 \), theoretically derived by Jaeger et al.[11] and Englert,[12] can be used to quantify the wave–particle duality, where \( D \) is the distinguishability and \( V \) is the visibility. This duality relation is valid even in a delayed-choice manner, and the setup for Wheeler’s delayed-choice experiment[13,14] is shown in Fig. 1(a). A particle is sent into a Mach–Zehnder interferometer (MZI) and split into two paths after the first beam splitter (BS1). The second beam splitter (BS2) is randomly either inserted or removed after the particle is already inside the interferometer. By inserting or removing BS2, we can observe the wave or particle behavior. The duality (complementarity) relation was confirmed experimentally.[15] Recently, a theoretical proposal[16] suggested that the second beam splitter, instead of being randomly inserted or not, can be controlled by an ancillary state \( \ket{\phi} = c_1 \ket{0}_a + c_2 \ket{1}_a \) (with \( |c_1|^2 + |c_2|^2 = 1 \) and \( a \ket{0}_a = 0 \); see Fig. 1(b). The second beam splitter is present (absent), when the ancillary state is \( \ket{1}_a \) (\( \ket{0}_a \)). That is to say, the second BS is in a superposition of presence and absence.[16,17] The second BS is also called a quantum beam splitter (Q-BS). The final state is a superposition of the particle and wave states, and consequently, we can test the particle and wave behaviors of the particle at the same time.[17–19]

In Fig. 1(b), the ancillary state can be considered to be the two dimensions of the internal degree of freedom of the particle.[17,18] The control of the presence and absence of the BS2 can be realized by controlling the two-dimensional internal degree of freedom. That is to say, we can use a \( 2 \times 2 \) transformation matrix to describe the action of the Q-BS. For a lossless beam splitter, the matrix is unitary. The second beam splitter in Fig. 1(a) will be replaced by a new device, \( U \), which transforms paths 1 and 2 to paths 1’ and 2’; see Fig. 2.

The two-dimensional internal degree of freedom of the ancillary state can be extended to an \( n \)-dimensional \((n > 2)\) internal degree of freedom. In this paper, we share an account of our theoretical study of the duality relation with an ancillary system involved, and we discuss the duality relation for a single particle with a general \( n \)-dimensional internal degree of freedom (components) that is sent to an MZI setup which has a \( U \) device. The \( U \) device can change both the paths and the internal degree of freedom, and can be represented by a \( 2n \times 2n \) unitary matrix if the loss is neglected. We confirm the duality relation \( D^2 + V^2 \leq 1 \) theoretically and find that this relation is still valid in the general situation.

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2. Duality of a single particle with an n-dimensional internal degree of freedom

In a Mach–Zehnder interferometer, the distinguishability used to quantify the particle-like behavior has two different aspects. First, the a priori distinguishability, also called the predictability, measures the which-way knowledge carried in the initial state of the single particle. Second, the a posteriori distinguishability measures the which-way knowledge we actually obtained in an experiment. This a posteriori distinguishability can be measured either by creating an entanglement between the particle and a which-way marker, or by using an interferometer with an output beam splitter.

Here we choose the second case to study the duality for a single particle with an n-dimensional internal degree of freedom; see Fig. 2. And we use the definition of distinguishability ($D$) given in Ref. [15] as

\[ D = \frac{D_1 + D_2}{2}, \]

\[ D_1 = |p_{11} - p_{12}|, \quad \text{path 2 blocked,} \]

\[ D_2 = |p_{21} - p_{22}|, \quad \text{path 1 blocked,} \]

where $p_{uv}$ is the probability that the particle follows path $u$ (the other path is blocked) and is detected by detector $v$ ($u, v = 1, 2$). The factor 1/2 in Eq. (1a) is due to the 50% probability, as one of the two paths is blocked.

Defined in Ref. [15], the visibility $V$ of the interference pattern, used to describe the wave-like information, is determined by the maximum and the minimum intensities of the interference fringes

\[ V = \frac{P_{max} - P_{min}}{P_{max} + P_{min}}, \]

where the maximum and the minimum values are obtained by scanning the phase $\phi$ (via a piezoelectric transducer, PZT).

For the MZI in Fig. 2, a single input particle with an n-dimensional internal degree of freedom is split by a 50:50 beam splitter into two paths. In path 2, a phase shift $\phi$ is introduced by the PZT. All particles from the two paths are sent to an unknown lossless device, which has two output paths, and finally detected by two detectors $P_1$ and $P_2$, which are used to record the particle numbers in paths $1'$ and $2'$. The initial state of the input particle with an n-dimensional internal degree of freedom is assumed to be a direct product of its internal degree of freedom and path state

\[ |\psi\rangle = \left( \sum_{i=1}^{n} c_i |\alpha_i\rangle \right) |1\rangle_{in} |0\rangle_u, \]

where \( \sum_{i=1}^{n} |c_i|^2 = 1 \), $n$ is an integer, and $|\alpha_i\rangle$ ($i = 1, 2, \cdots, n$) denote $n$ orthogonal bases of the internal degrees of freedom, for example, horizontal polarization and vertical polarization. The subscripts in and u denote the paths. After the 50:50 BS and the PZT, the state of the single particle becomes

\[ |\psi\rangle = \frac{1}{\sqrt{2}} \left( \sum_{i=1}^{n} c_i |\alpha_i\rangle \right) \left( |1\rangle_{1'} |0\rangle_2 + e^{i\phi} |0\rangle_1 |1\rangle_{2'} \right), \]

where the $2n$ basis

\[ \{|\alpha_1\rangle |1\rangle_{1'} |0\rangle_2, |\alpha_2\rangle |1\rangle_{1'} |0\rangle_2, \cdots, |\alpha_n\rangle |1\rangle_{1'} |0\rangle_2, |\alpha_1\rangle |0\rangle_1 |1\rangle_{2'}, |\alpha_2\rangle |0\rangle_1 |1\rangle_{2'}, \cdots, |\alpha_n\rangle |0\rangle_1 |1\rangle_{2'} \}, \]

can be rewritten as \( \{|a_1\rangle, |a_2\rangle, \cdots, |a_{2n}\rangle \} \).

The unknown device, described by a unitary transformation $U$ in the following, can be a simple beam splitter, a Q-BS, or the like. Its role is to exchange or mix the paths and the internal degree of freedom. Note the device $U$ must
be a unitary matrix for a lossless device, which is a $2n \times 2n$ matrix. The output state after the $U$ device is

$$|F\rangle = U|I\rangle.$$  

(5)

In the bases of the output state, $\{|b_1\rangle, |b_2\rangle, \ldots, |b_{2n}\rangle\}$, which actually represent the bases

$$|F\rangle = U|I\rangle = \begin{pmatrix} u_{11} e^{i\delta_1 a_1} & u_{12} e^{i\delta_1 a_2} & \ldots & u_{1n} e^{i\delta_1 a_n} \\ u_{21} e^{i\delta_2 a_1} & u_{22} e^{i\delta_2 a_2} & \ldots & u_{2n} e^{i\delta_2 a_n} \\ \vdots & \vdots & \ddots & \vdots \\ u_{n1} e^{i\delta_n a_1} & u_{n2} e^{i\delta_n a_2} & \ldots & u_{nn} e^{i\delta_n a_n} \end{pmatrix} \begin{pmatrix} u_{1(1+n)} e^{i\delta_1 a_1} & u_{1(2+n)} e^{i\delta_1 a_2} & \ldots & u_{1(2n)} e^{i\delta_1 a_n} \\ u_{2(1+n)} e^{i\delta_2 a_1} & u_{2(2+n)} e^{i\delta_2 a_2} & \ldots & u_{2(2n)} e^{i\delta_2 a_n} \\ \vdots & \vdots & \ddots & \vdots \\ u_{n(1+n)} e^{i\delta_n a_1} & u_{n(2+n)} e^{i\delta_n a_2} & \ldots & u_{nn} e^{i\delta_n a_n} \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} 2n \times 1.$$  

(6)

The expression of $U$ can be found in Appendix A, Eq. (A5).

2.1. Visibility

The wavelike information of the light field is obtained by measuring the visibility of the interference. Since the detectors record the number of particles regardless of their internal degree of freedom, the probability of particles at detector 1 is

$$p_1 = \sum_{i=1}^{n} |b_i\rangle \langle F| b_i\rangle = \sum_{i=1}^{n} |b_i|^2$$

$$= \frac{1}{2} [n(n+1)] 2 \sum_{i=1}^{n} (|A_i|^2 + |B_i|^2) + \sqrt{M^2 + N^2} \cos(\varphi - \gamma),$$  

(7)

where $A_i$, $B_i$, $M$, $N$, and $\gamma$ are some parameters associated with the elements of matrix $U$

$$A_i = \sum_{j=1}^{n} u_{ij} e^{i\theta_j} a_j, \quad B_i = \sum_{j=1}^{n} u_{i(n+j)} e^{i\theta_j} a_j, \quad (7a)$$

$$M = \sum_{i=1}^{n} |A_i||B_i| \cos \theta_i, \quad N = \sum_{i=1}^{n} |A_i||B_i| \sin \theta_i,$$  

(7b)

$$A_iB_i^* = |A_i||B_i| e^{i\theta},$$  

$$\cos \gamma = \frac{M}{\sqrt{M^2 + N^2}}, \quad \sin \gamma = \frac{N}{\sqrt{M^2 + N^2}},$$  

(7c)

$$\sum_{i=1}^{n} (|A_i|^2 + |B_i|^2) = 1.$$  

(7d)

Equation (7d) has been proven (see the details in Appendix B).

When all particles are detected by detector 1, an interference pattern can be observed, as the length of path 2 is varied.

The maximum and the minimum values can be obtained by adjusting the phase $\varphi$. Then we obtain the visibility $V$ for the single particle with an $n$-dimensional internal degree of freedom

$$V = \frac{p_{1\text{max}} - p_{1\text{min}}}{p_{1\text{max}} + p_{1\text{min}}}$$

$$= 2 \sum_{i=1}^{n} |A_i|^2 |B_i|^2 2 \sum_{i=1}^{n} \sum_{\ell=i+1}^{n} |A_i||B_i| |A_\ell||B_\ell| \cos(\theta_i - \theta_\ell).$$  

(8)

We obtain the same visibility if we detect all particles by detector 2.

2.2. Distinguishability

In order to obtain the distinguishability $D$, we block one path of the interferometer and measure the probabilities of particles on detectors $P_1$ and $P_2$ [18]. The two paths cannot be distinguished at all if $D = 0$, and can be fully distinguished if $D = 1$. First, we block path 2 after the 50:50 BS in Fig. 2. The states before and after $U$, respectively, become

$$|F\rangle = U|I\rangle = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_{2n} \end{pmatrix} 2n \times 1,$$  

(9)
with \(|b'_1|^2 + |b'_2|^2 + \cdots + |b'_{n+1}|^2 = 1\). The probabilities of particles being detected by detectors 1 and 2 (via path 1) can be obtained, with the probabilities \(p_{11}\) and \(p_{12}\) being

\[
\begin{align*}
p_{11} &= \sum_{i=1}^{n} |b_i|^2, \\
p_{12} &= \sum_{i=1}^{n} |b_{n+i}|^2.
\end{align*}
\]

By substituting Eq. (10) into Eq. (1b), we have

\[
D_1 = \left| 2 \left( \sum_{i=1}^{n} |A_i|^2 \right) - 1 \right|.
\]

For \(D_2\), a similar measurement is implemented when path 1 is blocked,

\[
D_2 = \left| 2 \left( \sum_{i=1}^{n} |B_i|^2 \right) - 1 \right|.
\]

By using Eq. (7d), we obtain the distinguishability

\[
D = \frac{D_1 + D_2}{2} = \left| \sum_{i=1}^{n} (|A_i|^2 - |B_i|^2) \right|.
\]

2.3. Duality

The combination of Eqs. (8) and (13) leads to the following complementarity relation:

\[
(D^2 + V^2) - 1 = (D^2 + V^2) - \left| \sum_{i=1}^{n} (|A_i|^2 + |B_i|^2) \right|^2 \\
= -4 \sum_{i,\bar{i}=1,1'\neq\bar{i}}^{n} |A_i|^2 |B_{i'}|^2 \\
+ 8 \sum_{i=1}^{n-1} \sum_{i'=1}^{n} |A_i| |B_{i'}| |A_{i'}| |B_i| \cos(\theta_i - \theta_{i'})
\]

Here, we discuss it from two aspects. First, if all the parameters \(|A_i|, |B_i| \neq 0\), we have

\[
(D^2 + V^2) - 1 \\
\leq -4 \sum_{i,\bar{i}=1,1'\neq\bar{i}}^{n} (|A_i| |B_{i'}| - |A_{i'}| |B_i|)^2 \leq 0,
\]

with the equal sign holding for

\[
\theta_i - \theta_{i'} = 2k\pi \quad (k \text{ is an integer}), \quad |A_i| |B_{i'}| - |A_{i'}| |B_i| = 0,
\]

\((i, \bar{i}' = 1, 2, \cdots, n; \ i \neq \bar{i}'\)\).

Second, if one or more than one of the parameters \(|A_i|, |B_i| \) (\(i = 1, 2, \cdots, n\)) is equal to 0, such as \(|A_j| = 0\), we have

\[
(D^2 + V^2) - 1 \\
\leq -4 \sum_{i,\bar{i}=1,1'\neq\bar{i}}^{n} |A_i|^2 |B_{i'}|^2 \\
+ 8 \sum_{i=1}^{n-1} \sum_{i'=1}^{n} |A_i| |B_{i'}| |A_{i'}| |B_i| \cos(\theta_i - \theta_{i'}) \leq 0,
\]

with the equal sign holding for

\[
|B_j|^2 \sum_{i=1,i \neq j}^{n} |A_i|^2 = 0,
\]

\[
\left\{ \begin{array}{l}
|A_i| |B_{i'}| - |A_{i'}| |B_i| = 0, \\
\theta_i - \theta_{i'} = 2k\pi,
\end{array} \right. \quad (\bar{i}' \neq i, \ k \text{ is an integer}).
\]

Equations (15a) and (16a) tell us that the duality relation

\[
D^2 + V^2 \leq 1
\]

is still valid for a single particle with an \(n\)-dimensional internal degree of freedom. Please note that we can have \(D^2 + V^2\) smaller than one even though the input state before the device \(U\) is a pure state (with the internal degree of freedom).

If the input particle is at one state of the internal degree of freedom, we can prove that \(D^2 + V^2 = 1\) is still valid. Let us assume that the state of the input particle is at internal degree of freedom state \(|\alpha_1\rangle \) \((c_1 = 1 \text{ and } c_j = 0 \quad (j > 1))\). \(|I\rangle = |\alpha_1\rangle |(1_1|0_2 + e^{i\pi}|0_1|1_2)/\sqrt{2}\). From Eq. (7a), we have \(|A_i| = |u_{i1}|, \ |B_i| = |u_{i(n+1)}|\), and \(\theta_i = \delta_{i1} - \delta_{i(n+1)} \quad (i = 1, 2, \cdots, n). \) According to Eq. (8), we get \(|u_{i1}| |u_{i'1}| = |u_{i(n+1)}| |u_{i'n}| \quad (i, i' = 1, 2, \cdots, n; \ i \neq i')\), which leads to \(|A_i| |B_{i'}| - |A_{i'}| |B_i| = 0\). According to Eq. (15b), we have \(D^2 + V^2 = 1\).

Now let us consider a simple example (a single particle with a two-dimensional internal degree of freedom). Assume the input state and the \(U\) matrix to be

\[
|I\rangle = \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2}} |\alpha_1\rangle + \frac{1}{\sqrt{2}} |\alpha_2\rangle \right) \left( |1_1|0_2 + e^{i\pi}|0_1|1_2\right),
\]

\[
U = \begin{pmatrix}
\frac{1}{\sqrt{2}} e^{i\delta_{a1}} & 0 & \frac{1}{\sqrt{2}} e^{i\delta_{a2}} & 0 \\
0 & 1 & 0 & 0 \\
-\frac{1}{\sqrt{2}} e^{i\delta_{a1}} & 0 & \frac{1}{\sqrt{2}} e^{i\delta_{a2}} & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}.
\]

which leads to \(|A_1| = 1/2, \ |B_1| = 1/2, \ |A_2| = 1/\sqrt{2}, \ |B_2| = 0, \ \delta_{1} = \delta_{1a1} - \delta_{1a2}, \) and \(\delta_{2} = 0\). Consequently, we have \(D^2 + V^2 = 0.5\), which is less than 1 even when the initial state is a pure state.
3. Quantum beam splitter (Q-BS)

The U device Q-BS is a special case of a particle with a two-dimensional internal degree of freedom,[17,18] as shown in Fig. 3. A particle is sent into an MZI setup and split into two paths after the first beam splitter (BS1). The first half-wave plate (HWP) is used to rotate the polarization in path 1 and path 2 by the same angle \( \alpha \). Then the particles are split by the first polarization beam splitter (PBS) into two components. One component goes through a closed MZI setup (without BS2), while the other goes through an open MZI setup (with BS2). In the end, they are recombined by the second PBS. Then the particles are detected by detectors \( P_1 \) and \( P_2 \). Here, vertical polarization and horizontal polarization are the two dimensions of the internal degree of freedom.

For this Q-BS scheme, the state before the Q-BS is

\[
|\psi\rangle = \frac{1}{\sqrt{2}} (|\alpha\rangle_H + \sin \alpha |\alpha\rangle_V) \times (|1\rangle_1|0\rangle_2 + e^{i\theta}|0\rangle_1|1\rangle_2), \tag{18}
\]

where \( |\alpha\rangle_H \) and \( |\alpha\rangle_V \) denote the horizontal polarization and the vertical polarization, respectively, and the subscripts denote the paths. The expression of \( U \) for this Q-BS is shown in Appendix C. Then the final state becomes

\[
|F\rangle = U|\psi\rangle = \cos \alpha |P\rangle |H\rangle + \sin \alpha |W\rangle |V\rangle, \tag{19a}
\]

with

\[
|W\rangle = \frac{1}{\sqrt{2}} \left[ e^{i\delta_1} (\sqrt{1-R} + \sqrt{R} e^{i(\delta_0 + \varphi)}) |1\rangle_1' - e^{i\delta_2} (\sqrt{R} - \sqrt{1-R} e^{i(\delta_0 + \varphi)}) |1\rangle_2' \right],
\]

\[
|P\rangle = \frac{1}{\sqrt{2}} \left[ |1\rangle_1' + e^{i\theta}|1\rangle_2' \right].
\]

After tracing out the internal degree of freedom, the final state becomes

\[
\rho = \text{Tr}_{\text{internal}}|F\rangle\langle F| = \sin^2 \alpha |W\rangle\langle W| + \cos^2 \alpha |P\rangle\langle P|. \tag{19b}
\]

We detect the probability of particles at detector \( P_1 \) or \( P_2 \). According to Eq. (2), the visibility can be obtained as follows:

\[
p_1 = v(1|\psi\rangle\langle 1| = \frac{1}{2} + \sqrt{R(1-R)} \cos(\phi + \delta_0) \sin^2 \alpha, \tag{20a}
\]

\[
p_2 = v(1|\psi\rangle\langle 1| = \frac{1}{2} - \sqrt{R(1-R)} \cos(\phi + \delta_0) \sin^2 \alpha. \tag{20b}
\]

\[
V = 2 \sqrt{R(1-R)} \sin^2 \alpha. \tag{21}
\]

For distinguishability, we block one path after BS1 in Fig. 3 and detect the probabilities of particles at detectors \( P_1 \) and \( P_2 \). Thus we obtain \( D_1 \) by using Eq. (1b), and \( D_2 \) can be obtained in the same way when we block the other path. According to Eq. (1a), the distinguishability is

\[
D_1 = |1-2R \sin^2 \alpha|, \quad D_2 = |1-2R \sin^2 \alpha|, \tag{22a}
\]

\[
D = \frac{D_1 + D_2}{2} = |1-2R \sin^2 \alpha|. \tag{22b}
\]

Consequently, we have the inequality for the duality of Q-BS

\[
D^2 + V^2 = 1 - 4R \sin^2 \alpha \cos^2 \alpha \leq 1. \tag{23}
\]

For \( R = 0 \) or \( \cos \alpha = 0 \) or \( \sin \alpha = 0 \), we have the equal sign. For \( R = 0.5 \), the BS2 in Fig. 3 is a 50:50 beam splitter. Thus we have \( D^2 + V^2 = \sin^2 \alpha + \cos^2 \alpha \leq 1 \). Figure 4 shows the results for \( D^2 \), \( V^2 \), \( D^2 + V^2 \) as a function of angle \( \alpha \). Please note that the curve in Fig. 4 of Ref. [18] is \( D + V \) (not \( D^2 + V^2 \)).

![Fig. 3. (color online) Schematic diagram of a particular Q-BS. A particle is sent into an MZI setup and split into two paths after BS1 (50:50 beam splitter). The first HWP is used to rotate the polarization in path 1 and path 2 by the same angle \( \alpha \). Then the particles are split by the first PBS into two components. One component goes through a closed MZI setup (without BS2), and the other is reflected to the other direction and goes through an open MZI setup (with BS2, which has reflectivity \( R \) and transmissivity \( 1-R \)). Finally, they are recombined by the second PBS.](image)

![Fig. 4. (color online) For \( R = 0.5 \) in the Q-BS device, we obtain \( D^2 + V^2 \leq 1 \) for all angles. The red, blue, and black lines show the respective results for \( V^2 \), \( D^2 \), \( D^2 + V^2 \) as functions of angle \( \alpha \).](image)

Here, equation (19b) is not the superposition state of \( |W\rangle \) and \( |P\rangle \), because \( |H\rangle|V\rangle = 0 \). In order to have the superposition state of \( |W\rangle \) and \( |P\rangle \), with constant coefficients, an additional device for polarization (as a projection) is needed, which results in the superposition state of \( |W\rangle \) and \( |P\rangle \) with certain probability. However, the projection results in particle loss (with certain probability). Consequently, the records at the two detectors will not be related to the distinguishability and visibility.
4. Conclusion

The duality of a particle with an $n$-dimensional internal degree of freedom passing through an MZI setup with a quantum device $U$ is studied. The duality relation $D^2 + V^2 \leq 1$ is always valid, regardless of the state of the internal degree of freedom. The experiments performed with Q-BS\textsuperscript{[17,18]} are a particular case of the $U$ device with $n = 2$. It is well known that for any pure state input without the internal degree of freedom, we have $D^2 + V^2 = 1$. However, with the internal degree of freedom, we find that $D^2 + V^2$ can be smaller than one for a pure state input. The case of a two-dimensional internal degree of freedom is a particular case of an $n$-dimensional internal degree of freedom, and the duality relation $D^2 + V^2 \leq 1$ is still valid for an internal degree of freedom with more than two dimensions.

Appendix A: The expression of $U$

Let us consider the expression for the $U$ matrix, whose role is exchanging or mixing of the paths and the states of the internal degree of freedom. This will be easy by considering the transfer of the annihilation (or creation) operators. The device of $U$ is lossless. Let us consider the annihilation operators before the $U$ device, which are $a_{1\alpha_1}, a_{2\alpha_2}$ ($i = 1, 2, \ldots, n$), $(a_{1\alpha_1}^+ | 0 | a_{1\alpha_1}) = (| \alpha_1 | j)$ with $j = 1, 2$, while the annihilation operators after the $U$ device are $a_{1\prime\alpha_1}$, $a_{2\prime\alpha_2}$ ($i = 1, 2, \ldots, n$), $(a_{1\prime\alpha_1}^+ | 0 | a_{1\prime\alpha_1}) = (| \alpha_1 | j')$ with $j' = 1, 2$. Here the subscripts of the operators represent the path and the internal information, $a_{\text{path}(\text{internal})}$. For the $U$ device in Fig. 2, these operators satisfy the following transformation:

$$
\begin{pmatrix}
    a_{1\prime\alpha_1} \\
    a_{1\prime\alpha_2} \\
    \vdots \\
    a_{1\prime\alpha_n} \\
    a_{2\prime\alpha_1} \\
    a_{2\prime\alpha_2} \\
    \vdots \\
    a_{2\prime\alpha_n}
\end{pmatrix}
= U
\begin{pmatrix}
    a_{1\alpha_1} \\
    a_{1\alpha_2} \\
    \vdots \\
    a_{1\alpha_n} \\
    a_{2\alpha_1} \\
    a_{2\alpha_2} \\
    \vdots \\
    a_{2\alpha_n}
\end{pmatrix},
$$
(A1)

which can be generally written as follows:

$$
a_{1\prime\alpha_1} = (u_{11} e^{i \delta_{\alpha_1}} a_{1\alpha_1} + u_{1(n+1)} e^{i \delta_{\alpha_1}} a_{2\alpha_1}) + (u_{12} e^{i \delta_{\alpha_1}} a_{1\alpha_2} + u_{1(n+2)} e^{i \delta_{\alpha_1}} a_{2\alpha_2}) + \cdots + (u_{1(n+1)} e^{i \delta_{\alpha_1}} a_{1\alpha_n} + u_{1(2n)} e^{i \delta_{\alpha_1}} a_{2\alpha_n}),
$$

$$
a_{1\prime\alpha_2} = (u_{21} e^{i \delta_{\alpha_1}} a_{1\alpha_1} + u_{2(n+1)} e^{i \delta_{\alpha_1}} a_{2\alpha_1}) + (u_{22} e^{i \delta_{\alpha_1}} a_{1\alpha_2} + u_{2(n+2)} e^{i \delta_{\alpha_1}} a_{2\alpha_2}) + \cdots + (u_{2(n+1)} e^{i \delta_{\alpha_1}} a_{1\alpha_n} + u_{2(2n)} e^{i \delta_{\alpha_1}} a_{2\alpha_n}),
$$

$$
a_{2\prime\alpha_1} = (u_{11} e^{i \delta_{\alpha_2}} a_{1\alpha_1} + u_{1(n+1)} e^{i \delta_{\alpha_2}} a_{2\alpha_1}) + (u_{12} e^{i \delta_{\alpha_2}} a_{1\alpha_2} + u_{1(n+2)} e^{i \delta_{\alpha_2}} a_{2\alpha_2}) + \cdots + (u_{1(n+1)} e^{i \delta_{\alpha_2}} a_{1\alpha_n} + u_{1(2n)} e^{i \delta_{\alpha_2}} a_{2\alpha_n}),
$$

$$
a_{2\prime\alpha_2} = (u_{21} e^{i \delta_{\alpha_2}} a_{1\alpha_1} + u_{2(n+1)} e^{i \delta_{\alpha_2}} a_{2\alpha_1}) + (u_{22} e^{i \delta_{\alpha_2}} a_{1\alpha_2} + u_{2(n+2)} e^{i \delta_{\alpha_2}} a_{2\alpha_2}) + \cdots + (u_{2(n+1)} e^{i \delta_{\alpha_2}} a_{1\alpha_n} + u_{2(2n)} e^{i \delta_{\alpha_2}} a_{2\alpha_n}),
$$

$$
a_{2\prime\alpha_n} = (u_{11} e^{i \delta_{\alpha_n}} a_{1\alpha_1} + u_{1(n+1)} e^{i \delta_{\alpha_n}} a_{2\alpha_1}) + (u_{12} e^{i \delta_{\alpha_n}} a_{1\alpha_2} + u_{1(n+2)} e^{i \delta_{\alpha_n}} a_{2\alpha_2}) + \cdots + (u_{1(n+1)} e^{i \delta_{\alpha_n}} a_{1\alpha_n} + u_{1(2n)} e^{i \delta_{\alpha_n}} a_{2\alpha_n}).
$$

where we have assumed that the phases are accumulated due to the propagation, and there is no phase accumulation for changing the internal degree of freedom, and $\delta_{\alpha_m}$ are real. Here $\delta_{\alpha_k}$ (with $j = 1, 2$ and $i = 1, 2, \ldots, n$) denotes the phase difference from path $j$ with internal degree of freedom state $\alpha_k$ to path $1'$; $\delta_{\alpha_k'}$ (with $j' = 1, 2$) denotes the phase difference from path $j$ with internal degree of freedom state $\alpha_k'$ to path $2'$.

In the MZI setup, the mixing of the two paths must comply with quantum mechanics, i.e., the commutation relation must be satisfied. The commutation relation can generally be written as

$$
\begin{aligned}
    a_{1\prime\Phi} &= \sin \theta a_{1\Phi} + \cos \theta a_{2\Phi}, \\
    a_{2\prime\Phi} &= -\cos \theta a_{1\Phi} + \sin \theta a_{2\Phi},
\end{aligned}
$$
(A3)

for the same state of the internal degree of freedom. According to the commutation relation, we can find

$$
\begin{aligned}
    u_{(n+1)1} &= -u_{(n+1)1}, & u_{(n+1)2} &= -u_{(n+1)2}, & \ldots, \\
    u_{(n+1)n} &= -u_{(n+1)n}, & u_{(n+1)(n+1)} &= u_{11}, \\
    u_{(n+1)(n+2)} &= u_{12}, & \ldots, & u_{(n+1)(2n)} &= u_{1n}, \\
    u_{(n+2)1} &= -u_{(n+2)1}, & u_{(n+2)2} &= -u_{(n+2)2}, & \ldots, \\
    u_{(n+2)n} &= -u_{(n+2)n}, & u_{(n+2)(n+1)} &= u_{21}, \\
    u_{(n+2)(n+2)} &= u_{22}, & \ldots, & u_{(n+2)(2n)} &= u_{2n}, \\
    \ldots \\
    u_{(2n)1} &= -u_{(2n)1}, & u_{(2n)2} &= -u_{(2n)2}, & \ldots, \\
    u_{(2n)n} &= -u_{(2n)n}, & u_{(2n)(n+1)} &= u_{n1}, \\
    u_{(2n)(n+2)} &= u_{n2}, & \ldots, & u_{(2n)(2n)} &= u_{nn}.
\end{aligned}
$$
(A4)

Based on Eqs. (A1) and (A4), the unitary matrix $U$ can be written as
with the normalization conditions $U^+ U = U U^+ = I$.

**Appendix B: The proof of** $\sum_{i=1}^{n} (|A_i|^2 + |B_i|^2) = 1$

As the normalization condition $U^+ U = U U^+ = I$, we can obtain the following coefficients’ relations:

1. $\sum_{j=1}^{2n} |u_{ij}|^2 = 1, (i = 1, 2, \ldots, 2n)$, \hspace{1cm} (B1)

2. $\sum_{i=1}^{2n} |u_{ij}|^2 = 1, (j = 1, 2, \ldots, 2n)$, \hspace{1cm} (B2)

3. $\delta_{i\alpha_i} - \delta_{j\alpha_j} = \delta'_{i\alpha_i} - \delta'_{j\alpha_j}, \text{ (with } i = 1, 2, \ldots, n)$, \hspace{1cm} (B3)

   $u_{p1}u_{m1} + u_{p2}u_{m2} + \cdots + u_{p(n)}u_{m(n)} = 0$,  
   \hspace{1cm} (here $p, m = 1, 2, \ldots, n; p \neq m$), \hspace{1cm} (B4)

   $u_{pq}u_{mn(q)} = u_{p(q)n}u_{mq}$,  
   \hspace{1cm} (here $p, q, m = 1, 2, \ldots, n; p \neq m$), \hspace{1cm} (B5)

   $u_{p1}u_{q1} + u_{p2}u_{q2} + \cdots + u_{np}u_{nq} = 0$,  
   \hspace{1cm} (here $p, q = 1, 2, \ldots, m; p \neq q$), \hspace{1cm} (B6)

   $u_{1(n+p)}u_{1(n+q)} + u_{2(n+p)}u_{2(n+q)} + \cdots + u_{n(n+p)}u_{n(n+q)} = 0$,  
   \hspace{1cm} (here $p, q = 1, 2, \ldots, m; p \neq q$), \hspace{1cm} (B7)

Based on Eqs. (B1), (B2), (B6), (B7), (A4), and (7a), we can obtain

$$
\sum_{i=1}^{n} (|A_i|^2 + |B_i|^2) = \sum_{i=1}^{n} (|A_i|^2 + |B_i|^2) + \cdots + |A_n|^2 + |B_n|^2
$$

$$
= (u_{11} + u_{21} + \cdots + u_{n+1}^2) |c_1|^2
+ (u_{12}^2 + u_{22}^2 + \cdots + u_{n+2}^2) |c_2|^2 + \cdots
+ (u_{1n}^2 + u_{2n}^2 + \cdots + u_{n+n}^2) |c_n|^2
+ \left[ \sum_{p=1}^{n-1} \sum_{q=p+1}^{n} u_{pq}u_{q} |c_p| |c_q| \cos(\delta_{ip} - \delta_{iq} + \alpha_{pq}) \right]
+ \left[ \sum_{p=1}^{n} \sum_{q=p+1}^{n} u_{pq}u_{q} |c_p| |c_q| \cos(\delta_{ip} - \delta_{iq} + \alpha_{pq}) \right]
+ \left[ \sum_{p=1}^{n} \sum_{q=p+1}^{n} u_{pq}u_{q} |c_p| |c_q| \cos(\delta_{ip} - \delta_{iq} + \alpha_{pq}) \right]
+ \left[ \sum_{p=1}^{n} \sum_{q=p+1}^{n} u_{pq}u_{q} |c_p| |c_q| \cos(\delta_{ip} - \delta_{iq} + \alpha_{pq}) \right]
+ \left[ \sum_{p=1}^{n} \sum_{q=p+1}^{n} u_{pq}u_{q} |c_p| |c_q| \cos(\delta_{ip} - \delta_{iq} + \alpha_{pq}) \right]
$$

$$
= 1
$$

\hspace{1cm} (B8)

**Appendix C: The expression of $U$ in Section 3**

Based on Eq. (A1), we can derive the expression of $U$ in Fig. 3 as follows. After the first PBS, the particles with horizontal polarization would go through a closed MZI setup (without beam splitter), while the particles with vertical polarization go through an open MZI setup (with beam splitter).

After the first PBS, we can find the relations

$$
a_{3H} = a_{1H},
$$
$$
a_{3V} = a_{1V},
$$
$$
a_{4H} = a_{2H},
$$
$$
a_{4V} = a_{2V},
$$

where the first subscript denotes the path, and the second subscript denotes the polarized information. Then after the second beam splitter (BS2), we have

$$
\begin{align*}
\begin{cases}
a_{3H} = a_{1H} & a_{3H} = a_{1H} \quad a_{3V} = \sqrt{1-R_{aV}} e^{i\delta_1} + \sqrt{R_{aV}} e^{i(\delta_1 + \delta_2)}, \\
a_{4H} = a_{2H} & a_{4H} = a_{2H} \quad a_{4V} = -\sqrt{R_{aV}} e^{i\delta_1} + \sqrt{1-R_{aV}} e^{i(\delta_1 + \delta_2)},
\end{cases}
\end{align*}
$$

where $\delta_1$ denotes the phase shift from path 5 to path 7, $\delta_2$ denotes the phase shift from path 5 to path 8, and $\delta_1$ denotes the phase difference between path 5 and path 6. Then the four
HWPs rotate the polarization by \(90^\circ\). We have

\[
\begin{align*}
  a_{9H} &= a_{3H}, \\
  a_{11V} &= a_{7V}, \\
  a_{10H} &= a_{4H}, \\
  a_{12V} &= a_{8V},
\end{align*}
\] (C3)

At last, they are recombined by the second PBS. So, we have

\[
\begin{align*}
  a_{1}'_{H} &= a_{9H}, \\
  a_{1}'_{V} &= a_{11V}, \\
  a_{2}'_{H} &= a_{10H}, \\
  a_{2}'_{V} &= a_{12V},
\end{align*}
\] (C4)

Combining Eq. (A1) and Eqs. (C1)–(C4), we obtain

\[
U = \begin{pmatrix}
  1 & 0 & 0 & 0 \\
  0 & e^{i\delta_1} \sqrt{1 - R} & 0 & e^{i(\delta_1 + \delta_0)} \sqrt{R} \\
  0 & 0 & 1 & 0 \\
  0 & -e^{i\delta_2} \sqrt{R} & 0 & e^{i(\delta_2 + \delta_0)} \sqrt{1 - R}
\end{pmatrix}.
\] (C5)

References

[1] Bohr N 1928 Naturwissenschaften 16 245